MOKA[1] - Many Body Physics

K. Enqvist and K. Kajantie

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[1] From Finnish for Many Body Physics: Monen Kappaleen fysiikka

0.1 Preface

This version contains the lectures of 2006 including the following files:

include preface
include equilibriumthermo ch1
include particle1 ch2sect1-7
include generfunc1 ch2sect8-, not covered in 2004,06
include idealFDBEgas ch3
include idealBE1 ch4sec1-2
include neutronstars ch4sec3
include beyondideal ch4sec4-7
include hydroplasmakinetic
include spin1 ch6sec1-5
include heatbath1 chsec6
include landau1input ch7
include 1plus2dphys ch8 not covered in 2006
include mokabibliography very incomplete!
appendix
include units
tableofcontents

These are notes from a graduate course in theoretical physics given at the University of Helsinki over the years. It contains basic material which, as we feel, should be known to everybody graduating in theoretical physics, from string theorists to ionospheric physicists. The material has been covered in four 45 min weekly lectures during thirteen weeks, with four hours of problem sessions each week.

This is not a course in ”many body quantum theory” with a detailed discussion of Green’s function techniques etc.

The guiding idea is a path integral defining statistical and quantum systems and various approximations to it: mean field plus fluctuations, coarse graining, integrating out irrelevant degrees of freedom.

It is assumed that the participants of the course have had some 50 hours of lectures in classical mechanics, electrodynamics, quantum mechanics and statistical physics each.

Chapter 1

Equilibrium thermodynamics

1.1 Basic concepts

Perhaps the most important concept in any course of many body physics is thermal equilibrium. One should have both a physical understanding of thermal equilibrium (one needs infinite systems, but in physics nothing is infinite) as well as an operative formal understanding (define a system by an action, compute the partition function, compute physics by partial derivatives of thermodynamic potentials). In this Chapter we shall remind the reader of the standard formulas of equilibrium thermodynamics.

The key object of study in many particle physics is the partition function

$$Z = e^{-\beta F} = \mathrm{Tr} e^{-\beta H} = \sum_{\text{n=all states}} e^{-\beta E_n}, \quad \beta \equiv \frac{1}{T}, \tag{1.1}$$

$$\langle \mathcal{O} \rangle = Z^{-1} \mathrm{Tr} \mathcal{O} e^{-\beta H} \equiv \mathrm{Tr} \mathcal{O} \rho \tag{1.2}$$

and its reformulation in terms of path integrals

$$Z = e^{-\beta F} = \mathrm{Tr} e^{-\beta H} \Rightarrow \int \mathcal{D}\Phi e^{-S[\Phi]/\hbar}, \tag{1.3}$$

$$\langle \Phi_1 \Phi_2 \ldots \Phi_N \rangle = \int \mathcal{D}\Phi \, \Phi_1 \Phi_2 \ldots \Phi_N e^{-S[\Phi]/\hbar}, \tag{1.4}$$

where Φ is a set of fields, degrees of freedom, and $S[\Phi]$ is the Euclidean action of the theory governing the dynamics of the fields Φ. We shall discuss path integrals in detail in Chapter 2. In Chapter 3 we move on to study "ideal gases" and the multitude of their physical applications.

Remember: in terms of eigenvalues a_n of a matrix A, $\mathrm{Tr}A = a_1 + a_2 + \cdots + a_N$, $\det A = a_1 a_2 \ldots a_N = \exp(\log a_1 + \log a_2 + \cdots + \log a_N) = \exp(\mathrm{Tr} \log A)$. This relation holds also for a general non-diagonal matrix since both Tr and det are invariant under $A \to UAU^{-1}$. From here one can further derive $\delta \det A = \det A \, \mathrm{Tr}(A^{-1} \delta A)$.

The difference between Eqs. (1.1) and (1.3) is that of the difference between quantum mechanics and quantum field theory. In the latter the sum is over all possible field configurations, not just over all the eigenstates of the Hamiltonian. The Euclidean action $S[\Phi]$ gives a weight also to the configurations that do not obey the classical equations of motion and hence takes into account all possible quantum fluctuations.

The word "partition" refers to the way the fundamental degrees of freedom of the system are arranged into the available states. It could be argued that partition is a more fundamental concept than, say, thermal equilibrium, which corresponds to a very special partitioning. Indeed, "partition" and "correlation" may be considered as describing the fundamental properties of the system while "entropy" and "temperature" are derived concepts.

To demonstrate this, let us consider a system that is divided up in j subsystems consisting of N_j identical particles. Each subsystem containing G_j states and each state has energy E_j. Let us further impose a global constraint: there can be only one particle per state. Then we have a problem which is identical to the combinatorial problem of putting N_j balls into G_j slots. Each ball should be delivered into a slot independently, i.e. without any correlation to past or future. This can be done in $Z_j = G_j(G_j-1)\cdots(G_j-N_j-1)/N!$ ways so that the number of possible partitions balls into slots in the subsystem is $Z_j = G_j!/N_j!G_j(-N_j)!$ and the total number of the partitions for the whole system is

$$Z = \Pi_j Z_j \ . \tag{1.5}$$

If we now define entropy as $S = \log Z$ it is clear it is just a measure of the number of partitions. Using $\log x! = x\log x/e$ for $x \gg 1$ we find

$$S = -\sum_j G_j\left[\bar{n}_j \log\bar{n}_j + (1-\bar{n}_j)\log(1-\bar{n}_j)\right] \tag{1.6}$$

where we have defined the mean occupation number $\bar{n}_j \equiv N_j/G_j$.

Let us consider a system whose total energy and total particle number is fixed: $N = \sum N_j = \text{const.}$, $E = \sum_j E_j N_j = \text{const.}$ What is the most probable partition? We maximize S subject to the energy and particle number constraint, writing

$$\frac{\partial}{\partial \bar{n}_j}(S - \alpha N - \beta E) = 0 \ , \tag{1.7}$$

where α and β are Lagrange multipliers. We then find that the most probable occupation number is given by the Fermi-Dirac distribution

$$\bar{n}_j = \frac{1}{\mathrm{e}^{\alpha+\beta E_j}+1} \ , \tag{1.8}$$

identifying $\alpha \equiv -\mu/T$, $\beta \equiv 1/T$. (Had we allowed many particles to occupy the same state, we would have obtained the Bose-Einstein distribution.) Thus thermal equilibrium is seen to correspond to the maximum entropy state or to the likeliest partition of completely uncorrelated degrees of freedom. If all other things are kept equal, adding correlations (i.e. interactions) will decrease the number of available partitions and hence entropy.

Note that if $G_j \gg N_j$ we could argue that when partitioning particles into the available states, there is a very small probability to hit a state that is already occupied so that we could write just $Z_j \approx G_j^N/N!$; the resulting most probable partition corresponds then to the Maxwell-Boltzmann distribution.

A similar line of argument can be carried over to quantum mechanics, where instead of classical energies one has to deal with operators. Recall that in quantum mechanics

$$E = \langle H \rangle = \mathrm{Tr}\rho H \ , \tag{1.9}$$

where ρ is the density matrix, and

$$S = -\sum p_n \mathrm{log} p_n = -\rho \ \mathrm{log}\rho \ . \tag{1.10}$$

Let us now vary S by requiring that E =const and $\mathrm{Tr}\rho = 1$:

$$\begin{aligned} 0 &= \delta(S - \beta\langle H\rangle - \alpha \mathrm{Tr}\rho) \\ &= \mathrm{Tr}\delta\rho(-\mathrm{log}\rho - I - \beta H - \alpha) \ . \end{aligned} \tag{1.11}$$

Here again β and α are Lagrange multipliers. Eq. (1.11) should hold for arbitrary variation so that we find the solution (taking now $\alpha = 0$)

$$\rho = \mathrm{const} \times \mathrm{e}^{-\beta H} \equiv Z^{-1}\mathrm{e}^{-\beta H} \ , \tag{1.12}$$

which, recalling that $\mathrm{Tr}\rho = 1$, reproduces Eq. (1.1).

1.2 Global versus local thermal equilibrium

Infinity is defined by a dimensionless number $\gg 1$, so effectively a spatially infinite system requires system size $\gg$ relevant length scale, which could be some correlation length ξ or some mean free path $\lambda \approx 1/(n\sigma)$. Here n = number density and σ = cross section. Alternatively temporal infinity would mean system life time $\gg$ relevant dynamical time scale, which could be the combination ξ/v_{sound} or the collision time $\tau_{\mathrm{coll}} = \lambda/v_{\mathrm{thermal}}$.

Exercise. Why $\lambda \approx 1/(n\sigma)$ is a good estimate of a mean free path and $\tau_{\mathrm{coll}} = \lambda/v_{\mathrm{thermal}}$ of collision time? Check dimensions.

Theoretically one can study a homogenous infinite system (say, T = constant everywhere), but in practice one always has gradients (say, $T = T(x)$ varies as a function of one spatial coordinate x). Nevertheless, there may exist local thermal equilibrium if the range in space or time within which T varies is $\gg$ some microscopic scale. Formally one could write as the conditions for local equilibrium $\lambda_{\mathrm{free}} \cdot \nabla \ll 1$ or $\tau_{\mathrm{coll}}\partial_t \ll 1$ (small λ_{free} or frequent collisions thermalise the system locally). Dynamically, this also induces hydrodynamics ($\nabla p \Rightarrow$ flow $= \mathbf{v}(t, \mathbf{x})$). The smaller the above dimensionless variables are, the better the assumption of ideal = adiabatic = entropy conserving = isentropic motion. This dynamics is built in the Euler equations. Corrections of $\mathrm{O}(\lambda_{\mathrm{free}}\nabla)$ give rise to dissipation ($\Delta S > 0$), viscosities, heat conductivity, etc, built in the Navier-Stokes equations. (See Ch. 5.)

1.3 Microcanonical ensemble

Let us now go through the pragmatic formal side of thermodynamics. We define various ensembles (microcanonical, canonical, grand canonical, etc) which are minimised in equilibrium. The value of the potentials at the minima is unspecified (this is the cosmological constant problem!), but partial derivatives (of first, second, etc order) give physics.

In the microcanonical ensemble the potential E depends on only *extensive* (proportional to the size of the system) variables: $E = E(S, V, A, B, N, ...)$, where, for generality, several different variables are indicated. These variables, together with their conjugate intensive variables, are

E = potential
S = entropy $\leftrightarrow T$ = temperature
V = volume $\leftrightarrow p$ = pressure
A = area $\leftrightarrow \sigma$ = interface tension
B = magnetic flux density $\leftrightarrow H$ = magnetic field
N = conserved particle number $\leftrightarrow \mu$ = chemical potential.

Then E is explicitly given by

$$\begin{aligned} E &= TS - pV + \mu N + \sigma A + V\mathbf{H}\cdot\mathbf{B} + \ldots \\ &= T(S,V,A,B,N)S - p(S,V,A,B,N)V + \mu(S,V,A,B,N)N + \ldots \end{aligned} \tag{1.13}$$

The aim is to use capital letters for extensive variables and small letters for intensive ones. For historical reasons, this does not work for T, H. We also define the intensive densities $\epsilon = E/V$, $s = S/V$ and $n = N/V$. Often $\epsilon \to \rho = mc^2 n$.

The combination $V\mathbf{H}\cdot\mathbf{B}$ is also somewhat special. It should really be written as $L\mathbf{H}\cdot A\mathbf{B}$ with $V = LA$ and $A\mathbf{B}$ symbolising the magnetic flux Φ_B (check dimensions!).

Differentiating Eq.(1.13) with respect to its variables gives

$$\begin{aligned} dE &= \frac{\partial E}{\partial S}dS + \frac{\partial E}{\partial V}dV + \frac{\partial E}{\partial N}dN + \ldots \\ &= TdS - pdV + \mu dN + \cdots \end{aligned} \tag{1.14}$$

Partial derivatives of E are physical and measurable:

1st derivatives $\Rightarrow T, -p, \mu, ...$
2nd derivatives $\Rightarrow C_v, C_p, v^2_{\text{sound}}, ...$

There are lots of relations among partial derivatives; use, choosing z, ω suitably,

$$\frac{\partial u}{\partial x}\Big|_y = \frac{\partial(u,y)}{\partial(x,y)} = \frac{\frac{\partial(u,y)}{\partial(z,\omega)}}{\frac{\partial(x,y)}{\partial(z,\omega)}} = \begin{vmatrix} \frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} \\ \frac{\partial y}{\partial x} & \frac{\partial y}{\partial y} \end{vmatrix} \tag{1.15}$$

Starting from E, many further potentials with various names (sometimes confusing!) can be defined by trading extensive $\leftrightarrow$ intensive variables by a Legendre transformation. A prototype Legendre transformation is that in Hamiltonian mechanics:

$$L(q,\dot{q}) = T - V \Rightarrow H(p,q) = p\dot{q} - L(q,\dot{q}), \quad p = \frac{\partial L}{\partial \dot{q}}. \tag{1.16}$$

Equally, starting from some $f(x,y)$ and defining $z = \partial f/\partial y$ one can define

$$g(x,z) = f(x,y) - yz \tag{1.17}$$

satisfying

$$dg = \frac{\partial f}{\partial x}dx + \frac{\partial f}{\partial y}dy - ydz - zdy = \frac{\partial f}{\partial x}dx - ydz = \frac{\partial g}{\partial x}dx + \frac{\partial g}{\partial z}dz \tag{1.18}$$

since $\frac{\partial f}{\partial y}dy - zdy$ cancels.

1.4 Canonical Ensemble

Starting from $E = TS - pV + \mu N = E(S, V, N)$ (omit possible other variables) trade extensive $S \to$ intensive T by inverting $T = \partial E/\partial S$ to give $S = S(T, ..)$. Relevant formulas are:

$$F(T, V, N) = E - TS = -p(T, V, N)V + \mu(T, V, N)N$$

$$\begin{aligned} dF &= \frac{\partial F}{\partial T}dT + \frac{\partial F}{\partial V}dV + \frac{\partial F}{\partial N}dN \\ &= -S\ dT - p\ dV + \mu dN. \end{aligned} \tag{1.19}$$

Thus the first derivatives are

$$\frac{\partial F}{\partial T} = -S, \quad \frac{\partial F}{\partial V} = -p, \quad \frac{\partial F}{\partial N} = \mu \tag{1.20}$$

For the pair T, V there are three second derivatives, which can be expressed in terms of three measurable quantities, two specific heats and the sound velocity ($\rho = mn$ is the mass density):

$$F_{TT} = -S_T = -\frac{1}{T}C_V, \quad VF_{VV} = \rho\frac{C_V}{C_p}{\nu_s}^2, \quad {F_{TV}}^2 = \frac{\rho}{TV}{C_V}^2{\nu_s}^2(\frac{1}{C_V} - \frac{1}{C_p})$$

To derive these, use (1.15).

F is computed from the partition function:

$$Z = e^{-\beta F} = \mathrm{Tr} e^{-\beta H} = \sum_{\text{n=all states}} e^{-\beta E_n}, \quad \beta \equiv \frac{1}{T}. \tag{1.21}$$

The fixed values of V, N are implicit in the definition of "all states". The quantity $\rho = e^{-\beta H}/Z$ is the density matrix which maximizes the entropy -Trρ logρ keeping $\langle H \rangle = \mathrm{Tr}\rho H = E$ fixed.

Eq. (1.21) presents an extremely general formula: H can be the Hamiltonian of any quantum system! Much of the work in statistical mechanics boils down to computing Z, exactly or approximately.

Example. An important special case is that of $p = nT$-gas, ideal gas of non-relativistic particles in Maxwell-Boltzmann statistics. Let us review the appropriate formulas.

¿From the definition of Z one obtains for N identical independent particles

$$Z(T, V, N) = \sum_i e^{-\beta E_i} = \frac{1}{N!}\left(\frac{V}{\lambda_{\text{th}}^3}\right)^N = \frac{1}{N!}Z(1)^N \tag{1.22}$$

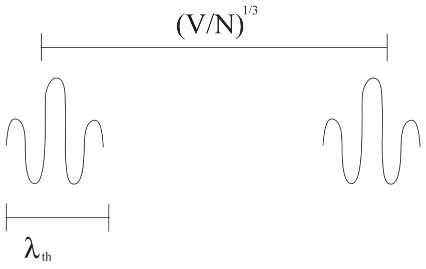

Figure 1.1: Particle wave packets should not overlap for MB statistics to be valid

where

$$Z(1) = \int \frac{d^3p\,d^3x}{h^3} e^{-p^2/(2mT)} \tag{1.23}$$

and

$$\lambda_{\rm th} = \hbar\sqrt{\frac{2\pi}{mT}} \tag{1.24}$$

is the thermal Compton wave length. In (1.23) one has applied the semiclassical rule that the volume $dxdp$ in phase space should be divided by h, Planck's constant. The rule is derived in (1.51) below. This statistics is valid if the distance between particles, $(V/N)^{1/3}$ is much greater than the size of wave packets, $\lambda_{\rm th}$. From (1.22), using Stirling, $N! \approx (N/e)^N$,

$$F = -NT\left(1 + \log\frac{V/N}{\lambda_{\rm th}^3}\right) \tag{1.25}$$

so that the validity criterion implies that the log here and below is a number of order 10, logs are never very big. The rest is now a mechanical application of the formulas given above. We have three first derivatives

$$\begin{aligned} S &= -\frac{\partial F}{\partial T} = N\left(\frac{5}{2} + \log\frac{V/N}{\lambda_{\rm th}^3}\right), & (1.26)\\ p &= -\frac{\partial F}{\partial V} = \frac{NT}{V}, & (1.27)\\ \mu &= -\frac{\partial F}{\partial N} = -T\log\frac{V/N}{\lambda_{\rm th}^3}. & (1.28) \end{aligned}$$

Inserting back to (1.25) one sees that $F = -NT + \mu N = -pV + \mu N = E - TS$, $E = \frac{3}{2}NT$. For the second derivatives in the T, V space one has $F_{TT} = -3N/2T$, $F_{TV} = -N/V$, $F_{VV} = NT/V^2$, compatible with $\gamma = C_p/C_V = 5/3$, $v_{\rm s}^2 = \gamma T/m$. We shall soon rederive these expressions in the full relativistic case from the complete BE and FD statistics.

As a quantitative application one may quote

$$\frac{S(\text{Argon})}{N} = 18.4 + \log[\frac{V}{22.4\text{l}}\cdot(\frac{T}{273\text{K}})^{3/2}]$$

These formulas illustrate the following properties of entropy:
- S is a pure number = (number of order 1)·N.
- S is additive (depends on V/N, resolution of Gibbs paradox).
- S(T=0) is undefined; it can be meaningfully discussed only in true Fermi-Dirac or Bose-Einstein statistics.

One difference between a physicist and a chemist is that the former counts particles microscopically and simply writes $pV = NT$ or even simpler $p = nT$. The latter measures amounts of gas of atomic number A by weighing macroscopically and thus has to convert mass to number by (g=gram)

$$N = \frac{M}{Am_p} \equiv \frac{M}{A\text{g}}N_A, \quad m_p \equiv \frac{1}{N_A}\text{g} \tag{1.29}$$

so that the gas law becomes $pV = (M/(A\mathrm{g})N_A T \equiv RT$, where R is the universal gas constant. Actually m_p here is replaced by mass of a ^{12}C atom divided by 12. The dimensionless number $M/(A\mathrm{g})$ is called the number of moles of the gas.

Exercise.Check that (room temperature/pressure)$^{1/3}$ gives the average distance between molecules in the air ≈ 3 nm.

Example: black hole entropy. For comparison, the black hole entropy is

$$S_{\mathrm{BH}} = \frac{4\pi G M^2}{\hbar c} \equiv 4\pi \frac{M^2}{M_{\mathrm{Pl}}^2} = \frac{c^3}{\hbar G}\frac{A}{4} \equiv \frac{A}{8\pi L_{\mathrm{Pl}}^2}, \tag{1.30}$$

where M is the black hole mass and $A = 4\pi r_{\mathrm{s}}^2$, $r_{\mathrm{s}} = 2GM/c^2$ are respectively its area and the Schwartzschild radius. For a ball of gas like the sun we would have $S_{\mathrm{sun}} \sim N \sim nV \sim M/m_p \sim 10^{57}$ since in the Sun there are about $(M_{\mathrm{Pl}}/m_p)^3 = 10^{57}$ (m_p= proton mass) nucleons. For a BH with the same mass

$$S_{\mathrm{BH}}(M = M_{\mathrm{sun}} = m_p (\frac{M_{\mathrm{Pl}}}{m_p})^3) = 4\pi (\frac{M_{\mathrm{Pl}}}{m_p})^4 \approx 10^{77}. \tag{1.31}$$

So the entropy of a solar mass black hole wins that of the sun by a factor $\sim 10^{20}$; collapse increases S tremendously. Similarly, the entropy of a single million solar mass BH in the center of a galaxy equals the entropy of the entire cosmic background radiation.

Actually even for a black hole $S \sim N$, but N is now the number of quanta in the Hawking radiation emitted by the black hole. If there is radiation at $T = T_{\mathrm{Hawk}}$ the energy of each quantum is $\sim T_{\mathrm{Hawk}}$ and one may argue that their number is

$$N \sim Mc^2/T_{\mathrm{Hawk}} \sim S \sim (M/M_{\mathrm{Pl}})^2 \tag{1.32}$$

so that (with correct factors inserted)

$$T_{\mathrm{Hawk}} = \frac{\hbar\kappa}{2\pi c} = \frac{\hbar c}{4\pi r_s} = \frac{\hbar c^3}{8\pi G M} = \frac{M_{\mathrm{Pl}}^2 c^2}{8\pi M}. \tag{1.33}$$

Here κ is the surface gravity $\kappa = GM/r_{\mathrm{s}}^2 = c^2/(2r_s)$. Many alternative expressions were given here.

Let us parametrically estimate the lifetime of a radiating BH. The radiation luminosity in J/m^2/s is $\sim T^4$ (derived later) so that the total power = mass loss is

$$\frac{dM}{dt} \sim -r_s^2 T_{\mathrm{Hawk}}^4 \sim -\frac{1}{r_s^2} \sim -\frac{M_{\mathrm{Pl}}^4}{M^2}. \tag{1.34}$$

Integration leads to $M^3(t) = M^3(0) - 3M_{\mathrm{Pl}}^2 t$ and the mass is gone when

$$t \sim \left(\frac{M(0)}{M_{\mathrm{Pl}}}\right)^3 \frac{1}{M_{\mathrm{Pl}}}. \tag{1.35}$$

A BH of mass 10^{12}kg would live as long as the present universe radiating at a temperature of ~ 10 MeV.

These results arise from considerations of virtual particle production near the event horizon, or more properly, from field theory in curved space. Entropy of a black hole seems rather puzzling considering that the black hole is pointlike; from a (classical) statistical perspective, it should not have entropy any more than, say, an electron. However, perhaps a black hole has a substructure? The key question then is, what exactly are the microscopic degrees of freedom that give rise to the entropy of a black hole? This is one of the deepest questions of today's physics. In string theory the answer would be that black holes are just certain string (or brane) configurations in extra dimensional spaces.

Modification: Tsallis statistics. The exponential function e^x permeates statistical physics. We know that $e^x = \lim_{n\to\infty}(1 + x/n)^n$. Tsallis statistics [1] introduces here one parameter q by defining

$$e_q(x) = \left(1 + \frac{x}{n}\right)^n, \qquad n \equiv \frac{1}{1-q} \tag{1.36}$$

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[1] see, e.g., http://www.ccsem.infn.it/issp2006/docs/Tsallis.pdf or http://tsallis.cat.cbpf.br/biblio.htm

Its inverse defines a q-logarithm

$$\log_q(x) = n(x^{1/n} - 1) = \frac{x^{1-q} - 1}{1-q}. \tag{1.37}$$

The crucial functional equations satisfied by log and exp are modified:

$$\log_q(xy) = \log_q(x) + \log_q(y) + (1-q)\log_q(x)\log_q(y). \tag{1.38}$$

Entropy will now be defined by

$$S_q(p) = \frac{1}{q-1}\left(1 - \sum_{i=1}^{N} p_i^q\right), \quad \sum_i p_i = 1 \tag{1.39}$$

and satisfies $S_q(p_i q_j) = S_q(p_i) + S_q(q_j) + (1-q)S_q(p_i)S_q(q_j)$; entropy is non-extensive. Proceeding from this one can develop q-thermodynamics with some interesting q-mathematics. In nature there are lots of distributions which are non-exponential, rather powerlike, and they can often be fitted with some value of q. Effectively one writes

$$e^{-E/T} \Rightarrow \frac{1}{(1+E/T_0)^{(T_0/T)}} \tag{1.40}$$

and fits the measured E-distribution. Note that one can write

$$e_q(x)^{-1} = \frac{1}{(1+x/n)^n} = \frac{1}{\Gamma(n)}\int_0^\infty dt\, t^n e^{-(n+x)t}, \tag{1.41}$$

which describes the q-exponential as a weighted integral over exponentials.

1.5 Grand Canonical ensemble

Going from microcanonical to canonical we replaced $E = TS - pV + \mu N \Rightarrow F = -pV + \mu N$. Now we clearly have two alternatives, either trade N for μ (get $\Omega = -pV = -Vp(T,\mu)$, the grand canonical ensemble) or trade V for p (get $G = \mu N = N\mu(T,p)$, the Gibbs ensemble). Chemists like the Gibbs energy but we shall concentrate on the grand potential Ω, since we often have a situation with some conserved (= commutes with the Hamiltonian, $[H,N]=0$) particle number N. The basic equation is

$$\mathcal{Z}(T,V,\mu) = e^{-\beta\Omega} = \mathrm{Tr} e^{-\beta(H-\mu N)} = \sum_{N=0}^{\infty}(e^{\beta\mu})^N \mathcal{Z}(T,V,N), \qquad [H,N]=0 \tag{1.42}$$

This is a "generating function of multiplicity moments", $Z(z) = \sum_{N=0}^{\infty} z^N Z(N)$, with $z = e^{\beta\mu}$ sometimes called fugacity. Since Ω is extensive and V is the only extensive variable, we must have

$$\Omega = -Vp(T,\mu)\ . \tag{1.43}$$

The remaining basic equations are

$$d\Omega = -SdT - pdV - Nd\mu, \quad S = -\frac{\partial\Omega(T,\mu)}{\partial T}, \quad N = -\frac{\partial\Omega(T,\mu)}{\partial\mu}, \tag{1.44}$$

which we write in terms of densities as

$$s(T,\mu) = +\frac{\partial p(T,\mu)}{\partial T}, \qquad n(\mu,T) = \frac{\partial p(T,\mu)}{\partial\mu} = \frac{N}{V}. \tag{1.45}$$

Here the first derivatives give averages, the second derivatives give fluctuations, widths of distributions, e.g.,

$$\langle N^2\rangle - \langle N\rangle^2 = -T\frac{\partial^2\Omega}{\mu^2} = TV\frac{\partial^2 p}{\partial\mu^2}. \tag{1.46}$$

Thus pressure is the fundamental quantity. It gives s and n and the energy density ϵ through

$$\epsilon = Ts - p + \mu n. \tag{1.47}$$

In thermal equilibrium, Ω is minimised and hence p is maximised. In particular, if the system has several different minima of Ω, the true stable ground state is the one with minimal Ω (maximal pressure); the other ones are metastable states. This is a very common situation (see Fig.**??** below).

1.6 Density of states

The general relation (1.21) can, by normalising $E \geq 0$, be written in the form

$$Z = e^{-\beta F} = \mathrm{Tr} e^{-\beta H} = \sum_{\text{n=all states}} e^{-\beta E_n} = \int_0^\infty dE\,\frac{dN}{dE}e^{-\beta E}, \tag{1.48}$$

where

$$\frac{dN}{dE} \equiv \rho(E) \equiv \rho(E,N) \tag{1.49}$$

is the density of states, the number of states of the system per unit E. The relation (1.48) implies that $Z(\beta)$ and $\rho(E)$ are Laplace transforms of each other. Both are as good in giving the full thermodynamics. The density of states is practical since it arises naturally in numerical simulations. It is also conceptually important: of there is an exponential density of states, there is a singularity in the partition function.

Example: Particle(s) in a box. This trivial case is a cornerstone. From periodicity (surface effects can usually be neclected) of a 3d box

$$\mathbf{k} = \frac{2\pi}{L}(n_1,n_2,n_3), \quad n_i = 0, \pm1, \pm2, .. \tag{1.50}$$

so that ($E^2 = k^2 + m^2$)

$$\sum_i = \int d^3n = \frac{V}{(2\pi)^3}\int d^3k = \int_m^\infty dE\frac{V}{2\pi^2}E\sqrt{E^2-m^2}. \tag{1.51}$$

Note that now we have derived the classical result (1.23):

$$\sum_i = \int \frac{Vd^3k}{(2\pi)^3} = \int \frac{d^3x\,d^3p}{h^3} \tag{1.52}$$

since $p = \hbar k$. In the ultrarelativistic (UR) limit, where $m << E$, and in the non-relativistic (NR) limits we thus obtain

$$\rho_{\rm UR}(E) = \frac{1}{2E}\frac{VE^3}{\pi^2}, \quad \rho_{\rm NR}(E) = \frac{V}{2\pi^2}m\sqrt{2mE}. \tag{1.53}$$

E	$N(E) = \log S(E)$
-200	1
-196	0
-192	100
-188	190
-184	5390
-180	19920
-176	226185
-172	1123330
-168	8441545
-164	46439270
-160	288232165
-156	1596503840
-152	9008597790
-148	48530806690
-144	258919598835
-140	1348085135068
-136	6918375532625
-132	34921952998720
-128	173864285141465
-124	853528946161100
-120	4131702217991006
-116	19598116107747500
-112	92337394182797240
-108	424635096183933970
-104	1910993686546702565
-100	8394325581182421100
-96	35900636024138056610
-92	149134699701274540190
-88	600434187444808042305
-84	2338237484656296289710
-80	8790991827530811266845
-76	31852806882802872810510
-72	111039862678342970767760
-68	371793726574328382611580
-64	1193670523583033542771745
-60	3668437423804485582262430
-56	10772807184138254585743365
-52	30174747119602748554894980
-48	80467250627920555722255415
-44	203904785227407787528278180
-40	490026517327332203099130689
-36	1114622254786255520262613920
-32	2974787743912498152267010800
-28	4849969799910449080522379200
-24	9239228193366464362451697155
-20	16521328755364544210468233924
-16	27673114057688890670065067455
-12	43328960149817735987320787580
-8	63289600282274727602148469440
-4	86076254527328476831763676120

E	$N(E) = \log S(E)$
0	108804232426376087683496097815
4	127615138775266749696010320050
8	138682226083589753382353631155
12	139467535997338317070747513220
16	129673265537564086898449474485
20	111398087687361442602934363604
24	88394194656000609637107306835
28	64789735278060885125545778420
32	43882526876091406802688842040
36	27484620182084875609413209920
40	15934677821408488316923097025
44	8562769731912107647661352420
48	4271377195758556988860024315
52	1981325557749994784540426400
56	856247175668720270761391354
60	345440085480687517414714344
64	130373941135805243213306725
68	46131131663242989983156880
72	15336949736067657882440975
76	4801625511818556981759340
80	1418746354667950902604900
84	396504230728933768862650
88	105044804469611713155910
92	26439076355718752657610
96	6336775057494900296995
100	1449347253869825330984
104	317184792213120157975
108	66590745159525686410
112	13450173814318534170
116	2621824707749641960
120	494837291835094171
124	90726699739843320
128	16209249292505960
132	2829255985524290
136	483344637121035
140	80889449574800
144	13259776474415
148	2126884521530
152	333319272600
156	50912615760
160	7565408818
164	1088231770
168	151489010
172	20119550
176	2579540
180	303762
184	35230
188	3340
192	350
196	20
200	2

Table 1.1: State counts for the Ising model on a 10 by 10 lattice (Stodolsky-Wosiek, Nucl.Phys. B413(94) 817)

But what if we have N MB particles in a box? Then by just counting the states one has

$$\rho(E,N) = \frac{1}{N!}\int \delta(E - \sum_i E_i)\prod_1^N \frac{V}{(2\pi)^3}\int d^3k_i, \tag{1.54}$$

which one can evaluate by introducing a Fourier representation for the δ function and using steepest descent. But let us compute $\rho(E,N)$ by inverting the Laplace:

$$\rho(E,N) = \frac{1}{2\pi i}\int_{-i\infty+\beta_c}^{i\infty+\beta_c} d\beta Z(\beta,N) \tag{1.55}$$

for the UR case

$$Z(\beta,N) = \frac{1}{N!}\left(\frac{VT^3}{\pi^2}\right)^N. \tag{1.56}$$

A saddle point calculation leading to $\beta_c = 3N/E$ gives

$$\rho(E,N) = \frac{1}{N!\,(3N-1)!}\frac{1}{E}\left(\frac{VE^3}{\pi^2}\right)^N, \tag{1.57}$$

a powerlike behaviour. Remember, though, that the exponent can be gigantic. However, if you do the same with the Grand potential $\Omega(T,\mu)$, using

$$Z(T,z) = \sum_{N=0}^{\infty} z^N Z(T,N) = \int_0^\infty dE\,\rho(E,z)e^{-\beta E} = \exp(zVT^3/\pi^2), \quad z = e^{\beta\mu} \tag{1.58}$$

and (1.55) in the saddle point approximation (with $\beta_c^4 = 3zV/(\pi^2 E)$), one finds

$$\rho(E,z) = \frac{1}{\sqrt{8\pi}}\left(\frac{3zV}{\pi^2}\right)^{\frac{1}{8}} E^{-\frac{5}{8}}\exp\left[\frac{4}{3}\left(\frac{3zV}{\pi^2}\right)^{\frac{1}{4}} E^{\frac{3}{4}}\right], \tag{1.59}$$

an exponential of a fractional power.

Example: particles in a harmonic potential. Instead of a box we can also have a smoother confinement by a harmonic oscillator potential $V = \frac{1}{2}m\omega^2\mathbf{x}^2$. This case will be important when discussing Bose-Einstein condensation. Then the energy spectrum is $(\omega_i = \omega)$

$$E = \hbar\omega(n_1 + n_2 + n_3 + \frac{3}{2}), \quad n_i = 0,1,2,\ldots \tag{1.60}$$

and we can write

$$\sum_{\text{states}} = \int d^3n = \int dE \int d^3n\,\delta(E - \hbar\omega(n_1+n_2+n_3)) \equiv dE\rho(E), \tag{1.61}$$

with (integrating first over n_3 and imposing the condition $n_3 > 0$

$$\rho(E) = \frac{1}{\hbar\omega}\int_0^\infty dn_1 dn_2 \Theta\left(\frac{E}{\hbar\omega} - n_1 - n_2\right) = \frac{E^2}{2(\hbar\omega)^3}. \tag{1.62}$$

More generally, in d dimensions,

$$\rho(E) = \frac{E^{d-1}}{(d-1)!\prod \hbar\omega_i}. \tag{1.63}$$

Example: Ising model. We shall later define the d-dimensional Ising model. For this one can numerically compute the exact numbers of states corresponding to a fixed total energy of the system. A concrete example for the 2d model is shown in Table 1.1. Huge numbers enter; more of them can be found in Paul D. Biele, Phys. Rev. Letters 76, 78, 1996 or F. Wang and D.P.Landau, Phys. Rev. E64, 056101, 2001.

Example: density of state and partitioning an integer. Some cute combinatorics enters here. See http://arxiv.org/ps/math-ph/0309020.

Let us now try to evaluate the expression Eq. (1.48) in suitable approximation. Since (or when) $\rho(E)$ increases extremely fast and since $e^{-\beta E}$ decreases fast the method of choice is the saddle point "semi-classical" approximation:

$$\begin{aligned}
\int_{-\infty}^{\infty} dx\, e^{-\frac{1}{\hbar}S(x)} &= \int_{-\infty}^{\infty} dx\, \exp\{-\frac{1}{\hbar}[S(\bar{x}) + S'(\bar{x})(x-\bar{x}) + \frac{1}{2}S''(\bar{x})(x-\bar{x})^2 + \frac{1}{6}S'''(\bar{x})(x-\bar{x})^3 + \\
&\qquad + \frac{1}{24}S''''(\bar{x})(x-\bar{x})^4 + \ldots]\} \\
&= e^{-\frac{1}{\hbar}S(\bar{x})} \int_{-\infty}^{\infty} dx\, \exp[-\frac{1}{2\hbar}\bar{S}''(x-\bar{x})^2 - \frac{1}{6\hbar}\bar{S}'''(x-\bar{x})^3 - \frac{1}{24\hbar}\bar{S}''''(x-\bar{x})^4 + \ldots] \\
&= e^{-\frac{1}{\hbar}S(\bar{x})}\sqrt{\frac{2\hbar}{\bar{S}''}} \int_{-\infty}^{\infty} dy\, e^{-y^2}[1 - \frac{\hbar}{6}\frac{\bar{S}''''}{(\bar{S}'')^2}y^4 + \frac{\hbar}{9}\frac{(\bar{S}''')^2}{(\bar{S}'')^3}y^6 \ldots] \\
&= e^{-\frac{1}{\hbar}S(\bar{x})}\sqrt{\frac{2\pi\hbar}{\bar{S}''}}\left\{1 - \hbar\left[\frac{\bar{S}''''}{8(\bar{S}'')^2} - \frac{5}{24}\frac{(\bar{S}''')^2}{(\bar{S}'')^3}\right] + \mathcal{O}(\hbar^2)\right\} \qquad (1.64)
\end{aligned}$$

We have gone through the various steps in some detail since there is lots of important physics behind the simple mathematics here:

- First, we have introduced $\hbar$ as a formal parameter and one observes that the outcome will be an expansion in $\hbar$.
- Second, we have expanded the integrand around some point $\bar{x}$ and chosen this point so that $S'(\bar{x}) = 0$ (the name saddle point fits better when this is done in the complex domain or with more than one degree of freedom). This is the analogue of finding classical equations of motion by extremizing the action; $S(x)$ is the action and $\bar{x}$ is the analogue of a solution of classical equations of motion.
- For the solution to be a stable minimum, one must have $\bar{S}'' \equiv S''(\bar{x}) > 0$. Then one can take $y = \sqrt{\bar{S}''/2\hbar}(x-\bar{x})$ as a new variable, expand in $\sqrt{\hbar}$ and do the y integral. The odd terms vanish and the result becomes an expansion in $\hbar$.
- In the result the first term has, in various connections, the names classical, tree level, mean field approximation. Its evaluation is relatively simple, one just finds the "classical field" $\bar{x}$ and finds the value of the action for this field. The second term is important in that it gives the correct dimensions (those of x) to the integral. It is called the fluctuation, Gaussian, one-loop term and its evaluation is often possible - it comes from a Gaussian integration - but may be technically very complicated. The corrections are, for example, called loop corrections. For the harmonic oscillator they vanish.

To apply Eq. (1.64), write the partition function (1.48) as (include $1/T$ to keep Z dimensionless and extend the lower limit to $-\infty$, what matters is anyway a small region around the saddle point)

$$Z = \int_{-\infty}^{\infty} dE \frac{dN}{dE} e^{-\beta E} \equiv \int_{-\infty}^{\infty} dE \frac{1}{T} e^{S(E)-\beta E}. \qquad (1.65)$$

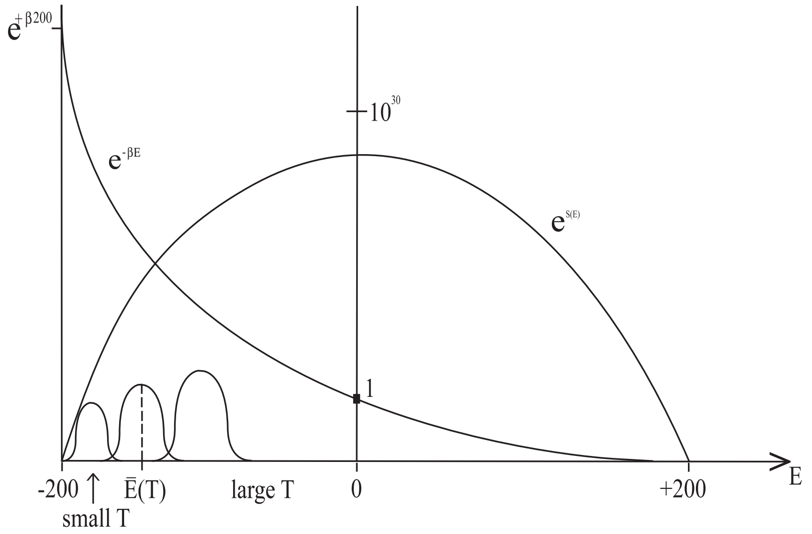

Figure 1.2: S, E competition in more detail (schematically)

In the saddle point approximation one solves $\bar{E}$ from $S'(\bar{E}) = \beta$ and expands the integrand around $\bar{E}$. Neglecting higher terms $S(E) - \beta E = S(\bar{E}) - \beta\bar{E} + S'(\bar{E}) - \beta + \frac{1}{2}(E-\bar{E})^2 S''(\bar{E})$ and

$$\begin{aligned} Z &= \frac{1}{T} e^{S(\bar{E})-\beta\bar{E}} \int_{-\infty}^{\infty} dE e^{-\frac{1}{2}S''(E-\bar{E})^2} \\ &= e^{S(\bar{E})-\beta\bar{E}} \sqrt{\frac{2\pi}{-T^2 S''(\bar{E})}} = e^{-\beta F}. \end{aligned} \tag{1.66}$$

What is happening is shown in Fig.1.6: rapidly increasing and decreasing terms together give a Gaussian. The saddle point equation further gives $S''(\bar{E}) \cdot d\bar{E}/dT = -1/T^2$ so that the specific heat $C_V = d\bar{E}/dT = -1/T^2 S''(\bar{E})$. From the above we can then read

$$F(T) = \bar{E}(T) - TS(\bar{E}(T)) - \frac{1}{2} T \log C_V \approx \bar{E}(T) - TS(\bar{E}(T)) \ . \tag{1.67}$$

($T \log C_V$ is tiny and can be neglected).

Thermodynamics is in derivatives of $F(T)$ (there is no N, μ in this simple example):

$$\begin{cases} F'(T) = \bar{E}'(T) - S(\bar{E}(T)) - TS'(E) \cdot \frac{d\bar{E}}{dT} = -S(\bar{E}(T)), \\ F''(T) = -S'(\bar{E}) \cdot \frac{d\bar{E}}{dT} = -\frac{1}{T} C_V. \end{cases}$$

The probability for a fixed E is

$$P(E) = \frac{1}{Z} \frac{dN}{dE} e^{-\beta E} \approx \sqrt{\frac{-S''}{2\pi}} e^{-\frac{(-S'')}{2}(E-\bar{E})^2} \tag{1.68}$$

The factor $(-S'')$ represents fluctuations in energy: $\langle (E-\bar{E})^2 \rangle = 1/\sqrt{-S''} = T\sqrt{C_V}$.

Example: negative temperature The competition between entropy and energy is manifest also for negative temperatures. (When finding the most likely partition, temperature is just a Lagrange multiplier that can be either positive or negative, see Eq. (1.7).) Negative temperature requires that there is a finite upper limit in the energy spectrum; otherwise the Boltzmann factor, i.e. the occupation probability, $\mathrm{e}^{-\beta E}$ would grow without limit for $\beta < 0$.

Consider a 2-state spin system in an external magnetic field $\mathbf{B}$ with

$$H = -\mu \cdot \mathbf{B} = \begin{cases} +\mu B \equiv +E_0 & \text{spin } \downarrow \\ -\mu B \equiv -E_0 & \text{spin } \uparrow \end{cases} \tag{1.69}$$

For fixed particle number N, the total energy and entropy can then be written as

$$\begin{aligned} E &= -n_1 E_0 + (N - n_1) E_0, \\ S &= -n_1 \log n_1 - (N - n_1) \log (N - n_1), \end{aligned} \tag{1.70}$$

where n_1 is the occupation number of the spin $\uparrow$ level.

Since $F = S - \beta E$, as $\beta \to 0_+$ the free energy is extremized by S, and $dS/dn_1 = 0$ implies $n_1 = N/2 = n_2$, a fully disordered state. The same holds when $\beta \to 0_-$. For $\beta \to \infty$, when F is extremized by E, we would find $n_1 = N, n_2 = 0$ so that at zero temperature the system is at its ground state. However, when $\beta \to -\infty$, we find $n_2 = N, n_1 = 0$ so that the system finds itself in the excited state.

Since the disordered state corresponds to both $T = \infty$ and $T = -\infty$, one can say that the jump from positive to negative temperatures goes by way of infinity. "Negative temperatures", i.e. certain partitions, have been observed in well isolated systems of e.g. silver and rhodium atoms[2].

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[2] See P.Hakonen and O.Lounasmaa, Science 265 (1994) 1821.

Chapter 2

Partition functions and path integrals

In the previous section we discussed how all the equilibrium thermodynamics can be computed from the partition function, defined by

$$Z = e^{-\beta F} = e^{-\beta E+S} = \mathrm{Tr} e^{-\beta H} = \sum_{\mathrm{states}} e^{-\beta E_i}, \tag{2.1}$$

where the sum goes over all the eigenstates i of the *Hamiltonian* of the system.

Now comes a very important technical step: we write the fundamental formula for the partition function as a path integral containing the *Lagrangian* of the system. Symbolically,

$$Z = e^{-\beta F} = \mathrm{Tr}\, e^{-\beta H} \Rightarrow \int \mathcal{D}\Phi\, e^{-S[\Phi]/\hbar}, \tag{2.2}$$

where Φ is a set of degrees of freedom defining the system, $\mathcal{L}[\Phi]$ is the Lagrangian density of the theory governing the dynamics of the degrees of freedom Φ and $S[\Phi] = \int d\tau d^3x \mathcal{L}[\Phi]$ is the *Euclidean* action. We shall see that thermodynamics leads to Euclidean spacetime with imaginary time which we shall, conventionally, define as $\tau = it$. The measure $\mathcal{D}\Phi \equiv \Pi d\Phi$ is defined so that in the path integral one is integrating over all possible field configurations $\Phi(\boldsymbol{x}, \tau)$ (which are functions). To get a proper Minkowskian quantum (field) theory, we need to Wick rotate $\tau \to it$ to obtain $e^{-S_E[\Phi]/\hbar} \to e^{iS_M[\Phi]/\hbar}$. (For rules of going from Minkowski to Euclidian space, see end of Section 2.2.)

The relation between quantum mechanics and field theory should be appreciated at this stage. In the simplest quantum mechanical case, particle in one dimension x, $\Phi = x$ so that one integrates over all possible paths $x(t)$ of the particle. This is straightforward to generalise first into one particle in many dimensions, $\Phi = \mathbf{x}$, then to N particles in many dimensions, $\Phi = \mathbf{x}_i$, $i = 1, .., N$, in just adds more indices. N can be arbitrarily large but it always obtains discrete values. However, in quantum field theory the index i corresponds to the value of some field ϕ (possibly with many components ϕ_a) in the spatial point $\mathbf{x}$, $\phi(t, \mathbf{x}) \equiv \phi_{i=\mathbf{x}}(t)$ so that effcectively $N \to$ continuum ∞. Then sums become integrals, $\sum_{i=1}^{N} \to \int d^dx$, functions of coordinates $\mathbf{x}_i$ become functionals of fields $\phi(t, \mathbf{x})$, etc.

The partition function is a powerful tool in many fields of physics and writing it in path integral form is an exercise one will never regret. All the correlators – and hence all physics – can be constructed as expectation values from the probability distribution defined by Z:

$$\langle \Phi_1 \Phi_2 \ldots \Phi_N \rangle = Z^{-1} \int \mathcal{D}\Phi \, \Phi_1 \Phi_2 \ldots \Phi_N e^{-S[\Phi]/\hbar}. \tag{2.3}$$

To compute them, one introduces the *generating functional*

$$Z[J] = e^{-W[J]} = \int \mathcal{D}\Phi e^{-S[\Phi] - \int dx J \Phi} \ , \tag{2.4}$$

where dx stands for $d\tau$ or $d\tau d^n x$, depending on the case at hand. One then takes (functional) derivatives with respect to J to obtain

$$\langle \Phi_1 \Phi_2 \ldots \Phi_N \rangle = (-1)^{N-1} \frac{\delta^N Z[J]}{\delta J(x_1) \delta J(x_2) \cdots \delta J(x_N)}\Big|_{J=0} \ . \tag{2.5}$$

A reminder: Functional differentiation. Let $E[f]$ be a functional of $f(x)$ (e.g. $E = \int dx\, f(x)$ etc.). Then functional derivation is defined as

$$\frac{\delta E[f(x)]}{\delta f(y)} = \lim_{\epsilon \to 0} \frac{E[f(x) + \epsilon \delta(x-y)] - E[f(x)]}{\epsilon} \ . \tag{2.6}$$

The chain rule

$$\frac{\delta E}{\delta f(y)} = \int dx' \, \frac{\delta E}{\delta F(x')} \frac{\delta F(x')}{\delta f(y)} \tag{2.7}$$

holds and so on. The functional Taylor series is defined by

$$E[f] = \sum_{n=0}^{\infty} \frac{1}{n!} \int dx_1 \ldots dx_n f(x_1) \ldots f(x_n) \frac{\delta^n E[f]}{\delta f(x_1) \ldots \delta f(x_n)}\Big|_{f=0} \ . \tag{2.8}$$

As a concrete example, let us consider the functional $E[J] = \int dx\, dy\, J(x) K(x-y) J(y)$; this is a functional of the function J, and K is a fixed *kernel function.* Then the functional derivative is

$$\begin{aligned} \frac{\delta E}{\delta J(z)} &= \int dx\, dy \, \underbrace{\frac{\delta J(x)}{\delta J(z)}}_{\delta(x-y)} K(x-y) J(y) + \ldots \\ &= \int dy\, K(z-y) J(y) + \int dx\, K(x-z) J(x) \\ &= 2 \int dx\, K(z-y) J(y) \ . \end{aligned}$$

Likewise, the second functional derivative is found to be

$$\frac{\delta^2 E}{\delta J(z) \delta J(u)} = 2 \int dx\, K(z-y) \underbrace{\frac{\delta J(y)}{\delta J(u)}}_{\delta(y-u)} = 2K(z-u) \ . \tag{2.9}$$

A practical way to approach functional derivation is to think of the function $f(x)$ as a variable f with an index x, never minding what the mathematicians say.

2.1 Partition function of a particle in a potential as a path integral

What is important and perhaps surprising in the path integral formulation is that the Lagrangian (or its integral, the action) appears, not the Hamiltonian. This is a great simplification at least when Lorentz covariance is needed. So let us first collect some simple Hamiltonian mechanics formulas relating $L(x,\dot{x})$ and $H(x,p)$ for a particle in a potential $V(x)$ in 1+1 dimensions (e.g., $V=\frac{1}{2}m\omega^2x^2$):

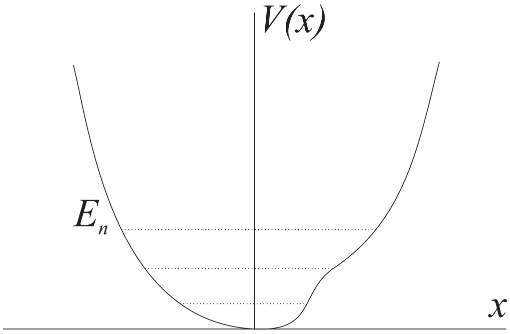


Figure 2.1: Particle in potential $V(x)$; discrete energy levels are known.

Classically, the Lagrangian is

$$L(x,\dot{x})=T-V=\frac{1}{2}m\dot{x}^2-V(x) \tag{2.10}$$

leading to the equation of motion (the solutions of which give the extrema of the action $\int dtL$)

$$\frac{\partial L}{\partial x}-\frac{d}{dt}\frac{\partial L}{\partial\dot{x}}=-V'(x)-m\ddot{x}=0 \quad\Rightarrow\quad m\ddot{x}=-V'(x)=F(x). \tag{2.11}$$

The Hamiltonian is obtained as the Legendre transform:

$$H=H(x,p)=p\dot{x}-L(x,\dot{x})=\frac{p^2}{2m}+V(x), \quad p=\frac{\partial L}{\partial\dot{x}}=m\dot{x} \tag{2.12}$$

so that

$$dH=\frac{\partial H}{\partial x}dx+\frac{\partial H}{\partial p}dp=\dot{x}dp+pd\dot{x}-\frac{\partial L}{\partial x}dx-\frac{\partial L}{\partial\dot{x}}d\dot{x} \tag{2.13}$$

from which follow the Hamiltonian equations of motion

$$\dot{p}=-\frac{\partial H}{\partial x}, \qquad \dot{x}=\frac{\partial H}{\partial p} \tag{2.14}$$

(and possibly $\partial L/\partial t=\partial H/\partial t$). In quantum mechanics $p\to -i\hbar\partial_x$ and $E\to i\hbar\partial_t$:

$$i\hbar\partial_t\Psi(x,t)=H\Psi(x,t)=\big[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\big]\Psi(x,t)=E_n\Psi(x,t) \tag{2.15}$$

$$\Psi(x,t) = e^{-\frac{i}{\hbar}E_n t}\Psi(x) \tag{2.16}$$

so that the evolution operator is

$$U(t,0) = e^{-iHt/\hbar} \tag{2.17}$$

and the amplitude for an infinitesimal step from x_1 to x_2 is given by

$$\langle x_2(t+\Delta t)|x_1(t)\rangle = \langle x_2|e^{-iH\Delta t/\hbar}|x_1\rangle \ . \tag{2.18}$$

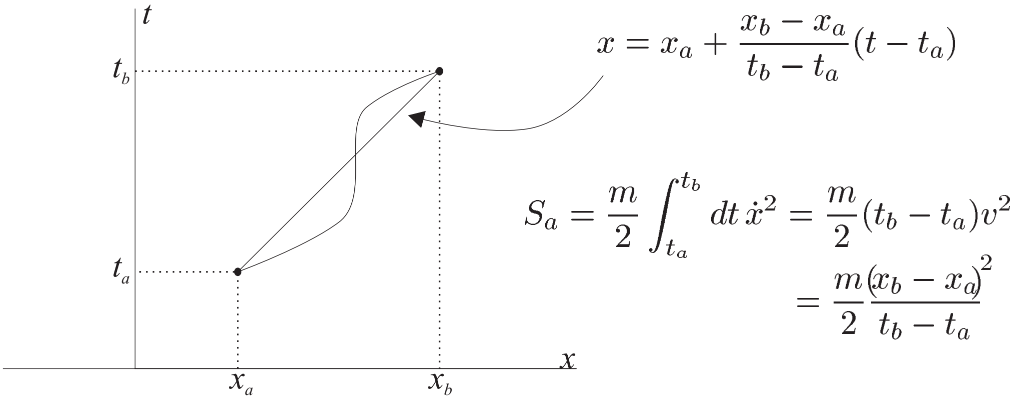
We observe that the Boltzmann factor is obtained from the evolution operator by taking $t = -i\hbar\beta$:

$$U(t=-i\hbar\beta,0) = e^{-\beta H}. \tag{2.19}$$

This hints at a the connection between imaginary time and thermodynamics (remember that there is no real time in equilibrium thermodynamics!) as well as at a connection between thermal averages and real-time amplitudes represented as sums over all possible paths.

In quantum mechanics, in important quantity is the matrix element $< x_b t_b | x_a t_a >$, the propagator from point x_a at time t_a to point x_b at time t_b. This can be evaluated exactly for the harmonic oscillator. First, for a free particle the result is

$$\langle x_b t_b | x_a t_a\rangle = \sqrt{\frac{m}{2\pi i\hbar(t_b - t_a)}}\exp[\frac{i}{\hbar}\overbrace{\frac{m}{2}\frac{(x_b-x_a)^2}{t_b-t_a}}^{\text{class. action}}] \tag{2.20}$$



$$x = x_a + \frac{x_b - x_a}{t_b - t_a}(t - t_a)$$

$$S_a = \frac{m}{2}\int_{t_a}^{t_b} dt\,\dot{x}^2 = \frac{m}{2}(t_b - t_a)v^2$$
$$= \frac{m}{2}\frac{(x_b - x_a)^2}{t_b - t_a}$$

Figure 2.2: Free particle with classical path and action.

For the harmonic oscillator, $V = \frac{1}{2}m\omega^2 x^2$:

$$\begin{aligned}
\langle x_b t_b | x_a t_a\rangle &= \sqrt{\frac{m\omega}{2\pi i\sin[\omega(t_b-t_a)]}}\exp\left\{\frac{im\omega}{2\hbar\sin[\omega(t_b-t_a)]}\left[(x_a^2+x_b^2)\cos[\omega(t_b-t_a)] - 2x_a x_b\right]\right\} \\
&= \underbrace{\sqrt{\begin{matrix}\text{determinant of gaussian fluctua-}\\ \text{tion (around classical solution)}\end{matrix}}}_{\begin{matrix}\text{can be calculated}\\ \text{exactly for harm. oscillator!}\end{matrix}} \cdot \exp\left\{\frac{i}{\hbar}S_a(\text{harm.osc.})\right\}
\end{aligned} \tag{2.21}$$

After these preliminaries, go back to the main problem, changing Tr$e^{-\beta H}$ to a "path" integral? What paths are there if there is no time? (Paths will be pariodic paths in imaginary time!).

We have one particle in 1+1d in some $V(x)$ (see fig.2.8) with the Hamiltonian $H = H(x,p) = \frac{p^2}{2m} + V(x)$. To evaluate the Trace we shall use two complete orthonormal sets of basic states $|x\rangle$ or $|p\rangle$:

$$|p\rangle = \underbrace{\sum_x |x\rangle\langle x|}_{=1,\quad \text{completeness}} p\rangle \equiv \int dx\, \underbrace{\langle x|p\rangle}_{e^{ipx}} |x\rangle \tag{2.22}$$

To normalize carefully one should use a finite box and let $L \to \infty$. Then simply

$$\mathrm{Tr}e^{-\beta H} = \int_{-\infty}^{\infty} dx_1\, \langle x_1|e^{-\beta H}|x_1\rangle. \tag{2.23}$$

Now comes the trick: write

$$e^{-\beta H} = e^{-\frac{\beta\hbar}{N}\cdot\frac{H}{\hbar}} \cdot e^{-\frac{\beta\hbar}{N}\cdot\frac{H}{\hbar}} \cdot \ldots \cdot e^{-\frac{\beta\hbar}{N}\cdot\frac{H}{\hbar}} \quad (N \text{ times}) \tag{2.24}$$

and put

$$\int dx|x\rangle\langle x| = 1 \tag{2.25}$$

to each of the $N-1$ intervals, calling the new variables $x_2, \ldots, x_N$ and renaming $x_1 \to x_{N+1}$ when it appears for the second time (see Fig.2.3). One obtains for Z

$$Z = \int_{-\infty}^{\infty} dx_1\, dx_2 \ldots dx_N\, \langle x_1|e^{-\epsilon\frac{H}{\hbar}} \underbrace{|x_2\rangle\langle x_2|}_{\text{new ones}}\, e^{-\epsilon\frac{H}{\hbar}}|x_3\rangle \ldots \langle x_{N-1}|e^{-\epsilon\frac{H}{\hbar}}|x_N\rangle\langle x_N|e^{-\epsilon\frac{H}{\hbar}}|x_{N+1} = x_1\rangle, \tag{2.26}$$

where $\epsilon = \beta\hbar/N$. The operator $e^{-\epsilon H}$ moves the state from x_1 to x_2 in the direction of *imaginary time* $\tau = it$ ($U(\tau,0) = e^{-\tau\frac{H}{\hbar}}$). The total motion will be $N\epsilon = \beta\hbar$. Since you integrate over all x_i (keeping $x_1 = x_{N+1}$) you are *summing over all periodic paths* (one such "configuration of $x(\tau)$" is shown in Fig. 2.3) for $N \to \infty$.

The idea now is that for $N \to \infty$ the amplitude $\langle x_{k+1}|e^{-\epsilon H}|x_k\rangle$ in the small interval $\epsilon \to 0$ can be reliably estimated by assuming that the potential V in that interval is essentially a constant: $\partial_x V \approx 0$ or equivalently $[p, V] \approx 0$. A single step can then be written as (put for a

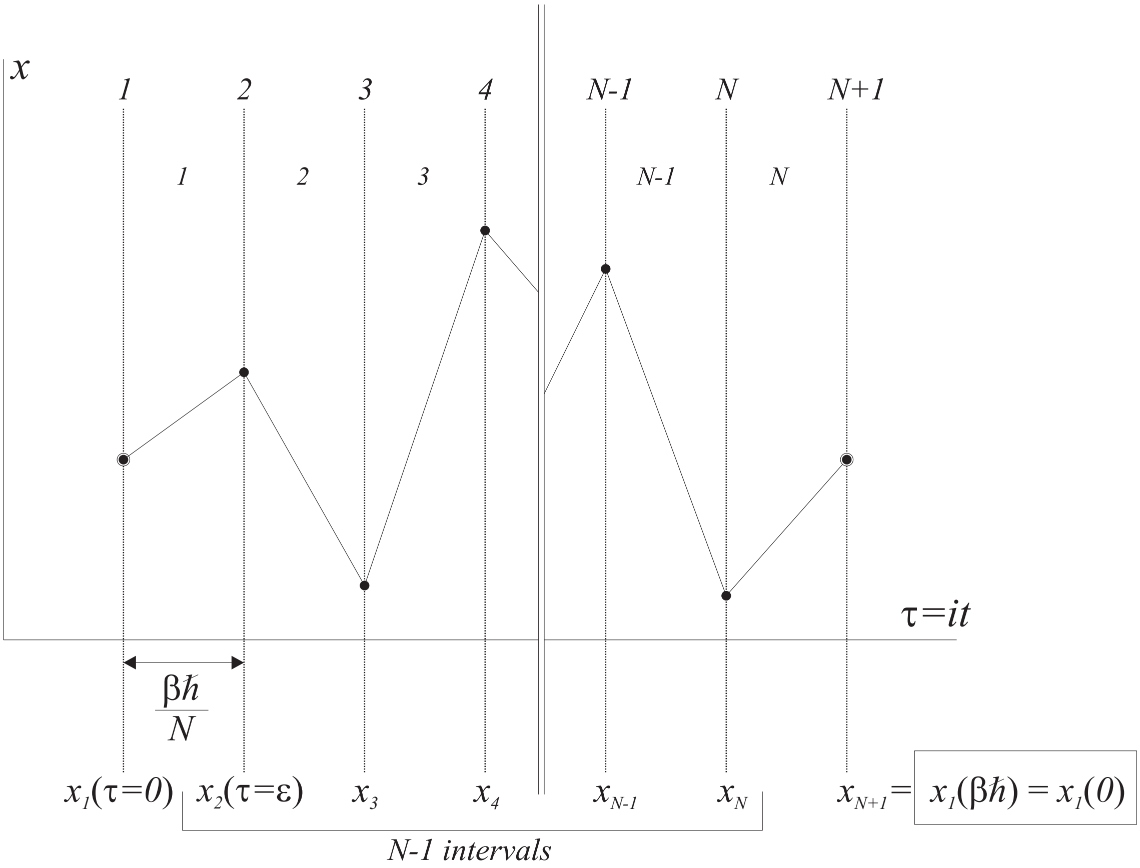


Figure 2.3: How a periodic path arises, $x_1 = x_{N+1}$.

while $\hbar = 1$):

$$\langle x_1 | e^{-\epsilon[\frac{p^2}{2m}+V(x)]} | x_2 \rangle \tag{2.27}$$

$$\approx \underbrace{\langle x_1 | e^{-\epsilon\frac{p^2}{2m}} | x_2 \rangle}_{\text{free motion in } \tau} \cdot e^{-\epsilon V(\overbrace{x_1}^{\text{or } \frac{x_1+x_2}{2}}) + \mathcal{O}([p,V])} \tag{2.28}$$

$$= \int \frac{dp_1}{2\pi}\frac{dp_2}{2\pi} \langle x_1 | p_1 \rangle \underbrace{\langle p_1 | e^{-\epsilon\frac{p^2}{2m}} | p_2 \rangle}_{2\pi e^{-\epsilon\frac{p_1^2}{2m}}\delta(p_1-p_2)} \overbrace{\langle p_2 | x_2 \rangle}^{e^{ip_2x_2}} e^{-\epsilon V} \tag{2.29}$$

$$= \int_{-\infty}^{\infty} \frac{dp}{2\pi} e^{ip(x_2-x_1)-\epsilon\frac{p^2}{2m}} e^{-\epsilon V} \tag{2.30}$$

where we have used

$$\int_{-\infty}^{\infty} dx\, e^{-\alpha x^2 - \beta x} = \sqrt{\frac{\pi}{\alpha}} e^{\frac{\beta^2}{4\alpha}} \tag{2.31}$$

Inserting, for each step, (2.30) to (2.26), we obtain an intermediate form for Z:

$$Z = \int dx_1 \dots dx_N \frac{dp_1}{2\pi\hbar} \cdots \frac{dp_N}{2\pi\hbar} \exp\Big\{\epsilon[ip_1\frac{x_2-x_1}{\epsilon} + ip_2\frac{x_3-x_2}{\epsilon} + \ldots - H(x_1) - \ldots - H(x_N)]\Big\} \tag{2.32}$$

$$\equiv \int \underbrace{\frac{\mathcal{D}x(\tau)\mathcal{D}p(\tau)}{2\pi\hbar}}_{\frac{\Delta x\Delta p}{h}} \exp\Big\{\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau[ip\dot{x} - H(x,p)]\Big\} \tag{2.33}$$

Note that the factor $ip\dot{x} - H(x,p)$ in the integrand is just the Lagrangian (remembering that $\tau = it$). Note also the basic phase space unit cell volume $\Delta x\Delta p = h = 2\pi\hbar = 2\pi$.

With $H = p^2/2m + V$ the p-integration can be done: Then

$$\int_{-\infty}^{\infty} \frac{dp}{2\pi} \exp\Big[ip(x_2-x_1) - \epsilon\frac{p^2}{2m}\Big] = \sqrt{\frac{m}{2\pi\epsilon}} \exp\Big[-\frac{m}{2\epsilon}(x_2-x_1)^2\Big] \tag{2.34}$$

and we get the free particle propagator

$$K(x_2, \tau = it; x, 0) = \sqrt{\frac{m}{2\pi\hbar\Delta(it)}} \exp\Big[-\frac{1}{\hbar}\frac{m}{2}\frac{(x_1-x_2)^2}{\Delta(it)}\Big] \tag{2.35}$$

and the matrix element

$$\langle x_1|\exp(-\epsilon H)|x_2\rangle = \sqrt{\frac{m}{2\pi\epsilon}} \exp\Big\{\underbrace{-\epsilon[\frac{m}{2}(\overbrace{\frac{x_2-x_1}{\epsilon})^2}^{\dot{x}(\tau)^2} + V(x_1)]}_{\text{Euclidean Lagrangian!!}}\Big\} \tag{2.36}$$

Putting everything together, we have an important (Feynman-Hibbs at the end of their book call it "amusing") result:

$$Z = \mathrm{Tr} e^{-\beta H} = \sum_{\text{states}} e^{-\frac{E_n}{T}}, \qquad H = \frac{p^2}{2m} + V(x)$$

$$= \int \prod_1^N \frac{dx_i}{\sqrt{\frac{2\pi\hbar\epsilon}{m}}} \exp\Big[-\frac{\epsilon}{\hbar}\Big\{\frac{m}{2}[(\frac{x_1-x_2}{\epsilon})^2 + \ldots + (\frac{x_N-x_{N-1}}{\epsilon})^2 + (\frac{x_1-x_N}{\epsilon})^2]$$

$$+ V_1 + V_2 + \ldots + V_N\Big\}\Big] \tag{2.37}$$

$$\underset{N\to\infty}{\equiv} \int_{x(0)=x(\beta\hbar)} \mathcal{D}x(\tau) \exp\Big\{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau\,[\frac{m}{2}\dot{x}^2(\tau) + V(x(\tau))]\Big\} \tag{2.38}$$

$$\equiv \int \mathcal{D}x(\tau) \exp\Big(-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau\, L(x,\tau)\Big) \equiv \int \mathcal{D}x(\tau) \exp\Big(-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau\, S_E[x]\Big)\ , \tag{2.39}$$

where S_E is the euclidean action. Note that Eq. (2.39) is defined as the $N \to \infty$ limit of Eq. ((B.1)). The partition function also has a similar limit, the thermodynamic limit

$V \to \infty$. We have now attained our goal, the partition function has been expressed in terms of the Euclidian Lagrangian of the system ($L_E(\tau) = -L_M(\tau = it)$). For curiosity, note that $\beta\hbar = 25$ps for T=300K. This is the amount of imaginary time you have to cover in room temperature!

There are several interesting computations one can do starting from Eq. (2.39). First, it is a very good exercise to work out the integrals in (B.1) for the harmonic oscillator potential and then take the limit $N \to \infty$ of the result, to again get the vibrational partition function. Second, one may calculate the same result directly from the gaussian functional integral, using functional methods. Third, one may evaluate the "fluctuation determinant around a classical solution". We shall return to these after some general remarks about finite T and imaginary time.

One more good application of the harmonic oscillator is to compute the finite T expectation value of the time dependent correlator $\langle x(t)x(0)\rangle$. Here we really have both real time t and finite T in the same quantity, which now can be exactly computed:

$$\langle x(t)x(0)\rangle_T = Z^{-1}\mathrm{Tr}e^{-\beta H}x(t)x(0) \tag{2.40}$$

$$= Z^{-1}\sum_{m,n=0}^{\infty} e^{-\beta\hbar\omega_n + it(\omega_n-\omega_m)}\langle n|x(0)|m\rangle\langle m|x(0)|n\rangle. \tag{2.41}$$

Insert here

$$E_n = \hbar\omega_n = \hbar\omega(n+1/2) \tag{2.42}$$

$$\langle n|x(0)|m\rangle = \sqrt{\frac{n}{2}}\delta_{m,n-1} + \sqrt{\frac{n+1}{2}}\delta_{m,n+1} \tag{2.43}$$

and obtain

$$\langle x(t)x(0)\rangle_T = \frac{\hbar}{2\omega}\frac{\cosh(\beta\hbar/2 - it)\omega}{\sinh(\beta\hbar\omega/2)} = \frac{\hbar}{\omega}\left[n_{\mathrm{BE}}(\beta\hbar\omega)\cos(\omega t) + \frac{1}{2}e^{-it\omega}\right]. \tag{2.44}$$

Plot this in imaginary time $\tau = it$! It is useful to separate a commutator and anticommutator:

$$\langle x(t)x(0)\rangle_T = \langle\frac{1}{2}\{x(t),x(0)\}\rangle_T + \langle\frac{1}{2}[x(t),x(0)]\rangle_T = \frac{\hbar}{\omega}\left[n_{\mathrm{BE}}(\beta\hbar\omega) + \frac{1}{2}\right]\cos(\omega t) + \frac{\hbar}{2i\omega}\sin(\omega t) \tag{2.45}$$

Thus the anticommutator is the real part, $\sim 1 + (\hbar\omega/T)^2/12 + ..$ and even in t while the commutator is the imaginary part, $\mathcal{O}(\hbar)$, and odd in t.

How does all this match with classical physics? Harmonic motion with some initial values $x_c(0), p_c(0)$ is

$$x_c(t) = x_c(0)\cos\omega t + \frac{p_c(0)}{\omega}\sin\omega t. \tag{2.46}$$

Thus

$$\langle x(t)x(0)\rangle_T = \langle x_c^2(0)\cos\omega t + \frac{p_c(0)x_c(0)}{\omega}\sin\omega t\rangle_T = \langle x_c^2(0)\rangle_T\cos\omega t \tag{2.47}$$

since the thermal average of the initial momentum is zero. But here we can insert the fact that the thermal energy per quadratic degree of freedom is $T/2$: $\langle\frac{1}{2}\omega^2x_c^2(0)\rangle_T = \frac{1}{2}T$ and obtain

$$\langle x(t)x(0)\rangle_T = \frac{T}{\omega^2}\cos\omega t. \tag{2.48}$$

Comparing with the exact quantum mechanics result (2.45) one sees that to order $\mathcal{O}(\hbar^2)$ the classical result (averaging over initial conditions, taking t dependence from classical equations of motion) = result from quantum theory. This seems rather trivial but actually forms the groundwork for many numerical attempts to compute field theory correlators $\langle O(t)O(0)\rangle$. There is no nonperturbative first-principle method for computing these correlators in gauge field theory and one thus has had to resort to the above approximation, separating

- Equilibrium average over initial conditions,
- Subsequent classical motion.

Applications range from baryon number generation in field theory (the correlator then is that of topological susceptibility, $F\tilde{F}$) to particle production in ultrarelativistic heavy ion collisions.

2.2 Finite T means compact imaginary time

We can summarize the properties of the result as follows:

- Thermodynamics is now formulated in terms of the “Euclidean” Lagrangian, which in many cases is much simpler than H. In particular, in gauge field theories the Lagrangian is Lorentz scalar and a simple singlet under gauge transformations, while defining H requires gauge fixing.
- The formulation is easy to generalize from one particle in 1d ⇒ N particles in d dimensions ⇒ Field theories in d dimensions = infinite number of particles.
- Very general, applies to any system the dynamics of which is expressed in terms of an action.
- Good starting point for numerics.
- One avoids computing the energy levels E_n, one gets directly the sum over them! For example, for QCD nobody can compute the full energy spectrum, i.e., the spectrum of hadrons (m_π, m_N, m_δ, ...) and it is inconceivable to compute Z by summing over states. In the path integral formulation this is entirely avoided and, in some sense, computing $Z(T)$ is as simple (difficult!) as computing a single mass.

We have thus the general result that thermal equilibrium means summing over all “periodic configurations”: $x(0) = x(\beta\hbar)$. Periodicity reflects the fact that one is computing a Trace. For fermions the configurations actually have to be antiperiodic. Graphically:

Because of the periodicity the usual continuous energy is replaced by a discrete sum over ”Matsubara frequences”. A physicist frequently wants to analyze time or space dependence in terms of Fourier modes. For usual real time ($-\infty < t < \infty$) one writes:

$$f(t) = \int_{-\infty}^{\infty} \frac{dk_0}{2\pi} e^{-ik_0 t} f(k_0)$$

and we have continuous energy modes. For real $f(t)$, $f^\star(k_0) = f(-k_0)$ and in terms of these, for example,

$$\int_{-\infty}^{\infty} dt\,[\dot{x}^2(t) + m^2 x^2(t)] = \int_{-\infty}^{\infty} \frac{dk_0}{2\pi} f(k_0)(k_0^2 + m^2) f(-k_0) \tag{2.49}$$

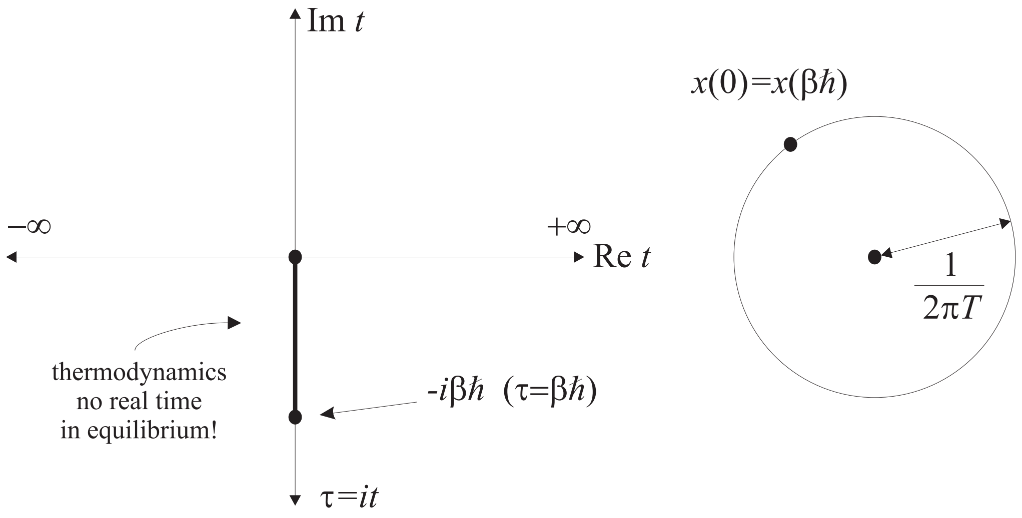


Figure 2.4: Complex time plane

and the whole theory can be formulated in terms of the Fourier components $f(k_0)$. Now we want to do Fourier in imaginary time, $e^{-ik_0t} = e^{-k_0\tau} \equiv e^{ik_4\tau}$ with real k_4. However, since τ now is varying over a finite interval, we must write a Fourier series to represent $f(\tau)$:

$$f(\tau) = T \sum_{n=-\infty}^{\infty} e^{i\omega_n\tau}\mathrm{f}(\omega_n) \tag{2.50}$$

and the requirement $f(0) = f(\beta\hbar)$ specifies $e^{i\hbar\omega_n\beta} = 1$ or

$$\hbar\omega_n = 2\pi nT, \quad n = 0, \pm 1, \pm 2 \tag{2.51}$$

These are the "Matsubara frequences", the modes $f(\omega_n)$ are "Matsubara modes". Going beyond the interval $0, \beta\hbar$, the function f is periodic, $f(\tau) = f(\tau + \beta\hbar)$, the τ space has become topologically a circle. The factor T in Eq. (2.50) follows from changing k_4 to $2\pi Tn$:

$$\int \frac{dk_4}{2\pi} \Rightarrow T\sum_n . \tag{2.52}$$

One the complex energy plane:

A parenthesis on Minkowskian ⇔ Euclidean: How do different quantities behave when $\tau = it$ or $x_0 = x^0 = -ix_4$? Clearly $x_\mu x^\mu = x_0^2 - \mathbf{x}^2 = -x_E^2$. Then $\partial_0 = i\partial_4$ and one also wants the covariant derivative to behave similarly. Thus $D_0 = \partial_0 + igA_0$ becomes $iD_4 = i(\partial_4 + igA_4)$ so that $A_0 = +iA_4$, $E^i = F_{0i} = iF_{4i} = iE_i^{\mathrm{E}}$ and

$$i\int dtd^3x\,\frac{1}{2}(\mathbf{E}^2 - \mathbf{B}^2) = -\int d^4x_{\mathrm{E}}\,\frac{1}{2}(\mathbf{E}_{\mathrm{E}}^2 + \mathbf{B}^2) \tag{2.53}$$

which tells how, for electrodynamics, iS_M transforms to $-S_E$. For fermions the obvious goal $\{\gamma_\mu^E, \gamma_\nu^E\} = 2\delta_{\mu\nu}$, replacing $\{\gamma_\mu, \gamma_\nu\} = 2g_{\mu\nu}$, is reached by

$$\gamma_0^E = \gamma^0, \quad \gamma_i^E = -i\gamma^i = i\gamma_i. \tag{2.54}$$

$$\Rightarrow \gamma_\mu^{E\dagger} = \gamma_\mu^E, \quad i\gamma^\mu D_\mu = -\gamma_\mu^E D_\mu^E \tag{2.55}$$

so that the fermionic Lagrangian

$$L_M = \bar{\psi}(i\gamma^\mu D_\mu - m)\psi = -\bar{\psi}(\gamma_\mu^E D_\mu^E + m)\psi = -L_E \tag{2.56}$$

where $\gamma_\mu^E D_\mu^E + m$ is the famous fermion matrix, also a subject of much mathematical research.

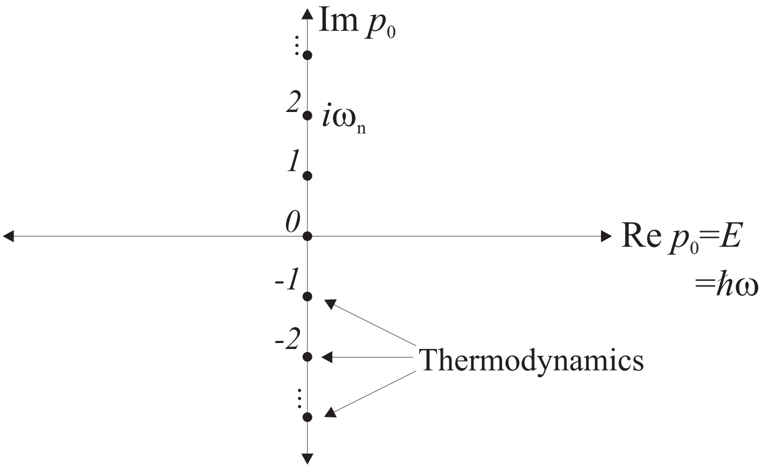


Figure 2.5: Complex energy plane

2.3 Finite T and $T = 0$

Usually the path integral is introduced for 1+1d quantum mechanics in real time. Then there is no T and no trace to evaluate. Instead of the sum (2.23) over diagonal matrix elements one has a single transition matrix element, for which slight modifications of the previous equations give

$$\langle x_b\, t_b | x_a\, t_a \rangle = \langle x_b\, 0 | \exp\big[-i\frac{H}{\hbar}(t_b - t_a)\big] | x_a\, 0 \rangle \tag{2.57}$$

$$= \int \mathcal{D}x\, \mathcal{D}p \,\exp\Big\{ i\frac{1}{\hbar} \int_{t_a}^{t_b} dt\, [p\dot{x}(t) - H(x,p)] \Big\} \tag{2.58}$$

$$= \int \mathcal{D}x \,\exp\Big\{ i\frac{1}{\hbar} \int_{t_a}^{t_b} dt\, L(x(t), \dot{x}(t)) \Big\}, \tag{2.59}$$

Because of the i this is mathematically badly behaved; one has to introduce $i\epsilon$:s which have a physics reason. Now the paths in real time arise as shown in Fig.2.6.

One usually also couples the system to an external current $J(t)$, some external force affecting the motion. Then the path integral becomes

$$\langle x_b\, t_b = \infty | x_a\, t_a = -\infty \rangle_{\mathcal{J}(t)} = \int \mathcal{D}x(t) \,\exp\Big\{ i\frac{1}{\hbar} \int_{-\infty}^{\infty} dt\, \big[L(x,\dot{x}) + \mathcal{J}(t)x(t)\big] \Big\} \tag{2.60}$$

$$\equiv Z(\mathcal{J}) \equiv e^{iW(\mathcal{J})} \tag{2.61}$$

Then the functional derivatives $\delta W/\delta \mathcal{J}(t)$, ..., give expectation values of products of $\hat{x}$-operators. We shall expand on this when discussing extension to field theory.

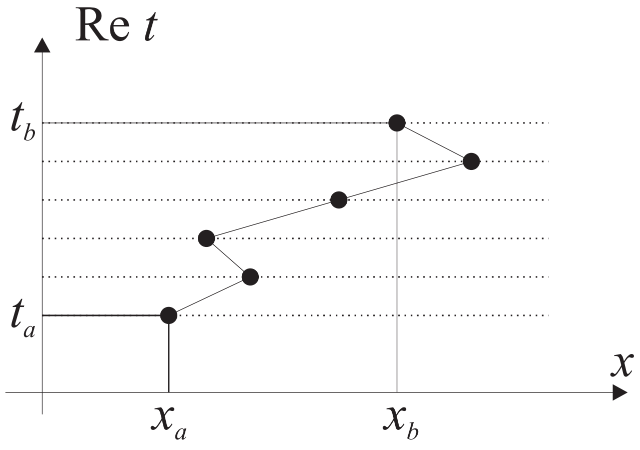


Figure 2.6: Real time paths

2.4 The path integral of harmonic oscillator using functional methods

Let us now return to the path integral for the 1d harmonic oscillator at finite T:

$$Z = \int_{x(0)=x(\beta)} \mathcal{D}x \exp\left[-\int_0^\beta d\tau \left(\frac{1}{2}m\dot{x}^2 + \frac{1}{2}m\omega^2 x^2\right)\right] \tag{2.62}$$

(here $\hbar = 1$) and complete the circle of arguments by directly showing that this reproduces the almost trivial vibrational partition function,

$$Z_{\text{vib}} = \sum_{n=0}^{\infty} e^{-\beta\hbar\omega(n+\frac{1}{2})} = \frac{1}{2\sinh\frac{\beta\hbar\omega}{2}}. \tag{2.63}$$

where we started from.

The harmonic oscillator is exactly solvable since the integral (2.62) is Gaussian, quadratic in x. A complication is the time derivative of x. The standard way of getting rid of this is by partial integration which casts the expression into the form $x[$ operator $]x$. So use $d(x\dot{x})/d\tau = \dot{x}^2 + x\ddot{x}$:

$$\int_0^\beta d\tau\ \dot{x}^2 = \underbrace{\Big/_{0}^{\beta} x\dot{x}}_{=0:\ x\text{ periodic}} - \int_0^\beta d\tau x\ddot{x}\ , \tag{2.64}$$

so that we get the explicitly Gaussian integral,

$$Z = \int_{x(0)=x(\beta)} \mathcal{D}x \exp\left[-\frac{1}{2}\int_0^\beta d\tau\ x\left(-m\frac{d^2}{d\tau^2} + m\omega^2\right)x\right] \tag{2.65}$$

A Gaussian integral can always be carried out using the fundamental formula

$$I = \int_{-\infty}^{\infty} \prod_1^N dx_i \exp\left(-\frac{1}{2}\sum_{ij} x_i A_{ij} x_j + \sum_i b_i x_i\right) = \frac{(2\pi)^{N/2}}{\sqrt{\det A}} \exp\left(\frac{1}{2}\sum_{ij} b_i A^{-1}_{ij} b_j\right), \tag{2.66}$$

which also leads to the Wick formulas for the correlators:

$$\langle x_1 x_2\rangle \equiv I^{-1}\int\prod_1^N dx_i\, x_1 x_2 \exp[-\frac{1}{2}xAx] == (A^{-1})_{12}, \tag{2.67}$$

$$\langle x_1x_2x_3x_4\rangle = (A^{-1})_{12}(A^{-1})_{34} + (A^{-1})_{13}(A^{-1})_{24} + (A^{-1})_{14}(A^{-1})_{23}, \tag{2.68}$$

etc. One should understand that the $\sum_{ij}$ in (2.66) is built in $\int d\tau$ in the path integral. Thus we can write

$$Z = \underbrace{\text{const}}_{\text{infinite!}} \times(\det\ K)^{-\frac{1}{2}}\ , \tag{2.69}$$

where now

$$K = m(-\frac{d^2}{d\tau^2} + \omega^2)\ . \tag{2.70}$$

To define and evaluate the determinant of this operator we have to find its eigenvalues k_n. Then

$$\det\ K = \prod k_n = e^{\sum \ln k_n} = e^{\text{Tr}\ \ln K} \tag{2.71}$$

The eigenvalues are obtained by solving the eigenvalue equation

$$Kf_n = k_n f_n\ , \tag{2.72}$$

where $f_n(\tau) = f_n(\tau+\beta)$ are the periodic eigenfunctions. Clearly, the solutions to

$$\left(-\frac{d^2}{dt^2} + \omega^2\right) f_n = k_n f_n \tag{2.73}$$

are of the form $f_n = e^{i\alpha\tau}$, and requiring periodicity $\tau \to t+\beta$ we find $f_n = e^{2\pi i n\tau/\beta}$ so that the eigenvalues are

$$k_n = \omega^2 + (2\pi n T)^2 \equiv \omega^2 + \omega_n^2; \tag{2.74}$$

the Matsubara frequences have reappeared and

$$Z(\omega) = \frac{\text{const}}{\sqrt{\prod_{-\infty}^{\infty}(\omega^2+\omega_n^2)}} = \frac{\text{const}}{\omega\prod_1^\infty(\omega^2+\omega_n^2)}. \tag{2.75}$$

The determinant is obviously infinite, but this need not worry us: in any case, we have to normalize to determine the constant. It is natural to normalise by the path integral of a free theory with $\omega = 0$. However, the $n = 0$ zero mode term in Eq. (2.75) diverges in this limit. The physical reason is that if $V = 0$ the particle is free to move anywhere in space which leads to this "infrared divergence". Mathematically, the problem is that the operator $d^2/d\tau^2$ has a zero eigenvalue, which clearly must be removed from the definition $\det K = \prod k_n$ for this to make sense. This situation is very common when evaluating functional determinants. Other arguments must be used to evaluate their contribution. Here we simply say that to keep Z_0 dimensionless, we must include a factor of dimension ω and there is just T. So we write

$$Z(\omega=0) \equiv Z_0 = \det\left(-\ m\frac{d^2}{d\tau^2}\right)^{-\frac{1}{2}} \times \text{const} = \frac{\text{const}}{T\prod_1^\infty \omega_n^2} \tag{2.76}$$

The properly normalized harmonic oscillator partition function Z_{HO} is thus

$$Z_{\mathrm{HO}} \equiv \frac{Z(\omega)}{Z(0)} = \frac{1}{\beta\omega \prod_{n=1}^{\infty}\left(1+\frac{\omega^2\beta^2}{4\pi^2 n^2}\right)} = \frac{1}{2\mathrm{sinh}\frac{\beta\omega}{2}} \ , \tag{2.77}$$

where in the last step $\sinh x = x\prod_1^\infty(1+x^2/(\pi n)^2)$ (Gradsteyn-Rydzik 1.431) was used. So we are back to Eq. (2.63) where we started from.

2.5 Generating functionals

By computing Z one obtains the thermodynamic potential of the system. In practise, for interacting systems, this is unfortunately a calculation we do not know how to do analytically (recall that physicists can, with some exceptions, do only gaussian integrals!). Therefore one has to resort to perturbation theory (i.e. assume that the interaction is weak) or numerics.

We need a path integral which generates correlators (=Green's functions). The task is then to evalute the correlators in perturbation theory. To this end, let us define the *generating functional* which in 1+1 dimensions can be written as

$$Z[J] = N\int \mathcal{D}x\, e^{-[S+\int_0^\beta d\tau\, J(\tau)x(\tau)]}, \tag{2.78}$$

where $J(\tau) = J(\tau+\beta)$ is an arbitrary (periodic) source functions so that formally

$$\begin{aligned}\frac{\delta Z}{\delta J(\tau_1)\ldots\delta J(\tau_n)}\Big|_{J=0} &= N\int \mathcal{D}x\; x(\tau_1)\ldots x(\tau_n)e^{-S}(-1)^n \\ &\equiv \langle x(\tau_1)\ldots x(\tau_n)\rangle(-1)^n \end{aligned} \tag{2.79}$$

with $N = Z[0]^{-1}$. For the harmonic oscillator we immediately obtain, using Eq.(2.66),

$$\begin{aligned} Z[J] &= N\int \mathcal{D}x \exp\Big[-\int d\tau(\frac{1}{2}m\dot{x}^2+\frac{1}{2}m\omega^2x^2) - \int d\tau\; J(\tau)x\Big] \\ &\propto \Big[\det\big(-\frac{d^2}{d\tau^2}+\omega^2\big)\Big]^{-\frac{1}{2}} \exp\Big[-\frac{1}{2m}\int_0^\beta d\tau\, d\tau'\; J(\tau')\big(-\frac{d^2}{d\tau^2}+\omega^2\big)^{-1}J(\tau)\Big] \ . \end{aligned} \tag{2.80}$$

The definition Eq. (2.78) is carried over to field theory where (for a scalar field ϕ)

$$Z[J] = N\int \mathcal{D}\phi\; e^{-S-\int d^4x\, J(x)\phi(x)} \ . \tag{2.81}$$

For an interacting scalar field theory $S = \int d^4x\,[\frac{1}{2}\partial_\mu\phi\partial^\mu\phi - V(\phi)]$. By computing $\delta Z/\delta J(x_1)\ldots\delta J(x_n)$ one finds the n-point functions (correlators). A similar procedure applies to QED, QCD and other gauge theories, but with some additional technicalities:

- gauge must be fixed (→ ghosts),
- fermions are Grassmann numbers: $\Psi_2\Psi_1 = -\Psi_1\Psi_2$.

2.6 Perturbation theory

The harmonic oscillator, $V(x) \sim x^2$, can be done exactly, as a Gaussian integral. For more complicated interactions various approximation methods have to be applied. We will outline two main methods. Both boil down to doing a Gaussian integral as a leading term and then computing corrections. Firstly, one may assume all the non-Gaussianity is a small effect and can be regarded as a perturbation. Secondly, one may attempt a semiclassical $\hbar \to 0$ saddle point computation.

The substance of perturbation theory is easy to formulate. Suppose we have a theory with action $S[\Phi] = S_0[\Phi] + S_1[\Phi]$, where Φ is a set of degrees of freedom, and S_0 contains all the quadratic terms. In the 1d case $S_0 = \int dt(\frac{1}{2}m\dot{x}^2 + \frac{1}{2}m\omega^2x^2)$. All the physics is in expectation values of operators $O(\Phi)$ and to compute them we expand in S_1:

$$\begin{aligned}
\langle O \rangle &= \frac{\int \mathcal{D}\Phi\, O \exp[-S_0 - S_1]}{\int \mathcal{D}\Phi \exp[-S_0 - S_1]} \\
&= \frac{\int \mathcal{D}\Phi\, O \exp[-S_0] \sum_0^\infty \frac{(-)^n}{n!} S_1^n}{\int \mathcal{D}\Phi \exp[-S_0] \sum_0^\infty \frac{(-)^n}{n!} S_1^n} \\
&\equiv \frac{\sum_0^\infty \frac{(-)^n}{n!} \langle O S_1^n \rangle}{\sum_0^\infty \frac{(-)^n}{n!} \langle S_1^n \rangle} \\
&= \frac{\langle O - OS_1 + \frac{1}{2} OS_1^2 - \ldots \rangle}{\langle 1 - S_1 + \frac{1}{2}S_1^2 - \ldots \rangle}
\end{aligned} \tag{2.82}$$

Thus perturbation theory boils down to computing Gaussian expectation values of powers of the interaction term and of the operator O multiplied by powers of S_1. Effectively, this is an application of the Gaussian master formula (2.66) with the correlator formulas (2.67), (2.68) and their generalisations.

Example: 1+1d interacting harmonic oscillator. Consider a theory defined by the Lagrangian

$$L(x) = \frac{1}{2}m\dot{x}^2 + \frac{1}{2}m\omega^2x^2 + \frac{1}{4}\lambda m\omega_0^4x^4; \quad \lambda \ll 1 \ . \tag{2.83}$$

Here ω, ω_0, λ are some constants. The constants are chosen such that in the units $\hbar = c = 1$, λ is a pure number and can be used as an expansion parameter. For general $\hbar, c$ one could write the interaction, e.g., in the form $+\lambda m^2\omega_0^4/\hbar x^4$, where ω_0 is a frequency. We may write down the path integral and, assuming a weak interaction, make an expansion in the small coupling constant λ:

$$\begin{aligned}
Z_\lambda &= \int \mathcal{D}x\, e^{-S_{\rm HO} - \frac{1}{4}\int_0^\beta d\tau\, \lambda m\omega_0^4 x^4} \\
&= \int \mathcal{D}x\, \exp\Big\{ - S_{\rm HO}\big[1 - \frac{\lambda}{4}\int_0^\beta d\tau\, m\omega_0^4 x^4 + \mathcal{O}(\lambda^2)\big]\Big\} \\
&= Z_{\rm HO} - \frac{\lambda}{4} m\omega_0^4 \int_0^\beta d\tau \int \mathcal{D}x\, e^{-S_{\rm HO}} x^4 \\
&= Z_{\rm HO} - \frac{\lambda}{4} m\omega_0^4 \int_0^\beta d\tau\, \underbrace{\frac{\delta^4 Z_{\rm HO}[J]}{\delta J(t) \ldots \delta J(t)}\Big|_{J=0}}_{\text{this can be computed}} + \mathcal{O}(\lambda^2) \ .
\end{aligned} \tag{2.84}$$

(2.85)

Thus we may write

$$\frac{Z_\lambda}{Z_{\lambda=0}} = 1 - \frac{\lambda}{4} m\omega_0^4 Z_{\mathrm{HO}}^{-1} \int_0^\beta d\tau \, \frac{\delta^4 Z_{\mathrm{HO}}}{\delta J^4}\Big|_{J=0} , \tag{2.86}$$

where the second term represents the first-order correction to the path integral of the ordinary harmonic oscillator.

Exercise: evaluate Z_λ.

2.7 Semiclassical approximation, Gaussian fluctuation determinant

Instead of expanding the potential with respect to some small dimensionless parameter, we may also use another, different method called the semiclassical approximation or the loop expansion, which does not require weak interactions. The following is equivalent to the saddle point evaluation of the integral $\int dx \exp[-S(x)/\hbar]$ in the first chapter, in the limit $\hbar \to 0$. Here $\hbar$ may be the Planck constant, but it can also be some formal parameter counting how many corrections are included. We discuss only the leading classical term and the first correction, the Gaussian fluctuation determinant.

Let us consider a general 1+1d Euclidean action

$$S = \int_0^\beta d\tau \left[\frac{1}{2} m\dot{x}^2 + V(x)\right] = \int_0^\beta d\tau \left[\frac{1}{2} m x(-\partial_\tau^2)x + V(x)\right] . \tag{2.87}$$

Here $V(x)$ is some arbitrary potential. In general, the configurations that contribute most to Z are those for which S is at its minimum. These are the saddle points $\delta S/\delta x = 0$ which correspond to the classical trajectories $x_{cl}(t)$ given by the equation of motion $V'(x) - m\ddot{x} = 0$. Therefore, it makes sense in the path integral to expand about the classical solution $x(t) = x_{cl}(t)$:

$$\begin{aligned} S[x] =& S[x_{cl}] + \int \underbrace{\frac{\delta S}{\delta x(\tau_1)}\Big|_{x=x_{cl}}}_{=0,\text{ eq. of motion}} (x(\tau_1) - x_{cl}) d\tau_1 \\ &+ \frac{1}{2} \int \frac{\delta^2 S}{\delta x(\tau_1)\delta x(\tau_2)}\Big|_{x=x_{cl}} (x(\tau_1) - x_{cl})(x(\tau_2) - x_{cl}) d\tau_1 d\tau_2 + \ldots \end{aligned} \tag{2.88}$$

Note that $-\partial_\tau^2$ is a linear operator so that we may write

$$\begin{aligned}
\frac{\delta S}{\delta x(\tau_1)} =& \frac{\delta}{\delta x(\tau_1)} \int d\tau \left(\frac{1}{2} m x(-\partial_\tau^2) x + V(x) \right) \\
=& \int d\tau \frac{\delta V(x)}{\delta x(\tau)} \underbrace{\frac{\delta x(\tau)}{\delta x(\tau_1)}}_{\delta(\tau-\tau_1)} - \frac{1}{2} m \int d\tau d\tau' x(\tau) \underbrace{K(\tau,\tau')}_{\text{symmetric kernel}} x(\tau') \\
=& V'(x(\tau_1)) - \frac{1}{2} m \int d\tau d\tau' \left[\delta(\tau-\tau_1) K(\tau,\tau') x(\tau') + \delta(\tau_1-\tau') K(\tau,\tau') x(\tau) \right] \\
=& V'(x(\tau_1)) - m \int d\tau K(\tau_1,\tau) x(\tau) \\
=& V'(x) - m\partial_\tau^2 x \ .
\end{aligned} \tag{2.89}$$

Then

$$\frac{\delta^2 S}{\delta x(\tau_1) \delta x(\tau_2)} = V\text{"} \delta(\tau_1 - \tau_2) - m K(\tau_1, \tau_2) \tag{2.90}$$

so that, defining $x - x_{cl} \equiv x_q$ (where "q" stands for quantum fluctuation), we find that

$$\begin{aligned}
S[x] =& S[x_{cl}] + \frac{1}{2} \int d\tau_1 d\tau_2 \left[V\text{"}(x_{cl}) \delta(\tau_1 - \tau_2) - m K(\tau_1,\tau_2) \right] x_q(\tau_1) x_q(\tau_2) + \mathcal{O}(x_q^3) \\
=& S[x_{cl}] + \frac{1}{2} \int d\tau_1 \left[x_q(\tau_1) \left(-m\partial_\tau^2 + V\text{"}(x_{cl}) \right) x_q(\tau_1) \right] + \mathcal{O}(x_q^3) \ .
\end{aligned} \tag{2.91}$$

If we neglect the terms of order $\mathcal{O}(x_q^3)$ and note that in the path integral measure we may perform the shift $\mathcal{D}x \to \mathcal{D}(x - x_{cl}) = Dx_q$ because x_{cl} is just a point in the space of all configurations, we again have a Gaussian integral. Hence the in the Gaussian approximation Z is obtained by an integration over small fluctuations:

$$Z = \int \mathcal{D}x e^{-S[x]} \simeq e^{-S[x_{cl}]} \int \mathcal{D}x_q e^{-\frac{1}{2}\int d\tau x_q K x_q} \propto e^{-S[x_{cl}]} [\det\ K]^{-\frac{1}{2}} \ . \tag{2.92}$$

So we again end up evaluating a functional determinant, now the determinant of the operator $K = -m\partial_\tau^2 + V\text{"}(x_{\rm cl})$. Evaluating $\det K$ is often tricky because unless x_{cl} is the trivial constant vacuum configuration (e.g. $x_{cl} = 0$), the determinant requires the solution of a complicated eigenvalue problem.

Example:. Assume the potential is of the double-well form $V(x) = \frac{1}{4}\lambda(x^2 - v^2)^2$ with minima at $x = \pm v$. Then the classical EOM has a "kink" solution, a solution of $\ddot{x} = V'(x)$, taking us from one minimum to the other:

$$x_{\rm cl}(\tau) = v \tanh \sqrt{\lambda/2} v(\tau - \tau_0) \tag{2.93}$$

with the classical action

$$S[x_{\rm cl}] = \frac{4}{3}\sqrt{\frac{\lambda}{2}} v^3 = \frac{m_H^3}{3\lambda}, \quad m_H^2 = V''(\pm v) = 2\lambda v^2 \tag{2.94}$$

and with

$$V''(x_{\rm cl}(\tau)) = \lambda v^2 [(3\tanh^2(\tau/\tau_1) - 1], \ \tau_1^2 \lambda v^2 = 2; \ \tau_0 = 0. \tag{2.95}$$

In (2.93) τ_0 is the "position of the kink" and we assume that $\beta\hbar$ and the parameters are such that the kink fits in the interval $0, \beta\hbar$, i.e., we can take $\tau \to \pm\infty$ in (2.93). A periodic configuration then is one in which one jumps from one minimum to the other and then returns, a kink + antikink. The nontrivial zero mode is easy to identify: by construction $x_{\rm cl}$ satisfies $\ddot{x}_{\rm cl} - V'(x_{\rm cl}) = 0$, take the derivative of this with respect to τ and find

$$[-\partial_\tau^2 + V''(x_{\rm cl})]\frac{dx_{\rm cl}}{d\tau} = 0 \tag{2.96}$$

so that the normalised zero mode is

$$x_0(\tau) = \sqrt{\frac{3}{4\tau_1}}\frac{1}{\cosh^2(\tau/\tau_1)}. \tag{2.97}$$

Finding the eigenvalues a_n of the operator $K = -m\partial_\tau^2 + V''(x_{\rm cl})$ we must, scaling variables suitably, solve

$$-\frac{1}{2}\ddot{x} + (3\tanh^2\tau - 1)x = \tau_1 a_n x \tag{2.98}$$

Astonishingly, these can be obtained analytically - not so many cases where analytic solutions of the eigenvalue equation can be given. There are two discrete eigenvalues and -functions:

$$\begin{aligned} a_0 &= 0 \quad x_0 = \frac{1}{\cosh^2\tau} \\ a_1 &= \frac{3}{2\tau_1^2} \quad x_1 = \frac{\sinh\tau}{\cosh^2\tau} \end{aligned} \tag{2.99}$$

and a continuum

$$\tau_1^2 a_p = 2 + \frac{1}{2}p^2, \quad x_p = e^{ip\tau}(3\tanh^2\tau - 1 - p^2 - 3ip\tanh\tau). \tag{2.100}$$

These may seem like very formal developments, but the applications are very practical: physics of the NH_3 molecule, symmetric and antisymmetric ground states and the tunneling between the two minima of the potential.

2.8 Path integrals in finite T field theory

In field theory one replaces x with the field $\phi(x)$. Let us focus here on scalar fields only. At $T = 0$, a classical free real scalar field obeys the equation of motion

$$(\Box + m^2)\phi = 0 \ , \tag{2.101}$$

where $\Box = \partial_\mu \partial^\mu = \partial_t^2 - \partial_{\mathbf{x}}^2$ The Klein-Gordon solutions are plane waves $\phi = e^{ik\cdot x}$ with a dispersion relation $k^2 - m^2 = 0$ (here $k = (k^0, k^i)$ is a 4-vector). The equation of motion follows from the action

$$S = \int d^4x \left[\frac{1}{2}\partial_\mu\phi\partial^\mu\phi - \frac{1}{2}m^2\phi^2 \right] . \tag{2.102}$$

As discussed previously, at $T \neq 0$, we take the euclidean action and periodic fields so that

$$Z = N \int \mathcal{D}\phi \ \exp\Big[- \int_0^\beta d\tau \int d^3x \big(\frac{1}{2}\partial_\mu\phi\partial^\mu\phi + \frac{1}{2}m^2\phi^2 \big) \Big] \ , \tag{2.103}$$

where $\phi(x, \tau + \beta) = \phi(x, \tau)$. Let us first note that

$$\begin{aligned} \int \underbrace{d^3\boldsymbol{x}\, d\tau}_{\text{periodic}} \ \frac{1}{2}\partial_\mu\phi\partial^\mu\phi &= \int d^4x \Big[\frac{1}{2}\partial_\mu(\phi\partial^\mu\phi) - \frac{1}{2}\phi\Box\phi \Big] \\ &= \underbrace{\frac{1}{2}\oint dS_\mu \, \phi\partial^\mu\phi}_{\substack{= 0 \text{ for } \phi(\boldsymbol{x}) \to 0 \text{ as} \\ \boldsymbol{x} \to \infty}} \quad -\frac{1}{2}\int d^4x\phi\Box\phi \ . \end{aligned} \tag{2.104}$$

The surface terms thus vanishes because there is no field at infinity. We can evaluate this, again using the fundamental Gaussian integral (2.66),

$$Z = N \int \mathcal{D}\phi \ \exp\big(- \int d^3\boldsymbol{x}\, d\tau \, \phi K \phi \big) \propto (\det K)^{-\frac{1}{2}} \tag{2.105}$$

where now

$$K = \Box + m^2 \ . \tag{2.106}$$

and where the box operator at $T \neq 0$ is euclidean: $\Box = \partial_t^2 + \nabla^2$.

Let us now compute

$$\det K = e^{\mathrm{Tr} \ln K} \tag{2.107}$$

for a massless scalar field. Taking a trace means summing over the diagonal matrix elements of the operator, and since K is continuous, we take an integral:

$$\begin{aligned}
\mathrm{Tr}\ln K &= \int \langle \boldsymbol{x}, \tau | \ln K | \boldsymbol{x}, \tau \rangle d^3x\, d\tau \ /V_4 \\
&= V_4^2 V_4^{-1} \int \frac{d^3\boldsymbol{k}}{(2\pi)^3} \frac{d^3\boldsymbol{k'}}{(2\pi)^3} e^{i\boldsymbol{k}\cdot\boldsymbol{x} - i\boldsymbol{k'}\cdot\boldsymbol{x}} \\
&\times \underbrace{\int \sum_{n,j=-\infty}^{\infty} \overbrace{e^{i2\pi n\tau/\beta - i2\pi j\tau/\beta}}^{\substack{\tau \text{ is compact} \\ L = 2\pi T\,:\, k \to k + L}} \left[\frac{2\pi T}{2\pi}\right]^2 d\tau}_{T^2\delta(n-j)} \\
&\times \langle \boldsymbol{k'}, n' | \ln(k_0^2 + \boldsymbol{k}^2 + m^2) | \boldsymbol{k}, n \rangle d^3\boldsymbol{x} \qquad (2.108)
\end{aligned}$$

Note the normalization factor $1/V_4$: for an identity operator the trace yields 1. For $\tau = \tau + \beta \to k_0 = \frac{2\pi n}{\beta}$, $n \in \mathbb{Z}$, so that

$$\mathrm{Tr}\ln K = V_3 \sum_{n=-\infty}^{\infty} \int \frac{d^3\boldsymbol{k}}{(2\pi)^3} \ln\left(4\pi^2 n^2 T^2 + k^2 + m^2\right) \qquad (2.109)$$

where we have used the fact that $V_3 \beta T = V_4 T$.

The result Eq. (3.28) obviously diverges, so we need to take into account the normalization in Z. Let it be such that $Z(T = 0) = 1$. Thus we wish to compute

$$\begin{aligned}
\Delta &\equiv \mathrm{Tr}\ln K - \mathrm{Tr}\ln K(T = 0) \\
&= \mathrm{Tr}\ln K - V_4 \int \frac{d^4\boldsymbol{k}}{(2\pi)^4} \ln\left(k_0^2 + k^2 + m^2\right) . \qquad (2.110)
\end{aligned}$$

Let us get rid of the infinity by first taking a derivative with respect to a parameter. We may then employ an extremely useful relation given by

$$T \sum_{n=-\infty}^{\infty} \frac{p}{4\pi^2 n^2 T^2 + p^2} = \frac{1}{2} + \frac{1}{e^{\beta p} - 1} \qquad (2.111)$$

which is often used in finite temperature field theory. Thus, let us consider

$$\begin{aligned}
\frac{\partial \Delta}{\partial m^2} &= V_4 \int \frac{d^3\boldsymbol{k}}{(2\pi)^3} \Big[\sum_{n=-\infty}^{\infty} \frac{T}{4\pi^2 n^2 T^2 + k^2 + m^2} - \int \frac{d^4\boldsymbol{k}}{(2\pi)^4} \frac{1}{k_0^2 + k^2 + m^2} \Big] \\
&= V_4 \int \frac{d^3\boldsymbol{k}}{(2\pi)^3} \Big[\big(\underbrace{\frac{1}{2E}}_{\text{diverges like } k^2} + \frac{1}{E} \frac{1}{e^{\beta E} - 1} \big) - \frac{1}{2\pi} \frac{1}{E} \underbrace{\Big/_{-\infty}^{\infty} \overbrace{\arctan \frac{k_0}{E}}^{\substack{\text{integrated} \\ \text{over } k_0}}}_{=\pi} \Big] \qquad (2.112)
\end{aligned}$$

where $E^2 \equiv k^2 + m^2$. Noting that $\frac{d}{dm^2} \ln(1 - e^{-\beta E}) = \frac{1}{e^{\beta E} - 1} \beta \frac{dE}{dm^2}$ we find

$$\Delta = 2V_4 \int \frac{d^3\boldsymbol{k}}{(2\pi)^3} \beta^{-1} \ln\left(1 - e^{-\beta E}\right). \qquad (2.113)$$

Thus we may write

$$Z = e^{-\Omega/T} = e^{-F/T} = e^{-\frac{1}{2}\Delta} \qquad \big(V_4 = V_3\beta\big)\ , \tag{2.114}$$

or

$$\Omega = VT\int \frac{d^3\boldsymbol{k}}{(2\pi)^3}\ln(1-e^{-\beta E})\ . \tag{2.115}$$

It should come to as no surprise that the final result is just ideal gas which by definition is non-interacting.

Note 1: that the beautiful formula (2.111) can even be generalised to

$$T\sum_{n=-\infty}^{\infty}\frac{1}{(2\pi nT+C)^2+E^2} = \frac{1}{2E}\bigg(1+\frac{1}{e^{\beta(E+iC)}-1}+\frac{1}{e^{\beta(E-iC)}-1}\bigg), \tag{2.116}$$

$$T\sum_{n=-\infty}^{\infty}\frac{1}{((2n+1)\pi T+C)^2+E^2} = \frac{1}{2E}\bigg(1-\frac{1}{e^{\beta(E+iC)}+1}-\frac{1}{e^{\beta(E-iC)}+1}\bigg). \tag{2.117}$$

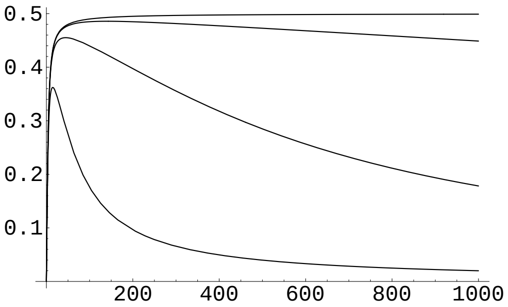


Figure 2.7: Top curve: limit, lower ones: sums up to 1000,100,10 terms.

Note 2, dimensional regularisation: Let us now evaluate the above sum

$$I(T,m) = T\sum_n\int\frac{d^dk}{(2\pi)^d}\frac{1}{\omega_n^2+k^2+m^2}, \qquad d = 3-2\epsilon \tag{2.118}$$

in the $T \gg m$ limit in a different way. As long as $\epsilon \neq 0$ all the integrals are finite, divergences are exposed by taking $\epsilon \to 0$. First, the zero mode term $n = 0$ has to be given special treatment:

$$I^{n=0}(T,m) = T\int\frac{d^dk}{(2\pi)^d}\frac{1}{k^2+m^2} = -\frac{Tm}{4\pi}. \tag{2.119}$$

Something seemingly positive has suddenly become negative: an infinite positive term has effectively been thrown away. Why this is justified has, of course, to be proven in theory of renormalisation. For the $n \neq 0$ terms one obtains

$$I^{n\neq 0}(T,m) = \frac{2T}{(4\pi)^{d/2}}\frac{1}{(2\pi T)^{2-d}}\sum_{l=0}^{\infty}\bigg(\frac{-m^2}{4\pi^2T^2}\bigg)^l\frac{\Gamma(l+1-d/2)}{\Gamma(l+1)}\zeta(2l+2-d). \tag{2.120}$$

Expanding for small ϵ and including terms up to $l = 2$:

$$I(T,m) = \frac{T^2}{12}-\frac{Tm}{4\pi}-\frac{m^2}{16\pi^2}\bigg(\frac{1}{\epsilon}+\log\frac{4\pi}{T^2}-2\log(2\pi)+2\gamma_E+\mathcal{O}(\epsilon)\bigg)+\frac{m^4\zeta(3)}{128\pi^4T^2}+\mathcal{O}(m^6/T^4). \tag{2.121}$$

2.9 Effective actions

An effective action is the fluctuation corrected action. The basic definition of the effective action *for a fixed background* x_b is

$$\Gamma(x_b) = W(J) - \int d\tau\, J(\tau) x_b(\tau) \ . \tag{2.122}$$

One may then trivially divide the effective action into kinetic and potential parts:

$$\Gamma(x_b) = \int_0^\beta d\tau \left[E_{\text{kin}}(x_b) + V_{\text{eff}}(x_b) \right] \tag{2.123}$$

so that for $x_b = \text{const} \equiv x_0$

$$\Gamma(x_0) = \frac{V_{\text{eff}}(x_0)}{T} \ . \tag{2.124}$$

The question one should then pose is: What is the value of the fixed background at which the effective action is minimized, i.e. what is the ground state of temperature-corrected system.

Here are a number of general equations on the effective potential in a compact notation. They may look very formal and boring but are actually very important for any computations in theories defined by path integrals. The basic definition is

$$\begin{aligned} Z(J) &= \int \mathcal{D}x\, e^{-S(\phi) - \int d\tau J x} = \\ &= e^{-W(J)} = e^{-\Gamma(\bar{x}) - \int d\tau J \bar{x}} \end{aligned}$$

($e^{\cdots + \int d\tau J \bar{x}}$ is perhaps nicer: then $J > 0 \to \bar{x} > 0$) where the *mean field* or the *expectation value* $\bar{x}$ is defined as

$$\bar{x}_J = \langle x \rangle_J = Z^{-1}(J) \int \mathcal{D}x e^{-S - \int d\tau J x} x = -\frac{1}{Z(J)} \frac{\delta Z(J)}{\delta J} = W'(J) \ , \tag{2.125}$$

where the subscript J reminds us that the expectation value depends on the fixed source. From (2.125)

$$\frac{\delta \bar{x}_{J_1}}{\delta J_2} = \frac{1}{Z(J)^2} \frac{\delta Z}{\delta J_1} \frac{\delta Z}{\delta J_2} - \frac{1}{Z(J)} \frac{\delta^2 Z}{\delta J_1 \delta J_2} = \bar{x}^2 - \langle x(\tau_1) x(\tau_2) \rangle \ . \tag{2.126}$$

Noting that $\langle (\bar{x} - x(\tau_1))(\bar{x} - x(\tau_2)) \rangle = -\bar{x}^2 - \langle x(\tau_1) x(\tau_2) \rangle$ we may also write

$$\frac{\delta \bar{x}_J}{\delta J} = W''(J) = \langle (\bar{x} - x)^2 \rangle \tag{2.127}$$

so that W'' is the fluctuation width.

Now perform a Legendre transformation and take $\bar{x}$ as a variable, instead of J:

$$\Gamma(\bar{x}) = W(J) - \int d\tau\, J \bar{x} \ . \tag{2.128}$$

Then

$$\Gamma'(\bar{x}) = \frac{\delta W}{\delta \bar{x}} - \frac{\delta}{\delta \bar{x}} \int d\tau\, J\bar{x} = \int \frac{\delta W}{\delta J}\frac{\delta J}{\delta \bar{x}} d\tau - J - \int \frac{\delta J}{\delta \bar{x}} \bar{x}\, d\tau = -J \tag{2.129}$$

and thus $\Gamma'(\bar{x}) = 0$ gives the true ground state (J=0). Further derivatives are

$$\Gamma''(\bar{\phi}) = -\frac{dJ}{d\bar{\phi}} = -\frac{1}{W''(J)}, \qquad \Gamma'''(\bar{\phi}) = W'''/(W'')^3,$$

$$\Gamma^{(4)}(\bar{\phi}) = W^{(4)}/(W'')^4 - 3(W''')^2/(W'')^5, ..$$

The physics behind this is that an external current J is used to tune $\langle\phi\rangle$ to the value $\bar{\phi}$; otherwise it relaxes to the value of $\bar{\phi}$ in the ground state.

Since Γ determines the ground state, it is very important to find methods to compute it. This can be done in the loop expansion (Jackiw74). Very schematically, taking $J(\tau) \equiv J$ and $x(\tau) \equiv \phi$ to be constants instead of functions so that we may perform the imaginary time integrals trivially, the following steps are needed:

1. Compute $W(J)$ expanding about the classical saddle point ϕ_c:

$$\begin{aligned} S(\phi) + J\phi &= S(\phi_c) + J\phi_c + [S'(\phi_c) + J)](\phi - \phi_c) + \frac{1}{2!}S''_c(\phi - \phi_c)^2 + \\ &+ \frac{1}{3!}S'''_c(\phi - \phi_c)^3 + + \frac{1}{4!}S^{(4)}_c(\phi - \phi_c)^4 + ... \end{aligned}$$

where the saddle point is chosen by

$$S'(\phi_c) + J = 0.$$

Then $W(J)$ is given by the Gaussian integral

$$\begin{aligned} e^{-W(J)} &= e^{-(S_c + J\phi_c)} \int \mathcal{D}\phi e^{-\frac{1}{2!}S''_c(\phi-\phi_c)^2 - ...} \\ &= e^{-(S_c+J\phi_c)} \int \mathcal{D}\chi e^{-\frac{1}{2!}S''_c\chi^2}\left[1 - \frac{1}{3!}S'''_c\chi^3 - -\frac{1}{4!}S^{(4)}_c\chi^4 + \frac{1}{2(3!)^2}(S'''_c)^2\chi^6 + ..\right] \\ &= e^{-(S_c+J\phi_c)}\sqrt{\frac{2\pi}{S''_c}}\left[1 - \frac{S^{(4)}_c}{8(S''_c)^2} + \frac{5}{24}\frac{(S'''_c)^2}{(S''_c)^3} + ...\right] \end{aligned}$$

leading to

$$\begin{aligned} W(J) &= S(\phi_c) + J\phi_c + \frac{\hbar}{2}\log S''(\phi_c) + \frac{\hbar^2 S^{(4)}_c}{8(S''_c)^2} - \frac{5\hbar^2}{24}\frac{(S'''_c)^2}{(S''_c)^3} + ... \\ &\equiv S(\phi_c) + J\phi_c + \Gamma_1(\phi_c). \end{aligned}$$

Here we have scaled $\phi - \phi_c = \sqrt{\hbar}\chi$ to demonstrate that we are dealing with an expansion in $\hbar$, the loop expansion ($\hbar$ is brought back into the equations by the scaling $S \to S/\hbar$). Thus $\Gamma/\hbar = S/\hbar + \frac{1}{2}\log S'' + \mathcal{O}(\hbar)$ and the gaussian contribution $\propto \log S''$ is thus of the order $\mathcal{O}(\hbar^0)$.

2. Compute $\Gamma(\bar{\phi})$, the effective action of the mean field ($\neq$ the saddle point ϕ_c if we go beyond the lowest order). ¿From $\bar{\phi} = W'(J)$ and the above result for $W(J)$ one finds that

$$\bar{\phi} = \phi_c - \frac{S_c'''}{2(S_c'')^2} \equiv \phi_c - \phi_1 .$$

Then write $W(J) - \bar{\phi}J$ in terms of $\bar{\phi} + \phi_1$, expand in ϕ_1 and find that

$$\begin{aligned} \Gamma(\bar{\phi}) &= S(\bar{\phi}) + \Gamma_1(\bar{\phi}) + \text{terms combining to } 1 - \text{particle reducible diagrams} \\ &= S(\bar{\phi}) + \Gamma_1(\bar{\phi})|_{\text{1-part.irred.diags}} \\ &= S(\bar{\phi}) + \frac{1}{2}\log S''(\bar{\phi}) + \frac{S^{(4)}}{8(S'')^2} - \frac{(S''')^2}{12(S'')^3)} \end{aligned}$$

Actually in $W(J)$

$$\frac{5}{24} = \frac{1}{8} + \frac{1}{12} = \text{spectacle} + \text{sunset}$$

and the 1/8 is cancelled by 1PI. **Some figure needed here!**

Compact form of the result:

$$V_{\text{eff}}(\phi) = V_0(\phi) - \frac{1}{V_3}\ln\int \mathcal{D}\phi e^{-S_0} - \frac{1}{V_3}\langle e^{-S_1}\rangle_{\text{1PI}}$$

where one has shifted one of the components ϕ_i by ϕ, neglected linear terms and grouped the quadratic terms in S_0 and the rest + counter terms in S_1.

Example: Inverted oscillator. Let us return to quantum mechanics and consider the 1+1 dimensional inverted oscillator with the Lagrangian

$$L = \frac{1}{2}m\dot{x}^2 + V(x), \qquad V(x) = -\frac{1}{2}m\omega^2 x^2 + \underbrace{\frac{1}{4}\lambda m\omega_0^4 x^4}_{\text{needed for stabilizing V}} . \tag{2.130}$$

Here we have chosen the coefficient of the x^4 such that λ is dimensionless.

Let us take a constant background $x_c = \text{const.}$; then $V''(x_c) = -m\omega^2 + 3\lambda m\omega_0^4 x_c^2$. From pages [49 prujussa] and [76] we find that the gaussian integration yields

$$\text{“det}K\text{”} = \text{const}\cdot e^{\sum_n \ln(3\lambda\omega_0^4\boldsymbol{x}^2 + 4\pi^2 n^2 T^2)} \tag{2.131}$$

so that for a constant background we may immeadiately write

$$\Gamma(x_c) = \frac{V_{\text{eff}}(x_c)}{T} = \frac{V(x_c)}{T} + \underbrace{\frac{1}{2}\sum_n \ln\left(3\lambda\omega_0^4\boldsymbol{x}^2 - \omega^2 + 4\pi^2 n^2 T^2\right)}_{\text{diverges}\rightarrow\text{ must renormalize}} . \tag{2.132}$$

The divergence is here due to the zero point quantum fluctuations, which are present already at $T = 0$. It is a theorem that no new divergences appear at finite T so that the infinities can be absorbed by the redefinition of the parameters of the $T = 0$ theory; this is just the usual renormalization procedure. Thus at large T we may write the effective potential as

$$V_{\text{eff}}(x_c) \simeq \frac{1}{2}T\sum_n \ln(3\lambda\omega_0^2 x_c^2 - \omega^2 + 4\pi^2 n^2 T^2) + \underbrace{\text{terms independent of } T}_{\text{these cancel the infinities}} . \tag{2.133}$$

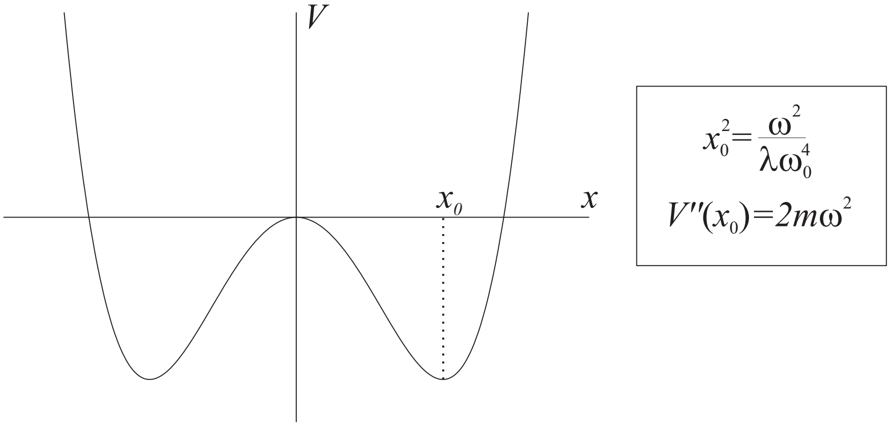


Figure 2.8: Potential of inverted oscillator

Strictly speaking, the expression is well defined only when

$$U \equiv 3\lambda\omega_0^4 x_c^2 - \omega^2 \geq 0 \; . \tag{2.134}$$

We may sidestep the issue of infinities by taking a derivative with respect to U (recall that x_c is just some fixed constant). Then

$$\begin{aligned} \frac{\partial V_{\text{eff}}}{\partial U} &= \frac{1}{2} T \sum_n \left[\frac{1}{U + 4\pi^2 n^2 T^2} \right] \\ &= \frac{1}{2} \frac{1}{\sqrt{U}} \sum_n \frac{T\sqrt{U}}{U + 4\pi^2 n^2 T^2} \\ &= \frac{1}{2} \frac{1}{\sqrt{U}} \left[\frac{1}{2} + \frac{1}{e^{\beta\sqrt{U}} - 1} \right] \; . \end{aligned} \tag{2.135}$$

Thus the T-dependent part of the effective potential close to the origin $x_c \approx 0$ is found from

$$\begin{aligned} \frac{\partial V_{\text{eff}}}{\partial \boldsymbol{x}^2} = \frac{\partial U}{\partial x_c^2} \frac{\partial V_{\text{eff}}}{\partial U} &= \frac{3}{2} \lambda \omega_0^4 \frac{1}{\sqrt{U}} \frac{1}{e^{\beta\sqrt{U}} - 1} \\ &\simeq \frac{3}{2} \lambda \omega_0^4 \frac{T}{U} \end{aligned} \tag{2.136}$$

i.e. $V_{\text{eff}} \propto x_c^2 T$ as $T \to \infty$. Thus, at very high temperatures, the term proportional to x_c would dominate over the zero temperature potential (at least close to $x_c \sim 0$). As a consequence, the high temperature ground state is $x_c = 0$. When the temperature decreases, eventually the vacuum term $-m\omega^2 x_c^2$ takes over and $x_c = 0$ becomes unstable, triggering a phase transition from $x_c = 0$ to $x_c \neq 0$.

2.10 Effective theories in general

Note that the notion of an effective action is not unique; there are an infinite number of effective actions. Starting with the path integral

$$Z = \int \mathcal{D}\phi \, e^{-S_E[\phi]} \tag{2.137}$$

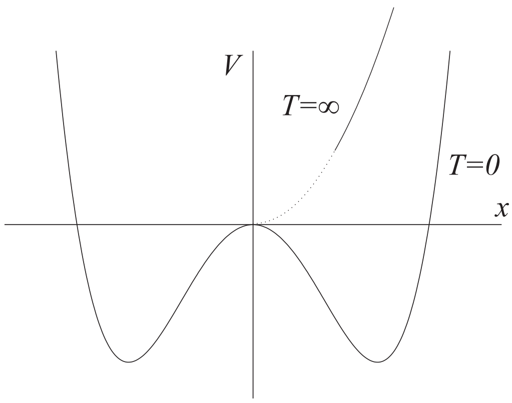


Figure 2.9: Phase transition

we may organize the degrees of freedom into different sets, for example

$$Z = \int \Pi \mathcal{D}\phi_L \, \mathcal{D}\phi_S \, e^{-S_E[\phi_L,\phi_S]} \tag{2.138}$$

where ϕ_L stands for long wavelengths and ϕ_S for shortwavelengths; integrating the latter out we find

$$Z = \int \mathcal{D}\phi_L \, e^{-S_E^{\text{eff}}[\phi_L]} \tag{2.139}$$

which is an effective action for the long wavelength degrees of freedom. How the division is actually done is of course dictated by the physical problem at hand. Nevertheless, this demonstrates a general principle of *coarse graining*: irrelevant degrees of freedom have been *averaged out.* An example is chemistry, which can be viewed as coarse grained QED with an integration over short wavelength modes.

Note that, because of nonlinearities, coarse graining gives rise to qualitatively new "laws" as the fundamental degrees of freedom q are replaced by the effective degrees of freedom $\langle q\rangle_{time,space,...}$. This means that the equations of motion, which typically are of the form $\mathcal{D}q = \lambda q^2 + \gamma q^3 + \ldots$ where $\mathcal{D}$ is some differential operator, gets replaced by

$$\mathcal{D}\langle q\rangle = \lambda\langle q^2\rangle + \gamma\langle q^3\rangle + \ldots \neq \lambda\langle q\rangle^2 + \gamma\langle q\rangle^3 \ . \tag{2.140}$$

As a consequence, even simple fundamental laws may give rise to complicated laws for the coarse grained quantities.

Example. Effective theories in quantum mechanics. Consider a quantum mechanical system (such as a two-particle spin system) in an entangled state:

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|+\rangle|-\rangle + |-\rangle|+\rangle\right). \tag{2.141}$$

The density matrix reads

$$\rho = |\phi\rangle\langle\phi| = \underbrace{\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}}_{++\ +-\ -+\ --} \tag{2.142}$$

and we are obviously dealing with a pure state: $\rho^2 = \rho$. An effective theory, describing only a reduced number of degrees of freedom (here = 1), is obtained by integrating out (= taking a trace over) the superfluous degrees of freedom. The effective density matrix reads

$$\rho_{\text{eff}} = \underbrace{\text{Tr}\rho}_{\text{over states 2}} = \langle +|\rho|+\rangle + \langle -|\rho|-\rangle$$
$$= \tfrac{1}{2}\left(|+\rangle\langle +| + |+\rangle\langle -|\right) \qquad (2.143)$$

which describes now a mixed state: $\rho_{\text{eff}}^2 = \rho_{\text{eff}}$.

The very interesting question is: given that at the fundamental level the world is quantum mechanical with $Z = \int \mathcal{D}x e^{iS}$, how come for large ensembles we nevertheless write $Z = \int \mathcal{D}x e^{-S_E}$?

The answer appears to be decoherence. Consider a quantum system that consist of a small subsystem $|a\rangle$, with possible states labeled by $|n\rangle$ so that $|a\rangle = \sum_n c_n|n\rangle$, and the environment $|\phi_0\rangle$. The total density matrix is $\rho_{\text{tot}} = |\phi_0\rangle|a\rangle\langle a|\langle\phi_0|$ The density matrix of the subsystem $\rho = \text{Tr}_{\text{env}}\rho_{\text{tot}} = |a\rangle\langle a|$ is subject to evolution, which has two sources, internal and interaction with the environment:

$$i\frac{\partial\rho}{\partial t} = [H_{\text{int}}, \rho] + i\frac{\partial\rho}{\partial t}\Big|_{\text{scatt}} \; . \qquad (2.144)$$

Let us assume slow internal dynamics. Then, with a single scattering event, the initial state $|a\rangle|\phi_0\rangle \to S|a\rangle|\phi_0\rangle$, where S is the S-matrix. Assuming no recoil the subsystem remains the same even after the scattering. Thus

$$S|a\rangle|\phi_0\rangle = \sum_n c_n|n\rangle|\phi_n\rangle \; , \qquad (2.145)$$

where $|\phi_n\rangle$ is the environment state corresponding to the subsystem state $|n\rangle$ (the environment could be considered as a measuring device with n pointer position; after scattering, the device would be in a superposition of the pointer positions). Thus, after scattering, the reduced density matrix of the subsystem

$$\rho = \sum c_m^* c_n|n\rangle\langle m| \to \sum c_m^* c_n\langle\phi_n|\phi_m\rangle|n\rangle\langle m| \qquad (2.146)$$

or

$$\rho_{nm} \to \rho_{nm}\langle\phi_m|\phi_n\rangle = \rho_{nm}\langle\phi_0|S_n^\dagger S_m|\phi_0\rangle \; . \qquad (2.147)$$

We now assume that a single scattering is not enough to resolve the different system states; the system remains in "almost unmeasured" state and $S_n^\dagger S_m \approx 1 - \epsilon$. The scattering rate $\Gamma = \sigma v n$ depends on the dynamics, but in general we may now write

$$\rho_{nm} \to \rho_{nm}(1-\epsilon)^{\Gamma t} \approx \rho_{nm}e^{-\epsilon\Gamma t} \qquad (2.148)$$

so that the non-diagonal elements of the density matrix vanish exponentially fast. Because of quantum entanglement, the subsystem is thus seen to become a statistical ensemble.

Here we may echo the sentiments of the French mathematician Emile Borel, who in 1914 wrote: "Statistical mechanics is not mechanics of large complicated systems, rather it is the mechanics of limited, not completely isolated systems".

2.11 Tunneling

Let us now apply path integral methods to tunneling, which relates directly to first order phase transitions (phase transitions will be discussed in detail in Ch. X). ¿From quantum mechanics we recall that in the WKB-approximation the tunneling rate Γ is given by

$$\Gamma = \frac{1}{\tau} \approx \frac{\omega}{2\pi} e^{-2\int_{x_1}^{x_2} dx K(x)} \; , \; K(x) = \frac{2m}{\hbar^2}\left(V_{\text{eff}} - E\right) \tag{2.149}$$

where V_{eff} is the effective potential. For example, for a 3-d problem with spherical symmetry $V_{\text{eff}} = V(r) + \hbar^2 l(l+1)/(2mr^2)$. Quantum mechanics gives directly the barrier penetration probability $e^{-2\int dxK}$; the prefactor ω is in general more difficult to compute. Quantum indeterminacy allows the system to go over (or rather, through) the barrier $V(x_0)$ even though the energy is less than the barrier height. **KUVA PUUTTUU**

For a thermal system the situation is analogous. However, since the probability for a thermal fluctuation is given by the Boltzmann factor $e^{-\beta E}$, the tail of the distribution may escape from the potential well simply by going classically over the wall. Let us consider the situation where at $x \approx 0$ the potential is given by $V \approx \frac{1}{2}m\omega_0^2 x^2$ while at the barrier $V \approx V(x_0) - \frac{1}{2}m\omega^2(x-x_0)^2$. We assume that $T \ll V(x_0)$. Then classically the differential probability for going over the wall is

$$\frac{d\Gamma}{dx\, dp} = \underbrace{P(E \geq V(x_0))}_{\propto e^{-\beta E} \approx e^{-\beta V(x_0)}} \; \underbrace{v\theta(v)\; \delta(x - x_0)}_{\text{rightmoving flux}} \; . \tag{2.150}$$

Then, assuming that most contribution to the path integral is obtained from $x \approx 0$, we may write

$$\Gamma = \frac{e^{-V(x_0)} \int dp\; \frac{p}{m}\theta(p) e^{-\beta p^2/2m}}{\int dp\; e^{-\beta p^2/2m} \underbrace{\int dx\; e^{-\frac{1}{2}m\omega_0^2 x^2 + \dots}}_{\sqrt{\frac{2\pi}{\beta m\omega_0^2}}}} \approx \frac{\omega_0}{2\pi} e^{-\beta V(x_0)} \; . \tag{2.151}$$

Note that here we closed our eyes to the fact that at $x \approx x_0$

$$e^{-V(x)} \approx e^{-V(x_0)} e^{+\frac{1}{2}m\omega^2(x-x_0)^2} \tag{2.152}$$

where the second factor is formally divergent but when analytically continued, gives rise to an imaginary contribution. In a proper treatment, it is really this imaginary part which is the source of non-zero tunneling rate. You should recall from quantum mechanics that the probability distribution decays if there is an imaginary component in energy:

$$|\psi(t)|^2 = |e^{-iHt}\psi(0)|^2 = |e^{-i\text{Re}Et + \text{Im}Et}\psi(0)|^2 = e^{2\text{Im}Et}|\psi(0)|^2 \tag{2.153}$$

so that $\Gamma = -2\text{Im}E$.

In a thermal system the instability of the (ground) state is signalled by a non-zero imaginary part of the free energy. Indeed, classically

$$\begin{aligned}\mathrm{Im}F &= -T\frac{\mathrm{Im}Z}{Z} = -T\frac{\mathrm{Im}\int dxdp\; e^{-\beta p^2/2m}e^{-\beta[V(x_0)-\frac{1}{2}m\omega^2(x-x_0)^2]}}{\int dxdp\; e^{-\beta p^2/2m}e^{-\frac{1}{2}m\omega_0^2 x^2}} \\ &= -T\frac{\mathrm{Im}\; e^{-\beta V(x_0)}\sqrt{\frac{2\pi T}{-\omega^2}}}{\sqrt{\frac{2\pi T}{\omega_0^2}}} \\ &= T\frac{\omega_0}{2\omega}e^{-\beta V(x_0)}\;, \end{aligned} \tag{2.154}$$

where we now have continued analytically the gaussian integral in the numerator. Thus we find

$$\Gamma = T\frac{\omega_0}{\omega}e^{-\beta V(x_0)} \tag{2.155}$$

which agrees with (2.151) if we choose $T = \hbar\omega/(2\pi)$ (see Affleck, Phys. Rev. Lett. 46 (1981) 388.)

In the quantum case we should again look for the imaginary part of F (or Z). Let us consider the potential shown in Figure XXXXX. We already know that integration about the trivial saddle point $x = x_0$ yields the usual result (2.77) for the harmonic oscillator. But what about other saddle points? These are given by the euclidean equation of motion

$$\frac{1}{2}m\ddot{x} - V'(x) = 0 \to \frac{1}{2}m\dot{x}^2 - V(x) = -E = \text{const.} \tag{2.156}$$

The question is: are there non-trivial solutions such that $x(0) = x(\beta)$? As can be seen from (2.156), these can be viewed as non-euclidean solutions for motion in an inverted potential starting from x_1 and coming to rest at x_2 (see Fig. XXXXX). At $x \approx x_0$ the potential is approximately harmonic with frequency ω, and $x_+ > x_2$ is defined by $V(x_+) = 0$. The period P of such a motion is given by

$$\begin{aligned}P(E) &= 2\int_{\tau_1}^{\tau_2} d\tau = 2\int_{x_1}^{x_2} dx\;\left[\frac{2}{m}\left(V(x)-E\right)\right]^{-1/2} \\ &\geq \int_{x_+-x_0}^{x_+} dx\,\sqrt{\frac{2}{m}}\underbrace{\left(V(x_0)-E-\frac{1}{2}m\omega^2(x-x_0)^2\right)^{-1/2}}_{\text{harmonic oscillator}} = \frac{2\pi}{\omega}\;. \end{aligned} \tag{2.157}$$

Thus we conclude that the motion is periodic, i.e. $P(E) = \beta$, whenever $\beta \geq 2\pi/\omega$. In that case there always exists an orbit $\bar{x}$ such that $\bar{x}(0) = \bar{x}(\beta)$ which is also a saddle point (if $T \geq \omega/(2\pi)$ the only solution is the classical $x = x_0$). We may call the solution $\bar{x}$ an *instanton*.

Expanding about the instanton we find

$$Z = N\left[\det\left(-\frac{d^2}{d\tau^2} + V''(\bar{x}(\tau))\right)\right]^{-1/2} e^{-S_E[\bar{x}]}\;. \tag{2.158}$$

The aim is then to show that the determinant has one negative eigenvalue, giving rise to an imaginary part of Z; this is a non-trivial task but can be done (see. Phys. Rev. D25 (1982) 330).

2.12 Tunneling in field theory

Tunneling in field theory is analogous to the quantum mechanical case considered in the previous Section. At high T we may simplify things by noting that as $\beta \to 0$, only the static modes with $\dot{\phi} = 0$ contribute to the action so that

$$S = \int_0^\beta d\tau d^3x \left[\frac{1}{2}\dot{\phi}^2 + \frac{1}{2}(\nabla\phi)^2 + V(\phi, T)\right] \approx \frac{1}{T}\int d^3x \left[\frac{1}{2}(\nabla\phi)^2 + V(\phi, T)\right] \equiv \frac{1}{T}S_3[T] \ . \tag{2.159}$$

The tunneling rate is then given by

$$\Gamma = Ae^{-S[\phi_*]/T} \tag{2.160}$$

where A is the fluctuation determinant (from a gaussian integration) and ϕ_* is the *critical field* configuration, which is the solution to the euclidean equation of motion that connects the two vacua.

In general there is an infinity of configurations connecting any two vacua. The issue then is, which of these has the lowest action and thus corresponds to the fastest tunneling rate? Usually the answer is: the most symmetric one. Let us therefore assume that the critical field configuration is spherically symmetric. The euclidean equation of motion reads then

$$\frac{d^2\phi_*}{dr^2} + \frac{2}{T}\frac{d\phi_*}{dr} = V'(\phi_*, T) \ . \tag{2.161}$$

The solution $\phi_* = \phi_*(r)$ is called the critical bubble.

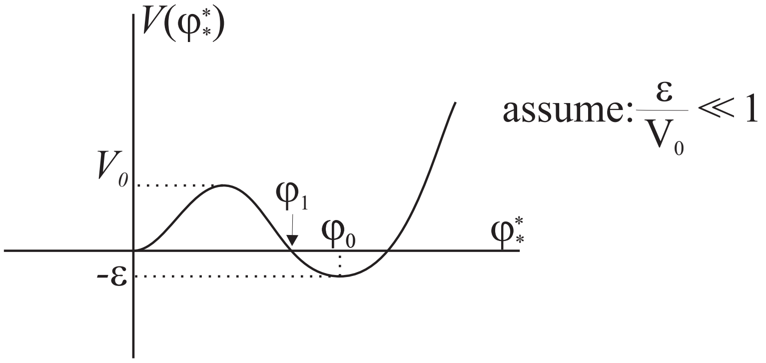


Figure 2.10: The potential appropriate for the thin wall approximation.

Thin wall approximation. The critical bubble can be found analytically in the thin wall approximation[1] which is appropriate for the potential of the type depicted in Fig. 2.10. There one assumes that the energy difference ϵ between the two vacua is small compared with the height of the potential wall V_0 that separates them. In that case we may seek for a solution where $\phi_* \approx \phi_0 = const$ when $r < R$, the size of the bubble, and $d\phi_*/dr \neq 0$ only in a narrow region $\ll R$, while outside the bubble we have $\phi_* \approx 0$ (see Fig. 2.11). Close to the thin wall r is large so that we may write

$$\frac{d^2\phi_*}{dr^2} \approx V'(\phi_*, T) = \frac{dV}{dr}\frac{dr}{d\phi_*} \tag{2.162}$$

---

[1] S. Coleman, Phys. Rev. D15, 2929 (1977).

so that $\phi_*'^2 \approx V(r)$ and

$$r \approx \int_{\phi}^{\phi_0} \frac{\phi_*}{\sqrt{V}} \; . \tag{2.163}$$

We then find that

$$\begin{aligned} S_3 &= 4\pi \int_0^\infty dr\, r^2 \left[\frac{1}{2} \frac{d^2\phi_*}{dr^2} + V(\phi_*, T) \right] \\ &= -\frac{4}{3}\pi R^3 \epsilon + 4\pi R^2 S_1(T) \; , \end{aligned} \tag{2.164}$$

where S_1 is the surface tension, which is the integral over the region where ϕ_* changes rapidly; it can be calculated explicitly once $V(\phi_*, T)$ is specified.

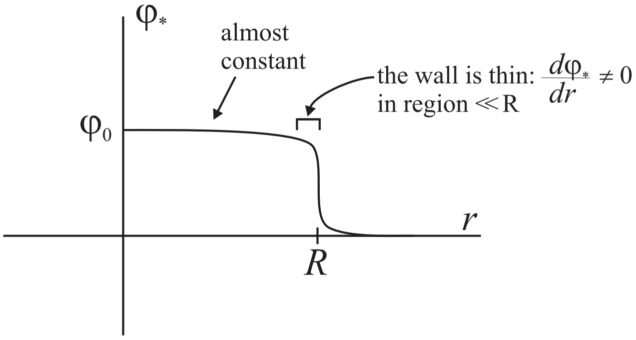


Figure 2.11: The critical field in the thin wall approximation.

The remaining task is now to minimize the action as a function of the free parameter R, the size of the critical bubble:

$$\frac{dS_3}{dR} = 0 \;\rightarrow\; R = \frac{2S_1}{\epsilon} \; . \tag{2.165}$$

Since ϵ is assumed to be small, the bubble is large, as it should for the thin wall approximation to be valid. We can also find the action, which reads

$$S_3 = \frac{16\pi S_1^3}{3\epsilon^2} \; . \tag{2.166}$$

Hence in the thin wall approximation the tunneling rate $\Gamma \sim e^{S_3/T}$ is small and the transition could be called slow boiling.

Finding the fluctuation determinant is again much more complicated. A good guess is always that $A \sim T^4$ since T is often the only relevant mass scale in the problem.

Chapter 3

Ideal Fermi-Dirac and Bose-Einstein gases

Here "ideal gas" will denote a collection of free particles within a system with known energy levels $E_1, E_2, \ldots$. For example, if the system is a box of volume $V = L^d$ (usually $d = 3$) with periodic boundary conditions and if the particles satisfy the dispersion relation $E^2(k) = (\hbar c k)^2 + (mc^2)^2 \equiv \mathbf{k}^2 + m^2$ the energy spectrum is

$$\begin{aligned}\mathbf{k} &= (k_1, k_2, k_3) = \frac{2\pi}{L}(n_1, n_2, n_3), \quad n_i = 0, \pm 1, \pm 2, ..., \\ E^2(k) &= \frac{4\pi^2}{L^2}(n_1^2 + n_2^2 + n_3^2) + m^2 \end{aligned} \tag{3.1}$$

and each set of n_i corresponds to a state of the system. A second example is free particles in a 3d harmonic oscillator potential with $E(\mathbf{n}) = \hbar\omega(n_1 + n_2 + n_3 + 3/2)$.

The crucial assumption is then the following: each state is occupied with equal probability, given by the usual FD or BE statistics. This is easy to implement formally (and the standard steps are reproduced below), but leaves completely open the dynamical issue of how this kind of state is actually attained, i.e. how the system thermalises. Paradoxically, as will be discussed in Ch. XXXXX, the stronger the interactions are, the faster and more efficiently they thermalise the system; however, at the same time the interactions should be weak enough so that the system is perturbatively close to the non-interaction ideal system. Therefore, in reality ideal gas system is not a collection of free particles even if confined in a box!

Very much physics is built in the ideal gas formulas. Therefore, in this and the next Chapters we shall discuss ideal gas systems from different angles and in various contexts.

3.1 Partition functions, counting states

Let us assume that the occupation number of each of the energy levels E_i is N_i. From the definition of grand canonical partition function $\mathcal{Z}$ we find that

$$\mathcal{Z}(T,V,\mu) \equiv \sum_{N=0}^{\infty} z^N Z(T,V,N) = \sum_{N=0}^{\infty} (e^{\frac{\mu}{T}})^N \sum_{\{N_1,N_2,\ ...\}} e^{-\frac{1}{T}(N_1E_1+N_2E_2+...)}. \tag{3.2}$$

Because of the condition $\sum N_i = N$, the summation in $Z(T,V,N)$ is hard to perform. Note however that the sum in $\mathcal{Z}$ goes over all accessible states, as depicted in Fig. 3.1. Therefore, by rearranging the order of the summation we may write:

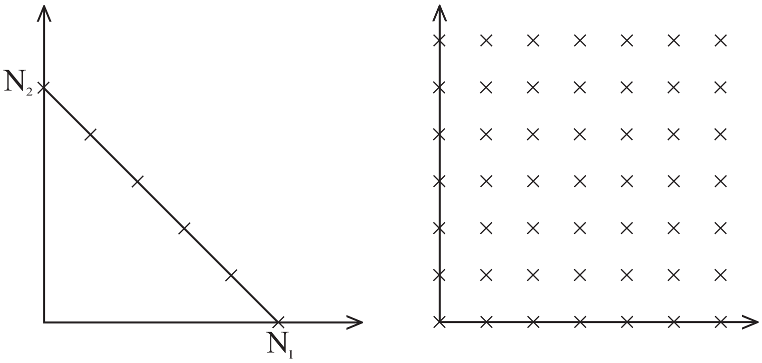


Figure 3.1: Z to the left and $\mathcal{Z}$ to the right.

$$\begin{aligned}
\mathcal{Z} &= \sum_{\{N_1,N_2,...=0\}}^{\infty} e^{\frac{\mu}{T}N_1} e^{\frac{\mu}{T}N_2} ... (e^{-\frac{1}{T}E_1})^{N_1} (e^{-\frac{1}{T}E_2})^{N_2} ... \\
&= \sum_{\{N_1,N_2,...=0\}}^{\infty} (e^{\frac{1}{T}(\mu-E_1)})^{N_1} (e^{\frac{1}{T}(\mu-E_2)})^{N_2} ... \\
&= \sum_{N_1=0}^{\infty} (e^{\frac{1}{T}(\mu-E_1)})^{N_1} \sum_{N_2=0}^{\infty} (e^{\frac{1}{T}(\mu-E_2)})^{N_2} ..., \qquad (3.3)
\end{aligned}$$

where the sums are now simple to evaluate:

$$\sum_{N=0}^{\infty} x^N = \left\{ \begin{array}{ll} 1+x & \text{FD} \\ \frac{1}{1-x} & \text{BE} \end{array} \right. . \tag{3.4}$$

Thus for FD we find

$$\mathcal{Z} = \prod_k [1 + e^{\frac{1}{T}(\mu-E_k)}], \qquad \Omega = -Vp(T,\mu) = -T\sum_k \log[1 + e^{\frac{1}{T}(\mu-E_k)}], \tag{3.5}$$

whereas for BE

$$\mathcal{Z} = \prod_k \frac{1}{1 - e^{\frac{1}{T}(\mu-E_k)}}, \qquad \Omega = -Vp(T,\mu) = T\sum_k \log[1 - e^{\frac{1}{T}(\mu-E_k)}], \tag{3.6}$$

From here one further derives, using $s(T,\mu) = \partial p/\partial T = S/V$, $n(T,\mu) = \partial p/\partial\mu = N/V$ and $\epsilon = Ts - p + \mu n = E/V$ that

$$\begin{aligned} N(T,\mu) &= \sum_k n_k, && (3.7)\\ S(T,\mu) &= \sum_k [-(1-n_k)\log(1-n_k) - n_k \log n_k] \qquad \text{FD}, && (3.8)\\ S(T,\mu) &= \sum_k [(1+n_k)\log(1+n_k) - n_k \log n_k] \qquad \text{BE}, && (3.9)\\ E(T,\mu) &= \sum_k E_k n_k, && (3.10) \end{aligned}$$

where the average occupation number of the level k is

$$n_k = \frac{1}{e^{\frac{1}{T}(E_k-\mu)} \pm 1} \left\{ \begin{array}{c} \text{FD} \\ \text{BE} \end{array} \right. . \tag{3.11}$$

The above is valid for any set of energy levels E_k. If we further take our free particles in a box, the energy levels are indexed by $E_k \equiv \sqrt{\mathbf{k}^2 + m^2}$ and the sums can be changed to integrals using the continuum limit of the density of states of particles in a 3d box:

$$\sum_k \to \frac{V}{(2\pi)^3} \int d^3k. \tag{3.12}$$

Then for FD the pressure reads as

$$p(T,\mu) = \frac{T}{(2\pi)^3} \int d^3k \log[1 + e^{\frac{1}{T}(\mu - E_k)}] \tag{3.13}$$

while for BE

$$p(T,\mu) = -\frac{T}{(2\pi)^3} \int d^3k \log[1 - e^{\frac{1}{T}(\mu - E_k)}]. \tag{3.14}$$

These expressions should be multiplied by g, the degeneracy of the momentum level k; g counts the internal degrees of freedom such as spin, colour, etc. One should also add the contribution of antiparticles. Since particles and antiparticles can annihilate, in equilibrium their chemical potentials are opposite and terms where $\mu \to -\mu$ should be added to Eqs. (3.13) and (3.14). Non-relativistically, however, their contribution is exponentially suppressed by the Boltzmann factor $\exp(-2\beta m)$ and thus negligible. To see this, write $E(k) = \sqrt{m^2 + \mathbf{k}^2} = \sqrt{(mc^2)^2 + (\hbar c k)^2} \approx mc^2 + \frac{\hbar^2 \mathbf{k}^2}{2m}$; then in the combination $\mu - E_k$ the rest energy mc^2 has to be combined with μ so that the chemical potential can be redefined as $\mu \to \mu' = \mu - mc^2$, which implies that the antiparticle occupation number goes like $1/(\exp(\beta(2m + \mu' + E_{\text{kin}}))$.

Partial integration permits one to eliminate the logarithm from the expressions (3.13) and (3.14) for p. Using the fact that the integrand is just a function of the absolute value of $\mathbf{k}$ and thus of the form $f(|\mathbf{k}|)$, one can write

$$\begin{aligned} p(T,\mu) &= \int d^3k f(|\mathbf{k}|) = 4\pi \int d(\frac{1}{3}k^3) f(k) \\ &= 4\pi \left[\Big|_0^\infty k^2 f(k) - \int dk \frac{df}{dk}\frac{1}{3}k^3 \right] = \int d^3k \frac{1}{3} k \left(-\frac{\partial f}{\partial k} \right), \end{aligned} \tag{3.15}$$

assuming that $f(k) \to \infty$ faster that $1/k^2$ when $k \to \infty$ as required by the finiteness of p. Thus, taking f from (3.13),

$$\frac{\partial f}{\partial k} = -\frac{1}{T}\frac{1}{e^{\frac{1}{T}(E-\mu)}+1}\frac{dE}{dk}$$

where $dE/dk = (\hbar c)^2 kdk$ and + stands for FD and - for BE. We then find

$$p(T,\mu) = \frac{(\hbar c)^2}{(2\pi)^3}\int d^3k \frac{k^2}{3E(k)}\frac{1}{e^{\frac{1}{T}(E-\mu)}\pm 1} \equiv \frac{(\hbar c)^2}{(2\pi)^3}\int d^3k \frac{k^2}{3E(k)} n_0(k). \tag{3.16}$$

with

$$n_0(k) = \frac{1}{e^{\frac{1}{T}(E(k)-\mu)}\pm 1}\left\{ \begin{array}{l} FD \\ BE \end{array} \right. .$$

From here one further derives, using $s(T,\mu) = \partial p/\partial T = S/V$, $n(T,\mu) = \partial p/\partial \mu = N/V$ and $\epsilon = Ts - p + \mu n = E/V$ that

$$n(T,\mu) = \frac{1}{(2\pi)^3}\int d^3k\, n_0(k) \tag{3.17}$$

$$s(T,\mu) = \frac{1}{(2\pi)^3}\int d^3k[(1-n_0)\log\frac{1}{1-n_0} + n_0 \log\frac{1}{n_0}] \qquad FD \tag{3.18}$$

$$s(T,\mu) = \frac{1}{(2\pi)^3}\int d^3k[-(1+n_0)\log\frac{1}{1+n_0} + n_0 \log\frac{1}{n_0}] \qquad BE \tag{3.19}$$

$$\epsilon(T,\mu) = \frac{1}{(2\pi)^3}\int d^3k E n_0(k) \tag{3.20}$$

3.2 Partition functions, free field theory

Let us next discuss how the above expression can be derived using other methods. In Eq. (2.77) we found that the partition function for harmonic oscillator using functional methods is given by $Z = Z(\omega) = \text{const}/(\prod_{-\infty}^{\infty}(\omega^2+\omega_n^2))^{1/2}$ so that

$$F = -T\log Z = \frac{1}{2}T\sum_{-\infty}^{\infty}((2\pi nT)^2+\omega^2). \tag{3.21}$$

It is quite automatic to transform this to a 3d system with massive particles: simply replace the oscillator frequency by the energy, $\omega^2 \to \mathbf{k}^2 + m^2$, and sum over $\mathbf{k}$. Then, writing d for 3,

$$f = -p = \frac{F}{V} = \frac{1}{2}\int d^{d+1}k\, \log(k_0^2+\mathbf{k}^2+m^2) = \frac{1}{2}T\sum_{n=-\infty}^{\infty}\int\frac{d^dk}{(2\pi)^d}\log[(2\pi nT)^2+\mathbf{k}^2+m^2]. \tag{3.22}$$

This result can be simply derived by reformulating the problem in the language of scalar field theory: free field theory is just a collection of harmonic oscillators. In field theory one replaces x with the field $\phi(x)$. At $T=0$, a classical free real scalar field obeys the equation of motion $(\Box + m^2)\phi = 0$,where $\Box = \partial_\mu\partial^\mu = \partial_t^2 - \partial_{\mathbf{x}}^2$. The

Klein-Gordon solutions are plane waves $\phi = e^{ik\cdot x}$ with a dispersion relation $k^2 - m^2 = 0$ (here $k^\mu = (k^0, k^i)$ is a 4-vector). The equation of motion follows from the quadratic action

$$S = \int d^4x \left[\frac{1}{2}\partial_\mu\phi\partial^\mu\phi - \frac{1}{2}m^2\phi^2\right] . \tag{3.23}$$

As discussed previously, at $T \neq 0$, we go to imaginary time with $\tau = it$ and require periodic fields so that

$$Z = N\int \mathcal{D}\phi \, \exp\Big[-\int_0^\beta d\tau \int d^3x \frac{1}{2}\big[(\partial_\tau\phi)^2 + (\partial_i\phi)^2 + m^2\phi^2\big]\Big] , \tag{3.24}$$

where $\phi(x, \tau + \beta) = \phi(x, \tau)$. Partial integration again groups the derivatives together with a - sign:

$$\begin{aligned}\int d^3\boldsymbol{x}\, d\tau\, \frac{1}{2}\partial_\mu\phi\partial_\mu\phi &= \int d^4x \Big[\frac{1}{2}\partial_\mu(\phi\partial_\mu\phi) - \frac{1}{2}\phi\Box\phi\Big] \\ &= \underbrace{\frac{1}{2}\oint dS_\mu\, \phi\partial_\mu\phi}_{=\,0 \text{ for } \phi(\boldsymbol{x})\to 0 \text{ as } \boldsymbol{x}\to\infty} \qquad -\frac{1}{2}\int d^4x\phi\Box\phi \ ,\end{aligned} \tag{3.25}$$

where now the box operator at $T \neq 0$ is euclidean: $\Box = \partial_t^2 + \nabla^2$ The surface terms vanish because there is no field at infinity. We can evaluate this, again using the fundamental Gaussian integral (2.66),

$$Z = N\int \mathcal{D}\phi \, \exp\big(-\int d^3\boldsymbol{x}\, d\tau\, \phi K\phi\big) \propto (\det K)^{-\frac{1}{2}} \tag{3.26}$$

where now $K = \Box + m^2$ and .

Let us now compute $\det K = e^{\mathrm{Tr}\ln K}$ for a massless scalar field. Taking a trace means summing over the diagonal matrix elements of the operator, and since K is continuous, we take an integral:

$$\begin{aligned}\mathrm{Tr}\ln K &= \int \langle \boldsymbol{x}, \tau|\ln K|\boldsymbol{x}, \tau\rangle d^3x\, d\tau\ /V_4 \\ &= V_4^2 V_4^{-1}\int \frac{d^3\boldsymbol{k}}{(2\pi)^3}\frac{d^3\boldsymbol{k'}}{(2\pi)^3} e^{i\boldsymbol{k}\cdot\boldsymbol{x} - i\boldsymbol{k'}\cdot\boldsymbol{x}} \\ &\quad \times \underbrace{\int \sum_{n,j=-\infty}^{\infty} \overbrace{e^{i2\pi n\tau/\beta - i2\pi j\tau/\beta}}^{\substack{\tau \text{ is compact} \\ L = 2\pi T\, :\, k\to k+L}} \Big[\frac{2\pi T}{2\pi}\Big]^2 d\tau}_{T^2\delta(n-j)} \\ &\quad \times \langle \boldsymbol{k'}, n'|\ln(k_0^2 + \boldsymbol{k}^2 + m^2)|\boldsymbol{k}, n\rangle d^3\boldsymbol{x}\end{aligned} \tag{3.27}$$

Note the normalization factor $1/V_4$: for an identity operator the trace yields 1. For $\tau = \tau + \beta \to k_0 = \frac{2\pi n}{\beta}$, $n \in \mathbb{Z}$, so that

$$\mathrm{Tr}\ln K = V_3 \sum_{n=-\infty}^{\infty}\int \frac{d^3\boldsymbol{k}}{(2\pi)^3} \ln\big((2\pi nT)^2 + \mathbf{k}^2 + m^2\big) \tag{3.28}$$

where we have used the fact that $V_3\beta T = V_4 T$. Thus we are back to Eq.(3.22).

To proceed further, we note that the integral is divergent, but the divergence is there already for $T = 0$, i.e., is T-independent. One can get rid of constants by taking derivatives, so let us improve the convergence by taking a derivative with respect to m^2:

$$I(m) \equiv 2\frac{df}{dm^2} = T\sum_{n=-\infty}^{\infty}\int \frac{d^dk}{(2\pi)^d}\frac{1}{(2\pi nT)^2 + \mathbf{k}^2 + m^2}. \tag{3.29}$$

Then apply a magic formula from 19th-century mathematics

$$\sum_{n=-\infty}^{\infty} \frac{x}{(2\pi n)^2 + x^2} = \frac{1}{x} + 2\sum_{1}^{\infty} \frac{x}{(2\pi n)^2 + x^2} = \frac{1}{2} + \frac{1}{e^x - 1}\ . \tag{3.30}$$

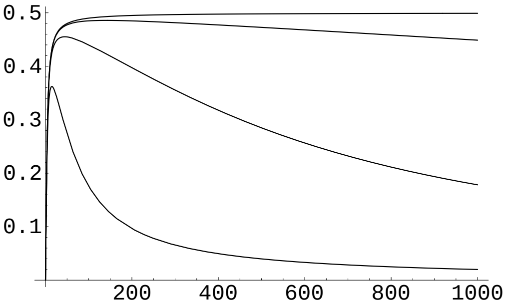


Figure 3.2: How the summation formula (3.30) works; the top curve shows the RHS -1/x as a function of x; the lower ones show respectively sums up to 1000, 100, and 10 terms.

and derive

$$I(m) = \int \frac{d^dk}{(2\pi)^d}\left[\frac{1}{2E(k)} + \frac{1}{E(k)}\frac{1}{e^{E(k)/T} - 1}\right]. \tag{3.31}$$

Further, by integrating over m^2 noting that $dm^2 = 2EdE$:

$$\begin{aligned} f(T) &= \frac{1}{2}\int_0^{m^2} dm^2\, I(m) = \int \frac{d^dk}{(2\pi)^d}\int^E dE\left(\frac{1}{2} + \frac{1}{e^{\beta E} - 1}\right) \\ &= \int \frac{d^3k}{(2\pi)^3}\left\{2E(k) + T\log[1 - e^{-\beta E(k)}]\right\}. \end{aligned} \tag{3.32}$$

Here all the divergences are dumped in the first term, which obviously sums over all the zero point energies. It is T-independent, as promised, and if we only are interested in T-dependence, we can forget it. And the second term is precisely Eq. (3.14) with $\mu = 0$.

However, if one really wants to find out the correct way of handling divergences, it is important to keep even the first term. Also, often m has an important dynamic significance (in symmetry breaking, for example) and cannot be forgotten. Then the simplest way of handling the divergence of the first term in Eq. (3.31) is to keep d arbitrary. As we want to be close to 3d we write $d = 3 - 2\epsilon$; then for small ϵ the integral is simply given by the expansion

$$\int \frac{d^dk}{(2\pi)^d}\frac{1}{2(\mathbf{k}^2 + m^2)^{1/2}} = -\frac{m^2}{8\pi^2}\left(\frac{1}{\epsilon} + 1 - \gamma_{\text{Euler}} + \mathcal{O}(\epsilon)\right) \tag{3.33}$$

so that the divergence is isolated in the $\frac{1}{\epsilon}$ singularity; this is an example of *dimensional regularisation.* We shall return to this in a moment when discussing the $T \gg m$-expansion of (3.14).

Why all this trouble with sums over n? The reason is that to include the effects of interactions perturbatively, you cannot avoid doing sums.

Note 1: that the beautiful formula (3.30) can even be generalised to

$$T\sum_{n=-\infty}^{\infty}\frac{1}{(2\pi nT+C)^2+E^2}=\frac{1}{2E}\left(1+\frac{1}{e^{\beta(E+iC)}-1}+\frac{1}{e^{\beta(E-iC)}-1}\right), \tag{3.34}$$

$$T\sum_{n=-\infty}^{\infty}\frac{1}{((2n+1)\pi T+C)^2+E^2}=\frac{1}{2E}\left(1-\frac{1}{e^{\beta(E+iC)}+1}-\frac{1}{e^{\beta(E-iC)}+1}\right). \tag{3.35}$$

The terms in the RHS here are distribution functions with chemical potential $= \pm iC$.

Note 2: Define $p^s(n)$ as the number of ways an integer can be expressed as a sum of sth powers of integers. For example, $p^1(5) = 7$ since the ways are 5, 4+1, 3+2, 3+1+1, 2+2+1, 2+1+1+1, 1+1+1+1+1. Similarly, $p^2(5) = 2$ since $5 = 2^2 + 1^2 = 1^2 + 1^2 + 1^2 + 1^2 + 1^2$. Assume now that the energy spectrum is $E_n = n^s$, $n \geq 1$, $s > 0$. If $x \equiv e^{-\beta}$, the bosonic partition function (3.5) with $\mu = 0$ is nothing but the generating function of $p^s(n)$:

$$Z(x=e^{-\beta})=\prod_{n=1}^{\infty}\frac{1}{1-x^{n^s}}=\sum_{n=1}^{\infty}p^s(n)x^n\approx\int_1^{\infty}dn\,p^s(n)e^{-\beta n}. \tag{3.36}$$

One can now invert this by saddle point methods to obtain the famous Hardy-Ramanujan formula (1918) for $p^s(n)$. For example, for the harmonic spectrum $s = 1$,

$$p(n)=\frac{1}{4\sqrt{3}N}e^{\pi\sqrt{2N/3}}. \tag{3.37}$$

In string theory, the spectrum of string excitations goes like $M^2 \sim 4N/\alpha'$ so that the number of states grows exponentially with mass.

3.3 Photon gas

Photons propagate with the velocity of light, but when a collections photons have velocities that are isotropic and momenta that are thermally distributed, the system is thermal gas. An example of photon gas which plays an important role in contemporary physics is the cosmic microwave background.

For the purposes of statistical physics, photons are bosons with with $m = 0$ and their degeneracy factor is 2 for the two helicities of massless vector bosons. In general, in the presence of interactions the number of photons is not conserved so that $\mu = 0$. Remembering that

$$\int_0^{\infty}dx\frac{x^{\alpha-1}}{e^x\mp 1}=\begin{cases}\zeta(\alpha)\Gamma(\alpha) & \text{BE}\\ (1-\frac{1}{2^{\alpha-1}})\zeta(\alpha)\Gamma(\alpha) & \text{FD}\end{cases} \tag{3.38}$$

we find the following expressions:

$$n_\gamma=\frac{N}{V}=2\cdot\frac{1}{(2\pi)^3}\int d^3k\frac{1}{e^{\frac{k}{T}}-1}=\frac{T^3}{\pi^3}\int_0^{\infty}dx\frac{x^2}{e^x-1}=\frac{2\zeta(3)}{\pi^2}T^3 \tag{3.39}$$

$$\epsilon_\gamma=\frac{E}{V}=2\cdot\frac{1}{(2\pi)^2}\int d^3k\frac{k}{e^{\frac{k}{T}}-1}=\frac{T^4}{\pi^2}\int_0^{\infty}dx\frac{x^3}{e^x-1}=\frac{\pi^2}{15}T^4=3p \tag{3.40}$$

$$s_\gamma=p'(T)=\frac{4}{3}\frac{\pi^2}{15}T^3=\frac{2\pi^4}{45\zeta(3)}n \tag{3.41}$$

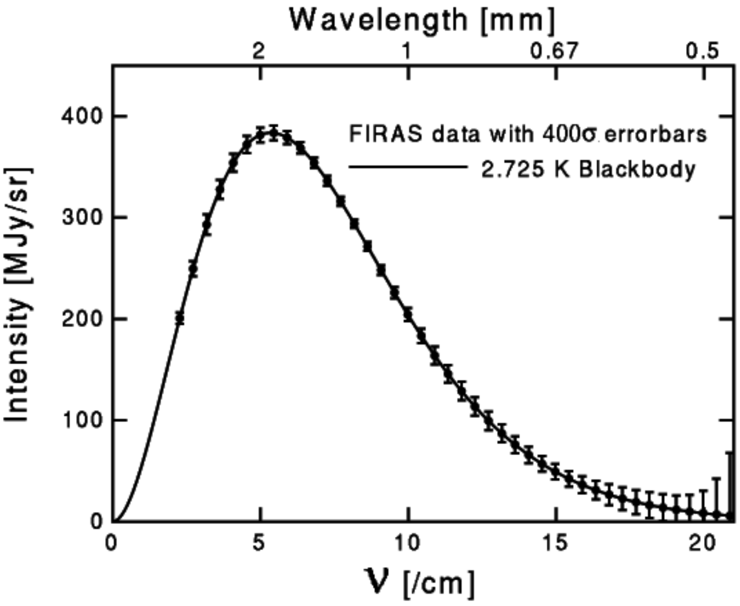


Figure 3.3: Spectrum of cosmic background radiation: perfect massless Bose-Einstein. Note that the error bars in the Figure are multiplied by 400.

From here one can derive various differential forms for $d\epsilon/d\omega$, $d\epsilon/d\lambda$, etc, using

$$\begin{aligned} E &= \hbar\omega = h\nu = pc = \hbar ck \qquad (3.42)\\ p &= \hbar k = \frac{h}{\lambda} \quad \text{(here p is momentum!)}. \qquad (3.43) \end{aligned}$$

For example, the energy density per unit frequency ν becomes

$$\frac{d\epsilon}{d\nu} = \frac{8\pi h}{c^3}\frac{\nu^3}{e^{h\nu/T}-1}. \qquad (3.44)$$

This is the celebrated black body spectrum, which is somewhat a misnomer since it does not actually refer to body which is black but to a body that does not absorb anything. The most perfect black body observed in Nature is the cosmic microwave background (see Fig. 3.3). Note also that "radiation emittance" = c/4× energy density.

In d spatial dimensions one finds

$$p(T) = \frac{1}{d}\epsilon(T) = \frac{2\Gamma(d+1)\zeta(d+1)}{d\Gamma(d/2)(4\pi)^{d/2}}T^{d+1}. \qquad (3.45)$$

Massless BE and FD gases; basic equations in early cosmology. Here we summarize the relevant ultrarelativistic expressions for Bose-Einstein and Fermi-Dirac gases emphasising unit choices. Both are very much needed in cosmology (units K, m), also in relativistic heavy ion collisions (units GeV, fm). The appropriate conversion relations are

$$\begin{aligned}
1\ \mathrm{eV} &= 1.602{\times}10^{-19}\ \mathrm{J};\\
\hbar &= 1 = 6.58{\times}10^{-22}\ \mathrm{MeVs} = 7.64{\times}10^{-12}\ \mathrm{Ks};\\
\hbar c &= 1 = 0.19733\ \mathrm{GeVfm} = 0.2290\ \mathrm{Kcm};\\
1\ \mathrm{K} &= 0.1532{\times}10^{-36}\ \mathrm{g}c^2.
\end{aligned}$$

Then $\epsilon = 3p$ with

$$\begin{aligned}
\epsilon &= \frac{g}{2}\cdot(\frac{7}{8})\cdot\frac{\pi^2}{15}T^4 = \frac{g}{2}\cdot(\frac{7}{8})85.633(\frac{T}{\mathrm{GeV}})^4\frac{\mathrm{GeV}}{\mathrm{fm}^3} = \frac{g}{2}\cdot(\frac{7}{8})\cdot 0.841\cdot 10^{-36}(\frac{T}{K})^4\frac{g}{\mathrm{cm}^3};\\
n &= \frac{g}{2}\cdot(\frac{3}{4})\cdot\frac{2\zeta(3)}{\pi^2}T^3 = \frac{g}{2}\cdot(\frac{3}{4})31.700(\frac{T}{\mathrm{GeV}})^3\frac{1}{\mathrm{fm}^3} = \frac{g}{2}\cdot(\frac{3}{4})\cdot 20.288(\frac{T}{\mathrm{K}})^3\frac{1}{\mathrm{cm}^3};\\
s &= \frac{g}{2}\cdot(\frac{7}{8})\cdot\frac{4\pi^2}{45}T^3 = (\frac{7}{6})\frac{2\pi^4}{45\zeta(3)}n.
\end{aligned} \tag{3.46}$$

For BE remove the bracketed fractions $(\frac{7}{8}),(\frac{3}{4}),(\frac{7}{6})$. Some further numerical relations are

$$\begin{aligned}
T_\gamma &= 2.725K \Rightarrow n_\gamma = 410\frac{1}{\mathrm{cm}^3};\\
T_\nu &= (\frac{4}{11})^{\frac{1}{3}}2.7K = 1.9K \Rightarrow n_\nu = 54\frac{1}{\mathrm{cm}^3}\quad\text{for } g_\nu = 1;\\
s_0 &= \frac{4\pi^2}{45}[1+\frac{2\cdot 3}{2}\cdot\frac{7}{8}\cdot\frac{4}{11}]{T_{0\gamma}}^3 = 2810\frac{1}{\mathrm{cm}^3}(\frac{T_{0\gamma}}{2.7K})^3 = 7.03n_{0\gamma}.
\end{aligned}$$

3.4 The non-relativistic limit: Maxwell-Boltzmann statistics

Maxwell-Boltzmann statistics is obtained in cases when we may approximate $1/(e^{\frac{1}{T}(E-\mu)}\pm 1)\approx e^{-\frac{1}{T}(E-\mu)}$, i.e., one can neglect the difference between BE and FD statistics. This requires that $e^{(E-\mu)/T} >> 1$ or $n_0 << 1$, which must hold for all values of k. Since $E=\sqrt{k^2+m^2}$ one should require $e^{(m-\mu)/T} >> 1$. All the thermodynamical functions can now be expressed in terms of the Bessel function $\mathrm{K}_\nu(z)$:

$$K_\nu(z) = \int_0^\infty e^{-z\cosh t}\cosh\nu t, \tag{3.47}$$

which for small x goes like

$$K_n(x) = \frac{\Gamma(n)}{2(x/2)^n},\quad K_0(x) = \log(2/x) \tag{3.48}$$

while for large x

$$K_n(x) = \sqrt{\pi/(2x)}e^{-x}. \tag{3.49}$$

From Eqs. (3.16)-(3.10) we obtain the expressions

$$\begin{aligned}
p &= \frac{m^2T^2}{2\pi^2}e^{\beta\mu}K_2(\beta m) = nT, \\
n &= \frac{m^2T}{2\pi^2}e^{\beta\mu}K_2(\beta m), \\
s &= \frac{m^3}{2\pi^2}e^{\beta\mu}\big[K_1(\beta m) + (4T-\mu)/m \cdot K_2(\beta m)\big], \\
\epsilon &= \frac{m^2T^2}{2\pi^2}e^{\beta\mu}\big[K_1(\beta m) + (3T/m)K_2(\beta m)\big]. \qquad (3.50)
\end{aligned}$$

Note that $p = nT$ holds also relativistically. In the non-relativistic limit $K_2(z) \to \sqrt{\pi/(2z)}\exp(-z)$ so that

$$n = (\frac{mT}{2\pi})^{\frac{3}{2}}e^{-\frac{m-\mu}{T}} \equiv \frac{1}{{\lambda_{th}}^3}e^{\frac{\mu-m}{T}} \ll \frac{1}{{\lambda_{th}}^3}. \qquad (3.51)$$

because $e^{\frac{m-\mu}{T}} \gg 1$. (Compare how we derived this result in Ch. 1 in reversed order: $\mu = \partial F/\partial N = -T\log 1/(n{\lambda_{th}}^3)$.) Thus Maxwell-Boltzmann statistics is valid if $n << 1/{\lambda_{\rm th}}^3$, that is, the mean particle distance is much larger than the thermal wavelength of the particles, which is the old condition that wavepackets not overlap, $\lambda_{\rm th} \ll n^{-1/3}$.

The ultrarelativistic limits $\beta m \to 0$ follow from $K_n(z) \approx \frac{1}{2}\Gamma(n)/(z/2)^n$.

3.5 Large T expansion

For $\mu = 0$ we may write for bosons from Eq. (3.14)

$$f(T,m) = \frac{T^4}{2\pi^2}\int_0^\infty dx\, x^2 \,\log[1 - e^{-\sqrt{x^2+y^2}}]|_{y=m/T} \,. \qquad (3.52)$$

The integral in Eq. (3.52) has the following expansions:

$$\begin{aligned}
\frac{f_{\rm BE}(T,m)}{T^4} &= -\left(\frac{y}{2\pi}\right)^{3/2} e^{-y} \qquad (y \gg 1) \qquad (3.53) \\
&= -\frac{\pi^2}{90} + \frac{y^2}{24} - \frac{y^3}{12\pi} - \frac{y^4}{32\pi^2}[\log y + \gamma_{\rm E} - \log 4\pi - \frac{3}{4}] + \frac{\zeta(3)y^6}{768\pi^4} + \ldots (3.54)
\end{aligned}$$

Similarly, for the FD free energy (3.13) one has the expansion

$$\frac{f_{\rm FD}(T,m)}{T^4} = -\frac{7\pi^2}{720} + \frac{y^2}{48} + \frac{y^4}{32\pi^2}[\log y + \gamma_{\rm E} - \log\pi - \frac{3}{4}] + \frac{7\zeta(3)y^6}{4\cdot 768\pi^4} + \ldots. \qquad (3.55)$$

Finding the small-y expansion is an interesting mathematical problem. Note that the integral seems to depend on y^2 but the expansion (3.54) contains the term y^3. There is no such in (3.55). The reason is that expanding the integrand for small y leads to a divergent integral

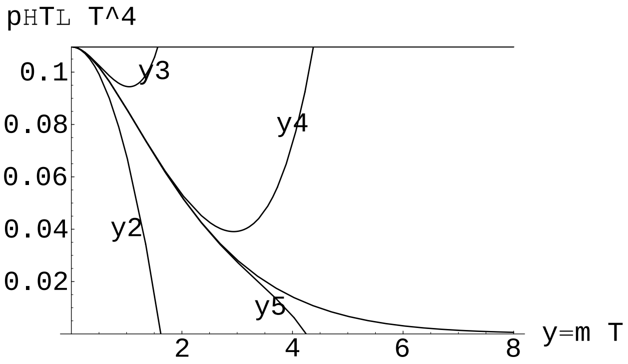


Figure 3.4: The exact result for $p(T)/T^4$ from (3.52) and the various terms of the large-T or small-y expansion in (3.54).

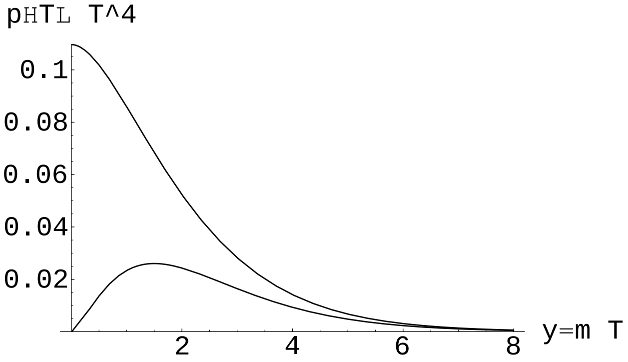


Figure 3.5: The exact result from (3.52) compared with the low-T approximation in (3.54).

for bosons. The physics reason is that the BE distribution function $1/(e^x - 1)$ diverges at $x \longrightarrow 0$, the FD distribution is finite. There are lots of infrared bosons at finite T!

To derive the $T \gg m$ expansion return to the m^2-derivative of f in Eq. (3.29). One sees that all the terms with $n \neq 0$ can be expanded for small m/T, the zero mode $n = 0$ is the dangerous one. So separate it:

$$\begin{aligned} I(T,m) &= I^{(n=0)}(T,m) + I^{n\neq 0}(T,m) \\ &= T\int \frac{d^dk}{(2\pi)^d}\frac{1}{\mathbf{k}^2+m^2} + 2T\sum_{n=1}^{\infty}\int\frac{d^dk}{(2\pi)^d}\frac{1}{(2\pi nT)^2+\mathbf{k}^2+m^2}\ . \end{aligned} \tag{3.56}$$

The zero mode term is seemingly a function of m^2 but actually is divergent for $d = 3$ so a consistent regularisation is needed. Try

$$\int\frac{d^3k}{(2\pi)^3}\frac{1}{\mathbf{k}^2+m^2} = \int_0^\infty \frac{dk}{2\pi^2}\frac{k^2+m^2-m^2}{k^2+m^2} = \int_0^\infty\frac{dk}{2\pi^2} - \frac{m^2}{2\pi^2}\int_0^\infty \frac{dk}{k^2+m^2}\ . \tag{3.57}$$

Thus

$$\int\frac{d^3k}{(2\pi)^3}\frac{1}{\mathbf{k}^2+m^2} = +\infty - \frac{Tm}{4\pi} \tag{3.58}$$

and an obviously positive function of m^2 has become a negative function of m – provided that the positive infinity can be disposed of. The second term in Eq. (3.56) can now be expanded for $T \gg m$:

$$\frac{1}{(2\pi nT)^2+\mathbf{k}^2+m^2}=\sum_{l=0}^{\infty}\frac{(-)^l(m^2)^l}{[(2\pi nT)^2+\mathbf{k}^2]^{l+1}} \tag{3.59}$$

and then integrated term by term over $\mathbf{k}$ using

$$d^dk=\frac{\pi^{d/2}}{\Gamma(d/2)}(\mathbf{k}^2)^{d/2-1}dk^2 \tag{3.60}$$

together with the definition of the gamma function:

$$\int\frac{d^dk}{(2\pi)^d}\frac{1}{(\mathbf{k}^2+m^2)^A}=\frac{1}{(4\pi)^{d/2}}\frac{\Gamma(A-d/2)}{\Gamma(A)}\frac{1}{(m^2)^{A-d/2}}. \tag{3.61}$$

After the integration the sum over n can be written as a zeta function and the final answer reads

$$I^{n\neq 0}(T,m)=\frac{2T}{(4\pi)^{d/2}}\frac{1}{(2\pi T)^{2-d}}\sum_{l=0}^{\infty}\left(\frac{-m^2}{4\pi^2T^2}\right)^l\frac{\Gamma(l+1-d/2)}{\Gamma(l+1)}\zeta(2l+2-d). \tag{3.62}$$

Expanding for small ϵ, including terms up to $l=2$, using the values of the zeta function, $\zeta(-1),\zeta(1+2\epsilon),\zeta(3)$ given below in Sect. 3.3 and adding the $n=0$ term (γ_E is the Euler constant) leads to

$$I(T,m)=\frac{T^2}{12}-\frac{Tm}{4\pi}-\frac{m^2}{16\pi^2}\left(\frac{1}{\epsilon}+\log\frac{4\pi}{T^2}-2\log(2\pi)+2\gamma_E+\mathcal{O}(\epsilon)\right)+\frac{m^4\zeta(3)}{128\pi^4T^2}+\mathcal{O}(m^6/T^4), \tag{3.63}$$

which ($\times 1/2$) still has to be integrated over m^2 to give (3.54).

The extremely accurate computations of the Standard Model in particle physics express their results in terms of the numbers $\log\pi,\gamma_E,\zeta(N)$ appearing here (plus further related ones). Why does Nature choose them?

3.6 Particle-antiparticle mixtures at large T

In relativistic plasmas one must include also the antiparticles. Since the two can annihilate to vacuum, the chemical potential of an antiparticle is $-\mu$. For a FD system one then has from (3.13) and the m^2-integral of (3.31):

$$p(T,\mu)=2\int\frac{d^dk}{(2\pi)^d}\left\{E(k)+T\left[\log(1+e^{-\beta(E(k)-\mu)})+\log(1+e^{-\beta(E(k)+\mu)})\right]\right\}, \tag{3.64}$$

where $E(k)=\sqrt{k^2+m^2}$, 2 counts the number of spin states and, for the first vacuum energy term, $d=3-2\epsilon$.

As for $\mu=0$, for the massless case the above result can be written in a very simple form. Dropping the vacuum term

$$\begin{aligned} p(T,\mu;m=0) &= \frac{T^4}{\pi^2}\int_0^{\infty}dx\,x^2\left[\log(1+e^{y-x})+\log(1+e^{-y-x})\right]\Big|_{y=\beta\mu} \\ &= \frac{T^4}{\pi^2}\left(\frac{7\pi^4}{180}+\frac{\pi^2}{6}y^2+\frac{1}{12}y^4\right) \\ &= \frac{7\pi^2}{180}T^4+\frac{1}{6}T^2\mu^2+\frac{1}{12\pi^2}\mu^4. \end{aligned} \tag{3.65}$$

Here the coefficient of the T^4 term is $2 \cdot 2 \cdot \frac{7}{8} \cdot \frac{\pi^2}{90}$ with obvious interpretations (2 for spin, 2 for particle+antiparticle at $\mu = 0$, 7/8 for relating fermions and bosons and $\pi^2/90$ the factor for one bosonic degree of freedom. For a quark-antiquark gas one would further have 3 for color and N_F for number of flavours). What is surprising here is that the sum of the two terms (which has to be even in y) is so simple while the log-terms separately just define some functions of y. Further analogous relations are

$$\int_0^\infty dx\, x\left(\frac{1}{e^{x-y}+1} + \frac{1}{e^{x+y}+1}\right) = \frac{\pi^2}{6} + \frac{1}{2}y^2 \tag{3.66}$$

$$\int_0^\infty dx\, x^2\left(\frac{1}{e^{x-y}+1} - \frac{1}{e^{x+y}+1}\right) = \frac{\pi^2}{3}y + \frac{1}{3}y^3 \tag{3.67}$$

$$\int_0^\infty dx\, x^3\left(\frac{1}{e^{x-y}+1} + \frac{1}{e^{x+y}+1}\right) = \frac{7\pi^4}{60} + \frac{\pi^2}{2}y^2 + \frac{1}{4}y^4 \tag{3.68}$$

Here the last is basically the same as (3.65), as shown earlier by partial integration. Note the minus sign in the middle equation, what is simple is the **net** fermion number, $n - \bar{n}$.

There are many ways of deriving the above integrals. Actually all the terms are polylogarithms $L_s(z)$:

$$\mathrm{L}_s(z) = \sum_{n=1}^\infty \frac{z^s}{n^s} = \frac{1}{\Gamma(s)}\int_0^\infty dx \frac{x^{s-1}}{z^{-1}e^x - 1}, \quad \mathrm{L}_s(1) = \zeta(s), \tag{3.69}$$

where z is a complex number and where the analytic continuation to the complex plane is quite non-trivial. Note, e.g., that the sum defines the function only for $|z| < 1$. The general result for an integral with arbitrary integer power of x is given later in (3.85). An elegant way of evaluating the integrals is Taylor expanding around $y = 0$. To calculate the derivatives with respect to y one should not work out $dn(x, y)/dy$ explicitly but note that this is equal to $\pm dn(x, y)dx$ and get rid of d/dx by partial integration, which simultaneously decreases the power of x. With proper sign between the terms one ultimately comes to constant derivative so that the expansion terminates.

Somewhat more laborious is to get the result by expanding the FD distributions using $1/(1-x) = \sum_0^\infty x^n$. Now $e^{x+y} \geq 1$ always, but $e^{x-y} \geq 1$ for $x \geq y$ so we have to expand differently for $0 < x < y$ and $y < x < \infty$. For the middle one we have

$$\begin{aligned}
&= \int_0^\infty dx\, x^2\Big\{-\Theta(x-y)\sum_1^\infty(-e^{-x+y})^n + \Theta(y-x)[1 + \sum_1^\infty(-e^{x-y})^n] + \sum_1^\infty(-e^{-x-y})^n\Big\} \\
&= \int_0^y dx\, x^2 + \sum_1^\infty(-)^n\Big\{-\int_y^\infty dx\, x^2 e^{-nx}e^{ny} + \int_0^y dx\, x^2 e^{nx}e^{-ny} + \int_0^\infty dx\, x^2 e^{-nx}e^{-ny}\Big\} \\
&= \frac{1}{3}y^3 + \sum_1^\infty(-)^n\Big\{\int_0^\infty dx\, x^2 e^{-nx}(e^{-ny} - e^{ny}) + \int_0^y dx\, x^2(e^{-nx}e^{ny} + e^{nx}e^{-ny})\Big\} \\
&= \frac{1}{3}y^3 + \sum_1^\infty(-)^n(-\frac{4y}{n^2}) = \frac{1}{3}y^3 + \frac{\pi^2}{3}y.
\end{aligned} \tag{3.70}$$

To get from the second to the third line we have added to the integrand of the last term $0 = e^{-nx}e^{ny} - e^{-nx}e^{ny}$. To get from the third to the last line, simple integrals were carried out explicitly, lots of terms then cancel.

3.7 Mathematical interlude: Properties of the ζ function

The ζ function appears frequently. It is defined by

$$\begin{aligned}\zeta(s) &= \sum_{n=1}^{\infty}\frac{1}{n^s} = \frac{1}{\Gamma(s)}\int_0^\infty dx\frac{x^{s-1}}{e^x-1} \quad \mathrm{Re}s>1\\ &= \frac{1}{1-2^{1-s}}\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n^s} = \frac{1}{(1-2^{1-s})\Gamma(s)}\int_0^\infty dx\frac{x^{s-1}}{e^x+1} \quad \mathrm{Re}s>0\\ &= 2(2\pi)^{s-1}\sin\frac{\pi s}{2}\Gamma(1-s)\zeta(1-s) = \prod_{p=\mathrm{prime}}\frac{1}{1-\frac{1}{p^s}}. \end{aligned} \tag{3.71}$$

The middle line follows from the indentity

$$\frac{1}{e^x+1} = \frac{1}{e^x-1} - \frac{2}{e^{2x}-1}. \tag{3.72}$$

From this analytic continuation we have a beautiful result of the sum of all positive integers:

$$\zeta(-1) = 1+2+3+4+... = \frac{2}{4\pi^2}\sin(-\frac{\pi}{2})\Gamma(2)\zeta(2) = -\frac{1}{12}. \tag{3.73}$$

This may look like something completely unphysical, but the contrary is the case. For example, when you hear that bosonic string theories are consistent only in a world of 26 dimensions, this number 26 is the solution of $1+2+3+4+.. = 2/(2-d)$.

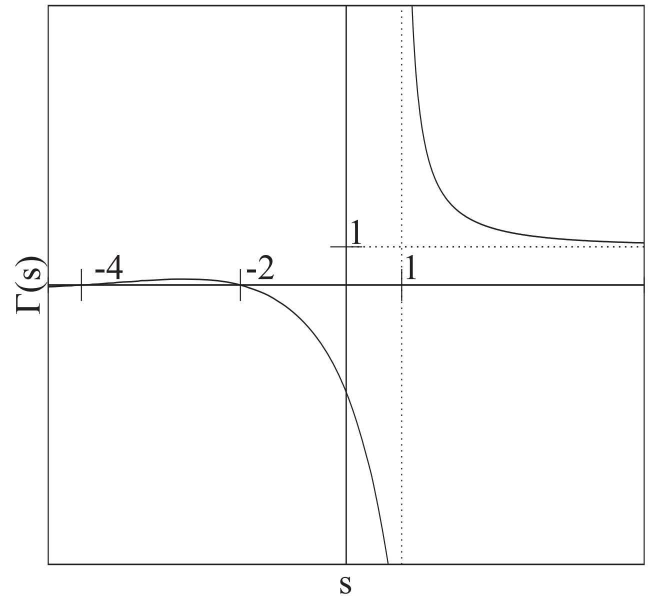


Figure 3.6: Plot of $\zeta(s)$.

What then is the product $1 \cdot 2 \cdot 3 \cdot 4 \cdots$ of all the integers? Now use

$$\zeta'(s) = \sum_{n=1}^{\infty} -\frac{\log n}{n^s} \Rightarrow \zeta'(0) = -\sum_1^{\infty} \log n = -\log \prod_1^{\infty} n$$

so that

$$\prod_1^{\infty} n = 1 \cdot 2 \cdot 3 \cdot 4 \cdots = e^{-\zeta'(0)} = \sqrt{2\pi}, \text{ since } \zeta'(0) = -\frac{1}{2}\log 2\pi.$$

A very important generalisation of this is the widely used "zeta function regularisation of functional determinants. Assume A is an operator with $Au_n = a_n u_n$, where a_n are its eigenvalues and u_n its eigenfunctions, $n = 1, 2, \ldots$. For any operator its determinant is an important quantity. In terms of the eigenvalues it is $\det A = a_1 \cdot a_2 \cdot a_3 \cdots$, but for infinite dimensional functional operators this product is most likely infinite. How do you regulate it? If one defines:

$$\zeta_A(s) = \sum_{n=1}^{\infty} \frac{1}{{a_n}^s} \qquad (3.74)$$

one has

$$\det A = a_1 \cdot a_2 \cdot a_3 \cdots = e^{-\zeta'_A(0)} \qquad (3.75)$$

and these equations define an analytic continuation of the product of eigenvalues from the region of large Res, where the product converges, to a region where one needs the value of the product. Since the eigenvalues of the harmonic oscillator are equally spaced, one notices that $\zeta(s)$ is essentially just the $\zeta_A(s)$ for $A =$ harmonic oscillator!

Some special values of $\zeta(s)$ are

$$\begin{aligned}
\zeta(-2n, n \geq 1) &= 0, \quad \zeta(-3) = \frac{1}{120}, \quad \zeta(-1) = -\frac{1}{12} \quad \zeta(0) = -\frac{1}{2}, && (3.76)\\
\zeta(2) &= \frac{\pi^2}{6}, \quad \zeta(3) = 1.20206, \quad \zeta(4) = \frac{\pi^4}{90}, && (3.77)\\
\zeta(1+\epsilon) &= \frac{1}{\epsilon} + \gamma_{\text{Euler}} + \mathcal{O}(\epsilon) \quad \text{the only singularity!.} && (3.78)
\end{aligned}$$

Riemann's hypothesis is that all the nontrivial zeroes of $\zeta(s)$ have Re$s = \frac{1}{2}$. Numerical verification has been extended up to 10^{12} zeroes, all of type $\frac{1}{2} + it$. Note that up to some value of t, there will be $t \cdot [\log(t/(2\pi e)/(2\pi) + \mathcal{O}(\log t/t)]$ zeroes, for example, the 10^{20}th zero is at $\frac{1}{2} + i1.52024...10^{19}$.

A function closely related to the ζ function is the polylogarithm

$$\mathrm{L}_s(z) = \sum_{n=1}^{\infty} \frac{z^s}{n^s} = \frac{1}{\Gamma(s)} \int_0^{\infty} dx \frac{x^{s-1}}{z^{-1}e^x - 1}, \quad \mathrm{L}_s(1) = \zeta(s), \qquad (3.79)$$

$$L_0(z) = \frac{z}{1-z}, \quad L_1(z) = \log\frac{1}{1-z}, \quad L_2(z) = -\int_0^z dt \frac{\log(1-t)}{t}, \ldots. \qquad (3.80)$$

If we define the integral

$$I(s) = \int_0^{\infty} dx\, x^{s-1} \left(\frac{1}{e^{x-y}+1} + (-)^s \frac{1}{e^{x+y}+1} \right) \qquad (3.81)$$

then from (3.79)

$$I(s) = -\Gamma(s)[L_s(-e^y) + (-)^s L_s(-e^{-y})]. \tag{3.82}$$

The polylog satisfies the functional relation

$$L_s(z) = (-)^{s-1} L_s(1/z) - \frac{(2\pi i)^s}{s!} B_s\biggl(\frac{\log(-z)}{2\pi i} + \frac{1}{2}\biggr), \tag{3.83}$$

where $B_s(x)$ is a Bernoulli polynomial,

$$\begin{aligned} B_1(x) &= \frac{1}{2} + x, \\ B_2(x) &= \frac{1}{6} - x + x^2, \\ B_3(x) &= x(\frac{1}{2} - x)(1-x), \\ B_4(x) &= -\frac{1}{30} + x^2(1-x)^2, \end{aligned} \tag{3.84}$$

etc. Using this one finds

$$I(s) = \frac{1}{s}(2\pi i)^s B_s(\frac{1}{2} + \frac{y}{2\pi i}), \tag{3.85}$$

which together with the explicit forms Eq. (3.84) reproduces the integrals Eq. (3.68).

Finally, are you interested in the 10 000 000th (hexadecimal) digit of $\zeta(3)$ (and who wouldn't)? From D. J. Broadhurst, math.CA/9803067 you find that $\zeta(3)$ goes like 1.202056903159594........CDA018F4E....., where the C is the 10Mth hexadecimal digit.

3.8 Casimir effect

As discussed in Ch. 2, at finite T the time direction is imaginary and of finite length, $0 < \tau < \beta$, while the spatial directions satisfy $0 < x < L \to \infty$. Let us now make one spatial direction of finite length, $0 < z < a$, while keeping the other two spatial directions and imaginary time infinite, $0 < x, y, \tau < L \to \infty$. From the symmetry of the problem it should be obvious that there is a physical quantity $\mathcal{E}(a)$ obtainable from $p(T)$ by $1/T \leftrightarrow 2a$ (for the factor 2, see below):

$$p(T)/T = -\mathcal{E}(a = \frac{1}{2T}), \quad \mathcal{E}(a) = -\frac{\pi^2}{720}\frac{\hbar c}{a^3}. \tag{3.86}$$

Take a look at Eq. (3.24): as it stands it would yield $Z = \exp(-F/T) = \exp(pL^3/T)$, and replacing $1/T \to 2a$ we have $Z = \exp(L \cdot L^2 \mathcal{E})$. The quantity $\mathcal{E}(a)$ is the *Casimir energy* [**?**], the energy per area between two infinite plates arising just from the fact that one has cut away a finite region from an infinite space. It is thus a macroscopic manifestation of the quantum mechanical zero point energy for field fluctuations, a "cosmological constant". Changing the shape of the region changes the constant, but as long as there is no other quantity with dimensions of mass (now $m_e = \infty$!), $\mathcal{E}(a)$ must behave as $\sim 1/a^3$. Since $\mathcal{E}(a) \sim -1/a^3$, the associated force $\mathcal{E}'(a)$ (which corresponds to entropy density at finite T) is attractive. That is, $\mathcal{E}(a)$ wants to be smaller and, since

$$\frac{\hbar c}{a^4} \approx 10^{-14}\frac{\mathrm{N}}{\mathrm{m}^2}\left(\frac{\mathrm{mm}}{a^4}\right),$$

the force is small indeed, but nevertheless measurable.

Let us derive the above result doing the mode sum explicitly using dimensional regularisation:

$$\begin{aligned} E &= \sum \frac{1}{2}\hbar\omega = \frac{1}{2}\hbar c \sum \sqrt{k_x^2 + k_y^2 + k_z^2} \\ &= \frac{1}{2}\hbar c \sum_{n=0,\pm1,\ldots} \int \frac{L^2}{(2\pi)^2} d^2k \sqrt{\mathbf{k}_T^2 + (\frac{\pi n}{a})^2}, \\ &= \frac{1}{2}\hbar c \sum_{n=0,\pm1,\ldots} \left(-\frac{L^2}{6\pi}\right)\left(\frac{\pi}{a}|n|\right)^3 \\ &= \frac{1}{2}\hbar c \left(-\frac{\pi^2}{6a^3}\right) L^2 \sum_{n=0,\pm1,\ldots} |n|^3 \\ &= -\frac{\pi^2 \hbar c}{720 a^3} L^2, \end{aligned} \tag{3.87}$$

where the momentum integral was done by setting $s = 0$ in

$$\int \frac{d^2k}{(2\pi)^2}(\mathbf{k}_T^2 + m^2)^{1/2-s} = \frac{m^{3-2s}}{4\pi}\frac{1}{s-3/2}$$

and where $\zeta(-3) = 1/120$ was used. Remarkably, the analytic continuation of a divergent integral (this even fixes the sign!) and the sum of a divergent series, properly done, gives a physical measurable result. Note that above the mode functions are those for a finite box, $\exp(ik_n z)$, $k_n = \pi/a\ n$, (both periodic and antiperiodic) while for finite T bosons one has to include only the periodic ones, $\omega_n = 2\pi/\beta\ n$, since the space is topologically a circle[1].

A recent review of the Casimir effect is, for example, http://arxiv.org/pdf/quant-ph/0609145

Since using zeta function regularization, which rather counterintuitively implies e.g. that $\sum |n|^3 = -1/60$, may look like magic, it is useful to check the calculation using the more "physical" momentum cutoff regularization. **Add calculation**

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[1] Actually, there is much discussion in the literature on the correct choice of modes.

Chapter 4

Degenerate physical systems

4.1 Bose-Einstein condensation

Bose-Einstein condensation, first discussed in an article by S. Bose in 1924 which he sent to Einstein who further elaborated on the subject in 1925, was first discovered 70 years after the theoretical prediction.

Let us first consider the case of non-relativistic Bose-Einstein gas. For an ideal non-relativistic boson system in thermal equilibrium the occupation number

$$n(E) = \frac{1}{e^{\beta(E-\mu)} - 1} \tag{4.1}$$

gives the thermodynamics via

$$\begin{aligned} \bar{N} &= \sum_k n(E_k) \equiv \int_0^\infty dE\, g(E) n(E), \\ E &= \int_0^\infty dE\, E\, g(E) n(E), \\ \Omega &= T \int_0^\infty dE\, g(E) \log[1 - e^{\beta(\mu - E)}] \ . \end{aligned} \tag{4.2}$$

where $g(E)$ is the density of states as discussed in Ch. 1.6, $g(E) \sim \sqrt{E}$ for a box and $g(E) \sim E^2$ for a harmonic trap.

Assume now we have some fixed number N of bosons in thermal equilibrium at some T, μ. One expects that these have to be related by

$$N = \bar{N} = \int_0^\infty dE\, g(E) \frac{1}{e^{\beta(E-\mu)} - 1}. \tag{4.3}$$

Consider now the RHS as a function of μ. Firstly, we clearly must have $\mu < 0$; otherwise the E-integral blows up at $E = 0$. At very large negative μ the integral is very small, as is made explicit below for Maxwell-Boltzmann statistics in Eq.(4.16). When μ approaches 0 from the negative side, the integral obviously grows monotonically. It thus reaches its maximum value at $\mu = 0$:

$$\bar{N}_{\max} = \int_0^\infty dE\, g(E) \frac{1}{e^{\beta E} - 1}. \tag{4.4}$$

For a given number N of bosons we shall define a critical temperature T_c by

$$N = \int_0^\infty dE\, g(E) \frac{1}{e^{E/T_c} - 1}. \tag{4.5}$$

This will be the temperature below which some of our N bosons will start condensing to the ground state.

To see the necessity of condensation, consider Eqs.(4.3) and (4.4). As long as $N < \bar{N}_{\max}$ we can solve μ from (4.3). However, when $N > \bar{N}_{\max}$ the difference $N - N_{\max}$ will condense to the ground state.

The problem arises because the occupation number $1/(\exp(-\beta\mu) - 1)$ of the $E = 0$ mode goes to infinity as $\mu \to 0_-$, and as a consequence the continuum approximation

$$\sum_k \to \int \frac{d^3k}{(2\pi)^3} \tag{4.6}$$

is not correct at $k = 0$. Instead we should take the continuum limit by

$$\sum_k \to \sum_{k=0} + \int_{k\neq 0} \frac{d^3k}{(2\pi)^3}\ . \tag{4.7}$$

(Note that removing the point $k = 0$ from the integration range does not change the outcome of the integral because of the measure.) This means that the density of states should be written as

$$g(E) = C_\alpha E^{\alpha-1} + \delta(E)\ , \tag{4.8}$$

where α labels the systems in which the gas is confined. We shall consider both a box and a harmonic trap, for which the density of states has been computed in Ch. 1.6: $g(E) = C\sqrt{E}$ for a box and $g(E) = CE^2$ for harmonic trap. The delta function in Eq. (4.8) takes care of the zero mode; because of it, the occupation number of ground state bosons can become macroscopic, i.e. bosons can condense in the ground state.

Inserting Eq. (4.8) into Eq. (4.2) we then find

$$N = \underbrace{C_\alpha \int_0^\infty dE\, \frac{E^{\alpha-1}}{e^{\beta(E-\mu)} - 1}}_{\text{usual thermal cloud}} + N_0(T) \tag{4.9}$$

where $N_0(T)$ is the number of particles in the ground state (≈ 0 for $T > T_c$). By expanding in powers of $e^{-\beta(E-\mu)} \leq 1$ one sees that the integral is a polylogarithm $\mathrm{L}_s(z) = \sum_{n=1}^\infty \frac{z^s}{n^s}$ discussed in Ch. 3.5:

$$N = C_\alpha \Gamma(\alpha) T^\alpha \mathrm{L}_\alpha(e^{\beta\mu}) + N_0(T), \tag{4.10}$$

If we start increasing N at some fixed temperature, then when it reaches $\bar{N}_{\max}$ the solution is $\mu = 0$. When it increases above $\bar{N}_{\max}$, μ remains at $\mu = 0$ and the surplus $N - \bar{N}_{\max}$ condenses in the ground state. From the definition of T_c in (4.5) we find that $N = C_\alpha \Gamma(\alpha)\zeta(\alpha) T_c^\alpha$ so that we can solve for $\mu = 0$, $T < T_c$ from (4.10)

$$N_0(T) = N\left(1 - \frac{T^\alpha}{T_c^\alpha}\right). \tag{4.11}$$

Consider now the two concrete cases, box and harmonic trap, explicitly. For a box we have $\alpha = 3/2$ so that

$$C_\alpha = \frac{V}{\hbar^3}\frac{m\sqrt{2m}}{2\pi^2} \Rightarrow \bar{n} = \frac{1}{\hbar^3}\frac{m\sqrt{2m}}{2\pi^2}\underbrace{\Gamma(\frac{3}{2})}_{\sqrt{\pi}/2}\zeta(\frac{3}{2})T_c^{\frac{3}{2}} \Rightarrow T_c = \frac{\hbar^2 \bar{n}^{\frac{2}{3}}}{m}\underbrace{\frac{2\pi}{(\zeta(\frac{3}{2}))^{\frac{2}{3}}}}_{\approx 3.3} \tag{4.12}$$

One can also get an estimate of T_c by demanding overlap between wave packets:

$$n^{-\frac{1}{3}} = \lambda_{th} = \hbar\sqrt{\frac{2\pi}{mT_c}} \Rightarrow T_c \simeq \frac{\hbar^2 n^{\frac{n}{3}}}{m} \tag{4.13}$$

Numerically, for the classic example of ^{4}He liquid with $n^{-\frac{1}{3}} \sim$ Å and $m \sim 4m_p$, one finds $T_c \sim 3K$ like the superfluid critical temperature. But ^{4}He is not a ideal dilute Bose gas!

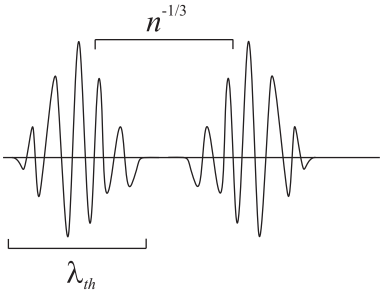

Figure 4.1: Estimating T_c.

A harmonic trap with $\alpha = 3$ is the relevant case for real experiments. Then

$$C_\alpha = \frac{1}{2}\frac{1}{(\hbar\omega)^3} \Rightarrow T_c = \underbrace{\frac{1}{(\zeta(3))^{\frac{1}{3}}}}_{\approx 0.94}\hbar\omega N^{\frac{1}{3}}. \tag{4.14}$$

Note, in particular, that there is no explicit volume V factor in C_α now. For $T \le T_c$ we can put $\mu = 0$ and all the thermodynamical quantities, from Eq. (4.2), become very simple:

$$\begin{aligned} \Omega &= \frac{T^4}{2(\hbar\omega)^3}\int_0^\infty dx\, x^2 \log(1 - e^{-x}) = -\frac{\pi^4}{90(\hbar\omega)^3}T^4 \\ S &= -\frac{\partial\Omega}{\partial T} = \frac{2\pi^4}{45(\hbar\omega)^3}T^3, \quad E = \frac{\pi^4}{30(\hbar\omega)^3}T^4 \\ N_0(T) &= N\left(1 - \frac{T^3}{T_c^3}\right) \end{aligned} \tag{4.15}$$

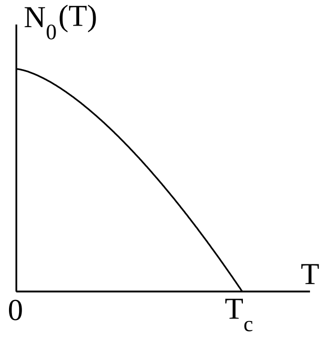

Figure 4.2: Condensate fraction

For $T > T_c$ exact expressions have to be used, but very simple expressions are obtained also at very large T since then one can apply the Maxwell-Boltzmann approximation and write

$$N = \frac{T^3}{(\hbar\omega)^3} e^{\beta\mu}, \quad E = \frac{3T^4}{(\hbar\omega)^3} e^{\beta\mu}. \tag{4.16}$$

Since $N \approx (T_c/\hbar\omega)^3$ we can invert from here $\mu = -3T\log(T/T_c)$.

Let us now consider more concretely the parameter values of BE condensation in a harmonic trap. This also illustrates why there is no explicit V factor in the density of states. The parameter values of atomic BEC experiments are quite different from those expected for liquids, since new trapping methods avoid formation of liquid or solid. Very roughly, one uses harmonic traps with $\omega \sim 1000$Hz, $\hbar\omega \sim 10^{-12}$eV $= 10^{-8}$K $= 10$nK and $N \sim 10^6$ atoms (early experiments had 10^4 atoms, one can go up to 10^7 atoms). Thus $T_c \sim 1000$nK but the systems are cooled down to 10 nK. The densities are of the order of $10^{14}/\text{cm}^3$ so that the "average distance between molecules" is ~ 1000 Å. Of course, this is not a real distance, actually the wave functions of the molecules overlap in the condensate. What is important is that this distance is larger than the scattering length $a \approx 100$Åof low energy scattering (see below); this implies that the system is dilute, it can be regarded as an approximately ideal gas. And clearly it is much larger than the size of molecules, ~ 1Å.

Assume we now have N atoms of mass m at some T in a harmonic oscillator potential $\frac{1}{2}m\omega^2\mathbf{x}^2$. How big is the system? If $T \gg \hbar\omega$ we know that very high states of the potential are occupied. Since $E_n = \hbar\omega(n+\frac{1}{2})$ we see that levels up to $n + \frac{1}{2} \sim T/\hbar\omega$ are occupied. Since for the nth excited state

$$\langle x^2 \rangle = \frac{\hbar}{m\omega}(n+\frac{1}{2})$$

we see that the size of the system is

$$R_{\text{highT}} = \sqrt{\frac{T}{m\omega^2}} = \sqrt{\frac{T}{\hbar\omega}}\sqrt{\frac{\hbar}{m\omega}}.$$

This can as well be obtained from classical equipartition (expectation values of potential and kinetic energies are essentially the same):

$$\frac{1}{2}m\omega^2R^2 \sim \frac{p^2}{2m} \sim \frac{3}{2}T \Rightarrow R \sim \sqrt{\frac{T}{m\omega^2}}, \quad p \sim m\omega R. \tag{4.17}$$

Condensation to ground state takes place when wave packets start overlapping:

$$\frac{\hbar}{p} \sim n^{-\frac{1}{3}} = \left(\frac{R^3}{N}\right)^{1/3} = \frac{R}{N^{1/3}} \sim \frac{\hbar}{m\omega R} \Rightarrow R_{\text{crit}} = \sqrt{\frac{\hbar}{m\omega}}N^{1/6} \tag{4.18}$$

corresponding to $T \sim \hbar\omega N^{1/3}$. At $T = 0$ all the bosons are finally condensed in the ground state and that has the width

$$R_{\text{cond}} = \sqrt{\langle x^2 \rangle} = \sqrt{\frac{\hbar}{2m\omega}} = \frac{1}{\sqrt{2A}} 20\mu\text{m} \tag{4.19}$$

for $m = Am_p$.

There is very much subtle and ingenious physics in BEC experiments. For the first, how does one create the trap $\frac{1}{2}m\omega^2\boldsymbol{x}^2$ for neutral atoms (or neutrons, or single ions and electrons)? Nobel prizes were given to Dehmelt & Paul (1989) for ion trap technique and to Chu, Cohen-Tannoudji, Phillips (1997) for cooling and trapping of atoms with laser light. Then one must find atoms that have suitable properties (such as Rubidium) and find methods for cooling them. Finally, one must be able to observe the formation of the condensate; this is done by releasing the atoms from the trap and measuring their velocity distributions. See, for example Bose-Einstein Condensation in Dilute Gases, C.J.Pethick and H. Smith, Cambridge University Press 2001, http://www.cambridge.org/uk/catalogue/catalogue.asp?isbn=0521665809

4.2 Condensate wave function

Let us next briefly discuss what one should do to go beyond the ideal gas situation. In the quantum mechanical treatment of the problem we should start with the wave function Ψ of N bosons in an external potential $V(\boldsymbol{r})$ (=box, $\frac{1}{2}m\omega^2 r^2$, ...), given in a one-particle factorised form by

$$\Psi = \Psi(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N) = \prod_{k=1}^{N} \Psi(\boldsymbol{r}_k) \ , \tag{4.20}$$

where $\Psi(\boldsymbol{r}_k) \equiv \Psi_k$ is the single particle wave function. Let us assume that we need to consider only pairwise interactions $U(\boldsymbol{r}_1 - \boldsymbol{r}_2)$ (=hard sphere, van der Waals, ...). The Schrödinger equation reads:

$$i\hbar\frac{\partial\Psi}{\partial t} = \sum_{i=1}^{N} \big[-\frac{\hbar^2}{2m}\nabla_i^2 + V(\boldsymbol{r}_i)\big]\Psi + \sum_{i<j} U(\boldsymbol{r}_i - \boldsymbol{r}_j)\Psi \ . \tag{4.21}$$

To proceed one uses the concept of scattering length a from low energy scattering theory, $\sigma_{\text{tot}}(E \longrightarrow 0) = 4\pi a^2$, $a > 0$ for repulsive, $a < 0$ for attractive interactions. Writing

$$U(\mathbf{r}) = \frac{4\pi\hbar^2 a}{m}\delta(\mathbf{r})$$

gives the correct cross section when used in potential scattering (with scattering amplitude $f(\theta) = -m/2\pi\hbar^2 \int d^3x \exp(i\mathbf{q}\cdot\mathbf{r})U(\mathbf{r})$, $\sigma = \int d\Omega |f|^2$). The combination na^3 (actually $\sqrt{na^3}$) is a dimensionless expansion parameter, a dilute gas has $na^3 \ll 1$.

What can one think of computing? The simplest situation is found at $T = 0$ when all the bosons are in the ground state $E = 0$. However, they interact via $U(\boldsymbol{r}_i - \boldsymbol{r}_j)$, which affects

E. Using first order perturbation theory one finds

$$\begin{aligned}
\Delta E &= \langle\Psi_0(\boldsymbol{r}_1)\dots\Psi_0(\boldsymbol{r}_N)| \underbrace{\sum_{i<j=1}^{N} U(r_i-r_j)}_{\frac{1}{2}N(N-1)\text{ equal terms}} |\Psi_0(\boldsymbol{r}_1)\dots\Psi_0(\boldsymbol{r}_N)\rangle \\
&= \frac{1}{2}N\underbrace{(N-1)}_{\approx N}\int d^3r_1 d^3r_2 |\Psi_0(\boldsymbol{r}_1)|^2|\Psi_0(\boldsymbol{r}_2)|^2 \underbrace{U(\boldsymbol{r}_1-\boldsymbol{r}_2)}_{\approx\frac{4\pi\hbar^2 a}{m}\delta^3(\boldsymbol{r}_1-\boldsymbol{r}_2)} \underbrace{\int d^3r_3|\Psi_0(\boldsymbol{r}_3)|^2\dots}_{=1} \\
&= \frac{2\pi\hbar^2 aN^2}{m}\underbrace{\int d^3r}_{V}\underbrace{|\Psi_0(\boldsymbol{r})|^2}_{\frac{1}{V}}\underbrace{|\Psi_0(\boldsymbol{r})|^2}_{\frac{1}{V}} \Rightarrow \epsilon = \frac{\Delta E}{V} = \frac{2\pi\hbar^2 an^2}{m} \qquad (4.22)
\end{aligned}$$

where $a > 0$ for repulsive and $a < 0$ for attractive interactions. This is how the low energy interactions change ground state energy (density) from the free value.

Calculating higher order corrections is a heroic chapter in quantum theory:

$$\epsilon = \frac{2\pi\hbar^2 an^2}{m}\Big\{1+\frac{128}{15\pi}\sqrt{na^3}+\big[\frac{8(4\pi-3\sqrt{3})}{3}\log na^3 + C\big]na^3+\dots\Big\} \qquad (4.23)$$

The first correction is from Lee-Yang (1957) (needs $a > 0$) and the second from Wu (1959). For C one needs more than the scattering length (cond-mat/9712041).

The computations are most conveniently carried out in the 2nd quantised field theory formulation:

$$\Psi_l(\boldsymbol{r}) = \sum_{\boldsymbol{k}=\frac{2\pi}{L}\boldsymbol{n}} a^l_{\boldsymbol{k}}\frac{1}{\sqrt{V}}e^{i\boldsymbol{k}\cdot\boldsymbol{r}}, \quad [a^l_{\boldsymbol{k}}, a^{l\dagger}_{\boldsymbol{k}'}] = \delta_{\boldsymbol{k}\boldsymbol{k}'} \qquad (4.24)$$

$$\Rightarrow \begin{cases} [\Psi_p,\Psi_l] = 0 \\ [\Psi_p,\Psi_l^\dagger] = \delta_{pl}\delta^3(\boldsymbol{r}-\boldsymbol{r}') \qquad \text{equal times!} \end{cases} \qquad (4.25)$$

The Schrödinger equation in this formulation is given by

$$\begin{aligned}
i\dot{\Psi} &= [H,\Psi]\ , \\
H &= H_0 + V^{(1)} + V^{(2)} + \cdots \\
V^{(1)} &= \int d^3r \Psi_k^\dagger V \Psi_k\ , \\
V^{(2)} &= \int d^3r d^3r' \Psi_k^\dagger(\boldsymbol{r})\Psi_l^\dagger(\boldsymbol{r}')\tilde{U}\delta(\boldsymbol{r}-\boldsymbol{r}')\Psi_k(\boldsymbol{r})\Psi_l(\boldsymbol{r}')\ , \qquad (4.26)
\end{aligned}$$

where we have now written the strength of the pairwise interaction as $\tilde{U}$. It is then an exercise to show that

$$[H,\Psi_k] = \tilde{U}|\Psi|^2\Psi_k - \frac{\nabla^2\Psi_k}{2m} + V(r)\Psi_k\ . \qquad (4.27)$$

Let us then assume that $\Psi = \Psi_0 + \Psi'$ with $\langle\Psi'\rangle = 0$ and $\Psi_0 = \sqrt{n_0}$. The ground state Ψ_0 has $E_0 = 0$ so that the time evolution is given by

$$\Psi_0(t) = e^{iHt}\Psi_0 = e^{i(E_0-\mu)t}\Psi_0 = e^{-i\mu t}\Psi_0\ . \qquad (4.28)$$

Then, using Eqs. (4.26) and (4.27), one arrives at the *Gross-Pitaevskii equation*:

$$-\frac{\nabla^2\Psi_0}{2m} + V(r)\Psi_0 + \tilde{U}|\Psi_0|^2\Psi_0 - \tilde{\mu}\Psi_0 = 0 \ , \tag{4.29}$$

where

$$\tilde{\mu} = \mu - 2n'\tilde{U}, \qquad n' = \langle \Psi'^{\dagger}\Psi \rangle \ll n_0 \ \text{ when } T < T_c \ . \tag{4.30}$$

In the case of harmonic trap $V = \frac{1}{2}m\omega^2 r^2$.

Another way of approaching this equation is to write the energy functional

$$E[\Psi] = \int d^3r \left[\frac{1}{2m}|\nabla\Psi(\mathbf{r})|^2 + V(r)|\Psi(\mathbf{r})|^2 + \frac{1}{2}\tilde{U}|\Psi(\mathbf{r})|^4\right]. \tag{4.31}$$

Finding the extrema of $E[\Psi]$ under the constraint that N is constant, i.e., computing $\delta(E - \mu N)/\delta\Phi^* = 0$ again results in Eq. (4.29). We shall later meet on several occasions functionals of this particular form.

If the interaction is weak (so that we may neglect the Ψ^4-term), the theory is Gaussian and we obtain an eminently sensible result for the condensate wave function:

$$\Psi_0 \approx \left(\frac{n_0}{\pi^{3/2} l_0^3}\right)^{1/2} e^{-\frac{r^2}{2l_0^2}} \ , \tag{4.32}$$

where $l_0 = (m\omega)^{-1/2}$) is the size of the condensate, i.e., the width of the harmonic oscillator ground state. This serves as the starting point for variational calculations when the interaction is switched on (exercise).

4.3 Neutron Star: A T = 0 Fermi System

Neutron star is a cold body consisting of essentially non-interacting fermions bound together by gravity. Hence it can be considered as a prime example of ideal Fermi gas at zero temperature.

Let us first review the relevant formulas for $T = 0$ degenerate fermion gas. The starting point is the FD expression for Ω, and we assume that there exist different fermions with μ_i, m_i. Then, as $T \to 0$, $\log[1 + e^{\beta(\mu-E)}] \to \beta(\mu - E)\Theta(\mu - E)$ so that we find (2 is for 2 spin states)

$$\begin{aligned}\Omega(T=0,\mu_i) &= -2\frac{V}{(2\pi)^3}\int d^3k \sum_i(\mu_i - E_i(k))\Theta(\mu_i - E_i(k)) \\ &= \sum_i 2\frac{V}{(2\pi)^3}\int d^3k(E_i(k)-\mu_i) = \sum_i(E_i - \mu_i N_i) = E - \sum_i \mu_i N_i \quad (4.33)\end{aligned}$$

where 2 is for 2 spin states and for any i, $k_F = \sqrt{\mu^2 - m^2}, \mu \equiv E_F$. Then

$$\begin{aligned}n &= \frac{1}{\pi^2}\int_0^{k_F} dk\, k^2 = \frac{1}{3\pi^2}k_F^3, & (4.34)\\ \epsilon &= \frac{1}{\pi^2}\int_0^{k_F} dk\, k^2\sqrt{k^2+m^2} = \frac{1}{8\pi^2}\left[k_F E_F(2k_F^2 + m^2) - m^4\log\frac{E_F + k_F}{m}\right] & (4.35)\\ &= mn + \frac{3}{5}\frac{k_F^2}{2m}n = mn + \frac{k_F^5}{10\pi^2 m}, \quad \text{NR} & (4.36)\\ &= \frac{1}{4\pi^2}k_F^4 = 3p \quad \text{ER} & (4.37)\\ p &= -\epsilon + \mu n = 2\int\frac{d^3k}{(2\pi)^3}\frac{k^2}{3E(k)}\Theta(\mu - E(k)) & \\ &= \frac{1}{8\pi^2}\left[k_F E_F(\frac{2}{3}k_F^2 - m^2) + m^4\log\frac{E_F+k_F}{m}\right] & (4.38)\\ &= \frac{k_F^5}{15\pi^2 m} = \frac{2}{3}(\epsilon - mn) = \frac{1}{15\pi^2 m}(3\pi^2 n)^{5/3}, \quad \text{NR.} & (4.39)\end{aligned}$$

Consider now bound states of neutrons, starting from a single one. A neutron is a uud-quark QCD bound state with mass $m_n = 939.565330 \pm 0.000038$ MeV. It decays to a proton with a mass $m_p = 938.271998 \pm 0.000038$ MeV via the beta decay $n \to p e^- \bar{\nu}_e$ $(d \to u e^- \bar{\nu}_e)$ with the energy release of $Q = m_n - m_p = 1.293318 \pm 0.0000005$ MeV and a lifetime $\tau_n = 885.7 \pm 0.8$ s (difficult to measure!). The maximum momentum of the decay electron is 1.19 MeV. Most of the neutron mass is QCD energy. It is heavier than the proton because for reasons nobody really knows, the d quark is heavier than the u quark (some 7 vs. 4 MeV in a certain scheme; no accurate number can be given since the quark mass is not a physical scheme independent quantity). All these numbers are crucial for the buildup of the nature around us.

Neutrons appear in bound states nucleons by virtue of the residual QCD forces that can be thought to "leak" out of the nucleons to within a distance of fm. Hence we have long-lived states like pn; pnn (but no nn!); $ppnn$=He^4, etc.

Question: why is *ppnn* stable but *nnnn* does not exist; why does n in He^4 not decay?

Stable or semistable states (i.e. elements and their isotopes) end at around A=250 with

$$E_A = (A-Z)m_n + Zm_p - 0.016A + 0.018A^{2/3} + 0.71Z^2A^{-1/3} + \ldots$$

including the masses, binding energy of nuclear matter, surface energy and Coulomb energy. Much work has been devoted to the study of cold nuclear matter with the binding energy $E/A - m_N = -16$ MeV at the nuclear matter matter density $n_{\rm nm} = 0.17\,1/{\rm fm}^3$. This is a degenerate Fermi gas with effects of nuclear force playing a significant role.

We shall, however, proceed to neutron stars. Residual QCD forces do not seem to be able to bind nucleons to (semi)stable states with $\gg 250$ neutrons, but if we have enough nucleons, gravitational forces will become important. Indeed, neutron stars can be considered as big nuclei with $A \approx 10^{57}$. They are possible end products of a stellar evolution whereby nuclei are burned in the core of the star through the chain H→He→C→$\cdots$Fe. The process ends in iron because it is the state of lowest energy in the space of nuclear configurations. When nuclear burning ceases, radiation pressure disappears and the star collapses under the weight of its own gravity. Depending on the mass of the star, the final state is a white dwarf, a neutron star, or a black hole. **Figure here with Chandrasekhar limit etc?????**

Why $A \approx 10^{57}$ for a neutron star? Assume a neutron star is a big nucleus with $R = A^{1/3}/m_n$ and mass $M = Am_n$, m_n giving the only energy scale. It is kept together by compensating the outward push from the Fermi pressure by gravitational attraction. The outward Fermi energy per neutron is also of the order of m_n (see below). The gravitational binding energy of a neutron is

$$m_n\frac{G\,Am_n}{R} \equiv \frac{m_n^2}{M_{\rm Planck}^2}\frac{A}{R} = \frac{m_n^3}{m_{\rm Planck}^2}A^{2/3}.$$

Equating this with m_n gives

$$A = \left(\frac{M_{\rm Planck}}{m_n}\right)^3 = (10^{19})^3 = 10^{57} \approx \frac{M_{\rm sun}}{m_n}.$$

In a collapse to a neutron star protons and elecrons merge in the weak process $pe^- \to n\nu_e$ and the neutrinos ν_e stream out of the star because of their very weak interactions, but only up to a point determined by the thermal and mechanical equilibrium conditions.

Let us now estimate the density of protons and electrons in a neutron star. The equilibrium conditions are:

1. $n_p + n_n \equiv n_B =$ const. This will be of the order of nuclear matter density and varies as a function of radius as given by the relativistic hydrostatic equilibrium equations. This variation is neglected here.

2. Electric neutrality, $n_p = n_{e^-} = n_B - n_n$.

3. We now have effectively only one free variable, n_n, and this is determined by finding the minimum of the energy density of the system by

$$\frac{d\rho}{dn_n} = 0 \Rightarrow \mu_n = \mu_p + \mu_e,$$

where $\mu^2 = k_F^2 + m^2$, and

$$\begin{aligned} k_{F,e} &= (3\pi^2 n_e)^{1/3} = [3\pi^2(n_B - n_n)]^{1/3} \\ k_{F,\mu} &= [3\pi^2(n_B - n_n)]^{1/3} \\ k_{F,n} &= [3\pi^2 n_n]^{1/3} = 1.71\text{fm}^{-1} = 338\,\text{MeV}, \quad \text{if } n = 0.17\text{fm}^{-3}. \end{aligned} \tag{4.40}$$

To verify that in equilibrium $\mu_n = \mu_p + \mu_e$ simply compute the derivative of $\rho = \rho_n + \rho_e + \rho_p$ with respect to n_n, taking $\rho \equiv \epsilon$ from Eq. (4.35). Then

$$\sum_i \frac{d\rho}{dk_{F,i}} \frac{dk_{F,i}}{dn_n} = \sum_i \frac{dk_{F,i}}{dn_n} {k_{F,i}}^2 E_i = 0, \quad \text{where } \frac{dk_{F,i}}{dn_n} \propto \frac{1}{k_{F,i}^2} \tag{4.41}$$

and the derivative vanishes when (abbreviating $C \equiv (3\pi^2)^{1/3}$)

$$\mu_n - \mu_p - \mu_e = \sqrt{C^2 n_n^{2/3} + m_n^2} - \sqrt{C^2(n_B - n_n)^{2/3} + m_p^2} - \sqrt{C^2(n_B - n_n)^{2/3} + m_e^2} = 0. \tag{4.42}$$

The minus signs for p, e follow since there is a $-n_n$ in their Fermi momentum k_F.

One can easily solve n_p/n_n from Eq. (4.42) numerically, but it is more illustrative to to find an approximate analytic solution. Let us therefore take p, n as non-relativistic and electrons as relativistic (for more accuracy, see Weinberg). For neutrons at nuclear matter density $k_F = 338$ MeV and $E_F = m_n + 61$ MeV so that this is qualitatively fine. Then Eq. (4.42) reads

$$m_n + \frac{1}{2m_n} C^2 n_n^{2/3} = m_p + \frac{1}{2m_p} C^2 (n_B - n_n)^{2/3} + C(n_B - n_n)^{1/2} \; . \tag{4.43}$$

For $n_n \approx$ nuclear matter density the order of magnitude of the terms is 939+60=938+2+60 and one sees that $m_n = m_p$ cancels, the Fermi kinetic energy of the proton contributes negligibly and we can equate the neutron Fermi kinetic energy and the electron Fermi energy and find $n_B - n_n = C^3 n_n^2/(2m_n)^3$ or

$$\frac{n_p}{n_n} = \frac{n_e}{n_n} = \frac{3\pi^2}{(2m_n)^3} n_n = 0.034 n_n \cdot \text{fm}^3, \tag{4.44}$$

since numerically $1/m_n^3 = 0.0083\,\text{fm}^3$. For real neutron stars the central density is few×nuclear matter density, n_e and n_p are a few % of n_n. Similarly,

$$k_{F,e} = C n_p^{1/3} = 197 \text{ MeV}(n_n \text{fm}^3)^{2/3} \tag{4.45}$$

which is $\geq$ the maximum decay momentum 1.19MeV of the beta decay electrons. Thus only part of the neutrons can beta decay, establishing the equilibrium as discussed above.

Summarising, at this very rough level of approximation, a neutron star is a $T = 0$ degenerate Fermi system of 10^{57} nucleons, with radius $R = A^{1/3}\text{fm} = M_{\text{Planck}}/m_n\,\text{fm} = 10^{19}\text{fm} = 10^4\text{km}$, with the n, p, e composition discussed above.

4.4 Degenerate Fermi gas with repulsive interactions

We got very far without saying anything about interactions. Let us now remedy this defect. Consider a dilute degenerate gas of fermions with a short range repulsive interaction near T = 0.

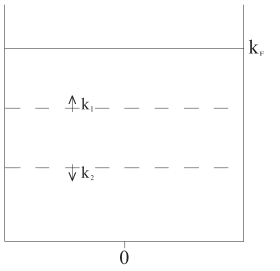

Figure 4.3: All states $\psi_k(r) = \frac{1}{\sqrt{V}}\chi_s e^{i\mathbf{k}\cdot\mathbf{r}}$ $(r \equiv \mathbf{r}, s)$ are filled up to k_F.

To leading order the energy is $E = E_0 = N \cdot \frac{3}{5}E_F$; for bosons $E = 0$. How do the low-energy scatterings of the fermion states within the Fermi sea affect E? A detailed discussion can be found in Landau-Lifshiz, Stat. Phys. 2, section 6; here we give a rough outline. To start with, let us apply again first-order perturbation theory with

$$\Delta E = \langle\Psi_0|H_I|\Psi_0\rangle \tag{4.46}$$

where we assume a pairwise interaction

$$H_I = \sum_{i<j=1}^{N} U(\mathbf{r_1} - \mathbf{r_0}); \qquad U(\mathbf{r}) = \frac{4\pi\hbar^2 a}{m}\delta(\mathbf{r}) \tag{4.47}$$

and where a, the scattering length, is the $k \to 0$ limit of the scattering amplitude so that

$$a = \frac{m}{4\pi\hbar^2}\int d^3r U(\mathbf{r}) \ . \tag{4.48}$$

This implies that the fermion interaction cross section is

$$\sigma = 4\pi a^2, \tag{4.49}$$

For dimensional reasons, one then expects that the expansion parameter should be ak_F.

The ground state wave function Ψ_0 is the antisymmetrizised state

$$\Psi_0 = \begin{vmatrix} \Psi_1(r_1) & \Psi_1(r_2) & ... & \Psi_1(r_N) \\ \Psi_2(r_1) & \Psi_2(r_2) & ... & \Psi_2(r_N) \\ . & . & . & . \\ . & . & . & . \\ \Psi_N(r_1) & \Psi_N(r_2) & ... & \Psi_N(r_N) \end{vmatrix} \tag{4.50}$$

where Ψ_k are single particle wave functions which also include the spin. Then

$$\begin{aligned}
\Delta E &= \langle\Psi_0|\sum_{i<j=1}^{N} U(\mathbf{r_i}-\mathbf{r_j})|\Psi_0\rangle && (4.51)\\
&\propto \sum_{\text{spin}}\langle\Psi_1(\mathbf{r_1})\Psi_2(\mathbf{r_2})|\delta(\mathbf{r_1}-\mathbf{r_2})|\Psi_1(\mathbf{r_1})\Psi_2(\mathbf{r_2})\rangle\langle\Psi_3\Psi_4\cdots|\Psi_3\Psi_4\cdots\rangle && (4.52)\\
&+ \text{ all combinations, properly antisymmetrized .} && (4.53)
\end{aligned}$$

As $\mathbf{r_1} \to \mathbf{r_2}$, the normalized antisymmetric spin combination is $(\psi_1^\uparrow\psi_2^\downarrow - \psi_1^\downarrow\psi_2^\uparrow)/\sqrt{2}$. Altogether there are $N = N_\downarrow + N_\uparrow$ states with $N_\downarrow = N_\uparrow = N/2$. As indicated above, the interaction Eq. (4.47) picks the terms spin$\uparrow$ $\times$spin$\downarrow$, each term contributing $\Delta E = 4\pi\hbar^2 a/m$. Thus altogether

$$\begin{aligned}
\Delta E &= N_\downarrow N_\uparrow \frac{4\pi\hbar^2 a}{m}\int \underbrace{d^3r}_{V}\underbrace{\langle\psi_1|\psi_1\rangle}_{1/V}\underbrace{\langle\psi_2|\psi_2\rangle}_{1/V} + \text{ all combinations, normalized} && (4.54)\\
&= \frac{N^2}{V}\frac{\pi\hbar^2 a}{m} = N\times\frac{k_F^3}{3\pi^2}\frac{\pi\hbar^2}{m}\left(\frac{k_F a}{k_F}\right) && (4.55)\\
&= E_0\left[1+\frac{10}{9\pi}k_F a\right] . && (4.56)
\end{aligned}$$

Adding next-to-leading order would result into

$$E = E_0[1+\frac{10}{9\pi}k_F a + \frac{4(11-\log 4)}{21\pi^2}(k_F a)^2 + ...] . \tag{4.57}$$

This is an academic case which should be contrasted with the case of attractive interactions, which will be discussed next.

4.5 Attractive interactions and the gap equation

Let us now assume the interaction is attractive. This seems like an unusual case since the Coulomb interaction between electrons is repulsive. However, when the electrons interact with the lattice vibrations of certain materials, there arises an effective attractive interaction between the electrons. Then one finds a remarkable instability of the usual fermionic $T = 0$ ground state, the Fermi sphere: if there is any attractive interaction between the fermions, then the energy E of two fermions with opposite momenta, $\mathbf{k}$ and $-\mathbf{k}$, just above the Fermi sphere, $k > k_F$, is less than $2E_F$ with $\Delta = 2E_F - E > 0$. Here Δ is called the mass (or energy) gap, and its existence is at the very heart of superconductivity.

Evaluating Δ, as will be done below, one finds that $\Delta \sim \exp(-1/\text{small})$. Hence the gap Δ is non-analytic when the small strength if the interaction $\to 0$ and hence the gap is genuinely non-perturbative: there is no (Taylor) expansion in the coupling strength. In contrast, the scattering corrections of the previous Section are perturbative and $\to 0$ smoothly as the scattering length $a \to 0$.

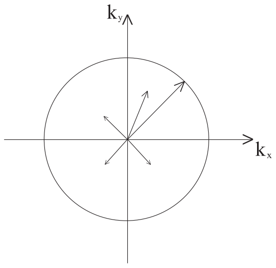

Figure 4.4: Leading order: states filled up to fermi surface $|k| \leq |k_F|$

To the leading order the states are filled up to Fermi surface and the energy of a pair at the surface is $2E_F$. Consider then two electrons in a spin zero antisymmetric state so that their momenta are $\mathbf{k}$ and $-\mathbf{k}$ and lie just above the Fermi sphere, $k > k_F$. Thus the spatial part of the wave function is $\sim e^{i\mathbf{k}\cdot\mathbf{x}_1}e^{-i\mathbf{k}\cdot\mathbf{x}_2}$, or when summing over all momenta ($\mathbf{x} = \mathbf{x}_1 - \mathbf{x}_2$),

$$\psi(\mathbf{x}) = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{x}} \psi(\mathbf{k})\theta(k - k_F) \ . \tag{4.58}$$

This should be solved from the Schrödinger equation

$$[-\frac{\hbar^2}{m}\nabla^2_{\mathbf{x}} + V(\mathbf{x})]\psi(\mathbf{x}) = E\psi(\mathbf{x}), \quad \mathbf{x} = \mathbf{x}_1 - \mathbf{x}_2, \tag{4.59}$$

where $m = 2m_{\text{reduced}}$. Since the conditions on ψ are formulated in momentum space, we also have to write the Schrödinger equation in momentum space, where the product $V(\mathbf{x})\psi(\mathbf{x})$ becomes a convolution:

$$\begin{aligned} (E - \frac{\hbar^2 k^2}{m})\psi(\mathbf{k}) &= \int \frac{d^3\mathbf{k}'}{(2\pi)^3} V(\mathbf{k} - \mathbf{k}')\psi(\mathbf{k}')\theta(k' - k_F), & (4.60) \\ V(\mathbf{x}) &= \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{x}} V(\mathbf{k}) \ . & (4.61) \end{aligned}$$

From here we see that the dimensions of $V(\mathbf{k})$ are energy·volume, the same as those of $4\pi\hbar^2 a/m$, where a is the scattering length. Eq. (4.60) should be solved for E with the expectation that $E = 2E_F - \Delta$.

Now insert the crucial information that V is attractive near Fermi surface:

$$V(\mathbf{k} - \mathbf{k}') = \begin{cases} -v_0 & \text{if } E_F < E_k, E_{k'} < E_F + \delta \\ 0 & \text{otherwise} \end{cases} \tag{4.62}$$

Here δ is a parameter which will turn out to be $\approx \hbar\omega_{\text{Debye}} \approx 100$ K. As we will see $\Delta \ll \delta$. The parameter $v_0 \sim 4\pi\hbar^2|a|/m$ (the attractive nature of the interaction, i.e. $a < 0$, is implemented in Eq. (4.62) by writing $-v_0$) characterises the strength of the interaction. Parametrically, it is the energy of the particle×volume of the particle. It should thus be compared with $E_F \times V/N$. Hence v_0 is small if $v_0 n/E_F \ll 1$ (typically 0.1...0.5).

Solving Eq. (4.60) we find

$$\psi(\mathbf{k}) = \frac{v_0}{2E_k - E} \int \frac{d^3k'}{(2\pi)^3} \theta(k' - k_F)\theta(E_F + \delta - E_{k'})\psi(\mathbf{k}') \tag{4.63}$$

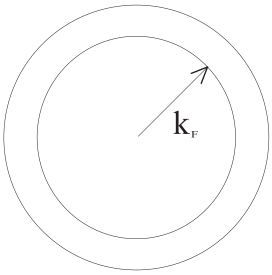

Figure 4.5: From (4.62) $k_F < k < k_F + m\delta/\hbar^2 k_F$.

Here $\int \frac{d^3k'}{(2\pi)^3}\theta(k'-k_F)\theta(E_F+\delta-E_{k'})\psi(\mathbf{k}')$ depends on k_F and δ, but not on k. Now multiply both sides by $\theta(k-k_F)\theta(E_F+\delta-E_k)$ and then integrate over d^3k; then factors of $\int \frac{d^3k}{(2\pi)^3}\theta(k-k_F)\theta(E_F+\delta-E_k)$ cancel and one finds

$$1 = v_0 \int \frac{d^3k}{(2\pi)^3}\theta(k-k_F)\theta(E_F+\delta-E_k)\frac{1}{2E_k-E}\ . \tag{4.64}$$

This is the famous gap equation.

To solve E from Eq. (4.64), let us write the density of states in a box in a conveniently normalised form:

$$\int \frac{d^3k}{(2\pi)^3} = \frac{1}{V}\sum_i = \int_0^\infty dE_k g(E_k), \quad g(E) = \frac{3}{4}\frac{N}{VE_F}\sqrt{\frac{E}{E_F}}. \tag{4.65}$$

Now, by convention, $g(E)$ is number of states per unit E per unit V. Then

$$v_0\int_{E_F}^{E_F+\delta} dE_k g(E_k)\frac{1}{2E_k-E} \approx \frac{v_0 g(E_F)}{2}\log(\frac{2E_F-E+2\delta}{2E_F-E}). \tag{4.66}$$

where we have assumed that the density of states $g(E_F)$ stays almost constant over the the narrow range $[E_F, E_F+\delta]$. Assuming further that the energy gap $\Delta = 2E_F - E =$ binding energy $\gg 2\delta$ one finds the solution

$$\Delta = 2\delta e^{-2/v_0 g(E_F)}. \tag{4.67}$$

Often the gap equation is written in a simplified prototype form:

$$1 = g^2\int_0^\Lambda \frac{dE}{\sqrt{E^2+\Delta^2}} = g^2\log\Big(\frac{\Lambda}{\Delta}+\sqrt{\frac{\Lambda^2}{\Delta^2}+1}\Big) \approx g^2\log\frac{2\Lambda}{\Delta}. \tag{4.68}$$

From this we see that

$$\Delta = 2\Lambda e^{-1/g^2}. \tag{4.69}$$

Remarkably, we have found a solution with $\Delta > 0$. Both forms of the solution emphasize the fact that the energy gap does not disappear in the weak interaction limit. It is not attainable from the ground state (Fermi sea) by small perturbations, and therefore an entirely new ground state has to be constructed: this is the BCS state.

To see in another way how the solution appears, rewrite (4.64) by going back to the sum over states and plot it as a function of E. The smallest value of $2E_k = \hbar^2 k^2/m$ is $2E_F$, above that but below $2E_F+\delta$ there are the states $2E^{(i)}$. Thus

$$\frac{1}{v_0} = \frac{1}{V}\sum_{\text{states}} \frac{1}{2E_k - E} = \frac{1}{V}\left[\frac{1}{2E_F - E} + \frac{1}{2E^{(1)} - E} + \frac{1}{2E^{(2)} - E} + ...\right]$$

and Fig. 4.5 shows how the solution is formed. Numerically, for superconductors, $E_F \approx$ 10000K, $\delta \approx \hbar\omega_{\text{Debye}} \approx 100$ K and $\Delta \approx 1$ K. These would correspond to $v_0 g(E_F) = \frac{3}{4}v_0 n/E_F \approx$ 0.4

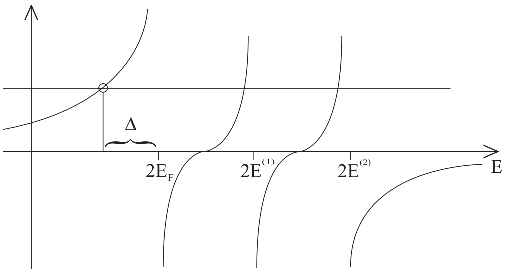

Figure 4.6: Gap equation plotted as a function of E.

The above is a simple discussion of quantum mechanics of one pair, both electrons outside the Fermi sphere. For a proper discussion one must include all possible pairs as well as fermions inside but still near the Fermi surface (see Landau-Lifshitz, Statistical Physics, Part 2, Chapter V). Then, at any T, the superconducting gap equation becomes

$$1 = gT\sum_{n=-\infty}^{\infty}\int \frac{d^3k}{(2\pi)^3}\frac{1}{(\hbar\omega_n)^2 + \xi_k^2 + \Delta^2}, \tag{4.70}$$

where $\hbar\omega_n = (2n+1)\pi T$, g is a four-fermion coupling ($=v_0$ previously), and $\xi_k = \hbar^2k^2/(2m) - E_F = (p+p_F)(p-p_F)/2m \approx v_F(p-p_F)$ is the energy measured from the Fermi surface. Note the simple one-loop structure of this: it is like the $I(T,m)$ discussed previously, now for fermions and with $\mathbf{k}^2 + m^2 \to v_F^2|p-p_F|^2 + \Delta^2$. Using

$$\sum_{n=-\infty}^{\infty} \frac{x}{(2n+1)^2\pi^2 + x^2} = \frac{1}{2} - \frac{1}{e^x+1} = \frac{1}{2}\tanh\frac{x}{2}$$

one derives from here the equation

$$\frac{1}{g} = g(E_F)\int_0^\delta \frac{d\xi}{\sqrt{\xi^2+\Delta^2}}\tanh\left[\frac{1}{2}\beta\sqrt{\xi^2+\Delta^2}\right]$$

for the T-dependence of the gap $\Delta(T)$; $\delta = \hbar\omega_{\text{Debye}}$ and $g(E_F)$ is the density of states on the Fermi surface. For $T=0, \beta=\infty$ one is back to (4.68). For any T, in the weak coupling limit

$\Delta \ll \delta$, one has

$$\log \frac{\Delta(0)}{\Delta(T)} = 2I(\frac{\Delta(T)}{T}),$$

where

$$I(y) = \int_0^\infty \frac{dx}{\sqrt{x^2+y^2}} \frac{1}{(\exp\sqrt{x^2+y^2}+1)}.$$

For large y, $I(y) \to \sqrt{\pi/2y}e^{-y}$ and for small y, $I(y) = \frac{1}{2}\log(\pi/y) - \frac{1}{2}\gamma_{\text{Euler}} + 7\zeta(3)/(16\pi^2)y^2 + \ldots)$. From here one finds that $(2e^\gamma/\pi \approx 1.13)$

$$T_c = \frac{e^\gamma}{\pi}\Delta(0) = \frac{e^\gamma}{\pi}2\delta e^{-2/g\cdot g(E_F)} \tag{4.71}$$

and

$$\Delta(T) = 1.74\Delta(0)(1-T/T_c)^{1/2}. \tag{4.72}$$

4.6 BCS theory

Using the usual fermionic creation and annihilation operators, $\{a, a^\dagger\} = \delta,\ \{a, a\} = \{a^\dagger, a^\dagger\} = 0$ the normal Fermi sphere could be written as $\prod_{k<k_F} a^\dagger_k a^\dagger_{-k}|0\rangle = |F\rangle$, writing the opposite momenta explicitly. As discussed above, this state is actually unstable if there is attractive interaction. The true ground state, replacing the Fermi sphere, is the BCS ground state (Nobel 1972)

$$|\Psi_{\text{BCS}}\rangle = \prod_{k>0}(\sqrt{1-v_k^2} + v_k a^\dagger_k a^\dagger_{-k})|0\rangle \qquad (k \equiv \mathbf{k}, s) \tag{4.73}$$

The last term implies that all electrons in the system are paired (with probability v_k^2) This ground state was a guess, ansatz, but it works very well! Let us briefly indicate how solving the Schrödinger equation with this wave function proceeds.

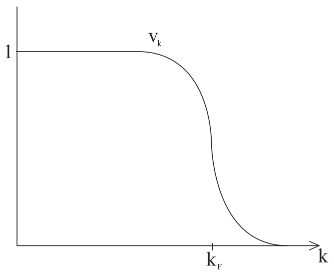

Figure 4.7: The superconducting solution for the weight v_k.

The Hamiltonian and the Schrödinger equation

$$\begin{cases} H = T + V = \sum_{i=0}^N T_i + \sum_{i<j=1}^N V(x_i - x_j) \\ i\hbar\partial_t\Psi(1,...,N) = H\Psi(1,...,N) \end{cases}$$

can in the occupation number representation

$$a|n\rangle = \sqrt{n}|n-1\rangle \quad a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$$

be written as

$$\begin{cases} H = \sum_{r,s=1}^{\infty} a_r^\dagger a_s \langle r|T|s\rangle + \frac{1}{2}\sum_{rs'lk} a_r^\dagger a_s^\dagger a_l a_k \langle ij|V|kl\rangle \\ i\hbar\partial_t|\Psi\rangle = H|\Psi\rangle \end{cases}$$

Here, in terms of one-particle states, $\langle r|T|s\rangle = \int d^3x \Psi_r^* T \Psi_s$, $\langle ij|V|kl\rangle = \int d^3x d^3x' \Psi_r^*(x)\Psi_s^*(x')V(x-x')\Psi_k(x)\Psi_l(x')$ and $|\Psi\rangle$ is a linear combination of states $= |n_1 n_2 n_3 .....\rangle \equiv (a_1^\dagger)^{n_1}...|0\rangle$. Further

$$H = \sum_k E_k a_k^\dagger a_k + \frac{1}{2}\sum_{k,q}\langle q-q|V|k-k\rangle a_q^\dagger a_{-q}^\dagger a_{-k} a_k, \tag{4.74}$$

$$N = \sum_k a_k^\dagger a_k, \tag{4.75}$$

where (there is interaction between pairs only)

$$\langle q-q|V|k-k\rangle = \frac{v_0}{V}\theta(\delta - |E_k-\mu|)\theta(\delta - |E_q-\mu|).$$

To solve $H|\Psi_{\mathrm{BCS}}\rangle = E|\Psi_{\mathrm{BCS}}\rangle$, where v_k in Ψ_{BCS} and E are unknown, one has to define new operators for which $|\Psi_{\mathrm{BCS}}\rangle$ is the "vacuum", $\alpha_k|\Psi_{\mathrm{BCS}}\rangle = \beta_k|\Psi_{\mathrm{BCS}}\rangle = 0$:

$$\begin{cases} \alpha_k = u_k a_k - v_k a_{-k}^\dagger \\ \beta_k = u_k a_{-k} - v_k a_k^\dagger \end{cases} \qquad u_k^2 + v_k^2 = 1$$

This is a canonical transformation $a, a^\dagger \Rightarrow \alpha, \beta$. Quite a bit of work leads to

$$H - \mu N = \sum_k \sqrt{(E_k-\mu)^2 + \Delta^2}(\alpha_k^\dagger \alpha_k + \beta_k^\dagger \beta_k) + ... \tag{4.76}$$

where $\sqrt{(E_k-\mu)^2+\Delta^2}$ gives the quasiparticle energy spectrum with gap "mass" and Δ is determined from the gap equation (4.70), essentially like the Δ for Cooper pairs.

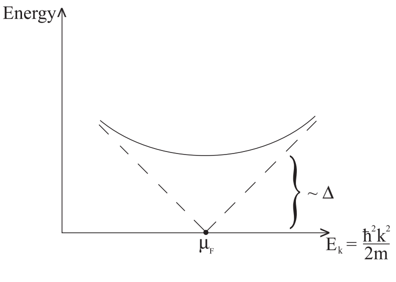

Figure 4.8: The gap function

The whole Fermi system can lower it's energy by going to the BCS state. Because of the gap this is a non-analytic transition.

What seems very surprising is how an attractive interaction between electrons can arise. For this one has to study carefully the collective behavior of electrons, including both the effects of electrons and ions. Allowing the ions to move in response to the motion of electrons one finds that there is firstly a static screening of a negative test charge, the Coulomb potential becomes

$$\int \frac{d^3k}{(2\pi)^3} \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{k^2 + 1/r_0^2} = \frac{1}{4\pi r} e^{-r/r_0}, \quad \frac{1}{r_0^2} = \frac{3}{2} \frac{e^2}{\epsilon_0} \frac{n}{\epsilon_F} \tag{4.77}$$

For a gas of electrons in a metal,

$$r_0 \sim \sqrt{\frac{a_0}{k_F}} \sim \frac{a_0}{\sqrt{a_0 k_F}} \sim \frac{a_0}{(a_0^3 n)^{1/6}},$$

where $a_0 = \hbar/(\alpha m_e c)$ is the Bohr radius. This is $\approx$ ionic lattice spacing so that the screening is very efficient. However, a closer analysis (see Ashcroft-Mermin, Eqs. (26.25) and (34.10)) shows that there is also dynamic screening, the electron-electron interaction becomes frequency dependent. The screening by ionic motion gives rise to a net attractive interaction between electrons with energies separated by less than $\hbar\omega_D$, the energy of lattice vibrations.

4.7 Quark matter

For electrons in metals the net attractive interaction arose in a rather complicated way via interactions with ions. For quarks at $T = 0$ the non-Abelian color interaction itself leads to an attractive interaction. Thus instabilities of the Fermi sea at $T = 0$ are expected to lead to remarkable effects for quark matter. However, so far they remain unobserved. This is a part of the more general issue of determining the phase diagram of strongly interacting matter on the T, μ plane, which we now briefly discuss.

Quarks have several quantum numbers, which we denote as q_{sif}, with $s = 1, .., 4$ for spin, $i = 1, 2, 3$ for color and $f = 0, 1, 2, .., N_f$ for flavor. The quark masses are not physical because they are always confined within hadrons. Hence the masses are convention dependent. In a certain scheme they are $m_u \sim 4$MeV, $m_d \sim 7$MeV, $m_s \sim 150$MeV, $m_c = 1.5\text{GeV}, m_b = 5\text{GeV}, m_t = 180\text{GeV}$.

The QCD coupling constant varies with the energy scale μ as given by the renormalization group equation

$$\mu \frac{dg(\mu)}{d\mu} = -bg^3 + \mathcal{O}(g^5) \tag{4.78}$$

the solution of which to lowest order is

$$g^2(\mu_2) = \frac{g^2(\mu_1)}{1 + 2bg^2(\mu_1)\log(\mu_2/\mu_1)} \equiv \frac{1}{2b\log(\mu_2/\Lambda_{\rm QCD})}\ , \tag{4.79}$$

where $16\pi^2 b = 11 - 2N_f/3$ and $\Lambda_{\rm QCD} = \mu e^{-1/(2bg^2(\mu))}$ is the integration constant of Eq. (4.79); note the analogy with the energy gap in Eq. (4.69) [1]

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[1] Proving in a way mathematicians accept as satisfactory that QCD has a gap is one of the famous million dollar problems, see http://www.claymath.org. Any physicist knows there is a gap.

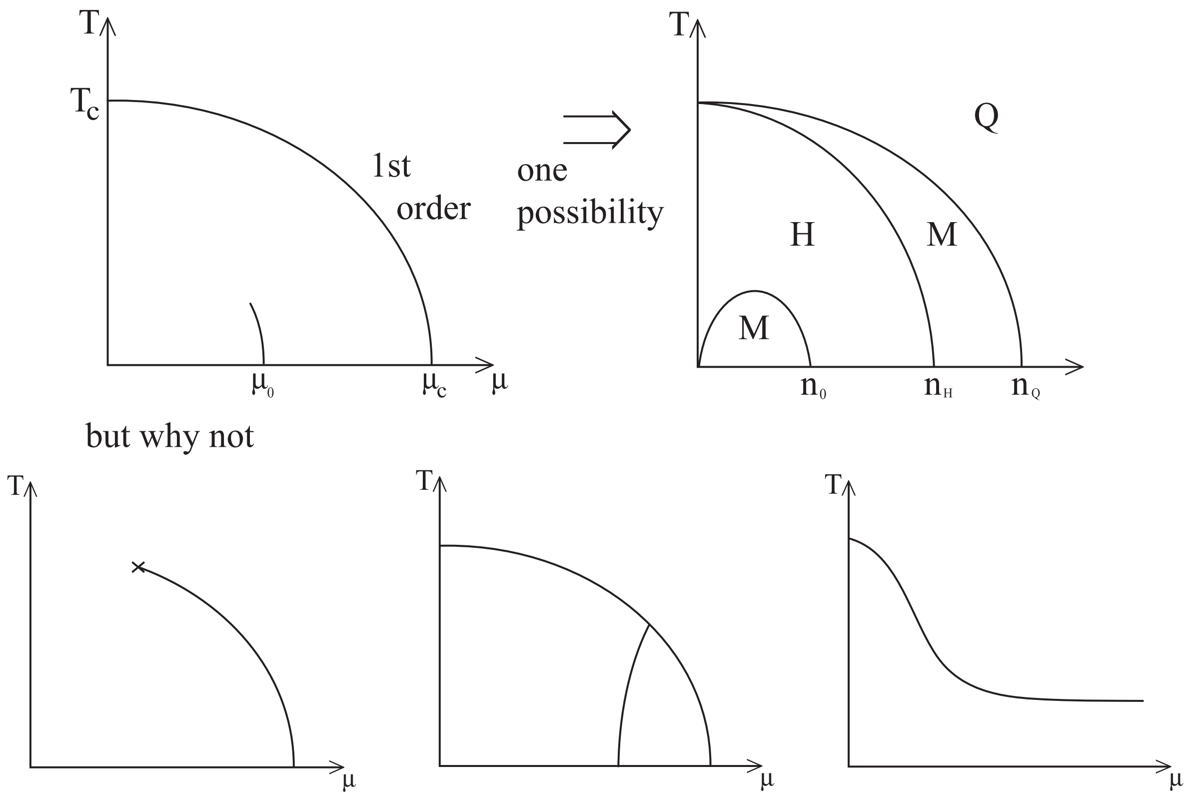

Figure 4.9: Some alternative phase diagrams on the (T, μ) or (T, n_B) plane.

The idea now is that if one heats ordinary matter up to $T \gg 200$ MeV $= 1/\text{fm}$ and/or compress it to densities $\rho \gg \rho_{\text{nuclmatt}} = 0.17/\text{fm}^3$ the quark-gluon structure of hadrons (strongly interacting particles) dissolves and a quark-gluon plasma is formed. The fundamental problems are then: what is $\Omega(T, \mu) = -Vp(T, \mu)$ for QCD matter? Is there a phase transition between the hadronic and quark-gluon phases?

Extensive theoretical and experimental work has been devoted to the study of $\Omega(T, \mu)$ for QCD matter. Note that theoretically there are different "QCDs" depending on what quark masses are assumed; there is only one physical QCD where quark masses are so fixed that the theory produces correct hadronic masses (such as m_n, m_p discussed earlier). Some possible alternatives are shown in Fig. 4.7

The bag model. A very simple, old (1974) phenomenological idea captures roughly some of the features of the quark-hadron phase differences. Gluons are massless and so are also relevant u and d quarks as is also, to some extent, the s quark. There is asymptotic freedom so interactions should be small at very large T so apply just ideal massless gas formulas. However, to represent all the unknown QCD interactions, include also a vacuum term $-B$ to the pressure. Then we have, from formulas of Chapter 3, for a system of massless gluons with 2 spin and 8 color states and N_F massless quarks and antiquarks with 2 spin and 3 color states in a quark chemical potential μ:

$$\begin{aligned} p_q(T,\mu) &= 2\cdot 8\frac{\pi^2}{90}T^4 + 3\cdot N_F\left(\frac{7}{8}\cdot 2\cdot 2\frac{\pi^2}{90}T^4 + \frac{1}{6}T^2\mu^2 + \frac{1}{12\pi^2}\mu^4\right) - B \\ &= \left(16 + \frac{21}{2}N_f\right)\frac{\pi^2}{90}T^4 + \frac{N_F}{2}T^2\mu^2 + \frac{N_F}{4\pi^2}\mu^4 - B, \end{aligned} \tag{4.80}$$

From here one further computes $s = \partial p(T,\mu)/\partial T$, $n = \partial p(T,\mu)/\partial\mu$,

$$\epsilon = Ts + \mu n - p = (T\partial/\partial T + \mu\partial/\partial\mu - 1)p = 3p + 4B.$$

As T (or μ) decrease, the system should go over to the hadron phase where

$$p_h = g_h\frac{\pi^2}{90}T^4 + \left(\frac{2mT}{\pi}\right)^{3/2} Te^{-m/T}\left(1 + \frac{1}{2}\frac{\mu^2}{T^2}\right), \tag{4.81}$$

where g_h can be assumed to count just the relativistic pions and where the nucleons of mass m are also included. The critical curve $T = T_c(\mu)$ is obtained at the phase equilibrium defined by equal pressures $p_h = p_q$.

For $\mu = 0$ we can write

$$p_q(T) = a_qT^4 - B, \quad \epsilon = 3a_qT^4 + B, \qquad p_h(T) = a_hT^4. \tag{4.82}$$

One now sees clearly how B operates. The critical temperature is determined by $a_qT_c^4 - B = a_hT_c^4$ and a solution is possible only if B exists, $T_c^4 = B/(a_q - a_h)$. One also sees that the bag constant acts just as a vacuum energy density, corresponding to an energy momentum tensor

$$T_{\mu\nu} = Bg_{\mu\nu}, \quad T_{00} = +B, \quad T_{ii} = -B. \tag{4.83}$$

Note that μ is the chemical potential associated with net baryon number, $n_B - n_{\bar{B}}$; this is the conserved quantity although pairs of $B\bar{B}$ or $q\bar{q}$ can appear/vanish. For a nucleon B(N) = 1 while for a quark B(q) = 1/3, and since in equilibrium the process $p \leftrightarrow qqq$ can take place, $\mu_N = 3\mu_q$.

The ideal gas formulas can, of course, be improved by computing higher order corrections in perturbation theory (see J. I. Kapusta and C. Gale, Finite-Temperature Field Theory, Cambridge University Press 2006).

Along the μ axis at $T = 0$ one might think that the net baryon number density $n = \partial p(0,\mu)/\partial\mu$ behaves as shown in Fig.4.7. One can directly apply the ideal gas formulas given above, but also higher order corrections can be computed with much effort over the entire T,μ plane (see Aleksi Vuorinen, thesis 2004). However, the Fermi sea instability leads to qualitatively new effects at $T = 0$. The point with $T = 0$ QCD matter is that the attractive interaction between fermions near the Fermi sea is obtained for free, from the colour symmetry. For electrons one needed a roundabout via interactions with positively charged ion oscillations.

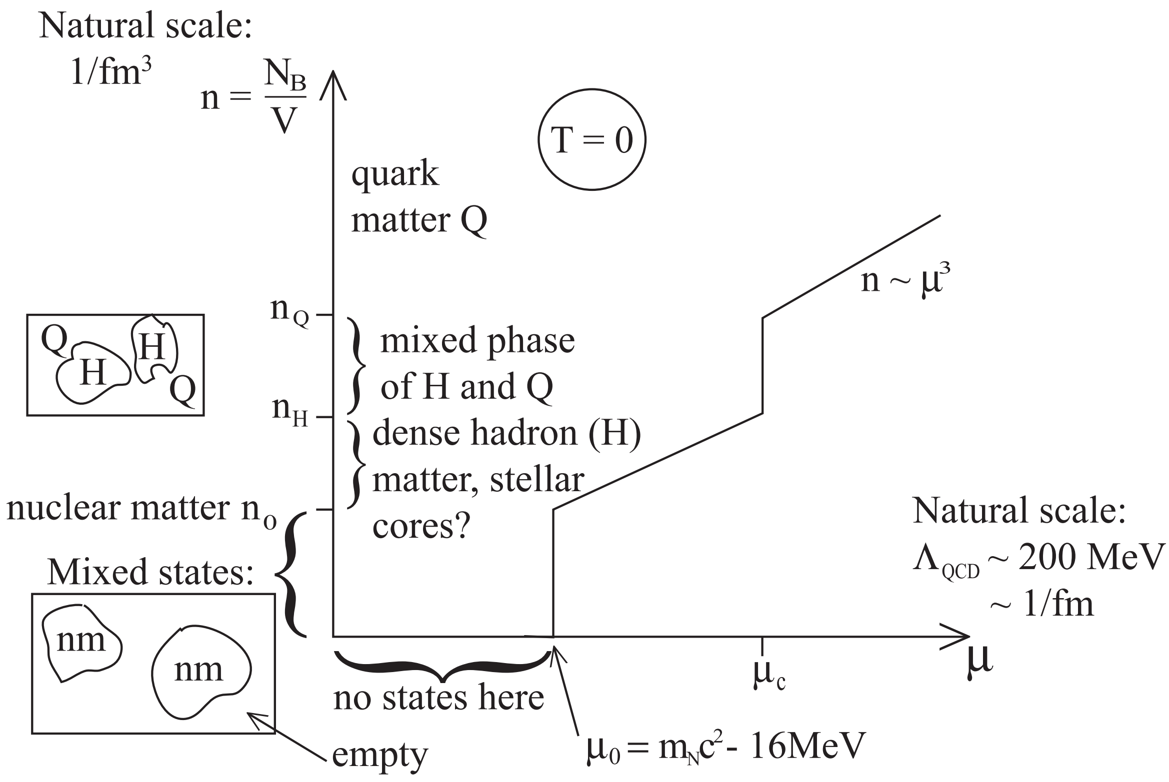

Figure 4.10: Net baryon number density at T = 0, μ increasing. The relation between μ and n is somewhat tricky at small μ!

Color superconductivity. To indicate where the attractive force between quarks comes from one needs some group theory. Consider the group SU(2) and the states of two spin 1/2 particles. Denote this state by (u, d), the fundamental representation of SU(2). The combined state reduces to a scalar and vector: $2 \times 2 = 1 + 3$, the singlet state is the antisymmetric state $(u_1 d_2 - d_2 u_1)/\sqrt{2}$ and the vector state is the symmetric set $(u_1 u_2, (u_1 d_2 + d_1 u_2)/\sqrt{2}, d_1 d_2)$. If the spin operator is $\mathbf{S}$, its eigenvalues are $\mathbf{S}^2/\hbar^2 = s(s+1) = 0, 3/4, 2$ for singlet, doublet and vector respectively. Assuming rotational symmetry, the potential between particles would be $V(r) = V_0(r) + V_1(r)\mathbf{S}_1 \cdot \mathbf{S}_2$, where

$$\begin{aligned}
\mathbf{S}_1 \cdot \mathbf{S}_2 &= \frac{1}{2}[|\mathbf{S}_1 + \mathbf{S}_2|^2 - |\mathbf{S}_1|^2 - |\mathbf{S}_2|^2 \\
&= -\frac{3}{4} \quad \text{singlet} \\
&= +\frac{1}{4} \quad \text{triplet} \qquad (4.84)
\end{aligned}$$

This simple argument has thus produced a sign change, change between attraction and repulsion, in the potential.

For the QCD color group SU(3) the quarks are in the fundamental representation 3 of SU(3). Taking two fundamental states q_i, p_j $(i, j = 1, 2, 3$ are color indices), the appropriate group theory relation is $3 \times 3 = \bar{3} + 6$ or in tensorial form

$$q_i p_j = \frac{1}{2}(q_i p_j - q_j p_i) + \frac{1}{2}(q_i p_j + q_j p_i). \tag{4.85}$$

Doing some SU(3) group theory as was done for SU(2) above shows that the antisymmetric two-quark state $\bar{3}$ is favoured by a factor -2 relative to the symmetric one 6.

This simple source of attraction has given rise to a large literature on the pairing instability of quark matter near $T = 0$. Since the quarks have many quantum numbers there can be complicated patterns of pairing: the order parameter would be $\langle q_{s,a,i} q_{s,b,j} \rangle$, where s(=left or right-handed) is a spin index, $a, b = u, d, s, c, ..$ is a flavor index and $i, j = 1, 2, 3$ is a color index. There is a very elegant result for the gap:

$$\Delta(\mu) = 514\pi^4 \left(\frac{2}{N_f}\right)^{5/2} \frac{1}{g^5(\mu)}\, \mu \exp\left[-\frac{3\pi^2}{\sqrt{2}} \frac{1}{g(\mu)} - \frac{\pi^2 + 4}{8}\right], \tag{4.86}$$

where N_f is the number of flavors and $g(\mu)$ is the dimensionless running coupling in (4.79). Note the dominant factor $\exp[-\text{const}/g(\mu)]$, due to special properties of QCD this really contains g, not g^2. Numerically, this has a huge effect; Δ is much bigger than expected by analogy with ordinary superconductivity, but still $\ll \mu$. Unfortunately, the only thinkable tests of these theoretical ideas are in observations of stellar compact systems and one has so far no empirical evidence of color superconductivity.

Chapter 5

Hydrodynamics and Kinetic Theory

5.1 Introductory remarks

Let us now move on from global to local thermal equilibrium, the dynamics of which is described by hydrodynamics, which is a set of equations describing continuous media. The degrees of freedoms are now fields: number density $n(\mathbf{x}, t)$, temperature $T(\mathbf{x}, t)$, pressure $n(\mathbf{x}, t)$, mass(energy) density $\rho(\mathbf{x}, t) = mn(\mathbf{x}, t)$ in the non-relativistic case, velocity $\mathbf{v}(\mathbf{x}, t)$, and so on. In order that we may treat matter as continuous naturally requires that the time scales $\delta t \gg \tau_c$, the collision time, and the length scales $\delta x \gg r$, the average distance between the particles (atoms, molecules). In terms of frequency and wave number the conditions are $\omega\tau_c \ll 1$, $k\lambda \ll 1$. Actually there will also be shock fronts with thickness λ, but these are treated as discontinuities conserving energy and momentum fluxes. One may also note that in magnetohydrodynamics a collisionless approximation with $\omega\tau_c \gg 1$ may be valid. Then the electric and magnetic fields $\mathbf{E}$ and $\mathbf{B}$ dominate the dynamics.

Thermal equilibrium	$\Rightarrow$	Local thermal equilibrium	$\Rightarrow$	No equilibrium
$\Delta t = \infty$		$\Delta t \gg$ something		
$\Delta x = \infty$		$\Delta x \gg$ something		
$T, p =$ constant		$p = p(t, \mathbf{x}), T = T(t, \mathbf{x})$		

Table 5.1: Equilibrium conditions.

There immediately arises two questions: (i) how do small perturbations about a given background evolve, and (ii) how is thermal equilibrium locally reached? The former issue leads to the study of the propagation of pressure and density waves, the latter to is related to dissipation and viscosity in general.

The third question would be: what is the microscopic origin of the hydrodynamics? This question is addressed by the *kinetic theory*, which yields hydrodynamics as a coarse grained description of the motion and interactions of point-like particles. Kinetic theory will be discussed in Sect. XX.

To get a feeling of the typical observables and their magnitudes, consider a simple example, air, which is mostly N_2 and O_2 molecules at $p = 10^5\mathrm{Pa}$ and $T = 273$ K. From $pV = NT$ we find that $n = p/T = 1/(33.5\text{Å})^3$ so that average distance between the air molecules is $n^{-1/3} = 33.5\text{Å} \gg$ radius of the molecule; here we may take the radius of the N_2 molecule $R = 1.9$ Å. The non-relativistic molecules obey the Maxwell distribution

$$f_0(\bar{v}) = n_0(\frac{m}{2\pi T})^{3/2} e^{-\frac{m}{2T}\bar{v}^2} \Rightarrow \langle v \rangle = \sqrt{\frac{8T}{\pi m}} = 453\mathrm{m/s}\ .$$

The mean free path can be estimated as $\lambda = 1/(n\sigma\sqrt{2}) = 1/(4\pi\sqrt{2}nr^2) = (33.5\text{Å})^3/(17.8 \cdot (1.9\text{Å})^2) = 586\text{Å}$, where the collision cross section was estimated by $\sigma \approx 4\pi R^2$. The collision frequency is then $\tau_c = \lambda/\langle v \rangle = 1.3 \cdot 10^{-10}\mathrm{s}$. A Nitrogen molecule thus collides, on the average, ten billion times in one second. Air can be described as continuous medium at scales $\delta t \gg 10^{-10}\mathrm{s}$ and $\delta x \gg 34\mathring{A}$.

In summary, for air $R : n^{-1/3} : \lambda = 1.9 : 33.5 : 586 \approx 1 : 17 : 17^2$; air at normal room temperature and density is a dilute, nearly ideal gas. However, what is of interest are not so much the static properties but rather the dynamical behaviour of air or fluids in general. In practise this means the fluid flow (e.g. the velocity field) or the propagation of perturbations (e.g. sound waves).

Flow is important! Consider an air molecule in front of a house, and suppose the street is 10 meters away. How long does it take for the molecule to find itself on the street? We may assume that the molecule travels with the velocity $v = \langle v \rangle$ and that in a collision its speed remains always the same although the direction to which it is travelling changes randomly (i.e. collisions are gaussian). After N collisions the mean distance traversed along any of the 3 dimensions is $\langle x \rangle = \sum_{i=1}^N x_i$, where $x_i \equiv L_0 = v\tau_c$ for all i. At each step positive and negative directions are as probable so that $\langle x_i \rangle = 0$ but $\langle x_i^2 \rangle = L_0^2$. Different steps are totally independent so that $\langle x_i x_j \rangle = \langle x_i \rangle \langle x_j \rangle = 0$ if $i \neq j$ The square of the total distance covered after N collisions is

$$\langle x^2 \rangle = \sum_{i=1}^N \sum_{j=1}^N \underbrace{\langle x_i x_j \rangle}_{L_0^2 \delta_{ij}} = L_0^2 N = (d\tau_c)^2 t/\tau_c = v^2 \tau_c t \equiv Dt.$$

so that

$$d \equiv \sqrt{\langle x^2 \rangle} = \sqrt{Dt}.$$

The time elapsed is $t = N\tau_c = d^2/(v^2\tau_c)$. Plugging in the appropriate numbers we verify that diffusion is a very slow process: $t(d = 10\text{ m}) \approx 1$ month. Flows, i.e. winds, are clearly of utmost importance. Here we have also defined a diffusion constant D and derived an expression for it. With the above numbers for air we have $d = 5\mathrm{mm}\sqrt{t/\mathrm{s}}$.

Similar considerations apply also to relativistic systems. An example would be the radiation dominated very early universe. Then $n \sim T^3$, $v = c = 1$ and $\sigma \approx \alpha^2/T^2$, where α is the appropriate (gauge) coupling strength squared, and the $1/T^2$-dependence of the cross section follows from dimensional considerations: $[\sigma] = \mathrm{cm}^2 = 1/\mathrm{energy}^2$ and in the ultrarelatvistic case the only energy scale is T. Thus the collision rate $\lambda = 1/(n\sigma v) \sim 1/(\alpha^2 T)$. The size of the system is now the Hubble distance $\sim M_{\mathrm{Planck}}/T^2$ and thus equilibrium can be achieved if $T \ll \alpha^2 M_{\mathrm{Planck}}$. This means that right after Big Bang, if the universe did not emerge in a thermal state, it did not reach thermal equilibrium until the Hubble rate had decreased sufficiently.

5.2 The basic equations of hydrodynamics

The local thermodynamical behavior of the fluid (= gas or liquid) is characterised by continuous fields such as the number density $n(\mathbf{x},t)$, temperature $T(\mathbf{x},t)$, mass density $\rho(\mathbf{x},t) = mn(\mathbf{x},t)$ and pressure $p(\mathbf{x},t)$. The hydrodynamic equations relate these to the velocity fields $\mathbf{v}(\mathbf{x},t)$, $\mathbf{j}(\mathbf{x},t) = \rho\mathbf{v}$. In terms of the microscopic theory, the fields are averages: they are moments of the phase space distribution function $f(\mathbf{x},\mathbf{v},t)$ of the (pointlike) particles that constitute the fluid:

$$n(\mathbf{x},t) = \int d^3v f(\mathbf{x},\mathbf{v},t), \qquad N(t) = \int d^3x n(\mathbf{x},t), \quad \mathbf{u}(\mathbf{x},t)\cdot n(\mathbf{x},t) = \int d^3v \mathbf{v} f(\mathbf{x},\mathbf{v},t).$$

The behavior of f is determined by kinetic theory, which will be discussed in Section 5.8. The averaged fields obey the hydrodynamic equations, which we first write down for the non-relativistic case.

- **Conservation of particle number or mass density**

Requiring the conservation of the mass density ρ we arrive at the continuity equation:

$$\frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x^k}\frac{\partial x^k}{\partial t}\rho = \frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\mathbf{v}) = 0 \tag{5.1}$$

which expresses the conservation of particle number. Relativistically, this is the net particle number, but non-relativistically there are no antiparticles in thermal equilibrium.

- **Conservation of momentum density**

By virtue of the continuity equation, the nonrelativistic force density can be written as

$$\mathbf{f} \equiv \frac{d\rho\mathbf{v}}{dt} = \rho\frac{d\mathbf{v}}{dt} = \rho\left(\frac{\partial \mathbf{v}}{\partial t} + \frac{\partial x^k}{\partial t}\frac{\partial}{\partial x^k}\mathbf{v}\right) . \tag{5.2}$$

On the other hand, for a time independent force $\mathbf{f} = -\nabla p$. Thus we arrive at the Euler equation:

$$\rho\left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v}\right) = -\nabla p + \mathbf{f}_{\text{ext}} , \tag{5.3}$$

where $\mathbf{f}_{\text{ext}}$ contains both internal forces such as viscosity, as well as external ones, such as gravity.

The Euler equation is simply the analogue of the newtonian force equation $\mathbf{F} = m\dot{\mathbf{x}} = \dot{\mathbf{p}}$ for fluids. On the left-hand-side one has $n\cdot m\times$ the convective time derivative of $\mathbf{v}$, i.e. the change of the velocity field when one follows the fluid flow, $\Delta\mathbf{x} = \mathbf{v}\Delta t$:

$$\mathbf{v}(\mathbf{x}+\Delta\mathbf{x}, t+\Delta t) - \mathbf{v}(\mathbf{x},t) = \Delta t\frac{\partial \mathbf{v}}{\partial t} + \Delta\mathbf{x}\cdot\nabla\mathbf{v} = \Delta t(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v}).$$

On the right-hand-side one has various forces causing the flow, starting from the pressure gradient. If only this is included, one has the Euler equation and the flow is adiabatic, entropy conserving, $\Delta S = 0$. For a viscous dissipative $\Delta S > 0$ one obtains the Navier-Stokes flow with

$$\mathbf{f}_{\text{viscosity}} = \eta \nabla^2 \mathbf{v} + (\zeta + \frac{1}{3}\eta)\nabla(\nabla \cdot \mathbf{v}),$$

with the proportionality constants that are called bulk and shear viscosities. Their role is to cause flow when, say, $v_x(y)$ depends on y, see Fig.5.2. We will return to viscosity and Navier-Stokes equation in Section 5.5

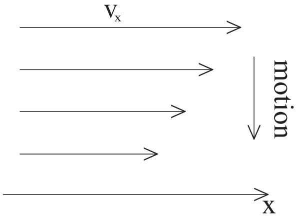

Figure 5.1: Dependence of v_x on y causes dissipative flow in y direction.

From the previous two equations and local thermodynamics, one further derives (LL, Fluids, §6)

- **Conservation equation for energy density**:

$$\frac{\partial}{\partial t}(\frac{1}{2}mnv^2 + U) + \nabla \cdot [\mathbf{v}(\frac{1}{2}mnv^2 + (U+p)) + \text{dissipation}] = 0 \qquad (5.4)$$

where $U = E/V = Ts - p$ is the internal energy density. Note the non-trivial structure of this equation. The energy density is obviously $(1/2)mnv^2 + U$. However, the corresponding current is not simply density $\times \mathbf{v}$ but one must also add the pressure to the energy density, the relevant potential is the enthalpy $E + pV$. Physically, when the system expands, it does $-pdV$ work. Energy, of course, is always conserved, but not the comoving energy density.

- **Entropy conservation**

Although energy density in the comoving volume is not conserved, entropy is. From previous equations and thermodynamic relations it follows that either

$$\frac{\partial s}{\partial t} + \nabla \cdot (s\mathbf{v}) = 0, \quad s = \frac{S}{V} \equiv \sigma n \qquad (5.5)$$

or

$$\frac{\partial \sigma}{\partial t} + \mathbf{v} \cdot \nabla \sigma = 0, \quad \sigma = \frac{S}{N} \equiv \frac{s}{n}. \qquad (5.6)$$

That both forms are equivalent, follows from the continuity equation for $\rho = mn$.

5.3 Relativistic hydrodynamics

Hydrodynamical equations can be written more symmetrically in the relativistic notation, where the starting point is the energy-momentum tensor, which for ideal fluids reads as

$$T^{\mu\nu} = (\epsilon + p)u^\mu u^\nu - p g^{\mu\nu} \tag{5.7}$$

while the current density is

$$j^\mu = n u^\mu \ . \tag{5.8}$$

Here ϵ is the relativistic energy density and $u^\mu = dx^\mu/d\tau = (dt/d\tau, d\mathbf{x}/d\tau) = (\gamma, \gamma\mathbf{v})$ is the four-velocity with $u^\mu u_\mu = \gamma^2 - \gamma^2 v^2 = 1$ (the proper time differential $d\tau = \sqrt{dt^2 - (d\mathbf{x})^2} = dt\sqrt{1-\mathbf{v}^2} = dt/\gamma$). In *comoving coordinates* which are definied by the rest frame of the flow $\mathbf{v} = 0$, the four-velocity $u^\mu = (1, 0)$.

In flat space with $g^{\mu\nu} = \mathrm{diag}(1, -1, -1, -1) \equiv \eta^{\mu\nu}$ we have then

$$T^{\mu\nu} = \begin{pmatrix} \epsilon & 0 & 0 & 0 \\ 0 & p & 0 & 0 \\ 0 & 0 & p & 0 \\ 0 & 0 & 0 & p \end{pmatrix} \tag{5.9}$$

and in any frame, when $\mathbf{v} \neq 0$, in block matrix notation,

$$T^{\mu\nu} = \begin{pmatrix} \gamma^2(\epsilon + p v^2) & \gamma^2(\epsilon + p)v^i \\ \gamma^2(\epsilon + p)v^i & (\epsilon + p)\gamma^2 v^i v^j + p\delta_{ij}. \end{pmatrix} \tag{5.10}$$

An interesting special case is the vacuum energy for which $\epsilon = -p \equiv \epsilon_{\rm vac}$ so that $T_{\mu\nu} = \epsilon_{\rm vac} g_{\mu\nu}$. Compare also Eq. (5.7) with energy momentum tensor of a collection of point particles at $\mathbf{x} = \mathbf{x}_i(t)$ for which

$$T^{\mu\nu} = \sum_i \frac{p_i^\mu p_i^\nu}{E_i} \delta^3(\mathbf{x} - \mathbf{x}_i(t)) = \sum_i \int d\tau \frac{p_i^\mu p_i^\nu}{m} \delta^4(x - x_i(\tau)). \tag{5.11}$$

The hydrodynamical equations (without dissipation) simply arise from the conservation of the energy-momentum tensor and of the particle number current:

$$\partial_\mu T^{\mu\nu} = 0,\ \nu = 0,1,2,3 \qquad \partial_\mu j^\mu = 0. \tag{5.12}$$

Note that when defining conservation one must take into account the change of the volume element with flow. In other words, what is conserved is

$$N(t) = \int_{V(t)} d^3x j^0(t, \mathbf{x})$$

in the comoving frame, defined by $\delta V = \mathbf{v}\delta t \cdot d\mathbf{A}$:

$$\begin{aligned} N(t + \delta t) &= \int_{V+\delta V} d^3x j^0(t + \delta t, \mathbf{x}) = N(t) + \int d^3x \frac{\partial j^0}{\partial t}\delta t + \int d\mathbf{A} \cdot \mathbf{v}\delta t j^0 = \\ &= N(t) + \int d^3x \left[\frac{\partial j^0}{\partial t} + \nabla \cdot (\mathbf{v}J^0)\right]\delta t = N(t) \end{aligned}$$

A particularly important point now is that entropy conservation again follows directly from the equations of motion (5.12). General thermodynamic relations are always valid so that

$$s = \frac{S}{V} = \frac{\partial p}{\partial T}, \quad n = \frac{N}{V} = \frac{\partial p}{\partial \mu}, \quad \epsilon(T,\mu) = Ts(T,\mu) - p(T,\mu) + \mu n(T,\mu),$$

where $T = T(t,\mathbf{x}), \quad \mu = \mu(t,\mathbf{x}), \quad \mathbf{v} = \mathbf{v}(t,\mathbf{x})$ are fields depending on $x^\mu = (t\mathbf{x})$. Using the definition (5.7) of $T^{\mu\nu}$ one finds that the projection of its conservation along u_ν can be written in the form

$$u_\nu \partial_\mu T^{\mu\nu} = T\partial_\nu(su^\nu) + \mu\partial_\nu nu^\nu. \tag{5.13}$$

Thus the conservation of $T^{\mu\nu}$ and j^μ also implies that

$$\partial_\mu s^\mu = 0, \qquad s^\mu = su^\mu \tag{5.14}$$

and entropy is conserved. With viscosities and thermal conductivity included, $\partial_\mu s^\mu > 0$. If one normalises to the net particle number N instead of V by defining $\sigma \equiv S/N$ then

$$\partial_\mu s^\mu = nu^\mu \partial_\mu \sigma + \sigma \partial_\mu nu^\mu = nu^\mu \partial_\mu \sigma = 0 \tag{5.15}$$

due to current coservation (5.12). Non-relativistically this was written in (5.5) and (5.6)

It is illuminating to study the non-relativistic limit of the relativistic equations (LL, Fluids, p.500). The subtle point here is that the NR equations are for a fixed volume element, while the relativistic equations refer to the proper frame. Thus one cannot only replace $\epsilon \to mn + \epsilon$ but instead $\epsilon \to mn/\gamma + \epsilon = \rho(1 - \frac{1}{2}v^2) + \epsilon$. Then, including c, the energy-momentum tensor becomes

$$T^{\mu\nu} = \begin{pmatrix} \rho c^2 + \epsilon + \frac{1}{2}\rho v^2 & \rho c v^i + (\epsilon + p + \frac{1}{2}\rho v^2) v^i/c \\ \text{Symmetric} & p\delta_{ij} + \rho v^i v^j \end{pmatrix} \tag{5.16}$$

where $v \ll c$ and ϵ is without the rest energy. Then $\partial_\mu T^{\mu 0} = \partial_0 T^{00} + \partial_i T^{i0} = 0$ yields

$$\begin{aligned} &\partial_t \rho + \partial_i(\rho v^i) = 0, && \text{to order } c \\ &\partial_t(\epsilon + \frac{1}{2}\rho v^2) + \partial_i[(\epsilon + p + \frac{1}{2}\rho v^2)v^i)] = 0, && \text{to order } 1/c \end{aligned}$$

while $\partial_\mu T^{\mu i} = \partial_0 T^{0i} + \partial_j T^{ji} = 0$ gives

$$\partial_t(\rho v^i) + \partial_j[(\rho v^i v^j + p\delta_{ij})] = 0, \quad \text{to order } 1 \tag{5.17}$$

Thus the 0-component gives both the particle number conservation and the energy density conservation equation, while the i-component gives the Euler equation.

5.4 Two practical applications

- **Sound**

Let us linearize around an obvious constant solution:

$$\epsilon = \epsilon_0 + \epsilon_1,\ p = p_0 + p_1,\ n = n_0 + n_1, \mathbf{v} = \mathbf{0} + \mathbf{v} \tag{5.18}$$

Then $u^\mu = (1,\mathbf{0}) + (0,\mathbf{v})$ and to order 1

$$T^{00} = \epsilon_0 + \epsilon_1,\ T^{0i} = (\epsilon_0 + p_0)v^i,\ T^{ij} = (p_0 + p_1)\delta_{ij},\ J^0 = n_0 + n_1,\ J^i = n_0 v^i. \tag{5.19}$$

As the problem is linear, one may go to Fourier space with $\partial_0 \to -i\omega$, $\partial_i \to ik^i$. The conservation equations then become

$$\begin{aligned}
&-\omega\epsilon_1 + (\epsilon_0 + p_0)\mathbf{k}\cdot\mathbf{v} = 0,\\
&-\omega(\epsilon_0 + p_0)\mathbf{v} + p_1\mathbf{k} = 0,\\
&-\omega n_1 + n_0\mathbf{k}\cdot\mathbf{v} = 0.
\end{aligned}$$

From the 2nd equation

$$\mathbf{v} = \frac{p_1}{\epsilon_0 + p_0}\frac{\mathbf{k}}{\omega} \to \mathbf{v}\,\text{is longitudinal} \tag{5.20}$$

and inserting this to the first one

$$\omega^2 = \frac{p_1}{\epsilon_1}\mathbf{k}^2. \tag{5.21}$$

In coordinate space this corresponds to an undamped wave moving with velocity

$$v_\text{sound} = \sqrt{\frac{p_1}{\epsilon_1}} = \sqrt{\left.\frac{dp}{d\epsilon}\right|_S}. \tag{5.22}$$

Here one has made the very important additional statement that local thermal equilibrium is always maintained so that small deviations ϵ_1, p_1 from constancy always go together adiabatically, conserving entropy. For example, when pressure increases, collisions are frequent enough to make also the internal energy to change as required by global thermodynamics. From the third equation, finally,

$$n_1 = \frac{n_0}{\epsilon_0 + p_0}\epsilon_1; \tag{5.23}$$

the net number oscillates together with energy density (though I do not seem to get $\partial n/\partial\epsilon = n/(\epsilon + p)$ at constant S, get $1/\mu = n/(\epsilon + p - Ts)$ instead).

- **Winds**

This is a very nice and truly practical application of hydrodynamic equations, showing also how one in physics has to proceed through different levels of approximation. One also has to mess up with rotating coordinate systems; anyone familiar with this can proceed directly to Eqs. (5.29)-(5.33).

(1) The rotation of the earth is essential:

$$\omega = \frac{\Delta p}{\Delta t} = \frac{v}{R} = \frac{2\pi}{P} = \frac{2\pi}{24\cdot 3600(1 - 1/365)} = 7.3\cdot 10^{-5}\frac{1}{s}$$

(2) In central motion:

$$v = \omega R\cos\varphi = 463\text{m/s}\cos\varphi, \quad a = \omega^2 R\cos\varphi = 0,0337\text{m/s}^2\cos\varphi \tag{5.24}$$

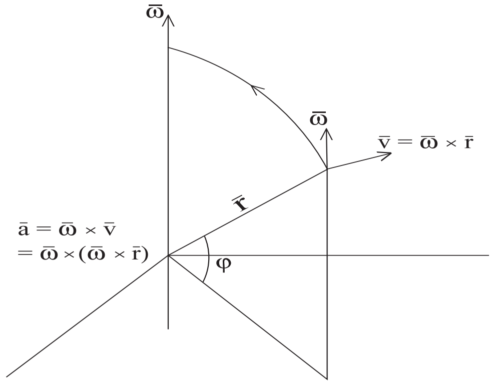

Figure 5.2: Coordinate system

(3) Coordinates fixed relative to space vs. coordinates fixed relative to the body:

$$\frac{d}{dt}|_{\text{space}} = \frac{d}{dt}|_{\text{body}} + \omega \times \quad | \,\mathbf{r}, \tag{5.25}$$

$$\Rightarrow \mathbf{v}_{\text{space}} = \mathbf{v}_{\text{body}} + \omega \times \mathbf{r} \tag{5.26}$$

$$\Rightarrow \frac{d}{dt}_{\text{space}} \mathbf{v}_{\text{space}} = \mathbf{a}_{\text{space}} = \mathbf{a}_{\text{body}} + \omega \times \mathbf{v}_{\text{body}} + \omega \times \frac{d\mathbf{r}}{dt}|_{\text{body}} + \omega \times (\omega \times \mathbf{r}) = \frac{1}{m}\mathbf{F} \tag{5.27}$$

($F = ma$ is valid in an inertial system!)

$$\Rightarrow \mathbf{a}_{\text{body}} = \frac{1}{m}\mathbf{F} - 2\omega \times \mathbf{v}_{\text{body}} - \omega \times (\omega \times \mathbf{r}) \tag{5.28}$$

(4) The coordinates on the surface of the earth

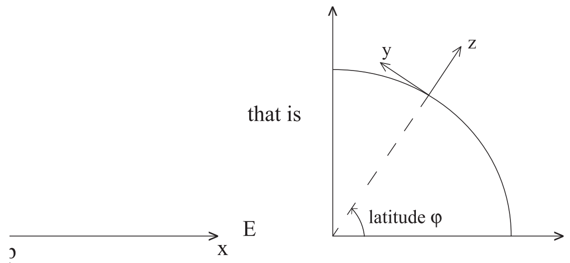

Figure 5.3: The coordinates on the surface of the earth

Then $\omega = \omega(\cos\varphi \mathbf{j} + \sin\varphi \mathbf{k}) = \omega(0, \cos\varphi, \sin\varphi)$

After this long preparation, the hydrodynamic equations can be written in the form:

$$\frac{d\mathbf{v}}{dt} = -\frac{1}{\rho}\nabla p + \mathbf{g} - \omega \times (\omega \times \mathbf{r}) - 2\omega \times \mathbf{v} \tag{5.29}$$

where one firstly can approximate $\mathbf{g} - \omega \times (\omega \times \mathbf{r}) \approx (0, 0, -g)$ and where the Coriolis force is, neglecting v_z:

$$-2\omega \times \mathbf{v} = -2\omega \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ 0 & \cos\varphi & \sin\varphi \\ v_x & v_y & v_z \end{vmatrix} = 2\omega(\sin\varphi\, v_y, -\sin\varphi\, v_x, \cos\varphi\, v_x). \tag{5.30}$$

Writing all the components separately one gets

$$\begin{aligned} \frac{dv_x}{dt}\ (10^{-4}) &= -\frac{1}{\rho}\frac{\partial p}{\partial x}\ (10^{-3}) + 2\omega\sin\varphi v_y\ (10^{-3}) && (5.31)\\ \frac{dv_y}{dt}\ (10^{-4}) &= -\frac{1}{\rho}\frac{\partial p}{\partial y}\ (10^{-3}) - 2\omega\sin\varphi v_x\ (10^{-3}) && (5.32)\\ 0 &= -\frac{1}{\rho}\frac{\partial p}{\partial z}\ (10) - g\ (10) + 2\omega\cos\varphi v_x\ (10^{-3}) && (5.33) \end{aligned}$$

The order of magnitude of the terms (in SI units) is written directly after each term, based on the estimates $v_x, v_y \sim 10$ m/s, $v_z \sim 10^{-2}$ m/s, $2\omega \sim 10^{-4}$ 1/s, $1/\Delta t \sim 1/\text{day} \sim 1/10^5$ 1/s.

The largest terms, of the order 10, give the equation

$$\frac{1}{\rho}\frac{\partial p}{\partial z} = -g. \tag{5.34}$$

If $\rho = m \cdot p/T$ then $dp/p = -gm/T \approx -g/v_s^2$ and one can solve this as

$$p(z) = p(0)e^{-\frac{g}{v_s^2}\cdot z} \tag{5.35}$$

This, of course, just gives the height of the atmosphere $\langle z\rangle \sim v_s^2/g \sim 10^4$ m. For a neutron star with the surface $T = 5$ keV and $v_s \sim \sqrt{T/m_p} \sim 6 \cdot 10^5$m/s and surface gravity $10^{11}\times$ that of earth one would have an atmosphere of height 10 cm.

The next-to-leading order terms of order 10^{-3} imply for the first that $dv_x/dt \approx dv_y/dt \approx 0$ (nearly steady state state) so that

$$\mathbf{v} = \frac{1}{2\omega\sin\varphi\cdot\rho}\left(-\frac{\partial p}{\partial y}, \frac{\partial p}{\partial x}, 0\right) = \frac{1}{2\omega\sin\varphi\cdot\rho}\,\mathbf{k}\times\nabla p \tag{5.36}$$

This is the "geostrophic equilibrium" in which the pressure force $-\nabla p$ and the Coriolis force balance each other. It cannot be reached near the equator, where $\varphi \sim 0$. Note that the wind velocity is perpendicular to the gradient of pressure, wind does not blow in the direction of decreasing pressure.

The next-to-next-to leading order terms include also $dv_x/dt, dv_y/dt$ of order 10^{-4}. Assuming 2d circular symmetry in the x, y plane and putting time dependence in $d\theta/dt = v/r$ the components are

$$\begin{cases} v_x = v(r)(-\sin\theta) \\ v_y = v(r)(\cos\theta) \end{cases} \quad \begin{cases} \frac{dv_x}{dt} = v(r)(-\sin\theta)\frac{v}{r} & \frac{\partial p(r)}{\partial x} = p'(r)\cos\theta \\ \frac{dv_y}{dt} = v(r)(-\sin\theta)\frac{v}{r} & \frac{\partial p(r)}{\partial y} = p'(r)\sin\theta \end{cases}$$

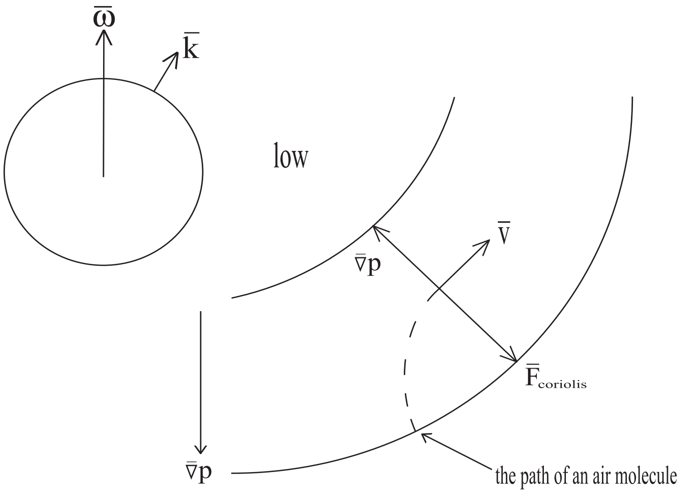

Figure 5.4: The pressure and the Coriolis force stabilize each other!

and the equations (5.31) and (5.32) become

$$-\frac{v^2(r)}{r} = -\frac{1}{\rho}p'(r) + 2\omega\sin\varphi \cdot v(r). \tag{5.37}$$

Going to the northerm hemisphere with $f \equiv 2\omega\sin\varphi > 0$ we can write

$$fv(r) = \frac{1}{\rho}p'(r) - \frac{v^2(r)}{r}. \tag{5.38}$$

For a low atmospheric pressure, a cyclone, $p'(r) > 0$, $0 < v(r) < v_{\text{gs}}(r) = p'(r)/(f\rho)$ and the rotation is anticlockwise, $d\theta/dt = v/r > 0$.

For high atmospheric pressure, anticyclone: $p'(r) < 0$, $v_{\text{gs}} < 0$ and the rotation is clockwise. However, now (5.38) implies that $|v(r)| > |v_{\text{gs}}(r)|$, but actually v cannot grow so winds are light around an anticyclone.

As a final application of (5.37), go to the equator, where $2\omega\sin\varphi = 0$ and

$$\frac{v^2(r)}{r} = \frac{1}{\rho}\frac{dp}{dr}.$$

Approximate here $r \approx \Delta r \sim 100$ km, $\Delta p \sim 30\,\text{mbar} \sim 0.03 \cdot 10^5$ Pa and ρ =1 kg/m^3. Then

$$v(r) = \sqrt{\frac{r}{\rho}\frac{\Delta p}{\Delta r}} \approx \sqrt{\frac{\Delta p}{\rho}} \approx 50\text{m/s}. \tag{5.39}$$

This is a tropical cyclone or hurricane. I still would love to understand why it is that the surface temperature of the ocean has to be > 27 C before a hurricane can be formed (Erik Palmen, 1948).

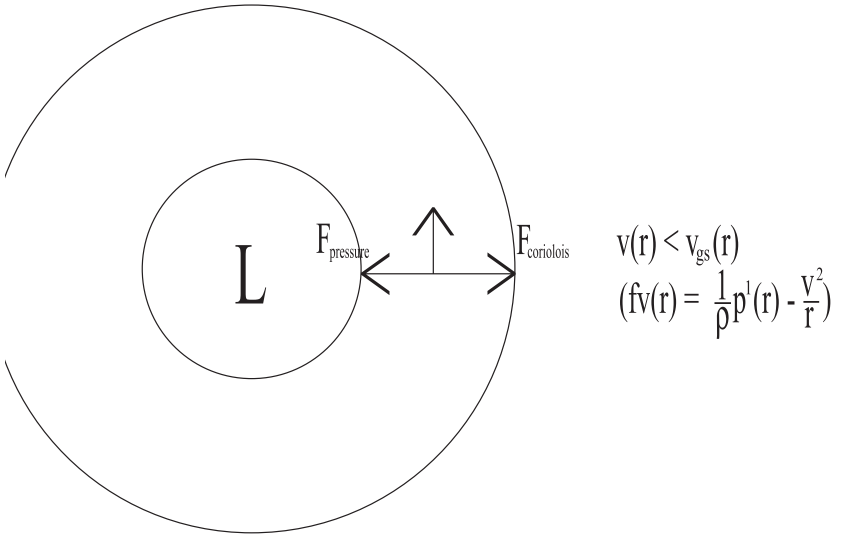

Figure 5.5: A cyclone

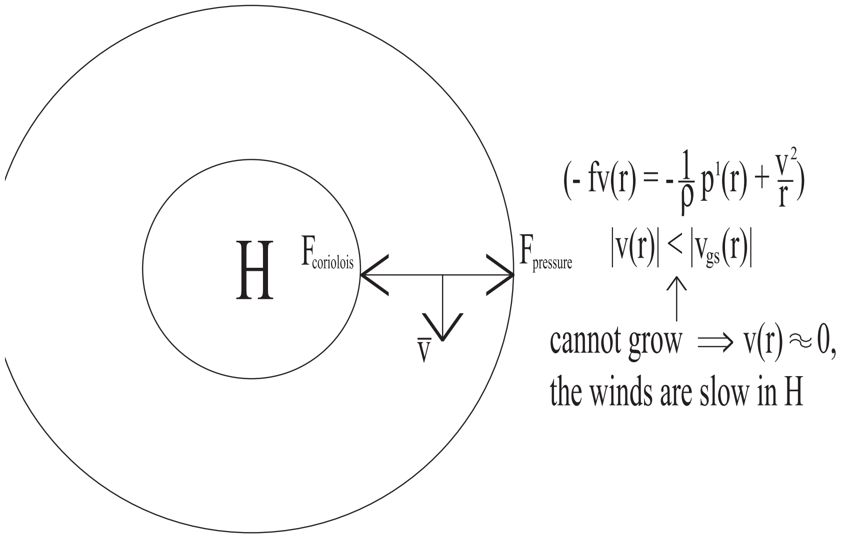

Figure 5.6: An anticyclone

5.5 Dissipation and the Navier-Stokes equation

The Euler equation conserves entropy (5.5), but in reality the entropy always grows. This can be taken into account by adding to the Euler equation dissipative terms, or viscosity, which physically arise because the collisions between fluid particles scatter them out of the flow. Because of the collisions, the fluid is no longer ideal. The Euler equation with viscosity terms is called the Navier-Stokes equation and is conventionally written as

$$\rho(\frac{\partial v}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v}) = -\nabla p + \eta \nabla^2 \mathbf{v} + (\zeta + \frac{1}{3}\eta)\nabla(\nabla \cdot \mathbf{v}), \tag{5.40}$$

where η is the shear and ζ the bulk viscosity. This is basically a phenomenological but an extremely well verified equation. There is no fundamental derivation of this, but one may use physically motivated arguments to arrive at Eq. (5.40). Writing

$$\Pi_{ik} = p\delta_{ik} + \rho v_i v_k + \Delta\Pi_{ik} \tag{5.41}$$

we may ask, what is the general form of the non-ideal stress energy $\Delta\Pi_{ik}$?

- If $\mathbf{v} = 0$, there is no flow and hence no dissipation so that $\Delta\Pi_{ik}(\mathbf{v} = 0) = 0$.
- It then makes sense to expand about $\mathbf{v} = 0$ so that when the velocity gradients are small, $\Delta\Pi_{ik} \propto \partial v_i/\partial x_k + \mathcal{O}(v^2)$.
- Uniform rotation has no friction. Thus, if the velocity field is of the form $\mathbf{v} = \omega \times \mathbf{r}$, we find
  $$\frac{\partial v_i}{\partial x_k} = \frac{\partial}{\partial x_k}\epsilon_{ijl}\omega^j x^l = -\epsilon_{kji}\omega^j \equiv -\frac{\partial v_k}{\partial x_i}$$
  where ϵ_{ijl} is the completely antisymmetric unit tensor with $\epsilon_{123} = +1$. Note also that if $i = k$, then $\partial v_i/\partial x_k = 0$. Thus we conclude that
  $$\Delta\Pi_{ik} = \alpha\left(\frac{\partial v_i}{\partial x_k} + \frac{\partial v_k}{\partial x_i}\right) + \beta\delta_{ik}\frac{\partial v_i}{\partial x_i}$$

where α and β are independent parameters (transport coefficients). It is however useful to rearrange the terms into a traceless and a non-traceless part, rename the independent parameters and write

$$-\Delta\Pi_{ik} = \eta(\partial_k v_i + \partial_i v_k - \frac{2}{3}\delta_{ik}\nabla\cdot\mathbf{v}) + \zeta\delta_{ik}\nabla\cdot\mathbf{v}. \tag{5.42}$$

Now $\mathrm{Tr}\Delta\Pi_{ik} = -\eta(2\partial v_i/\partial x_i - 2/3 \times 3\partial v_i/\partial x_i) + 3\zeta\partial v_i/\partial x_i = 3\zeta\partial v_i/\partial x_i$. Like the Euler equation, the Navier-Stokes equation is obtained from the conservation of $\mathbf{\Pi}$ in Eq. (5.41) so that we arrive at

$$-\nabla\cdot\Delta\mathbf{\Pi} = \eta\nabla^2\mathbf{v} + (\zeta + \frac{1}{3}\eta)\nabla(\nabla\cdot\mathbf{v}) \equiv \mathbf{f}_{\text{viscosity}}\ . \tag{5.43}$$

Note that the second term on the RHS is zero if the fluid is incompressible: by virtue of the continuity equation (5.1) $\nabla\cdot\mathbf{v} = 0$ if $\rho = \text{const}$.

Thermal conductivity. Thermal flow is also characterized by a trasport coefficient, the thermal conductivity κ, defined by

$$\mathbf{j}_q = -\kappa\nabla T\ .$$

Thermal flow affects the $0i$ components of the energy momentum tensor. Defining the densities $s = S/V$ and $\sigma = S/N$ one finds that thermal flow increases entropy:

$$\begin{aligned} T\left(\frac{\partial s}{\partial t} + \nabla\cdot(s\mathbf{v})\right) &= Tn\left(\frac{\partial\sigma}{\partial t} + \mathbf{v}\cdot\nabla\sigma\right) \\ &= \frac{1}{2}\eta(\partial_k v_i + \partial_i v_k - \frac{2}{3}\delta_{ik}\nabla\cdot\mathbf{v})^2 + \zeta(\nabla\cdot\mathbf{v})^2 + \nabla\cdot(\kappa\nabla T). \end{aligned} \tag{5.44}$$

Also the T-term, together with the T in the LHS gives a positive contribution to entropy production (LL, Fluids, §49).

The question of what to add to the non-dissipative terms is actually far from trivial. The standard non-dissipative terms, like those in Eq. (5.42) work extremely well in most practical instances, but lead to conceptual difficulties. For example, the diffusion equation is parabolic and the signal propagates with infinite velocity (if you start with $\delta(x)$ at $t = 0$, the solution extends to any x at $t > 0$). This can be corrected by introducing second-order corrections to the entropy current and hyperbolic dissipative hydrodynamic equations can be written down. A full account with references can be found in Azwinndini Muronga, arxiv.org/ps/nucl-th/0309055.

Historically, η is measured by the friction force on a spherical object moving in a fluid:

$$\mathbf{F}_{\text{friction}} = -6\pi R \cdot \eta \cdot \mathbf{v}$$

from where one can read the dimensions of η as kg/(ms). Some numerical values for η and the kinematic viscosity η/ρ are given in the Table.

	$\eta, \frac{Ns}{m^2}$	$\nu = \frac{\eta}{\rho}, \frac{m^2}{s}$
Water 20°C	$1.00 \cdot 10^{-3}$	$1.00 \cdot 10^{-6}$
Air 20°C	$1.8 \cdot 10^{-5}$	$1.5 \cdot 10^{-8}$
Hg 20°C	$1.56 \cdot 10^{-3}$	$1.2 \cdot 10^{-7}$

Table 5.2:

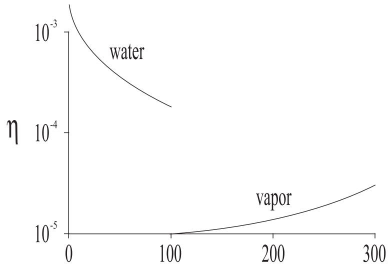

Figure 5.7: η for water

One of the most interesting results coming from string theory (some would suggest the only result, others like extra dimensions and supersymmetry also come from other arguments) is that viscosity for any substance should satisfy

$$\frac{\eta}{s} \geq \frac{\hbar}{4\pi}, \tag{5.45}$$

where $s = S/V$ is the entropy density. The equality sign applies to all 4d field theories obtainable from string theory in a certain well defined way. For all normal matters the inequality is usually violated by a wide margin. Note the factor $\hbar$; there is no c in this relation.

Note also that mathematically it has not yet been proven that physically reasonable solutions exist for the Navier-Stokes equation. Proving this is one of the Millenium problems, see http://www.claymath.org/millennium/Navier-Stokes_Equations/navierstokes.pdf

5.6 Turbulence and Reynolds number

It is of great theoretical and practical interest to consider the circumstances under which the viscosity terms in the Navier-Stokes equation (5.40) are important. To this end, to simplify the discussion, let us assume that the fluid is non-compressible with $\rho =$ const. so that $\nabla \cdot \mathbf{v} = 0$ and the dissipative part depends on η alone, which we assume to be a constant. Then we may define

$$\omega = \nabla \times \mathbf{v} \tag{5.46}$$

and operate with $\nabla\times$ on the Navier-Stokes equation[1]. We then find

$$\frac{\partial \omega}{\partial t} = -\nabla \times (\mathbf{v} \cdot \nabla)\mathbf{v} - \frac{1}{\rho} \underbrace{\nabla \times \nabla}_{\epsilon^{ijk}\partial_k \partial_l = 0} p + \frac{\eta}{\rho} \underbrace{\nabla \times \nabla \times \nabla^2 \mathbf{v}}_{\epsilon^{ijk}\partial_j (\nabla^2 v)_k = \nabla^2 (\nabla \times v)^i} \quad . \tag{5.47}$$

We further note that

$$\begin{aligned} \mathbf{v} \quad & \times(\nabla \times \mathbf{v}) = -(\mathbf{v} \cdot \nabla)\mathbf{v} + \frac{1}{2}\nabla \mathbf{v}^2 \\ \rightarrow \quad & -\nabla \times (\mathbf{v} \cdot \nabla)\mathbf{v} = \underbrace{\nabla \times \mathbf{v} \times (\nabla \times \mathbf{v})}_{=\nabla \times (\mathbf{v} \times \omega)} + \frac{1}{2} \underbrace{\nabla \times \nabla}_{=0} \mathbf{v}^2 \ . \end{aligned} \tag{5.48}$$

Thus we arrive at

$$\frac{\partial \omega}{\partial t} = \frac{\eta}{\rho} \nabla^2 \omega + \nabla \times (\mathbf{v} \times \omega) \tag{5.49}$$

where $\eta/\rho \equiv \nu$ is often called the kinematic viscosity.

Let us now defined the dimensionless variables $\tau = t/t_0$ and $u = v/v_0$, where t_0 is a typical time scale in the problem and $v_0 = L/t_0$ is a typical velocity with L is a typical length scale. With the dimensionless variables $\nabla \to \nabla' = L\nabla$ and $\omega \to \mathbf{\Omega} = L\omega/v_0$ and

$$\frac{\partial \mathbf{\Omega}}{\partial \tau} = \frac{1}{R} \nabla'^2 \mathbf{\Omega} + \nabla' \times (\mathbf{u} \times \mathbf{\Omega}) \ , \tag{5.50}$$

where

$$R = \frac{L v_0}{\nu} = \frac{\rho L v_0}{\eta} \tag{5.51}$$

is the *Reynolds number.*

Clearly, if $R \ll 1$, the evolution of $\mathbf{\Omega}$ is dominated by the diffusive term, which for a given Fourier mode k yields the equation $\dot{\mathbf{\Omega}} = -k^2 \mathbf{\Omega}/R$ so that $\Omega \to 0$ as $\tau \to \infty$. Thus for a small

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[1] This would also be the appropriate description for vorticity in the fluid

Reynolds number, viscosity damps the velocity field. If $R \gg 1$, viscosity is unimportant and the evolution of $\mathbf{\Omega}$ is dominated by the non-linear term in Eq. (5.50), which can then lead to fluid motion which is highly non-perturbative or turbulent. In other words, the flow develops an internal length scale $\delta \ll L$ and the magnitude of the viscosity term is rather $\eta/\rho \cdot v/\delta^2$ which equals the inertia term of $\delta = L/\sqrt{Re}$.

For an airplane with a wing length of 10 m, taking $\nu_{\mathrm{air}} \sim 0.15\ \mathrm{cm}^2/\mathrm{s}$ and typical velocity as $v_0 \approx 200$ m/s we find $R \sim 10 \cdot 100/10^{-5} \sim 10^8 \gg 1$; hence the motion of an airplane wing through air can be expected to generate turbulence (as it does). For a bug in water we take $L \approx 0.1$ cm, $\nu_{\mathrm{water}} = 0.01\ \mathrm{cm}^2/\mathrm{s}$ and $v_0 \approx 1$ cm/s to find $R \sim 10^{-3} \cdot 10^{-3}/10^{-3} = 10^{-3}$; hence water bugs live a pastoral and non-turbulent (but short) life at a small Reynolds number.

5.7 Magnetohydrodynamics

When hydrodynamics is supplemented by the Maxwell equatios, we obtain magnetohydrodynamics. The fluid elements are charge carriers and are therefore subject to the Lorentz-force $\mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B})$. Then there are two possibilities:

- **Collisionless plasma.** In this case, the electrons and the ions are separate. As a consequence, there are sources for electric fields and plasma oscillates. This case could be called plasmaphysics proper. **Will be discussed ????**
- **Collision dominate.** If collisions dominate such that the collision rates between the charged fluid elements (particles) are much faster than the rate of change of elecromagnetic fields, the charge densities effectively average out and there are no sources for electric fields. This case is magnetohydrodynamics proper (MHD for short).

Let us now focus on plasma dominated by collisions. Although there is no charge density, there nevertheless exists a current

$$\mathbf{j} = \sigma(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \ , \tag{5.52}$$

where σ is the conductivity. The Maxwell equations read

$$\begin{aligned} \nabla \times \mathbf{E} &= -\frac{\partial \mathbf{B}}{\partial t} \ , \\ \nabla \cdot \mathbf{B} &= 0 \ , \\ \nabla \times \mathbf{B} &= \mu_0 \mathbf{j} \ , \end{aligned} \tag{5.53}$$

where we have neglected the induced current $\partial\mathbf{E}/\partial t \ll \mathbf{j}$. Hitting the last of the Maxwell equations with $\nabla\times$ we obtain

$$\nabla \times (\nabla \times \mathbf{B}) = -\nabla^2 \mathbf{B} = \mu_0 \sigma(\nabla \times \mathbf{E} + \nabla \times (\mathbf{v} \times \mathbf{B})) \tag{5.54}$$

or

$$\frac{\partial \mathbf{B}}{\partial t} = \frac{1}{\mu_0 \sigma} \nabla^2 \mathbf{B} + \nabla \times (\mathbf{v} \times \mathbf{B}) \ , \tag{5.55}$$

which is the basic MHD equation. Note that Eq. (5.55) has the same form as the hydrodynamical description of non-compressible fluid (vorticity), Eq. (5.50). Therefore we may use Eq. (5.55) to define a magnetic Reynolds number R_M. Let us define the magnetic diffusivity $\eta_M \equiv (\mu_0\sigma)^{-1}$ and let $L_0 \sim \nabla^{-1}$ and v_0 be respectivley the typical length and velocity scales in the problem. Then, as before,

$$R_M = \frac{L_0 v_0}{\eta} \ . \tag{5.56}$$

Clearly, $R_M \ll 1$ corresponds to the limit of vanishing conductivity, $\sigma \to 0$. Conductivity vanishes if the charged particles in the flow scatter away; hence low conductivity means a large collision cross section or equivalently, a mean collision time $\tau_c \to 0$. Likewise, $R_M \gg 1$ implies high conductivity and a small collision cross section. These two case give rise to a qualitatively different magnetohydrodynamic behaviour of the plasma:

- **Low conductivity,** $R_M \ll 1$**.** If $\sigma \to 0$ in Eq. (5.55), we may write

  $$\frac{\partial \mathbf{B}}{\partial t} \approx \frac{1}{\mu_0\sigma}\nabla^2\mathbf{B} \tag{5.57}$$

  and choosing eg. $\mathbf{B} \uparrow\uparrow \hat{\mathbf{e}}_z$ we find at large t

  $$\mathbf{B} = \mathbf{B}_0 e^{-\frac{\mu_0\sigma z^2}{4t}} \ . \tag{5.58}$$

  Thus there is diffusion: the plasma cannot sustain B because of collisions. Note that the current dies out starting at small scales: defining the diffusion length r_D through $\mu_0\sigma r_D^2/4t \sim 1$ we find

  $$r_D \simeq 2\sqrt{\mu_0\sigma t} \ . \tag{5.59}$$

  At time t at length scales less than r_D there is no current and hence no magnetic field; the "microscopic" motion is random. However, at larger scales there still is bulk motion, and hence a current, and hence a magnetic field. When the ∇^2 - term dominates, $\mathbf{B}$ (and $\mathbf{\Omega}$ in Eq. (5.50)) spread diffusively, as depicted in Fig. **??**.

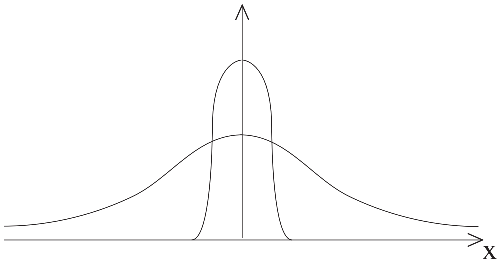


Figure 5.8: The ∇^2 - term, diffusive spreading

- **High conductivity,** $R_M \gg 1$**.** Now we approximate Eq. (5.55) by

  $$\frac{\partial \mathbf{B}}{\partial t} \approx \nabla \times (\mathbf{v} \times \mathbf{B}) \ , \tag{5.60}$$

which clearly admits the solution $\mathbf{B} \approx$ const., $\mathbf{B} \uparrow\uparrow \mathbf{v}$. Hence in this limit the magnetic field follows the motion of fluid; the magnetic field is said to be frozen in the plasma: $\frac{d}{dt}\oint_C \mathbf{v}\cdot d\mathbf{l} = \frac{d}{dt}\int \mathbf{B}\cdot d\mathbf{A} = 0$. This can lead to complicated entangled magnetic field lines as charge carriers move around in the plasma; this is an example of magnetic turbulence.

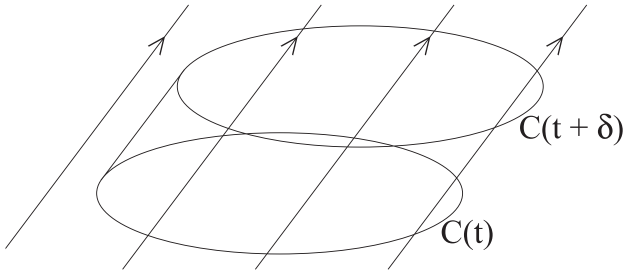


Figure 5.9: The curve C moves with the current!

Magnetic dynamo Because conductivity is high in many astrophysical situations, such as in the Sun and in galaxies, the magnetic field can be assumed to be highly entangled and to follow the velocity field lines. This has been used as a starting point to explain the magnetic fields of galaxies, which are typically of the order of 10^{-6} G with a coherence scale of about 1 kpc. In the magnetic dynamo model one assumes an initial small seed field, which is then enhanced exponentially by the differential rotation of the galaxy and by the coriolis drift of particles (and hence the magnetic field) from the galactic plane.

The diffusion equation for the temperature field is given by

$$\frac{\partial T}{\partial t} = k\nabla^2 T \tag{5.61}$$

Derivation: $\begin{matrix} T = \text{heat field} \\ \mathbf{j} = \text{heat current} \end{matrix} \quad \begin{cases} \dim T = \frac{J}{m^2} \\ \dim \mathbf{j} = \frac{J}{m^2 s} \end{cases} \quad \begin{cases} \mathbf{j} = -k\nabla T \\ \frac{\partial T}{\partial t} + \nabla\cdot\mathbf{j} = 0 \end{cases} \quad \Rightarrow \frac{\partial T}{\partial t} = k\nabla^2 T$

So $\begin{cases} \dim k = \frac{m^2}{s} \\ \dim \frac{1}{\mu_0\sigma} = \frac{c^2}{mkg}\cdot\frac{V}{A}m = \frac{m^2}{s} \end{cases} \qquad [\frac{1}{\mu_0\sigma} = \text{The magnetic diffusion constant}]$

With the initial condition $T(x, t \to 0) = T_0\delta(x)$, a heat pulse at $x = 0$, the solution is analogous to the case of magnetic diffusion with

$$T(x,t) = T_0\frac{1}{\sqrt{4\pi kt}}e^{-\frac{x^2}{4kt}}\ . \tag{5.62}$$

5.8 Kinetic theory

In hydrodynamics and in magnetohydrodynamics we assume continuous matter. The task of the kinetic theory is to explain both at the level of constituents. To this end one starts with the probability distribution $f(\mathbf{x}, \mathbf{p}, t)$ of a given particle species in the phase space volume element d^3xd^3p. Then the particle density is

$$n(\mathbf{x}, t) = \int d^3p f(\mathbf{x}, \mathbf{p}, t) \tag{5.63}$$

while the total particle number is $N(t) = \int d^3xn(\mathbf{x},t)$. The current density reads

$$\mathbf{u}(\mathbf{x},t)\cdot n(\mathbf{x},t) = \int d^3p\mathbf{v}f(\mathbf{x},\mathbf{p},t), \tag{5.64}$$

where $\mathbf{u}(\mathbf{x},t)$ is the velocity of the flow.

Example: MB statistics In the non-relativistic limit

$$f(\mathbf{x},\mathbf{v}) = n(\mathbf{x})(\frac{m}{2\pi T(\mathbf{x})})^{3/2}e^{-\frac{m}{2T(\mathbf{x})}(\mathbf{v}-\mathbf{u}(\mathbf{x})^2)}, \tag{5.65}$$

where $T, n, \mathbf{u}$ depend on $\mathbf{x}$. Relativistically, one would write

$$\begin{aligned} 1/n_f(p,x) &= \exp[u^\nu(x)p_\nu/T(x) - \mu(x)/T(x)] + 1, \\ 1/n_b(p,x) &= \exp[u^\nu(x)p_\nu/T(x)] - 1, \end{aligned} \tag{5.66}$$

where now all thermodynamic quantities depend on $x^\mu = (t,\mathbf{x})$ and the single quantity E is replaced by $p^\mu = (E,\mathbf{p})$. In the comoving frame, $u^\mu(x) = (1,\mathbf{0})$ the eqs. (5.66) reduce to the standard FD, BE distributions.

The phase space dynamics is dictated by the Liouville theorem, according to which, in the absence of collisions, $f =$ constant along its trajectory in phase space. Hence

$$\begin{aligned} 0 = \frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x^k}\frac{\partial x^k}{\partial t} + \frac{\partial f}{\partial p^k}\frac{\partial p^k}{\partial t} &= 0 \\ \to \frac{\partial f}{\partial t} + \nabla f\cdot\mathbf{v} + \nabla_p f\cdot\mathbf{F} &= 0\ , \end{aligned} \tag{5.67}$$

where $\mathbf{F}$ is the external force (e.g. the Lorentz force).

In the presence of collisions, the Liouville equation (5.67) is written formally as

$$\frac{\partial f}{\partial t} + \nabla f\cdot\mathbf{v} + \nabla_p f\cdot\mathbf{F} = \left.\frac{\partial f}{\partial t}\right|_{\text{coll}}\ , \tag{5.68}$$

where the RHS term is called the *collision integral* and the equation itself the *Boltzmann equation*. Note that this is a complicated non-linear equation even without collisions. For example, if f is the distribution of a charged particle, then the force term itself will depend on f via the Lorentz force: $\mathbf{F} = e(\mathbf{E} + \mathbf{v}\times\mathbf{B})$, where $\mathbf{E}$ and $\mathbf{B}$ depend on f.

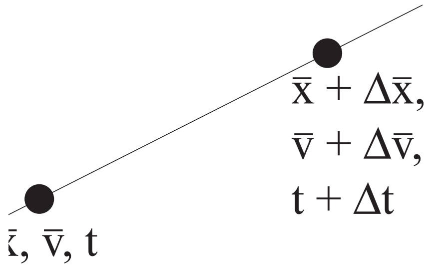


Figure 5.10: Moving with the flow means $\Delta\mathbf{x} = \mathbf{v}\Delta t$ and $\Delta\mathbf{v} = \mathbf{a}\Delta t$.

In a somewhat different formulation, to get the change while moving with the flow we have to take $\Delta\mathbf{x} \to \mathbf{v}\Delta t$ and $\Delta\mathbf{v} \to \mathbf{a}\Delta t$ so that the convective derivative of f becomes

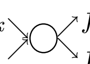
$$\frac{\Delta f}{\Delta t} = \left.\frac{f(\mathbf{x}+\Delta\mathbf{x},\mathbf{v}+\Delta\mathbf{v},t+\Delta t)-f(\mathbf{x},\mathbf{v},t)}{\Delta t}\right|_{\Delta\mathbf{x}=\mathbf{v}\Delta t,\Delta\mathbf{v}=\mathbf{a}\Delta t} .$$

Expanding in Δt and inserting $\mathbf{a}=\mathbf{F}/m$ one obtains the kinetic equation

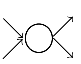
$$\frac{\partial f}{\partial t} + \mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{x}} + \frac{\mathbf{F}}{m}\cdot\frac{\partial f}{\partial \mathbf{v}} = \left.\frac{\partial f}{\partial t}\right|_{\text{coll}} . \tag{5.69}$$

The collision terms has two obvious components since collisions can in principle both destroy or produce a given state f_i. In this context there are several levels of approximation. The simplest approach is to ignore multiple scattering and $2 \to 3$, $2 \to 4$, and other higher order processes and focus only on the effect of 2→2 collisions to the distribution f_i of species i. Then there are collisions $k+l \to i+j$ which produce more particles while the collisions $i+j \to k+l$ reduce their number. In equibrium, $f_i = f_0$ so that the effect of collisions should vanish. Thus we may try to write in the relaxation time approximation

$$\left.\frac{\partial f_i(\mathbf{x},\mathbf{v},t)}{\partial t}\right|_{\text{coll}} = \sum_{k,l,j}\Bigg(\begin{matrix} f_k \\ f_l \end{matrix}$$



$$\begin{matrix} f_i \\ f_j \end{matrix} \; - \; f_i$$



$$\Bigg) \approx -\frac{1}{\tau_c}(f_i - f_0),$$

where $\tau_c =$ is the collision time $\approx$ constant. A more precise approach would be to compute the transition amplitudes $M(k+l \to i+j)$ and $M(i+j \to k+l)$ from theory (e.g. QED) and then integrate (possibly numerically) over the momenta of the particles of type k, l and j.

Example: two particle species. Let us assume there are only two particle species, denoted by A and B. Here A is the species the evolution of which we wish to follow. Then, apart from normalization factors,

$$\begin{aligned} \left.\frac{\partial f}{\partial t}\right|_{\text{coll}} \sim & - \int f_A(p_1)f_B(p_2)|M_d(AB\to AB;p_1)|^2 d^3p_2\, \underbrace{d^3p_3 d^3p_4}_{\text{final state}} \\ & + \int f_A(p_3)f_B(p_4)|M_p(AB\to AB;p_1)|^2 d^3p_3 d^3p_4 \; \underbrace{d^3p_2}_{\text{final state}} , \end{aligned} \tag{5.70}$$

where M_d (M_p) is respectively the matrix element for destroying (producing) particle A in the momentum state p_1. Let us now assume that the species B, which contributes to the thermal bath in which A propagates, is in near equilibrium so that $f_B = f_B^0$, where $f_B^0 \sim \exp(-\beta E)$ is the equilibrium distribution. Then, by virtue of energy conservation,

$$f_A(p_3)f_B(p_4) \approx e^{-\beta(E_3+E_4)} = e^{-\beta(E_1+E_2)} \approx f_A^0(p_1)f_B^0(p_2) . \tag{5.71}$$

Thus we may write

$$\left.\frac{\partial f}{\partial t}\right|_{\text{coll}} \sim -f_A(p_1)\Gamma_d(p_1) + f_A^0\Gamma_p(p_1) , \tag{5.72}$$

where Γ_d and Γ_p are the collision rates for destruction and production. In near equilibrium the matrix elements $M_d \approx M_p$ so that we may write $\Gamma_d \approx \Gamma_p \approx 1/\tau_c$.

Note that in the relaxation time approximation

$$df(t)/dt = -1/\tau_c[f(t) - f_0] \tag{5.73}$$

we may easily obtain the solution for the distribution function as

$$f(t) = f_0 + e^{-\frac{t}{\tau_c}} \tag{5.74}$$

so that due to collisions, f approaches equilibrium exponentially fast.

The hydrodynamic equations can now be derived from the kinetic equations. We start from the Liouville equation (5.67) and integrating over the momenta we find

$$\frac{\partial}{\partial t}\underbrace{\int d^3p f}_{\rho/m} + \nabla \cdot \underbrace{\int d^3p \, \mathbf{v} f}_{\langle \mathbf{v}\rangle \rho/m} + \int d^3p \, \mathbf{F} \cdot \nabla_p f = \int d^3p \left. \frac{\partial f}{\partial t}\right|_{\text{coll}} , \tag{5.75}$$

where we have defined the mean velocity field as

$$\langle \mathbf{v} \rangle = \frac{\int d^3p \, \mathbf{v} f}{\int d^3p f} . \tag{5.76}$$

For a single fluid the collision integral vanishes for 2 → 2 collisions:

$$\int d^3p \left. \frac{\partial f}{\partial t}\right|_{\text{coll}} \propto \int d^3p d^3p_2 d^3p_3 d^3p_4 |M|^2 \left(f(p)f(p_2) - f(p_3)f(p_4)\right) = 0 \tag{5.77}$$

since the p, p_2 etc are just integration labels. Moreover, the force term also vanishes:

$$\int d^3p \, F_k \frac{\partial}{\partial p^k} f = \underbrace{\oint d\mathbf{S} \cdot \mathbf{F} f}_{\to 0 \text{ since } f \to 0 \text{ as } |p| \to \infty} - \int d^3p f \underbrace{\nabla_p \cdot \mathbf{F}}_{\frac{\partial}{\partial p^k} \frac{\partial p^k}{\partial t} = 0} = 0 . \tag{5.78}$$

Thus from Eq. (5.75) we arrive at the continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \langle \mathbf{v} \rangle = 0 . \tag{5.79}$$

The continuity equation is the zeroth momentum moment of the Liouville equation; the Euler equation can be obtained by taking the first moment:

$$\frac{\partial}{\partial t}\underbrace{\int d^3p p_i f}_{\langle v_i \rangle \rho} + \nabla \cdot \int d^3p \, \mathbf{v} v_i m f + \int d^3p \, \mathbf{F} \cdot \nabla_p f p_i = \int d^3p p_i \left. \frac{\partial f}{\partial t}\right|_{\text{coll}} . \tag{5.80}$$

It is an exercise to show that the first moment of the collision integral vanishes for a single fluid. As for the other terms, let $v_i = \langle v_i \rangle + v_i'$ with $\langle v_i \rangle = 0$. Then

$$\begin{aligned} & m \int d^3p f \left[\langle v_i \rangle \langle v_j \rangle + \underbrace{v_j' \langle v_i \rangle}_{\to 0} + \underbrace{v_i' \langle v_j \rangle}_{\to 0} + v_i' v_j' \right] \\ = \;& \rho \langle v_i \rangle \langle v_j \rangle + \frac{1}{3} \delta_{ij} \langle v^2 \rangle m n . \end{aligned} \tag{5.81}$$

Since

$$\frac{1}{2}m\langle v^2\rangle = \langle E\rangle = \frac{3}{2}T \approx \frac{3}{2}p\frac{V}{N} = \frac{3}{2}p/n \ , \tag{5.82}$$

where p is now the pressure, we find

$$\begin{aligned}\frac{\partial\rho\langle\mathbf{v}\rangle}{\partial t} &+ \nabla\cdot[\rho\langle\mathbf{v}\rangle\langle\mathbf{v}\rangle + pI] \\ &= -\int d^3p\ \mathbf{pF}\cdot\nabla_p f \\ &= -\underbrace{\oint d\mathbf{S}\cdot\mathbf{Fp}}_{\to 0} + \int d^pf\ \underbrace{\frac{\partial}{\partial p^k}\mathbf{p}F_k}_{\mathbf{F}} \\ &= \langle\mathbf{F}\rangle\ . \end{aligned}\tag{5.83}$$

Thus we have obtained the Euler equation for the mean velocity and force fields.

Note that we get all the important basic equations by destroying information, i.e. integrating out inessential degrees of freedom. This is a concrete example of "weak emergence", new phenomena (hydrodynamic behavior, local thermal equilibrium) are obtained by coarse graining, integrating out parts of higher-level theories. Proponents of "strong emergence" hold that these new phenomena have an independent existence and are not obtained by integrating out degrees of freedom. This certainly is not the case here.

5.9 Transport coefficients

We now study a situation in which there are small gradients in $n(\mathbf{r}), T(\mathbf{r})$ or the flow velocity $\mathbf{u}(\mathbf{r})$ (small means $l_{\text{free}}\cdot\nabla n(\mathbf{r}) \ll n$, etc.). These small gradients cause a transport of particles, temperature or momentum and we define response = transport coefficient · gradient; these measure the viscosity, diffusivity and thermal conductivity of the fluid. Because of the smallness of the gradients, this approach is called linear response theory. The transport coefficients can now simply be estimated from kinetic theory. In fact, the equiblibrium distribution is of the form:

$$f_0(\mathbf{r},\mathbf{v}) = n(\mathbf{r})\left(\frac{m}{2\pi T(\mathbf{r})}\right)^3 \exp\left(-\frac{m}{2T(\mathbf{r})}[\mathbf{v}-\mathbf{u}(\mathbf{r})]^2\right) \tag{5.84}$$

From the transport equation in the relaxation time approximation it follows that

$$f - f_0 \equiv f_1 = -\tau_c[\mathbf{v}\cdot\frac{\partial f_0}{\partial\mathbf{r}} + \mathbf{a}\cdot\frac{\partial f_0}{\partial\mathbf{v}}], \tag{5.85}$$

where the RHS can be calculated with the help of $\nabla n, \nabla T, \nabla\mathbf{u}$ and the kinetic coefficients can be identified.

Some details. The starting point for the linear response theory is to consider small fluctuations about the local thermodynamical equilibrium and write

$$f_0(\mathbf{x},\mathbf{p},t) = f_0(E^*_{\mathbf{p}}/T(\mathbf{x},t))\ , \tag{5.86}$$

where $E^*_{\mathbf{p}}$ is the energy in the rest frame of the fluid, and T is the temperature field.

Let us consider small deviations from the local equilibrium:

$$f(\mathbf{x},\mathbf{p},t) = f_0 + \delta f(\mathbf{p}) \ . \tag{5.87}$$

Assume a stationary viscous flow, i.e. time-independent δf; then the Euler equation reads

$$\frac{\partial \rho V_i}{\partial t} + \partial_k(\Pi_{ik} + \Delta\Pi_{ik}) = 0 \tag{5.88}$$

with $V_i \equiv \langle v_i \rangle$ and

$$\begin{aligned} \Pi_{ik} &= m\int d^3p\ v_i v_k f_0 = \rho V_i V_j + p\delta_{ik}\ , \\ \Delta\Pi_{ik} &= m\int d^3p\ v_i v_k \delta f \equiv -\eta(\partial_i V_k + \partial_k V_i - \frac{2}{3}\delta_{ik}\nabla\cdot\mathbf{V}) - \zeta\delta_{ik}\nabla\cdot\mathbf{V}\ . \end{aligned} \tag{5.89}$$

In the relaxation time approximation we write the Boltzmann equations as

$$\frac{\partial f}{\partial t} + \frac{\mathbf{p}}{m}\cdot\nabla f = \left.\frac{\partial f}{\partial t}\right|_{\text{coll}} = -\frac{f-f_0}{\tau_c} = -\frac{\delta f}{\tau_c}\ . \tag{5.90}$$

For stationary flow $\partial f/\partial t = 0$ and we find

$$\delta f \approx -\tau_c \frac{\mathbf{p}}{m}\cdot\nabla f\ . \tag{5.91}$$

A comoving observer sees locally a velocity field $\mathbf{V} = 0$ with $f = f_0(E^*/T)$. In the laboratory coordinates the velocity field $\mathbf{v} = \mathbf{V} + v^*$ and

$$f_0(E^*) = f_0(E) + \frac{\partial f_0}{\partial E_{\mathbf{p}}}(E^* - E) \tag{5.92}$$

where $E = \frac{1}{2}mv^2 = \frac{1}{2}m(v^{*2} + 2\mathbf{v}^*\cdot\mathbf{V} + V^2) = E^* + \mathbf{p}^*\cdot\mathbf{V} + \mathcal{O}(V^2) = E^* + \mathbf{p}\cdot\mathbf{V} + \mathcal{O}(V^2)$. Thus

$$\begin{aligned} f_0(E) &= f_0(E^*) - \mathbf{p}\cdot\mathbf{V}\frac{\partial f_0}{\partial E_{\mathbf{p}}} \\ &\rightarrow\ \ \nabla f_0(E) = -\frac{\partial f_0}{\partial E_{\mathbf{p}}}\nabla\mathbf{p}\cdot\mathbf{V} \end{aligned} \tag{5.93}$$

and

$$\begin{aligned} \Delta\Pi_{ik} = m\int d^3p\ v_i v_k \delta f &= -\tau_c\int d^3p\ v_i v_k \frac{\mathbf{p}}{m}\cdot\nabla(\mathbf{p}\cdot\mathbf{V})\frac{\partial f_0}{\partial E_{\mathbf{p}}} \\ &= \frac{-\tau_c}{m}\int d^3p\ v_i v_k v_j \partial_j V_l v_l \frac{\partial f_0}{\partial E_{\mathbf{p}}}\ . \end{aligned} \tag{5.94}$$

From this expression one can in principle read off the properly symmetrized coefficient of $\partial_j V_l$, or the shear viscosity η, in an integral form.

• Viscosity

As an example, let us consider a simple physical situation in which $\mathbf{u}(\mathbf{x},t) = \int d^3v\mathbf{v}f(\mathbf{x},\mathbf{v},t) = (u_x(y),0,0)$, i.e., $\partial_y u_x \neq 0$.

Define now

$$\text{The density of momentum flow } = -\eta\frac{du_x}{dy}\ .$$

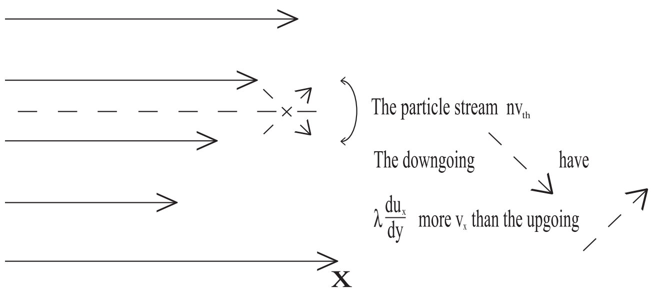


Figure 5.11: Shear viscosity

The flow is the transport, η is the transport coefficient and $\frac{du_x}{dy}$ is the reason for the transport.

(a) Let us first try to argue that

$$\frac{\text{The transported momentum}}{\text{m}^2\text{s}} = m\Delta v \cdot \text{flux} = m\lambda \frac{du_x}{dy} \cdot n v_{\text{th}} \ .$$

Thus

$$\eta = m\lambda n v_{\text{th}} = m\tau_c n \frac{T}{m} = T n \tau_c = p\tau_c \ .$$

Thus we have a very simple result

$$\eta = p\tau_c \ , \tag{5.95}$$

and if one puts in the numbers for the air $\eta = 10^5 \cdot 1,3 \cdot 10^{-10} = 1,3 \cdot 10^{-5}\text{Ns/m}^2$. Not bad!

(b)For this type of flow

$$f_0 = n_0 \big(\frac{m}{2\pi T}\big)^{3/2} \exp\big\{-\frac{m}{2T}[(v_x - u_x(y))^2 + v_y^2 + v_z^2]\big\}.$$

so that only the spatial derivatives remain in the kinetic equation:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f + \mathbf{a} \cdot \nabla_{\mathbf{v}} f = \mathbf{v} \cdot \nabla f = -\frac{1}{\tau_c}(f - f_0).$$

The density of momentum flow now expresses how the momentum p_x in the x-direction flows via v_y in the y-direction:

$$\int d^3v p_x v_y f(v) = \int d^3v p_x v_y [f(v) - f_0] = -\tau_c \int d^3v p_x v_y \mathbf{v} \cdot \nabla f_0, \tag{5.96}$$

where we inserted $\int_{-\infty}^{\infty} dv_y v_y f_0 = 0$. Inserting further

$$\mathbf{v} \cdot \nabla f_0 = v_y \frac{df_0}{dy} = v_y \cdot \frac{m}{T}[v_x - u_x(y)] \frac{du_x}{dy} \cdot f_0$$

Eq. (5.96) becomes

$$= -\tau_c m \frac{m}{T} \cdot \int d^3v v_x v_y^2 [v_x - u_x(y)] f_0 \cdot \frac{du_x}{dy} = -\tau_c T n \frac{du_x}{dy} \equiv -\eta \frac{du_x}{dy}$$

from where we again obtain $\eta = \tau_c T n$. Here we also used the fact that

$$\int d^3v v_x v_y^2 [v_x - u_x(y)] f_0 = \langle v_y^2 v_x^2 \rangle n = \frac{T}{m} \cdot \frac{T}{m} \cdot n \ .$$

Note the paradox: η grows or the fluid becomes more viscous when τ_c grows, that is the interactions become weaker. This may look strange, but the resolution is that τ_c gives the scale; we have to observe phenomena for which $\Delta t \gg \tau_c$.

- **The diffusion coefficient D**

Let us define the particle current

$$\mathbf{J} = \int d^3v \mathbf{v} f(\mathbf{r}, \mathbf{v}, t) = -D \nabla n \ ,$$

where $f = f_0 + f_1$ and

$$f_0 = n(\mathbf{r}) (\frac{a}{\pi})^{3/2} e^{-a\mathbf{v}^2}, \quad a \equiv \frac{m}{2T}.$$

From the kinetic equation

$$f_1 = -\tau_c \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} = -\tau_c (\frac{a}{\pi})^{3/2} e^{-a\mathbf{v}^2} \mathbf{v} \cdot \nabla n(\mathbf{r})$$

so that

$$\mathbf{J} = -\tau_c (\frac{a}{\pi})^{3/2} \int d^3v \mathbf{v}\mathbf{v} \cdot \nabla n(\mathbf{r}) e^{-a\mathbf{v}^2} = -\tau_c \langle v_x^2 \rangle \nabla n(\mathbf{r}) = -D \nabla n.$$

Here we used

$$\int d^3v v_i v_j F(\mathbf{v}^2) = \int d^3v v_i^2 F(\mathbf{v}^2) \delta_{ij} = \frac{1}{3} \delta_{ij} \int d^3v \mathbf{v}^2 F(\mathbf{v}^2)$$

and $\langle v_x^2 \rangle = \frac{1}{3} \langle v^2 \rangle = \frac{T}{m}$. Thus we finally obtain the diffusion coefficient as

$$D = \tau_c \langle v_x^2 \rangle = \tau_c \frac{T}{m}. \tag{5.97}$$

- **Thermal conductivity**

Let us define heat current by $\mathbf{q} = -\kappa \nabla T$ with

$$f_0 = n(\mathbf{r}) \left(\frac{m}{2\pi T(\mathbf{r})} \right)^{3/2} \exp\left(-\frac{m}{2T(\mathbf{r})} \mathbf{v}^2 \right).$$

Note that f_0 has both $n(\mathbf{r})$ and $T(\mathbf{r})$ to keep $p = n(\mathbf{r}) T(\mathbf{r}) =$ const.. From here, after some computation,

$$\mathbf{q} = \int d^3v \mathbf{v} \frac{1}{2} m v^2 (f_0 + f_1) = -\tau_c \frac{5}{2} n \frac{T}{m} \nabla$$

and

$$\kappa = \frac{5}{2} n \tau_c \frac{T}{m} = \frac{5}{2} \cdot \frac{1}{\sigma} \sqrt{\frac{T}{m}} \ . \tag{5.98}$$

The diffusion equation of heat with the thermal diffusivity is then given by

$$\frac{\partial T}{\partial t} = \frac{\kappa}{(C_p/N)n} \nabla^2 T \ . \tag{5.99}$$

Chapter 6

Spin models

6.1 Generic features

In spin models space is discretized by a regular crystalline lattice, and each lattice site is assigned a discrete variable, the spin. Different spin models are specified by different types of spins and the way they are coupled. Originally spin models were constructed to describe magnetism, and in particular the transition between magnetic and non-magnetic phases as the material is heated past its critical temperature. However, their field of application is much wider, including modeling of discretized field theories, and they can be considered as simple prototypes for critical phenomena and models for phases and phase transitions in general. Spin models provide very illustrative examples of the computation of the partition function $Z = \mathrm{Tr} e^{-\beta H} = e^{-\beta F}$. The advantage over continuous theories is that now the degrees of freedom are almost trivial (numbers, often integers, on a lattice) and their number are finite; moreover, the spin-spin interactions are simple (nearest neighbour, nnn,...). Spin models are also pedagocical in the sense that they, like most things in the real world, can seldom be solved analytically so that numerical methods are essential.

A generic spin model has a Hamiltonian of the form

$$H = -\sum_i H_i S_i - \sum_{i,j} J_{i,j} S_i S_j - \sum_{i,j,k} K_{ijk} S_i S_j S_k - \dots \ , \tag{6.1}$$

where the sum is over all the sites of the lattice that has a dimensionality d. At each site the spin variables S_i can take some values $0, 1, \dots, q-1$; we thus speak of d-dimensional q state models. The interactions J_{ij} etc may operate over the nearest neighbours only so that the range of interactions is finite; or we may have an infinite range models. In the first term H_i is an external field (e.g. magnetic field).

Simplest example: infinite range Ising model in 1 dimension. Let us assume that

$$H = -B \sum_i S_i - \frac{J}{2N} \sum_{i,j} S_i S_j \tag{6.2}$$

so that the interactions between all pairs have the same strength no matter what the distance $|i-j|$. We further assume that

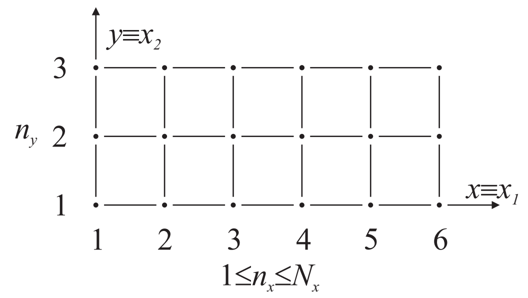


Figure 6.1: 3 × 6 rectangular lattice

- there are only two states: $S_i = \pm 1$
- the lattice is one dimensional and has N sites

Then there are 2^N possible spin configurations.

The great (and only?) virtue of the $d = 1$ infinite range Ising model is that, in contrast to almost any other spin model, it can be solved analytically. We want to compute the weighted sum over all configurations:

$$\begin{aligned} Z &= \sum_{\{S_i\}} e^{-\beta H} \\ &= \sum_{\{S_i\}} \int_{\infty}^{\infty} \frac{d\mu}{\sqrt{\frac{2\pi}{N\beta J}}} e^{-\frac{N\beta J\mu^2}{2}+\beta J\mu \sum_i S_i} e^{B\beta \sum_i S_i} \ , \end{aligned} \tag{6.3}$$

where we have used a trick: we have introduced an auxiliary (i.e. non-propagating) field μ such that when integrated over, we regain the original sum over configurations. The advantage of such an auxiliary field is seen by rearranging the the terms in Eq. (6.3) to obtain

$$\begin{aligned} Z &= \int_{\infty}^{\infty} \frac{d\mu}{\sqrt{\frac{2\pi}{N\beta J}}} e^{-\frac{N\beta J\mu^2}{2}} \underbrace{\sum_{\{S_i\}} e^{(\beta J\mu+\beta B)\sum_i S_i}}_{\prod_i^N \left[e^{\beta(J\mu+B)}+e^{-\beta(J\mu+B)}\right]} \\ &= \int_{\infty}^{\infty} \frac{d\mu}{\sqrt{\frac{2\pi}{N\beta J}}} e^{-\beta N\mathcal{L}(\mu,B)} \ , \end{aligned} \tag{6.4}$$

where the we have defined the Lagrangian density

$$\mathcal{L}(\mu, B) = \frac{J}{2}\mu^2 - \frac{1}{\beta}\log[2\cosh\big(\beta(B+\mu J)\big)] \ . \tag{6.5}$$

Note that the Lagrangian is volume × density = $N\mathcal{L}$. (For an auxialiary field Hamiltonian = −Lagrangian.)

Thus the infinite range Ising model is equivalent to a continuous theory that instead of discrete spins has a single degree of freedom μ. The stationary points, i.e. the metastable minima, are obtained by setting

$$\begin{aligned} \frac{d\mathcal{L}}{d\mu} &= 0 = J\mu - \frac{1}{\beta}\frac{\sinh\big(\beta(B+\mu J)\big)}{\cosh\big(\beta(B+\mu J)\big)}\beta J \\ \rightarrow \mu &= \tanh\big(\beta(B+\mu J)\big) \ . \end{aligned} \tag{6.6}$$

KUVAT!! If the external field $B = 0$, we see that there is a trivial solution $\mu = 0$; other solutions exist if

$$\frac{d\tanh\left(\beta\mu J\right)}{d\mu}|_{\mu=0} = \beta J > 1 \ . \tag{6.7}$$

Clearly, for $T > J \equiv T_c$ the minimum is at $\mu = 0$ whereas for $T < T_c$ the minimum jumps (adiabatically) to $\mu = \mu_0 \neq 0$. Hence there are two phases and μ is an *order parameter*.

6.2 Mean field approximation

The spin S_i is a quantum mechanical operator with a discrete set of eigenvalues; because of that, computing Z is often quite impossible. However, if we replace the operator S_i by its expectation value $\langle S_i \rangle \equiv s_i$, or make a mean field approximation, we obtain a variable which is a number that can take continuous values in a given range (e.g. $0 \leq \langle S_i \rangle \leq q-1$).

To illustrate the mean field approximation, let us consider the Heisenberg model. It is a short-range Ising model with

$$H = -\frac{J}{2} \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - g\mu_B \sum \mathbf{S}_i \cdot \mathbf{B} \ , \tag{6.8}$$

where the constants are according to the usual conventions, and $\langle i,j \rangle$ denotes a sum over the nearest neighbours only. Note that $\mathbf{S}_i$ is a vector with some dimensionality n so that $\mathbf{S}_i = (S_1, \ldots . S_n)_i$ with $\mathbf{S}_i^2 = 1$; here we take $n = 1$ for simplicity so that in the mean field approximation, adopting the boundary condition $S_{N+1} = S_1$, we may write

$$\begin{aligned} Z &= \sum_{\{S_i\}} \exp \left(\beta J \sum_{l=1}^{N} s_l s_{l+1} + \beta h \sum_{l=1}^{N} s_l \right) \\ &= \sum_{\{S_i\}} T_{s_1 s_2} T_{s_2 s_3} \cdots T_{s_N s_1} \equiv \mathrm{Tr}\; T^N \ , \end{aligned} \tag{6.9}$$

where $h \equiv g\mu_B B$ and we have introduced a 2×2 transfer matrix T, given by

$$T_{ss'} = \exp \ (\beta J s s' + \beta h (s + s')/2) \ . \tag{6.10}$$

The transfer matrix is yet another trick but well suited for the Heisenberg model. The eigenvalues of T are

$$\lambda_{1,2} = e^{\beta J} \cosh \beta J \pm \sqrt{e^{2\beta J} \sinh^2 \beta J + e^{-2\beta J}} \tag{6.11}$$

and

$$Z = \mathrm{Tr}\; T^N = \lambda_1^N + \lambda_2^N \ . \tag{6.12}$$

Let $\lambda_1 \geq \lambda_2$. Then the free energy density of the Heisenberg model can be written as

$$f = F/N = -\frac{1}{N} T \ln \left(\lambda_1^N + \lambda_2^N \right) = -T \ln \left(\lambda_1 \right) - \frac{1}{T} \frac{1}{N} \left(\frac{\lambda_2}{\lambda_1} \right)^N \ldots \tag{6.13}$$

Magnetization is given by

$$M = -\frac{\partial f}{\partial h} > 0 \ \text{ for } h \neq 0, \ \beta J \neq \infty \ . \tag{6.14}$$

However, for fixed h, β one finds that $M \to 0$ as $J \to 0$. This means that at $T = 0$ magnetization vanishes and there is a phase transition at zero temperature from ordered high T state to a disordered $T = 0$ state.

The details of the phase transition in the Heisenberg model are not as such terribly interesting. However, it is very illustrative to compute the correlators. Consider the 2-point function

$$\begin{aligned}\langle s_i s_j\rangle &= Z^{-1}\sum s_i s_j \exp\left(\beta J\sum_{l=1}^{N} s_l s_{l+1} + \beta h\sum_{l=1}^{N} s_l\right)\\ &= Z^{-1}\sum_{s_1,\ldots,s_N} T_{s_1 s_2}\cdots T_{s_{i-1}s_i}s_i\cdots T_{s_{j-1}s_i}s_j\cdots T_{s_N s_1}\\ &= Z^{-1}\mathrm{Tr}\; T^{i-1}\sigma_3 T^{j-i}\sigma_3 T^{N-j+1}\ ,\end{aligned} \tag{6.15}$$

where

$$\sigma_3 = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \tag{6.16}$$

is the usual Pauli matrix.

We may now use a unitary transformation U to diagonalize T:

$$U^{-1}TU = \tilde{T};\quad U = \begin{pmatrix}\cos\phi & -\sin\phi\\ \sin\phi & \cos\phi\end{pmatrix}\ . \tag{6.17}$$

Then

$$U^{-1}\sigma_3 U = \begin{pmatrix}\cos 2\phi & -\sin 2\phi\\ -\sin 2\phi & \cos 2\phi\end{pmatrix} \equiv \tilde{\sigma_3} \tag{6.18}$$

and using these, we find

$$\begin{aligned}\langle s_i s_j\rangle &= Z^{-1}\mathrm{Tr}\begin{pmatrix}\lambda_1^{N-j+1} & 0\\ 0 & \lambda_2^{N-j+1}\end{pmatrix}\tilde{\sigma_3}\begin{pmatrix}\lambda_1^{j-i} & 0\\ 0 & \lambda_2^{j-i}\end{pmatrix}\tilde{\sigma_3}\\ &= \left[\lambda_1^N\cos^2 2\phi + \lambda_1^N\left(\frac{\lambda_2}{\lambda_1}\right)^{j-i} + \lambda_2^N\left(\frac{\lambda_1}{\lambda_2}\right)^{j-i}\sin^2 2\phi + \lambda_2^N\cos^2 2\phi\right]/(\lambda_1^N+\lambda_2^N)\\ &\to \cos^2 2\phi + \left(\frac{\lambda_1}{\lambda_2}\right)^{j-1}\sin^2 2\phi \ \text{ as }\ N\to\infty\ .\end{aligned} \tag{6.19}$$

It is also easy to show that

$$\langle s_i\rangle = M = Z^{-1}\mathrm{Tr}\; T^{i-1}\sigma_3 T^{N-i+1} \to \cos 2\phi \ \text{ as }\ N\to\infty\ . \tag{6.20}$$

The pair correlator function is defined as

$$g_{ij} = \langle s_i s_j\rangle - \langle s_i\rangle\langle s_j\rangle = \sin^2 2\phi\,\exp\,[-(j-i)\ln\frac{\lambda_1}{\lambda_2}] \equiv \sin^2 2\phi\,\exp\,[-\xi^{-1}(j-i)]\ , \tag{6.21}$$

where ξ is the correlation length and measures the coherence of the spin alignment. (The exponential form is just a convention.)

It is now straightforward to see that if $h \neq 0$, then $\xi < \infty$ because $|\lambda_1/\lambda_2| > 1$; if however $h = 0$, $|\lambda_1/\lambda_2| = (\tanh \beta J)^{-1} \to 1$ as $T \to 0$ so that $T = 0$ is a critical point at which the correlation length becomes infinite. This is a sign of a second order phase transition: because of infinite range correlations, all the sites adjust their spins simultaneously; for first order phase transition, the correlation length is finite.

6.3 Potts model

The Potts model is a generalised Ising model and a useful tool for studying phase transitions. We take a d-dimensional $N_1 \cdot N_2 \cdot \ldots \cdot N_d$ - lattice ($= N^d$ if $N_i = N$) with the boundary conditions that are usually taken to be periodic (hypertorus, see Fig. 6.2). Other alternatives are fixed bondary conditions (which enhance finite size effects) or twisted boundary conditions (which are used to force the system to generate dynamically some effect such as an interface). There are N^d sites, dN^d links (or bonds) and $1/2 \cdot d(d-1)N^d$ plaquettes.

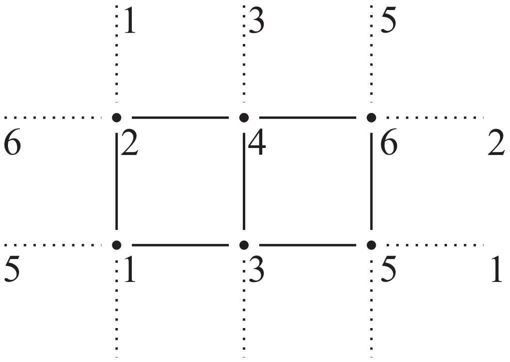


Figure 6.2: Lattice with periodic boundary conditions

In the Potts model each site is assigned a spin $\sigma = 0, 1, 2, \ldots, q-1$ (q-state Potts model) and one assumes a ferromagnetic (favors parallel spins) nearest neighbor (nn) interaction between the spins so that

$$H = -K \sum_{\langle i,j \rangle} \delta_{\sigma_i,\sigma_j} \tag{6.22}$$

where sum is over nearest neighbors. Thus if the spins of two adjacent sites are the same, the contribution of the pair (or the link between them) to the total energy is $-K$, if the spins are different, the contribution is zero. For the partition function one then has

$$Z = \sum_{\{\sigma_i\}} e^{\beta K \sum_{\langle i,j \rangle} \delta_{\sigma_i,\sigma_j}} = Z(T, N) \equiv e^{-F/T} \ , \tag{6.23}$$

where sum is over all states of the system, i.e., over all spin configurations. Solving the Potts model "simply" means evaluating Z (for $N \to \infty$).

The Ising model in d dimensions has 2 states, “spins” $s_i = \pm 1$:

$$\begin{array}{cccc} s_i s_j & & & \delta_{s_i s_j} \\ + & \overset{+}{\cdot} & \overset{+}{\cdot} & 1 \\ + & \overset{-}{\cdot} & \overset{-}{\cdot} & 1 \\ - & \overset{+}{\cdot} & \overset{-}{\cdot} & 0 \\ - & \overset{-}{\cdot} & \overset{+}{\cdot} & 0 \end{array} \quad \Rightarrow \delta_{s_i s_j} = \frac{1}{2}(1 + s_i s_j) \tag{6.24}$$

and one can alternatively write

$$H = -K \sum_{dN^d \text{pairs}} \delta_{s_i s_j} = -K \sum_{\text{pairs} \equiv \langle i,j \rangle} (\frac{1}{2} + s_i s_j) = -\widetilde{K} \sum_{\text{pairs}} s_i s_j + \text{const}, \tag{6.25}$$

where the constant is irrelevant.

Even for relatively small N, spins models have a vast number of states, the Ising model has 2^{N^d} states. Thus also many states can have the same energy, as already discussed in Chapter 1 in case of the Ising model.

For more details on the Ising model, see P. Beale, Phys. Rev. Lett. 76 (1996) 78, F. Wang and D. P. Landau, Phys. Rev. E, 64 (2001) 056101. For the Potts model see Alves, Berg, Villanova, Phys. Rev. B41 (1989) 383. Google gives 125000 hits for Ising model and 92500 hits for Potts model. One also learns that the Potts model partition function generates the Jones polynomial $V(t)$, important for knot theory, with $q-2 = t+1/t$!

In the discussion of the Potts model it is, for both physical and mathematical reasons, appropriate to also introduce a “magnetic field” h coupling to the total “spin” $\sum s_i$ just like in electrodynamics, where $E_B = -\boldsymbol{M} \cdot \boldsymbol{B}, \quad \boldsymbol{M} = e/2m\boldsymbol{S}$:

$$Z = \sum_{2^{N^d} \text{configs}} \exp\left[\beta \sum_{dN^d \text{pairs}} s_i s_j + \beta h \sum_{N^d \text{sites}} s_i\right] = e^{-\beta F(\beta,h)}. \tag{6.26}$$

This is physically important since clearly magnetic effects as such are very relevant. Mathematically the magnetic field serves as a generating function parameter, by taking derivatives of Z or F with respect to h one can evaluate expectation values of spins. The same applies to partial derivatives with respect to β. ¿From Eq.(6.26):

$$\frac{\partial Z}{\partial \beta} = (-F - \beta \partial_\beta F) \cdot Z = \sum_{\text{states}} (\sum_{i,j} s_i s_j + h \sum_i s_i) e^{-\beta H} \tag{6.27}$$

$$= -E + TS - TS = -E \ , \tag{6.28}$$

where $-E = \left\langle \sum_{i,j} s_i s_j + h \sum_i s_i \right\rangle$ is the total internal energy. Moreover,

$$\frac{\partial Z}{\partial h} = -\beta \frac{\partial F}{\partial h} \cdot Z = \sum_{\text{states}} \left[\beta \sum_i s_i \, e^{-\beta H}\right] \ , \tag{6.29}$$

where $-\partial F/\partial h = \left\langle \sum_i s_i \right\rangle \equiv M$ is the magnetisation.

Thermodynamics with possible phase transition singularities is obviously obtained only in the thermodynamic limit, $N \to \infty$. How can we sort this out when we can do numerics only at finite N? To analyse the situation we have to understand the V-dependence. To keep track of the volume factors, we shall now rewrite the Hamiltonian as follows:

$$\beta h \sum_i s_i \Rightarrow h \int_V d^d x\, a(x) \equiv hA, \quad \int d^d x = V \ , \tag{6.30}$$

where h is an external force which couples to $a(x)$, a degree of freedom of the system. Then

$$\beta H = \beta H_0 - hA \tag{6.31}$$

and

$$Z = Z(h) = \mathrm{Tr} e^{-\beta H_o + hA} = \sum_{\text{states}} e^{-\beta E_n + hA} \tag{6.32}$$

so that the derivatives become

$$\frac{\partial Z}{\partial h} = \mathrm{Tr} A e^{-\beta H} \equiv Z\langle A\rangle \Rightarrow \langle A\rangle = \frac{\partial \log Z}{\partial h} = \frac{Z'}{Z}, \tag{6.33}$$

$$\frac{\partial^2 Z}{\partial h^2} = \mathrm{Tr} A^2 e^{-\beta H} \equiv Z\langle A^2\rangle \Rightarrow \langle A^2\rangle = \frac{Z''}{Z}. \tag{6.34}$$

The susceptibility now expresses how the expectation value depends on h:

$$V\chi = \frac{\partial\langle A\rangle}{\partial h} = \overbrace{\frac{\partial^2 \log Z}{\partial h^2}}^{\sim F''} = \frac{Z''}{Z} - (\frac{Z'}{Z})^2 = \langle A^2\rangle - \langle A\rangle^2 = \langle(A - \langle A\rangle)^2\rangle, \tag{6.35}$$

where V is included since A is extensive, $\sim V$. Thus, simulating at some fixed T, h and finite V one will see something as depicted in Fig. 6.3: there is a peak at the position of $\langle A\rangle$ and the width of the peak is given by the susceptibility, $\sim F''(h)$.

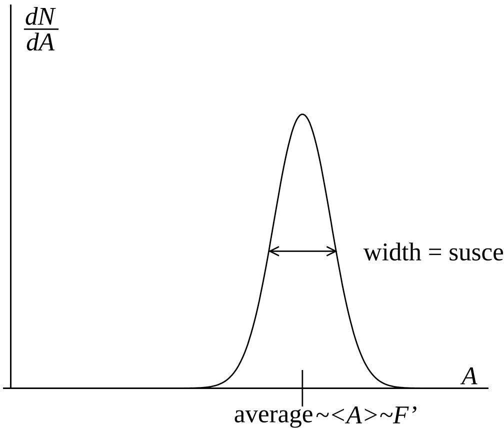


Figure 6.3: Distribution of A obtained at finite V at fixed T, h.

For an intensive variable, the volume average $a \equiv \int \frac{dx}{V} a(x) = A/V$, $dx \equiv d^d x$, and generalising in an obvious way $ha(x) \to h_i a_i(x)$ one has

$$\begin{cases} \langle a_i \rangle = \frac{1}{V} \frac{\partial \log Z}{\partial h_i} \\ \chi_{ij} = \frac{\partial \langle a_i \rangle}{\partial h_j} = V \left[\langle a_i a_j \rangle - \langle a_i a_j \rangle \right] = \frac{1}{V} \frac{\partial^2 \log Z}{\partial h_i \partial h_j} \ . \end{cases} \tag{6.36}$$

If one further defines a *correlation function*

$$C(x-y) = \langle a(x) a(y) \rangle - \langle a(x) \rangle \langle a(y) \rangle \tag{6.37}$$

then also, from Eq. (6.35),

$$\begin{aligned} \chi &= \frac{1}{V} \int dx \int dy \left[\langle a(x) a(y) \rangle - \langle a(x) \rangle \langle a(y) \rangle \right. \\ &= \frac{1}{V} \int dx\, dy\, C(x-y) = \int dx\, G(x) = \int dx\, e^{ikx} G(x)|_{k=0} \equiv \widetilde{G}(k=0) \ . \end{aligned} \tag{6.38}$$

Hence susceptibility is the Fourier transform of the correlation function at zero momentum.

One may now define the order of the phase transtions as follows:

- 1st order transition: jumps in some $\langle A \rangle$
- 2nd order transition: $\langle A \rangle$ is continuous, χ has a singularity

6.4 Phases, critical phenomena

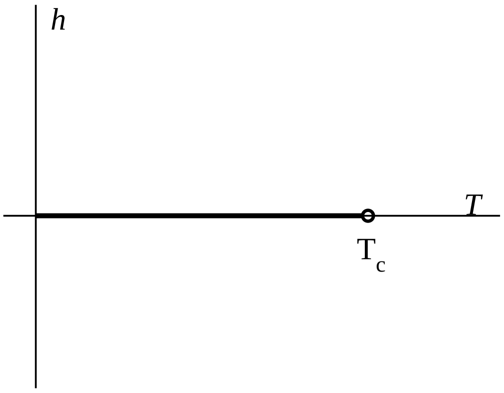


Figure 6.4: First order line ending in a 2nd order critical point at $T = T_c$.

Intuitively, one expects the T, h plane phase diagram as shown in Fig. 6.4 for the Ising model (Potts model with $q = 2$): M jumps from a negative to a positive value when one crosses the 1st order line. For $T < T_c$ the spins order and the symmetry $s_i \to -s_i$ of the theory, i.e., the

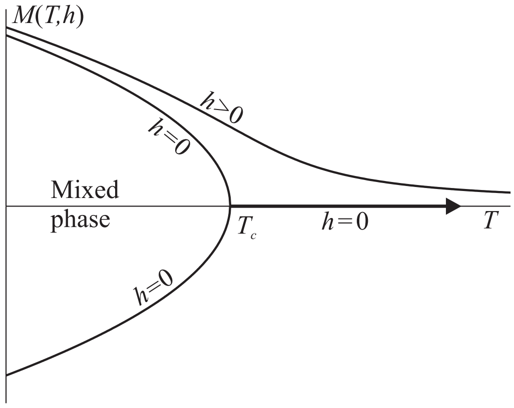


Figure 6.5: Magnetisation in the Ising model; for $0 \leq T < T_c$ and $h = 0$ two values, $\pm|M(T)|$ are possible.

symmetry of its Hamiltonian, is spontaneously broken (SSB, meaning that the theory has the symmetry but its solutions not).

The situation above holds in the $V \to \infty$ thermodynamic limit, but at finite V all discontinuities are smoothed. Simulating the system one will see distributions like those shown in Fig.6.6. With increasing V it makes more and more difficult to make system jump from a peak to another, SSB occurs for $V \to \infty$.

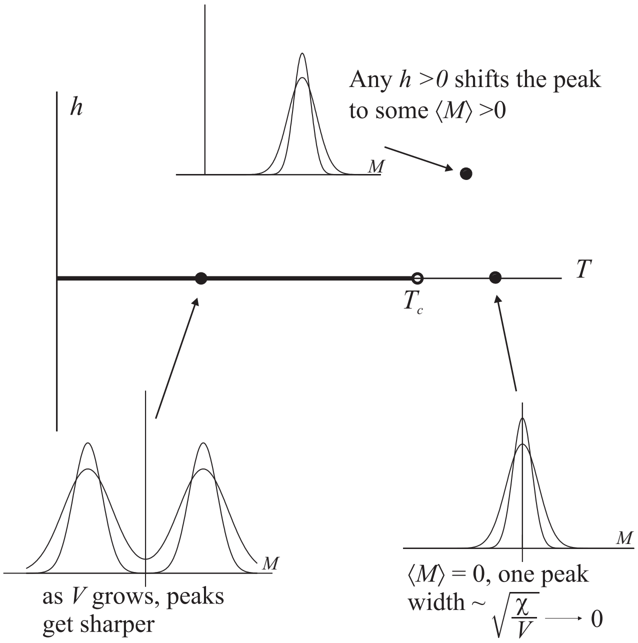


Figure 6.6: Types of distributions observed at finite V at three different regions of the h, T plane.

Thus, to solve the properties of a statistical system (like the Ising model) you simulate it on finite lattice (see section on Monte Carlo simulations) and plot (in one or even two dimensions) distributions in various variabels (like $\sum s_i s_j$ or $\sum s_i$). One will observe three different types of behavior as V increases:

- Usually, in a regular point of the phase diagram one obtains a Gaussian distribution of width $\sim \sqrt{\chi/V}$ which gets narrower when $V \to \infty$ (Fig. 6.7).

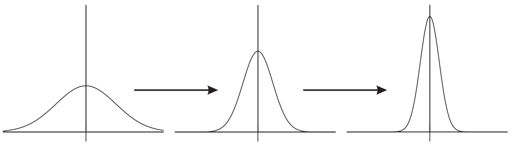


Figure 6.7: Usually distributions get narrower when $V \to \infty$.

- In case of a first-order transition, one has a two-peak distribution which survives in the $V \to \infty$ limit, see Fig. 6.8. Thus it approaches the characteristics of a 1st order transition: order parameter discontinuity, latent heat, interface tension, and correlation lengths which are finite.

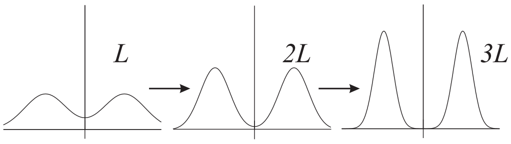


Figure 6.8: 1st order, peaks remain when $V \to \infty$.

- In the case of a 2nd order or continuous phase transition, the critical region is characterised by a diverging correlation length ξ. The situation is very subtle and much work has been devoted to the study of critical phenomena. In particular, one defines critical indices which describe describe how various quantities $\to \infty$ or $\to 0$ when $T \to T_c$ or $t = 1 - T/T_c \to 0$ (0^+ or 0^-):

$$\begin{aligned} \xi &\sim t^{-\nu}, \qquad M \sim t^{\beta} \text{ when } h = 0, \\ M &\sim h^{1/\delta} \text{ when } t = 0, \qquad \chi_M \sim \frac{\partial M}{\partial h} \sim F''(h) \sim t^{-\gamma}, \\ C_V &\sim F''(t) \sim t^{-\alpha}, \qquad C(r) \sim \frac{1}{r^{d-1+\eta}}, \text{ when } t = 0. \end{aligned}$$

  Note here the relation (6.35) between susceptibilities and 2nd derivatives of F. The logic behind these definitions becomes clearly when we soon derive from the Landau theory their mean field values.

To give a concrete example, we show data on 20000 configurations of the 3d Ising model on a 58^3 lattice at the infinite volume critical point $\beta_c = 0.221654$, $h = 0$. In the first plot the horizontal axis is $-58^3 < \sum s_i < 58^3 = 195112$ and the vertical axis shows $0 \le \sum_{\text{pairs}} \delta_{ij} \le 3 \cdot 58^3 = 585336$. In the second plot the axes are scaled by maximum values (and the vertical axis is changed to energy) so that the distribution is on the energy/link ($-1 < -\sum_{\langle ij\rangle} s_i s_j/3 \cdot 58^3 < 1$) vs. magnetization ($-1 < \sum_i s_i/58^3 < 1$) plane. The following figures show the projections on the axes of Fig.6.10. Note, in particular, that even here one observes a two-peak structure. However, now it is observed to *scale*, for example width $\sim L^{\gamma/\nu}$ for the peak in Fig.6.11.

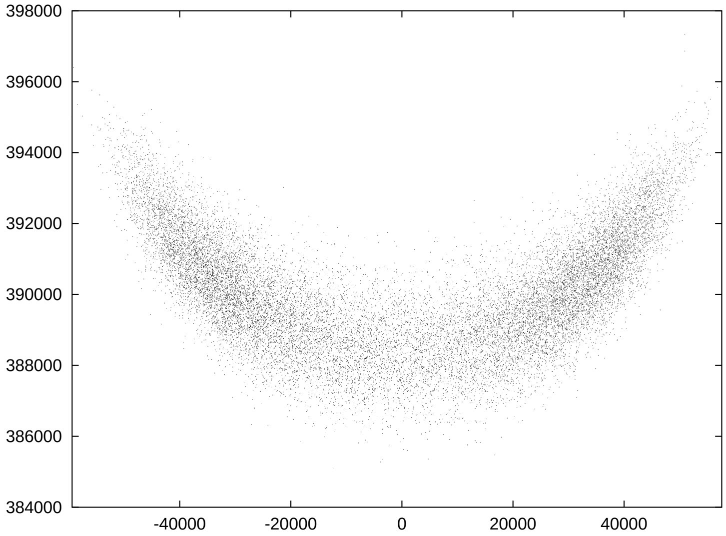


Figure 6.9: Distribution of points at T_c on the $\sum s_i$ vs $\sum_{\text{pairs}} \delta_{ij}$ plane of the 58^3 Ising model.

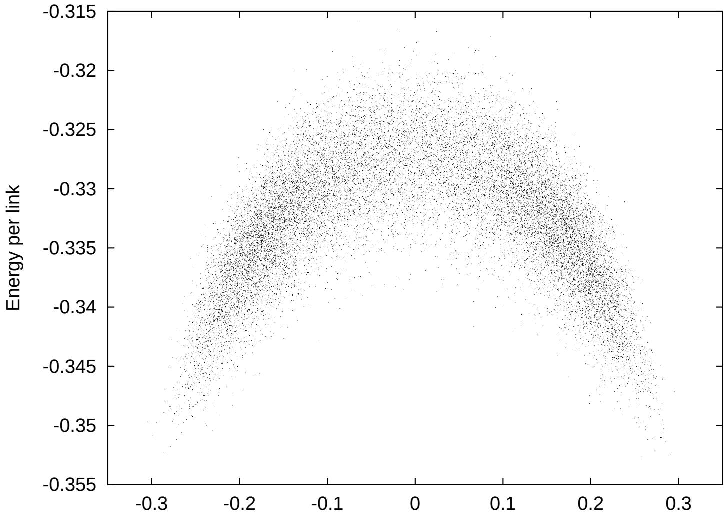


Figure 6.10: Distribution of points at T_c on the energy per link ($-1 < -\sum_{\langle ij\rangle} s_i s_j/3 \cdot 58^3 < 1$) vs. magnetization ($-1 < \sum_i s_i/58^3 < 1$) plane

The FSS (finite size scaling) analysis of these distributions (together with those at different $V = L^3$) now goes as follows. Since we are at T_c, the correlation lengths are formally infinite, but because L is the largest scale, we must have $\xi \sim L$. But since $\xi \sim t^{-\nu}$ (this was the

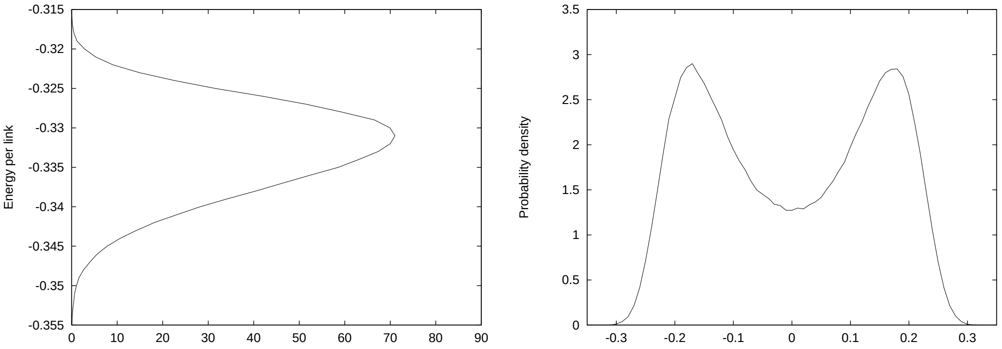


Figure 6.11: Projections of Fig.6.10

definition of ν), one has $t \sim L^{-1/\nu}$. Thus

$$\begin{aligned} C_V &\sim& F''(t) \sim \text{width of energy peak} \sim t^{-\alpha} \sim L^{\alpha/\nu} \\ \chi_M &\sim& F''(h) \sim \text{width of magnetisation peak} \sim t^{-\gamma} \sim L^{\gamma/\nu} \end{aligned}$$

Thus one plots the distributions in Fig.6.11 at different L and fits from them the values of the critical indices.

6.5 Mean field approximation for the Potts model

Considering the Potts model in the mean field approximation teaches us something about how first order transitions may arise. The ddqs (d dimensional q state) Potts model is defined by the Hamiltonian

$$H = -K \sum_{\langle ij \rangle} \delta_{\sigma_i,\sigma_j} \equiv -K \sum_n \sum_{\mu=1}^{d} \delta_{\sigma_n,\sigma_{n+\mu}} \tag{6.39}$$

where $\langle ij \rangle$ represents nearest neighbor links between sites n, $\mu = 1,2,...,d$ is a direction and $\sigma_n = 0,1,\ldots,q-1$ (q different values). An example of a typical configuration at T_c is shown in Fig. 6.12.

Let us now try the following mean field model. On each site n we just replace $\sigma_0,\ldots,\sigma_{q-1}$ by their expectation values $x_0,\ldots,x_{q-1}$, which have to satisfy $x_0 + x_1 + \ldots + x_{q-1} = 1$. One might first expect that by symmetry all the x_i have to be equal – but wait, there is symmetry breaking which is just what we hope to understand analytically! Since each site is treated independently, $\sum_n$ in Eq. (6.39) just gives the number of sites, N^d. Then the total energy is, due to Eq. (6.39),

$$E = -K \cdot N^d \Big[x_0(x_0 + \ldots + x_0) + x_1(x_1 + \ldots + x_1) + x_{q-1}(x_{q-1} + \ldots + x_{q-1}) \Big],$$

where $x_0 + \ldots + x_0$, etc, correspond to links in each of the d dimensions. Thus the energy per site becomes

$$\frac{E}{\text{site}} = \frac{E}{N^d} = -Kd(x_0^2 + \ldots + x_{q-1}^2). \tag{6.40}$$

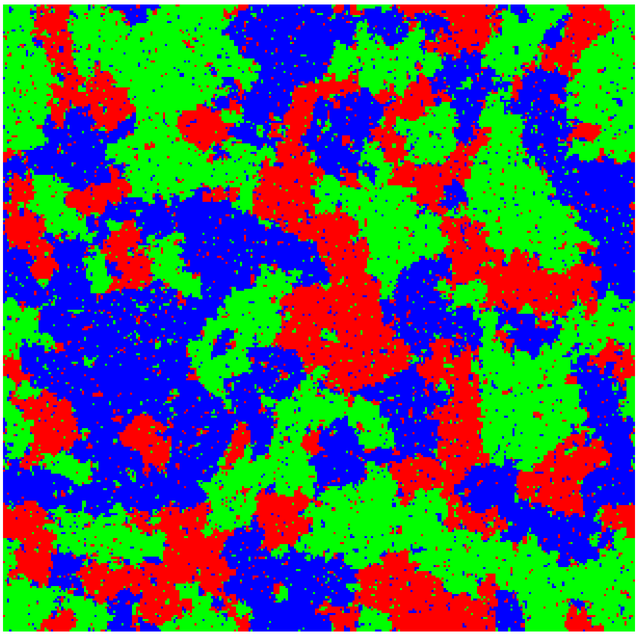


Figure 6.12: Example of a configuration of a 2d 3 state Potts model at T_c on a 128×128 lattice. Note the clustering.

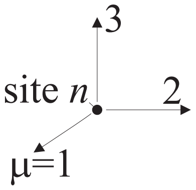


Figure 6.13: Site n and directions μ pointing to the adjacent sites in 3d.

But we do not want to minimize only energy but need also the entropy that competes against energy. The standard expression for the entropy is $S = -\sum p_i \log p_i$, $\sum_i p_i = 1$ so that

$$\frac{S}{\text{site}} = \frac{S}{N^d} = -(x_0 \ln x_0 + \ldots + x_{q-1} \ln x_{q-1}) \ . \tag{6.41}$$

Hence the free energy (per site) reads

$$\beta f \equiv \frac{F/T}{\text{site}} = \frac{E/T - S}{\text{site}} = x_0 \ln x_0 + \ldots + x_{q-1} \ln x_{q-1} - \beta K d(x_0^2 + \ldots + x_{q-1}^2) \ . \tag{6.42}$$

So where is the minimum? To illustrate how Eq. (6.42) operates, let us plot it for $q = 2$, the Ising model. Then $x_0 + x_1 = 1$ and it is convenient to define $x = x_0 - x_1 \Rightarrow x_0 = \frac{1}{2}(1+x), \quad x_1 = \frac{1}{2}(1-x)$. In terms of x

$$\beta f(x) = \frac{1+x}{2} \ln \frac{1+x}{2} + \frac{1-x}{2} \ln \frac{1-x}{2} - \beta K(1+x^2) \equiv h(x) + g(x). \tag{6.43}$$

In Fig. 6.14 we plot the entropy and energy terms $h(x)$, $g(x)$ in Eq. (6.43) separately. One sees again how the entropy and energy terms compete: energy wants to minimise itself, entropy to maximise. Their joint effect produces a minimum.

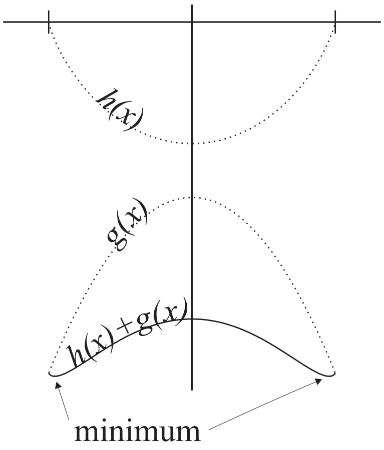


Figure 6.14: Minimum of βf. Here $h(x)$ and $g(x)$ are the first and second terms of (6.43).

For a general q we expect the following (see Fig. 6.15). For $T > T_c$ the system is disordered, $x_k = 1/q$, and each state is equally probable. For $T < T_c$ the system orders itself to any of the states, 0 for example.

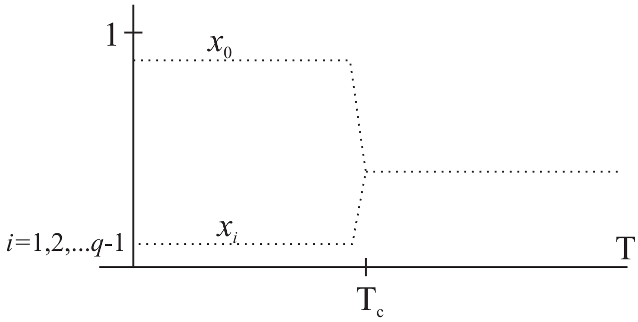


Figure 6.15: Expect: for $T > T_c$ the system is disordered, $x_k = 1/q$, each state is equally probable

Let us write βf as a function of an order parameter s defined by

$$x_i = \frac{1-s}{q}, \qquad i = 1, 2, \ldots, q-1, \qquad s \geq 0, \tag{6.44}$$

$$x_0 + (q-1)x_i = 1 \qquad \Rightarrow x_0 = \frac{1+(q-1)s}{q} \ , \tag{6.45}$$

where $s = 0$ when $T > T_c$. Then the free energy density in Eq. (6.42) can be written as

$$\begin{aligned}\beta f(s) = {}& \frac{1+(q-1)s}{q}\ln\frac{1+(q-1)s}{q} + (q-1)\frac{1-s}{q}\ln\frac{1-s}{q} \\ & - \beta K d\frac{1}{q^2}\left\{\left[1+(q-1)s\right]^2 + (q-1)(1-s)^2\right\}\end{aligned} \tag{6.46}$$

which satisfies $\beta f(0) = -\log q - \beta K d/q$, $\beta f(1) = -\beta K d$. Furthermore,

$$\begin{aligned}\beta[f(s) - f(0)] &= \frac{1+(q-1)s}{q}\ln[1+(q-1)s] + \frac{q-1}{q}(1-s)\ln(1-s) - \frac{q-1}{q}\beta K d s^2 \\ &= \frac{q-1}{2q}(q - 2d\frac{K}{T})s^2 - \frac{1}{6}(q-1)(q-2)s^3 + \frac{1}{12}(q-1)(q^2-3q+3)s^4 + \ldots \\ &= \left\{\begin{array}{llll} \frac{1}{2}(1-d\frac{K}{T})s^2 & & +\frac{1}{12}s^4 & \text{for } q=2 \\ (1-\frac{2}{3}d\frac{K}{T})s^2 & -\frac{1}{3}s^3 & +\frac{1}{2}s^4 & \text{for } q=3 \\ \frac{3}{2}(1-\frac{1}{2}d\frac{K}{T})s^2 & -s^3 & +\frac{7}{4}s^4 & \text{for } q=4 \end{array}\right.\end{aligned} \tag{6.47}$$

```
In[1]:=
f[q_,s_,k_]:=(1+(q-1)s)*Log[1+(q-1)s]/q+(q-1)(1-s)*Log[1-s]/q-(q-1)k*s^2/q

In[2]:=
Plot[{f[7,s,2],f[7,s,2.15],f[7,s,2.5],f[7,s,3]},{s,0,1},AspectRatio 1,
  PlotRange {{0,1},{-0.25,0.25}}]
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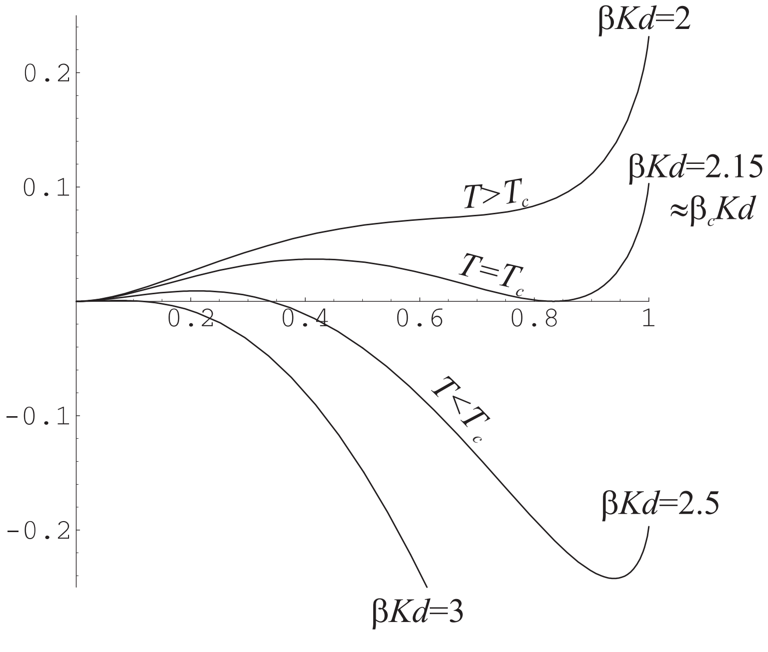

Table 6.1: Plotting $\beta[f(s) - f(0)]$ for $q = 7$ with Mathematica. The typical structure of a first order phase transition is evident.

What are β_c, s_c? Let us minimize $\beta f(s)$:

$$\beta f'(s_c) = \frac{q-1}{q}\Big[\ln\frac{1+(q-1)s_c}{1-s_c} - 2\beta K d s_c\Big] = 0. \tag{6.48}$$

There is always the solution $s = 0$, but there is also a second one, see Fig. 6.5, which corresponds to a second, albeit a metastable, minimum of the potential. At T_c this metastable minimum must be on the same level with the one at $s = 0$. Thus T_c is determined by the condition

$$\beta_c[f(s_c) - f(0)] = 0 \tag{6.49}$$

$$\Rightarrow (1+(q-1)s_c)\ln(1+(q-1)s_c) + (q-1)(1-s_c)\ln(1-s_c) = (q-1)\beta_c K d s_c^2\ . \tag{6.50}$$

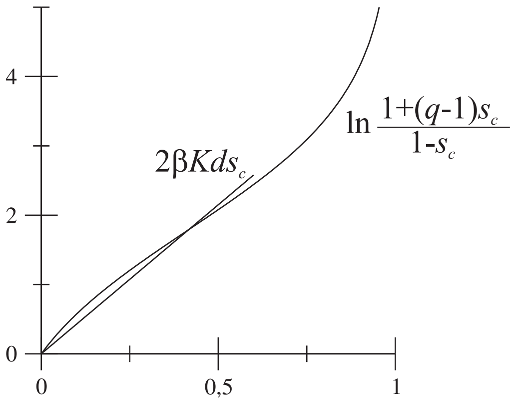

Figure 6.16: Solving Eq.(6.48): $s = 0$ and another solution.

Simultaneous solutions to both equations are:

$$\text{for } q=2: \qquad \ln\frac{1+s_c}{1-s_c} = 2\beta K d s_c \qquad \Rightarrow \beta_c K d = 1 \tag{6.51}$$

$$s_c = \tanh \beta K d s_c \tag{6.52}$$

$$\text{for } q \geq 3: \qquad s_c = \frac{q-2}{q-1}, \qquad \beta_c K d = \frac{q-1}{q-2}\ln(q-1) \tag{6.53}$$

$$T_c = \frac{q-2}{(q-1)\ln(q-1)} K d \tag{6.54}$$

Inspection shows that the exact result for $d = 2$ is

$$\begin{cases} T_c = \frac{1}{\log(1+\sqrt{q})} \rightarrow \frac{2}{\log q} K \\ T_c^{\text{mean field}}(q \rightarrow \infty) \rightarrow \frac{d}{\log q} K \end{cases} \tag{6.55}$$

so that both agree for large q.

What happens in the present mean field approximation is summarised in Fig. 6.5. At low T the system is ordered in state 0 (by choice). At non-zero temperature other spins are also

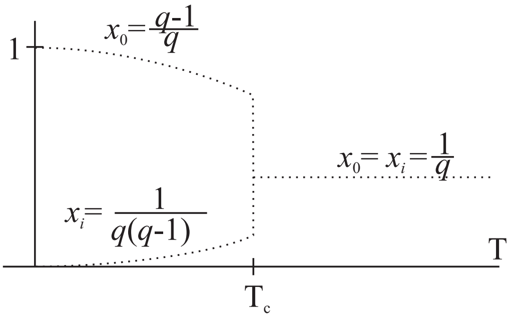

Figure 6.17: Mean field states of the q-state Potts model. Values of x_i given for $T \leq T_c$ refer to $T = T_c$.

around, but if we decrease temperature, at $T = 0$ all the spins are aligned and there is only the state 0. At $T > T_c$ there is complete disorder as all spins are equally probable.

In the mean field approximation the transition to a new minimum does not take place at $T = T_c$ for $q > 2$ because the of the local maximum in the free energy, which traps the system into the metastable vacuum at $s = 0$. However, eventually at $T < T_c$ the system will either tunnel or fluctuate over the barrier. Since now the new minimum has lower free energy, the phase transition is associated with a release of latent heat. In the Potts model one finds for the latent heat

$$L = \frac{T_c[S(T > T_c) - S(T < T_c)]}{N^d} = Kd\frac{(q-2)^2}{q(q-1)} \ . \tag{6.56}$$

Note that for $q = 2$, for which the transition is of second order, $L = 0$, as it should.

6.6 Monte Carlo simulations

Monte Carlo integration is based on the approximation

$$I=\int_0^1 dx\, f(x)\approx \bar{m}=\frac{1}{N}\sum_{k=1}^{N} f(r_k) \tag{6.57}$$

where r_k is a random number $(0\geq r_k\geq 1)$.

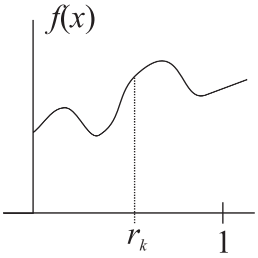

Figure 6.18: MC integration: generate random numbers evenly within 0,1 and take the average of $f(r_k)$.

The result would be quoted as $I=\bar{m}\pm\bar{\sigma}$, where an unbiased estimate of the error $\bar{\sigma}$ would be:

$$\bar{\sigma}^2=\frac{1}{N-1}\sum_1^N[f(r_k)-\bar{m}]^2. \tag{6.58}$$

Generating random numbers is a vast chapter of numerics, often they are obtained from congruences of the type $I_{j+1}=aI_j+c \mod m, \qquad r=\frac{I_j+1}{m}$

Importance sampling is a way to improve the efficiency of MC: you generate numbers mainly where the integrand is big. For example, if $f(x)=e^{-ax}g(x)$, where $g(x)\approx$ const, one should generate random numbers mainly for small x, preferably with the distribution e^{-ax}. Here it is simple, just take e^{-ax} as variable ($t=e^{-ax}$, $x=1/a\cdot\ln(1/t)$):

$$\begin{aligned}\int_0^1 dx\, e^{-ax}g(x) &= \int_{e^{-a}}^1 dt\,\frac{1}{a}g(\frac{1}{a}\ln\frac{1}{t})\\ &= \int_0^1 dr\,\frac{1}{a}(1-e^{-a})g\big(\frac{1}{a}\ln\frac{1}{(1-e^{-a})r+e^{-a}}\big)\end{aligned} \tag{6.59}$$

($t=(1-e^{-a})r+e^{-a}$). More generally, choosing $h(x)$ so that $f(x)/h(x)$ is so close to constant as possible,

$$\int_{x_-}^{x_+} dx f(x)=\int_{x_-}^{x_+} dx h(x)\frac{f(x)}{h(x)}=\big[H(x_+-H(x_-)\big]\int_0^1 dr\,\frac{f(x(r))}{h(x(r))}, \tag{6.60}$$

where one has defined

$$x=x(r)=H^{-1}\big[H(x_-)+r(H(x_+)-H(x_-))\big] \tag{6.61}$$

$$H(x)=\int_{-\infty}^{\infty} dt\, h(t). \tag{6.62}$$

This is useful only if both $H(x)$ and $H^{-1}(x)$ are known analytically, for example, if $h(x) \sim e^{ax}, 1/(x^2+a^2), 1/x^n, 1/(e^x+1)$.

The previous was in 1d and is, formally, straightforward to generalize to Nd. In spin models, discretised path integrals, $\ldots$, $N \to \infty$. For them there is one important simplification: we are interested in mean values (where the physics is) rather than the numerical values of integral Z:

$$\langle \mathcal{O} \rangle = \frac{\sum_{\{E\}} \mathcal{O} e^{-\beta E}}{\sum_{\{E\}} e^{-\beta E}} \tag{6.63}$$

The great idea now is to generate ”configurations”, sets of the spin variables σ_i, with probability $e^{-\beta E(\{\sigma_i\})}$. Then simply

$$\langle \mathcal{O} \rangle = \frac{1}{N_{\text{config}}} \sum_{\{\sigma_i\}} \mathcal{O}(\{\sigma_i\}) \tag{6.64}$$

Generation of random numbers is a “great algorithmic challenge” and there are many methods: Metropolis, heat bath, Langevin, overrelaxation, cluster, etc.

6.6.1 Metropolis

Let us as an example consider the 2d7s Potts model on a 3 × 4 lattice with periodic boundary conditions. An example of a configuration $\{\sigma_i\}$ could be:

$$\begin{array}{c|cccc|c} & 0 & 1 & 3 & 1 & \\ \cline{2-5} 1 & 1 & 2 & 1 & 1 & 1 \\ 1 & 1 & 4 & 4 & 1 & 1 \\ 1 & 0 & 1 & 3 & 1 & 0 \\ \cline{2-5} & 1 & 2 & 1 & 1 & \end{array} \tag{6.65}$$

On each site we have one of the numbers 0,...,6 (or 1,....,7 with the understanding that 0=7) and the numbers outside the rectangle follow from periodicity. The energy of a configuration is $H = -J \sum_{\langle i,j \rangle} \delta_{\sigma_i \sigma_j}$, where the sum goes over nearest neighbours (watch for a factor 2 depending on whether all neighbours or only those in positive direction are included), but we will need only changes of H.

Now proceed as follows. You want to replace one configuration on the lattice by a new one. Sweep through lattice site by site.

- Assume one has come to site **4**:

$$\begin{array}{|cccc|} \hline 1 & 2 & 1 & 1 \\ 1 & \mathbf{4} & 4 & 1 \\ 0 & 1 & 3 & 1 \\ \hline \end{array} \tag{6.66}$$

- Randomly generate new $q = 0, 1, 2, \ldots, 6$.

- Calculate change in H. The part of the old H which may change was

$$H_{\mathrm{old}} = \begin{array}{ccc} & 2 & \\ 1 & \mathbf{4} & 4 \\ & 1 & \end{array} = -J + 0 + 0 + 0 = -J (+\text{unchanged part}) \tag{6.67}$$

and the new possibilities are ($\Delta H \equiv H_{\mathrm{new}} - H_{\mathrm{old}}$)

$$\begin{array}{cccccccc}
 & \begin{array}{ccc} & 2 & \\ 1 & \mathbf{1} & 4 \\ & 1 & \end{array} & \begin{array}{ccc} & 2 & \\ 1 & \mathbf{2} & 4 \\ & 1 & \end{array} & \begin{array}{ccc} & 2 & \\ 1 & \mathbf{3} & 4 \\ & 1 & \end{array} & \begin{array}{ccc} & 2 & \\ 1 & \mathbf{4} & 4 \\ & 1 & \end{array} & \begin{array}{ccc} & 2 & \\ 1 & \mathbf{5} & 4 \\ & 1 & \end{array} & \begin{array}{ccc} & 2 & \\ 1 & \mathbf{6} & 4 \\ & 1 & \end{array} & \begin{array}{ccc} & 2 & \\ 1 & \mathbf{0} & 4 \\ & 1 & \end{array} \\
\text{new=} & & & & & & & \\
 & & & & & & & \\
H_{\mathrm{new}} = & -2J & -J & 0 & -J & 0 & 0 & 0 \\
 & & & & & & & \\
\Delta H = & -J & 0 & J & 0 & J & J & J
\end{array}$$

- How comes the heart of the algorithm. Accept new q always if $\Delta H \leq 0$ and with probability $e^{-\beta \Delta H}$ if $\Delta H > 0$. In other words, energy decreases are always accepted, but also energy increases:

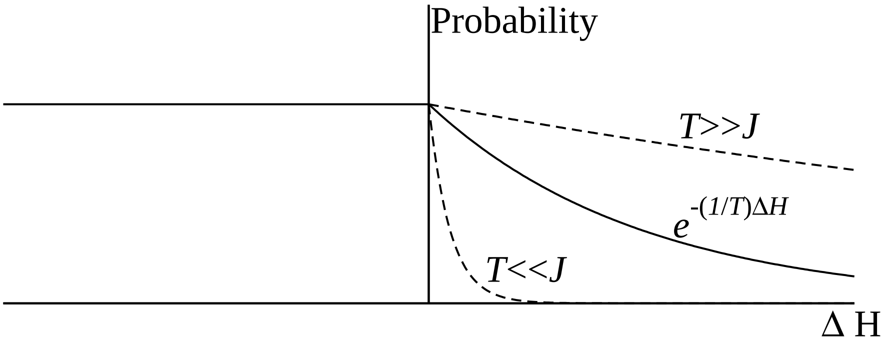

Figure 6.19: Energy increases are also accepted!

If one accepted only energy decreases, the system would soon be driven into the $T = 0$ ground state. The effect of T is precisely to excite higher state. This algorithm implements this by making changes that increase H acceptable with high probability if $T \gg J$ (disorder) and with low probability if $T \ll J$ (order). In the above example $q_{\mathrm{new}} = 1, 2$ and 4 would be always accepted. If $q_{\mathrm{new}} = 3, 5, 6, 0$ (with $\Delta H = +J$) then $0 \geq r \geq 1$ will be generated and q_{new} will be accepted if $e^{-J/T} > r$.

Why the above works and produces configurations distributed with desired probability clearly requires proof.

We want to generate a Markov sequence (C_{n+1} depends only on C_n) of configurations $C_0, C_1, C_2, ...$ with an update probability $P(C \to C')$ so that $P(C_n) \to e^{-S(C_n)}$ with some given action of Hamiltonian S. Two conditions must be satisfied, ergodicity (one must be able to reach all configurations) and microreversibility. To understand the latter note that you clearly want that if the desired probability distribution of configurations

$$P_{\mathrm{eq}}(C) \equiv e^{-S(C)} \tag{6.68}$$

is attained, you stay there. It is obvious that the following kinetic equation holds:

$$\frac{dP(C,t)}{dt} = \underbrace{-\sum_{C'} P(C)P(C \to C')}_{\text{out}} + \underbrace{\sum_{C'} P(C')P(C' \to C)}_{\text{in}}, \tag{6.69}$$

where dt is a computer "time" unit, i.e., one step in updating C. This should vanish for $P = P_{\text{eq}}$, so that the in- and out-probabilities should satisfy

$$\frac{P(C \to C')}{P(C' \to C)} = \frac{P_{\text{eq}}(C')}{P_{\text{eq}}(C)} = e^{-[S(C')-S(C)]} \equiv e^{-\Delta S}. \tag{6.70}$$

Different algorithms amount to constructing different forms for $P(C \to C')$. In this one must compromise between getting nowhere fast (accept frequently, but only small changes) and getting somewhere slowly (you may need big changes in C near phase transitions). For example you cannot

$$\boxed{\begin{matrix} + & + & + & + \\ + & + & + & + \\ + & + & + & + \\ + & + & + & + \end{matrix}} \quad \Rightarrow \quad \boxed{\begin{matrix} - & - & - & - \\ - & - & - & - \\ - & - & - & - \\ - & - & - & - \end{matrix}}$$

by "local update" (changing one spin at a time). Needs a lot of algorithmic development!

6.6.2 Heat bath:

Heat bath is effectively Metropolis with infinite number of tries at the same site. Assume we have again come to point **4** in the 2d7s Potts configuration

$$\begin{matrix} 1 & 2 & 1 & 1 \\ 1 & \mathbf{4} & 4 & 1 \\ 7 & 1 & 3 & 1 \end{matrix}$$

Now the previous value does not matter, one just generates a new q to replace the 4 with the probability

$$p_q = e^{-\frac{1}{T}H}\begin{pmatrix} 1 & 2 & 1 & 1 \\ 1 & q & 4 & 1 \\ 7 & 1 & 3 & 1 \end{pmatrix} \tag{6.71}$$

from which one explicitly evaluates

$$\begin{aligned} p_1 &= p_0 e^{2J/T} = \frac{z^2}{z^2+2z+4}, \qquad z \equiv e^{J/T} \\ p_2 = p_4 &= p_0 e^{J/T} = \frac{z}{z^2+2z+4}, \\ p_3 = p_5 = p_6 = p_7 &= p_0 = \frac{1}{z^2+2z+4}, \end{aligned} \tag{6.72}$$

fixing p_0 by normalising the sum of probabilities to one:

$$p_0[z^2+z+1+z+1+1+1] = 1 \quad \Rightarrow p_0 = \frac{1}{z^2+2z+4} \tag{6.73}$$

For small T, $z \gg 1$, q is most likely to be 1 (ordering, two neighbours are already 1). For large T, $z \to 1$, all q are equally probable (disorder). In practice, at some fixed T, order the p_i's on the interval (0,1). Then generate uniformly the random number $0 < r < 1$ and choose that q for which r lies in p_q:

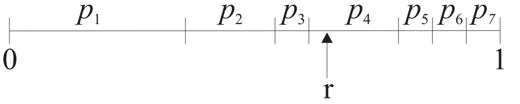

Figure 6.20: Here the generated random number r lies in p_4 and thus $q = 4$ is the new value (by chance the same as the old one).

6.6.3 Langevin, stochastic quantisation

Langevin equation: one particle, one dimension, mass m, no potential, damping force γv, stochastic force $\xi(t)$:

$$m\ddot{x} + m\gamma\dot{x} = \xi(t). \tag{6.74}$$

"Stochastic" clearly means that the force fluctuates with time. It is natural to assume that the average force is zero, $\langle\xi(t)\rangle = 0$. What about magnitude? One may specify the magnitude but it is also important to know how different times are correlated. The simplest assumption clearly is $\langle\xi(t)\xi(t')\rangle = I\delta(t - t')$, I is some constant, soon to be determined. It would seem that $\langle\xi^2(t)\rangle \sim \delta(0) \sim \infty$ and a careful limiting procedure can be invoked (replace δ by a Gaussian with a small width in time, one is saying that the values of the force are correlated only over this short time, over larger times thermal equilibrium is established). Now integrate Eq. (6.74) for $p = \dot{x}$:

$$p(t) = \int_0^t dt' e^{-\gamma(t-t')}\xi(t') + e^{-\gamma t}p(0)$$

and compute $\langle p^2(t)\rangle$ using the ξ correlator:

$$\langle p^2(t)\rangle = \frac{I}{2\gamma}(1 - e^{-2\gamma t}) + e^{-2\gamma t}\langle p^2(0)\rangle. \tag{6.75}$$

Now one knows that for each quadratic dof the energy $\langle p^2(t)/2m\rangle$ is $T/2$ so that for large t:

$$\langle p^2(t \to \infty)\rangle = \frac{I}{2\gamma} = \frac{1}{2}T \cdot 2m \tag{6.76}$$

so that the required magnitude of the fluctuation has been determined:

$$I = 2\gamma T m. \tag{6.77}$$

If one now solves Eq.(6.74) with a stochastic $\xi(t)$, this one coordinate $x(t)$ is "thermalised", energies are distributed $\sim \exp(-\beta E)$.

How could one convert this to a numerical algorithm for producing thermalised configurations? Now we know that we do not want to end up in classical field configurations, which are the extrema of the action:

$$\frac{\delta S[\Phi(x)]}{\delta \Phi} = 0. \tag{6.78}$$

So now simply again introduce a stochastic force and write

$$\frac{\partial \Phi(\tau, x)}{\partial \tau} = -\Gamma \frac{\delta S[\Phi]}{\delta \Phi} + \xi(\tau, x), \tag{6.79}$$

where τ is a fictitious computer time and ξ is constructed so that for large τ the probability distribution of Φ configurations is $\exp(-S[\Phi])$. ....

This numerical method can also be formulated as a method to quantize general field theories, in 4d one then introduces an extra fictitious 5th dimension, the τ in (6.79). This is stochastic quantisation, see P. Damgaard and H. Hüffel, Phys. Rept. 152 (1987) 227.

Chapter 7

Landau theory

7.1 Formulation of the Landau theory

Spin models teach us that in many cases one can describe the various phases of the system by an order parameter (or a set of order parameters), which gauges the properties of the system in some average sense. Hence we have an effective description: one can imagine a more complete theory containing a large number of degrees of freedom ϕ, part of which are integrated over under the condition that one of their combinations $M(\phi)$ be kept fixed:

$$e^{-\beta F(T,V,M)} = \int \mathcal{D}\phi \, e^{-\beta H(\phi)} \delta(M - M(\phi)) \; . \tag{7.1}$$

If one further integrates over M one obtains the partition function of the full theory:

$$Z = e^{-\beta F(T,V)} = \int \mathcal{D}\phi \, e^{-\beta H} = \int \mathcal{D}M[\mathrm{x}] \, e^{-\beta F(T,V,M[\mathrm{x}])}. \tag{7.2}$$

Effective approaches are guided by simplicity and symmetry principles and best justified by their workings. A formal *derivation* of e.g. $F(T, V, M[\mathrm{x}])$ in Eq. (7.2) is often very difficult if not impossible (cf. BCS-theory ⇒ Ginzburg-Landau-theory). Therefore we have to be satisfied with reasonable, physically motivated assumptions. To this end, let us write the free energy of a statistical system as a functional of some order parameter $M(\boldsymbol{x})$ (assumed here to be real for simplicity):

$$\begin{aligned} F[M(\boldsymbol{x})] &= \int d^3x [\frac{K}{2}|\boldsymbol{\nabla} M|^2 + \frac{1}{2}aM^2(\boldsymbol{x}) + \frac{1}{4}bM^4(\boldsymbol{x}) - hM(\mathrm{x}) + cM^6(\mathrm{x}) + \ldots] && (7.3) \\ &\equiv \int d^3x \big[\frac{K}{2}|\boldsymbol{\nabla} M|^2 + V(M(\mathrm{x}))\big], && (7.4) \end{aligned}$$

where the parameters satisfy

$$K > 0, \qquad a, \lesseqgtr 0 \qquad b > 0 \text{ (if } c = 0), \qquad h \gtrless 0, \qquad c > 0 \ldots,$$

Eq. (7.4) defines the Landau model. We have used here a condensed matter notation: in particle physics one would write $K = 1$ (the "canonical normalisation of the kinetic term", which can always be done in case of a constant K by the field redefinition $M \to M/\sqrt{K}$), $a = m^2$, $b = \lambda$, etc. The parameters may in general depend on T.

We could as well think of Eq. (7.4) as defining a 3d field theory with the action F. The functional integral

$$Z[J] = e^{-F(J)} = \int \mathcal{D}M[\mathbf{x}]\, e^{-F(M[\mathbf{x}])+\int d^3x J(\mathbf{x})M(\mathbf{x})} \tag{7.5}$$

would then give all the Green's functions or operator expectation values, i.e., all the physics content, of this theory. In the original Landau theory the argument for the validity of (7.4) was that near the phase transition M is small and higher powers can be neglected. In effective field theories it often happens that, even for dimensional reasons, higher powers come together with inverse powers of some mass scale and can thus be neglected when this mass scale is large.

If $h = 0$, the only symmetry of the action Eq. (7.4) or the theory Eq. (7.2) is $M \to -M$ (the group Z(2)). This is not accidental but rather reflects the fact that we have not included odd terms like M^3 in the free energy. Thus imposing a symmetry limits the possible form of the free energy in an essential manner. Instead on Z(2), we could impose a global U(1) symmetry, in which case the order parameter has to be complex $M = M_1 + iM_2$. If we gauge the U(1) symmetry, i.e. demand that it is local and valid at each point $\mathbf{x}$ separately, we have to introduce a gauge field so that effectively we arrive at a theory describing the interaction of an order parameter with a massless gauge field (photon); this is the Landau-Ginzburg theory of superconductivity. We could also have an order parameter which is a vector or a tensor.

Scaling to dimensionless variables. Clearly F/T is dimensionless, but

$$\frac{1}{T}F[M(\boldsymbol{x})] = \int d^3x\left(\frac{K}{2T}|\boldsymbol{\nabla} M|^2 + \frac{1}{2}\frac{a}{T}M^2 + \frac{1}{4}M^4\right) \tag{7.6}$$

contains quantities which are known but vary from problem to problem ($K = \frac{\hbar^2}{2m}$ or 1, M = magnetisation or wave function, ...). It is very useful to scale out dimensions. From dim$(F/T) \equiv [F/T]$=1 one finds that the dimensionalities are

$$[a] = [\frac{K}{x^2}], \quad [M^2] = [\frac{T}{Kx}], \quad [b] = [\frac{K^2}{Tx}] \quad \text{(this depends of } d = 3!).$$

Using these units we have the simple dimensionless form

$$\int d^3x\left(\frac{1}{2}|\boldsymbol{\nabla} M|^2 + \frac{1}{2}aM^2 + \frac{1}{4}bM^4\right). \tag{7.7}$$

7.2 Z(2) symmetry: the minimum energy configurations

We now have the theory defined by the path integral

$$Z = e^{-\beta F} = \int \mathcal{D}M(\mathbf{x})\, e^{-\beta F(M(\mathbf{x}))}. \tag{7.8}$$

To minimize F one should minimize the whole integral. In Landau theory one usually assumes that it is a good approximation to minimize the integrand, i.e., find the extrema of $F(M(\mathbf{x}))$. This approximation has many names: saddle point, tree level, mean field, classical field approximation, as already discussed in some detail in Chapter 1. So let us simply take the first functional derivative of F with respect to $M(\mathbf{x})$ (do first a very common partial integration based on $(f')^2 = -f \cdot f'' + d(f \cdot f')/dx$ and assume that the boundary term vanishes). Thus, as before, we arrive at the equation of motion

$$\begin{aligned}\frac{\delta F[M(\boldsymbol{x})]}{\delta M(\boldsymbol{y})} &= \frac{\delta}{\delta M(\boldsymbol{y})} \int d^3x \Big[\frac{K}{2} M(\boldsymbol{x})(-\boldsymbol{\nabla}^2) M(\boldsymbol{x}) + V(M(\boldsymbol{x}))\Big] \\ &= -K\boldsymbol{\nabla}^2 M(\boldsymbol{y}) + V'(M(\boldsymbol{y})) = 0\end{aligned} \tag{7.9}$$

Equally, one may use the equation of motion derived from the Lagrangian $L(M, \partial_i M)$:

$$\frac{\partial L}{\partial M} - \partial_i \frac{\partial L}{\partial \partial_i M} = V'(M) - \partial_i[K\partial_i M]) = 0. \tag{7.10}$$

To find the physical configuration $M(\mathbf{x})$, we can either *numerically* minimize

$$\int d^3x [\frac{K}{2}(\boldsymbol{\nabla} M)^2 + V(M)] \tag{7.11}$$

or solve, most likely also numerically, the equation of motion

$$K\nabla^2 M = V'(M).$$

Remark. In searching for the classical solution one may also start from the "Langevin-type" kinetic equation discussed in connection with numerical methods and neglect the stochastic term there, i.e., apply the equation

$$\frac{dM(\boldsymbol{x},t)}{dt} = -\Gamma \frac{\delta F(M(\boldsymbol{x},t))}{\delta M(\boldsymbol{x},t)} \tag{7.12}$$

where $\Gamma > 0$ is some constant and t is a fictitious computer time. This just expresses the natural fact that as long one is not in equilibrium, $\delta F/\delta M \neq 0$, the time derivative of M is proportional to the deviation from equilibrium. The role of the stochastic term was to thermalise the system and to keep it from falling into the classical solution.

To solve the equation of motion (7.2) one needs the boundary conditions (BC). These define the physical system one is considering. We shall go through a number of alternatives.

- **Simplest case, no BC forces $M(\boldsymbol{x})$ to vary**

  In this case any variation of M increases the action and F clearly is minimised by $\nabla^2 M = 0$. $M(\boldsymbol{x}) =$ constant at least satisfies this. Then the equation of motion reads

  $$V'(M) = aM + bM^3 - h = 0. \tag{7.13}$$

  Writing here (phenomenologically) $a = \alpha(T - T_c)$ (Landau's notation) and taking in turn $a = 0$, $b = 0$ and $h = 0$ we can motivate the existence and evaluate the mean field values of three relevant critical indices.

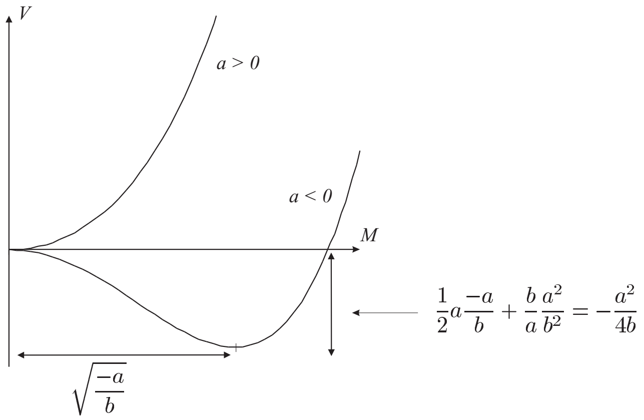

Figure 7.1: The potential for positive and negative a.

(i) Take first $h = 0$ and plot the potential for $a > 0$ and $a < 0$ as in Fig. 7.1.

This describes phenomenologically spontaneous symmetry breaking (SSB), a cornerstone of modern theoretical physics. If $\langle M \rangle$ is the value of M at the minimum, the expectation value of M, one has

$$\begin{array}{lll} a > 0 : & \langle M \rangle = 0 & \text{symmetric under } M \leftrightarrow -M \\ a < 0 : & \langle M \rangle = \sqrt{\dfrac{-a}{b}} & \text{symmetry} M \leftrightarrow -M \text{ broken} \end{array}$$

In the symmetry broken phase $a = \alpha(T - T_c)$ and

$$T < T_c : \quad \langle M \rangle = \sqrt{\frac{\alpha}{b}}\sqrt{T_c - T} \sim t^{\frac{1}{2}} \tag{7.14}$$

which expresses the fact that the mean field value of the critical index β, $\langle M \rangle \sim |T_c - T|^{\beta}$ near T_c is 1/2. Pictorially:

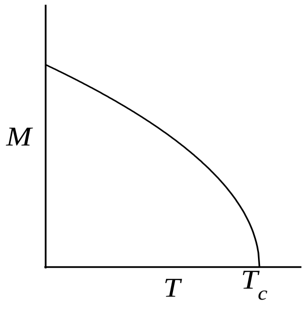

Figure 7.2: $M \sim \sqrt{T_c - T}$. Note this is valid only near $M \approx 0$, near T_c.

(ii) Next take $b = 0$ so that the potential is $V = \frac{1}{2}aM^2 - hM$ and the condition for the minimum becomes $aM - h = 0$. Now the Z_2 symmetry $M \to -M$ is broken, h is

a symmetry breaking parameter. Even the smallest non-zero h is enough to break the symmetry. There are many instances of this phenomenon, e.g., in QCD the smallest non-zero quark masses break the chiral symmetry.

For $a > 0$ the potential looks as shown in Fig.7.3 and the value at the minimum becomes

$$\langle M\rangle = \frac{h}{a} \approx \frac{h}{T - T_c}$$

so that the susceptibility, i.e., the response of the system to a small magnetic field becomes

$$\chi_M = \frac{\partial M}{\partial H} \sim \frac{1}{T - T_c} \sim t^{-\gamma}, \quad \gamma = 1. \tag{7.15}$$

Again we have derived the mean field value of one critical index, that corresponding to magnetic susceptibility, $\gamma = 1$.

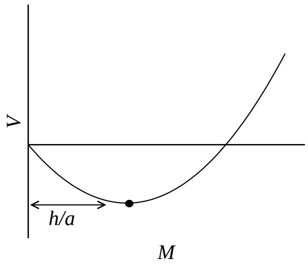

Figure 7.3: The potential near $M = 0$ for $b = 0, a > 0$.

(iii) Finally, take $a = 0$. Then the condition for the minimum is $h = bM^3$ so that

$$\langle M\rangle \sim h^{1/3} \sim h^{1/\delta}$$

where we have defined the third critical index δ and found its mean field value $\delta = 3$.

- **The case with boundary conditions: interface**.

  Take now $h = 0$ so that

$$\langle M\rangle = \pm\sqrt{\frac{-a}{b}} \equiv M_0 \tag{7.16}$$

and assume that one of the directions is special so that for $x \to +\infty$ the system is in the minimum $\langle M\rangle = +\sqrt{-a/b}$ and for $x \to -\infty$ in $\langle M\rangle = -\sqrt{-a/b}$. These two minima are shown in Fig.7.2 and we can set the BC so that the system moves from one minimum to another, i.e., $M(x, y, z) \equiv M(x)$ to varies as a function of x, Fig. 7.2.

It is easy to solve the equation of motion $-K\nabla^2 M + aM + bM^3 = 0, \quad a < 0$, analytically. Introducing the dimensionless variables

$$\begin{cases} M = \sqrt{\frac{-a}{b}}\hat{M} \\ x = \sqrt{\frac{K}{-a}}\hat{x} \end{cases}$$

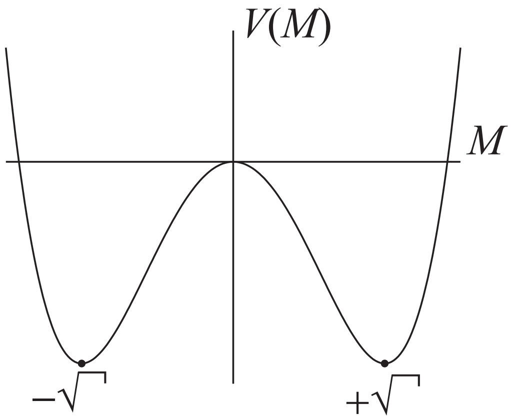

Figure 7.4: Double well

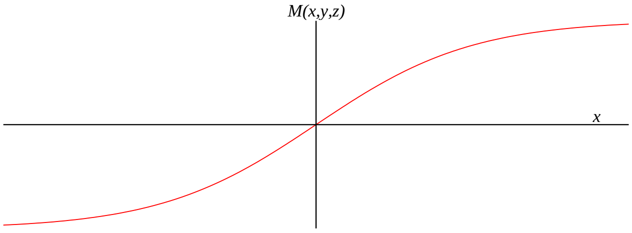

Figure 7.5: Variation $\sim \tanh(x)$.

the equation of motion becomes

$$\hat{M}''(\hat{x}) + \hat{M}(\hat{x}) - \hat{M}^3(\hat{x}) = 0. \tag{7.17}$$

This is solved by

$$\hat{M}(\hat{x}) = \tanh \frac{\hat{x}}{\sqrt{2}} \equiv \hat{M}_{\text{extr}}(\hat{x}). \tag{7.18}$$

Physically, what we have obtained is an interface or a domain wall.

Evaluating the free energy (7.4) for this particular form of M gives the free energy of the interface ($F = -\rho V + \sigma A$), often called the interface tension σ:

$$\begin{aligned} F[M_{extr}(\boldsymbol{x})] &= \int_{-\infty}^{\infty} dx\, \overbrace{dy\, dz}^{area} \left[\frac{K}{2}(M'_{\text{extr}}(\boldsymbol{x}))^2 + V(M_{\text{extr}})\right] \\ &= \text{Area} \cdot \frac{2\sqrt{2}}{3} \frac{(-a)^{3/2}}{b} \equiv A \cdot \sigma. \end{aligned} \tag{7.19}$$

This is the "classic", "saddle point", "tree level", "mean field", extremal solution. The effect of quantum fluctuations around it has been computed for small b (Münster, Nucl. Phys. B324(1989)630):

$$\sigma \rightarrow \sigma[1 - \frac{b}{16\pi^2}(\frac{3}{4} + \frac{\pi\sqrt{3}}{2} + \mathcal{O}(b^2)]. \tag{7.20}$$

Both quantum and thermal fluctuations can be important near the critical temperature. To demonstrate this, let us ask what is the probability for the system to fluctuate back to $M = 0$ from the minimum energy state $M = M_0$ in Eq. (7.16) at $T < T_c$. Since the probability is proportional to the Boltzmann factor, and for a constant order parameter the free energy is density × volume so that we may write

$$P(M = 0; T < T_c) \sim e^{-\beta V[f(M_0) - f(0)]} \ . \tag{7.21}$$

Hence the fluctuation probability is vanishingly small with $P(M = 0; T < T_c) \ll 1$ when the exponent is smaller than 1. To be concrete, let us take $a = \mu_0^2(1 - T/T_c)$ whence we find that fluctuations back to the unbroken phase end when

$$\begin{aligned} \beta V \frac{\mu_0^4}{4b}\left(1 - \frac{T}{T_c}\right)^2 &\gg 1 \\ \rightarrow \quad T_c - T \gg \frac{16b^2T_c^3}{K^3\mu_0^2} &\equiv \Delta T_c \ , \end{aligned} \tag{7.22}$$

where we have taken the volume factor V to be given by the correlation volume ξ^3, where $\xi = \sqrt{-K/a}$ as this is the spatial scale where the order parameter solution connecting the two phases changes by a relative amount of $\mathcal{O}(1)$. Thus very close to the critical temperature, in a region ΔT_c, the behaviour of a system is typically difficult to compute because the fluctuations are large.

Order parameter coupled to gravity. In the normal laboratory environment gravity plays no role. However, at very large scales gravity is important and one has to consider phase transitions in the presence of gravity. Perhaps the most striking example can be found in cosmic inflation, which is a period of superluminal expansion in the very early universe. It is driven by a coherent scalar field $\phi = \phi(t)$, the inflaton, which can be viewed as an order parameter of some early phase transition. If the potential is flat enough, as depicted in Fig. XXXXXX, the inflaton rolls slowly from $\phi \approx 0$ towards the minimum of the potential at $\phi = \phi_0$. Slow rolling means that the kinetic energy is much less than the potential energy, $\dot{\phi}^2 \ll V(\phi) \approx V_0$, which will hold until ϕ has grown to some value ϕ_* at $t = t_*$, after which the inflaton field starts to oscillate. During the slow roll the energy and the pressure are given by

$$\begin{aligned} \rho &= \frac{1}{2}\dot{\phi}^2 + V \approx V \\ p &= \frac{1}{2}\dot{\phi}^2 - V \approx -V \end{aligned} \tag{7.23}$$

so that the equation of state is $\rho \approx -p$; effectively, there is a large cosmological constant. Then, assuming a flat universe with a Friedmann-Robertson-Walker metric $ds^2 = dt^2 - R^2(t)d\mathbf{x}^2$ the Einstein equation reads

$$H^2 \equiv \left(\frac{\dot{R}}{R}\right)^2 = \frac{8\pi G}{3}\rho \approx \text{const.} \equiv H_0^2 \ , \tag{7.24}$$

the solution to which is

$$R(t) = R_0 e^{H_0 t} \ . \tag{7.25}$$

Thus the "size" of the universe becomes exponentionally large with the number of e-folds of the scale factor R given by $N = H_0 t_*$. For an adiabatic expansion $RT =$ const. so that during inflation the temperature of the universe $T \rightarrow 0$. After inflation ends at $t \approx t_*$, the inflation energy is assumed to be dissipated by decay, and as a consequence the universe reheats.

Inflation was initially introduced (in 1981) because it solves some of the naturalness problems of the Big Bang theory. However, its most important feature is that it can expalain the origin of structure in the universe. During inflation ϕ is subject to quantum fluctuations $\delta\phi$, which give rise to a calculable spectrum of density perturbations since (schematically) $\delta\rho = V'\delta\phi$. The spectrum can be measured from the temperature fluctuatations of the cosmic microwave background since $\rho_\gamma \propto T^4$ implies that $4\delta T/T = \delta\rho_\gamma/\rho_\gamma$. The temperature fluctuatations have been measured very accurately e.g. the WMAP satellite, and the results agree well with the inflationary predictions.

7.3 U(1) symmetry: complex order parameter

Let us now consider a complex order parameter with $M = \frac{1}{\sqrt{2}}(M_1 + iM_2)$. We write the free energy (or the action) in a form which is invariant under rotations in the complex plane. Instead of Z(2) the symmetry then is U(1), defined by

$$M \to e^{i\chi} M. \tag{7.26}$$

As long as the parameter χ is constant, this is called a *global* U(1) symmetry. In Sect. 8.5 we shall assume χ to be some arbitrary function $\chi(\mathbf{x})$ which leads to local or gauged U(1).

In case of the global U(1) symmetry, the free energy of the Landau model reads

$$F = \int d^3x \Big[K \boldsymbol{\nabla} M^* \cdot \boldsymbol{\nabla} M + a|M|^2 + b|M|^4 \Big] \ . \tag{7.27}$$

Note that the factors $\frac{1}{2}, \frac{1}{4}$ are built in the definition of M in terms of real variables. The parameter K could be absorbed into the definition of M by rescaling $M \to M/\sqrt{K}$. From Eq. (7.27) one derives the EOM

$$\frac{\delta F}{\delta M^*} = 0 \quad \Rightarrow -K\nabla^2 M + aM + 2b|M|^2 M = 0 \ . \tag{7.28}$$

For $a < 0$ this has a particularly interesting special solution: a vortex line or a string. For the global U(1) symmetry these are called global vortices. These are cylindrical configurations. Hence it is natural to use the cylindrical coordinates $\mathbf{x} \to r, \phi, z$, see Fig. 7.6.

In order to find the string solution let us adopt the Ansatz

$$M(\boldsymbol{x}) = \frac{1}{\sqrt{2}} f(r) e^{in\phi} \quad n = \text{ integer} \tag{7.29}$$

with the boundary conditions

$$f(0) = 0, \quad f(\infty) = \sqrt{\frac{-a}{b}}. \tag{7.30}$$

Due to $f(0) = 0$ one needs not to worry about ϕ being undefined there. Using

$$\nabla^2 = \frac{1}{r}\frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2} \tag{7.31}$$

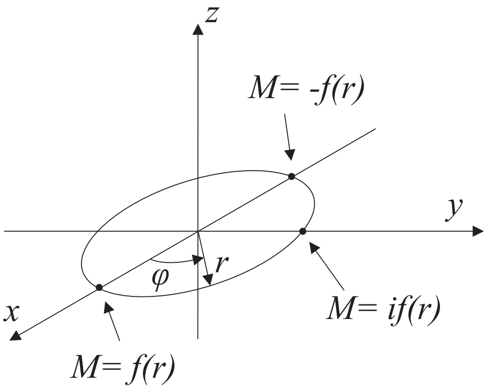

Figure 7.6: Coordinates for a global string

the EOM becomes

$$-K\frac{1}{r}\frac{d}{dr}(r\frac{dM(r)}{dr}) + \frac{Kn^2}{r^2}M(r) + aM(r) + 2bM^3(r) = 0 \ . \tag{7.32}$$

Introducing again dimensionless variables by $M = \sqrt{-a/b}\hat{M}$ and $r = \sqrt{K/(-a)}\hat{r}$ yields

$$-K\frac{-a}{K}\frac{1}{r}\frac{d}{dr}(r\hat{M})\underline{\sqrt{\frac{-a}{b}}} + Kn^2\frac{-a}{K}\underline{\sqrt{\frac{-a}{b}}}\frac{\hat{M}}{\hat{r}^2} + \underline{\sqrt{\frac{-a}{b}}}a\hat{M} + b\frac{-a}{b}\underline{\sqrt{\frac{-a}{b}}}\hat{M}^3 = 0. \tag{7.33}$$

Cancelling some terms and omitting now hats from the dimensionless variables gives

$$-\frac{1}{r}\frac{d}{dr}(rM') + n^2\frac{M}{r^2} - M + M^3 = 0 \tag{7.34}$$

or

$$\frac{1}{r}\frac{d}{dr}(rM'(r)) + (1 - \frac{n^2}{r^2})M - M^3 = 0 \tag{7.35}$$

and finally

$$M'' + \frac{1}{r}M' - \frac{n^2}{r^2}M + M - M^3 = 0 \ . \tag{7.36}$$

Comparing with Eq. (7.17) one notices that two new terms have appeared (the 2nd and 3rd terms). These imply that $\tanh(r/\sqrt{2})$ is not a solution. One has to find the solution numerically, and the outcome is an $M(r)$ growing monotonically from 0 at $r = 0$ to 1 at $r = \infty$, somewhat resembling the $r > 0$ half of $\tanh(r)$ (see, e.g., Fig. 55.1 of Fetter-Walecka).

Now the free energy of the extremal configuration is proportional to the string length; it is the string tension. It has to be computed numerically, but it is even more important to estimate

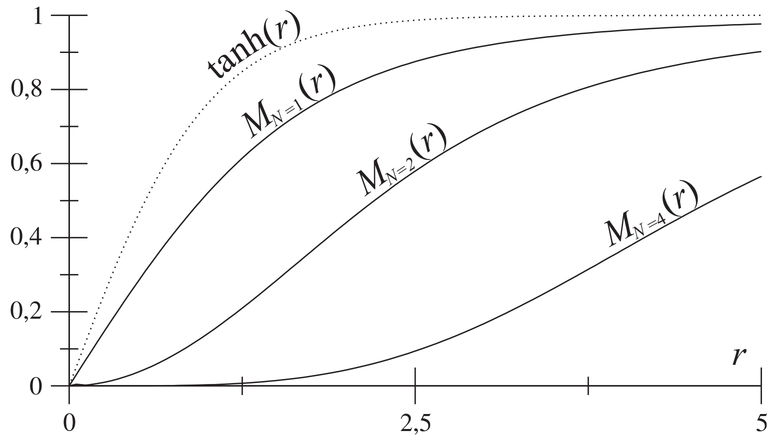

Figure 7.7: Radial dependences of a global string.

it parametrically:

$$\begin{aligned} F_{\text{extr}} &= \int dz \int dx\,dy\,\left[K|\boldsymbol{\nabla} M_{\text{extr}}|^2 + V(M_{\text{extr}})\right] \\ &= \text{Length} \;\cdot\; \text{Area} \;\cdot \text{free energy density} \cdot \text{number}. \end{aligned} \tag{7.37}$$

For Area we have the natural estimate Area $= K/(-a)$ (see the definitions of $\hat{r}$ above, one can also say Area = correlation length^2). Similarly free energy density = the value of $V(M)$ at the broken minimum $= -a^2/(4b)$. Thus we estimate

$$\frac{F}{\text{Length}} \equiv \text{Tension} = \text{number} \;\cdot K \cdot \frac{-a}{b} = \underbrace{\text{number}}_{\mathcal{O}(1)} \cdot K \cdot \langle M \rangle^2. \tag{7.38}$$

Example: Rotation of a bucket of superfluid. Because of superfluidity, the system cannot rotate as a whole, but if it is forced to rotate, it carries the angular momentum along global vortex lines, distributed in a hexagonal lattice (compare Abrikosov vortices in type II superconductors and magnetic fields) in the center of which the matter is in the normal symmetric state. If the superfluid wave function is $\psi = f(r)e^{i\theta}$, the superfluid density n_s and velocity of the matter $\mathbf{v}_s$ are given by

$$n_s = f^2(r), \qquad \mathbf{v}_s = \frac{\hbar}{m}\nabla\theta.$$

Note that this implies $\nabla \times \mathbf{v}_s = 0$ everywhere except at $r = 0$ (Feynman 1955). If simply $\theta = \phi$, the azimuthal angle, one has

$$|\mathbf{v}_s| = \frac{\hbar}{mr}, \qquad \frac{h}{m_{\text{He}}} = 1.0 \cdot 10^{-7}\frac{\text{m}^2}{\text{s}}.$$

Thus the velocity decreases with r, in contrast to rigid rotation. More generally, $\theta = n\phi$, n = integer, but only $n = 1$ is stable. For the tension of a superfluid vortex one obtains

$$\frac{E}{\Delta z} = \int d^2x \frac{1}{2} m n_s v_s^2 \approx \frac{\pi\hbar^2 n_s}{m} \log\frac{L}{\xi},$$

where L is the size of the system or the distance between vortices and ξ is the correlation length, width of the vortex. For He$_4$ the tension is some 10^{-12} N, in a neutron star the tension can be 10^4 N. One also has, for one vortex,

$$\oint \mathbf{v}_s \cdot d\mathbf{l} = \int \nabla \times \mathbf{v}_s \cdot d\mathbf{A} = \frac{h}{m}.$$

7.4 Symmetry currents

Imposing a *symmetry* on the theory means that the Lagrangian $L(\phi_k, \partial_i\phi_k)$ is invariant under the infinitesimal symmetry transformation

$$\phi_k \to \phi_k + i\chi T_{kl}\phi_l, \tag{7.39}$$

where T_{kl} are numbers defining the symmetry and $\chi \ll 1$ is an infinitesimal parameter; for mathematically minded, T is the generator of the symmetry algebra. The infinitesimal change induced into the Lagrangian by the symmetry transformation is

$$\begin{aligned}\delta L &= \frac{\partial L}{\partial\phi_k}\delta\phi_k + \frac{\partial L}{\partial\partial_i\phi_k}\partial_i\delta\phi_k \\ &= (\frac{\partial L}{\partial\phi_k} - \partial_i\frac{\partial L}{\partial\partial_i\phi_k})\delta\phi_k + \partial_i\big[\frac{\partial L}{\partial\partial_i\phi_k}\cdot\underbrace{\delta\phi_k}_{\sim T_{kl}\phi_l}\big].\end{aligned} \tag{7.40}$$

The last term is a surface one, which is neglected when deriving the EOM. However, if now $\phi_k^{\text{extr}}(\boldsymbol{x})$ satisfies the classical EOM, so that

$$\frac{\partial L}{\partial\phi_k} - \partial_i\frac{\partial L}{\partial\partial_i\phi_k} = 0\ ,$$

requiring invariance $\delta L = 0$ we can conclude that

$$\partial_i\mathcal{J}_i = 0, \tag{7.41}$$

where

$$\mathcal{J}_i = \frac{\partial L}{\partial\partial_i\phi_k}\cdot T_{kl}\phi_l\bigg|_{\phi_k=\phi_k^{\text{extr}}} \tag{7.42}$$

is the *Noether current.*

For global U(1) symmetry the infinitesimal transformation is

$$M \to M + i\chi M, \quad M^* \to M^* - i\chi M^*. \tag{7.43}$$

Since the partial derivative needed in Eq. (7.42) is

$$\frac{\partial L}{\partial\partial_i M} = K\partial_i M^* \tag{7.44}$$

we have the symmetry current for the global U(1) symmetry:

$$\mathcal{J}_i = iK[\partial_i M^*\cdot M - \partial_i M\cdot M^*] = -2K\,\mathrm{Im}(\partial_i M^*\cdot M) \tag{7.45}$$

which for the vortex ansatz $M = f(r)e^{i\phi}$ becomes

$$= -2K\,\mathrm{Im}(\partial_i f\cdot e^{-i\phi} - i\partial_i\phi\cdot fe^{-i\phi})fe^{i\phi} \ = 2Kf^2(r)\partial_i\phi(x,y). \tag{7.46}$$

Note the dimensions: $\left[\boldsymbol{\mathcal{J}}\right] = \left[T/x^2\right] =$ energy/area.

7.5 Ginzburg-Landau theory of superconductivity

Let us now make the U(1) symmetry in Eq. (7.27) *local*, i.e., demand that the free energy (or action) be invariant under the **x**-dependent transformation

$$M \equiv \phi(\boldsymbol{x}) \to e^{i\chi(\boldsymbol{x})}\phi(\boldsymbol{x}) \simeq (1+\chi(\boldsymbol{x}))\phi(\boldsymbol{x}) \ . \tag{7.47}$$

$V(\phi^*\phi)$ is still invariant but $\partial_i\phi^*\,\partial_i\phi$ is not. However, if we replace ∂_i by the covariant derivative

$$\partial_i \to \partial_i + ie_3A_i \equiv D_i \ , \tag{7.48}$$

where we have introduced a gauge field $A_i(\boldsymbol{x})$ which is required to transform as

$$A_i \to A_i - \frac{1}{e_3}\partial_i\chi \qquad (\partial_i \equiv \frac{\partial}{\partial x^i} \equiv \nabla_i) \ , \tag{7.49}$$

then

$$\begin{aligned} D_i\phi(\mathbf{x}) &\to [\partial_i + ie_3(A_i - \frac{1}{e_3}\partial_i\chi)]e^{i\chi(\boldsymbol{x})}\phi(\boldsymbol{x}) \\ &= i\partial_i\chi\cdot e^{i\chi}\phi + e^{i\chi}\partial_i\phi + ie_3A_i\cdot e^{i\chi}\phi - i\partial_i\chi\cdot e^{i\chi}\phi \\ &= e^{i\chi}D_i\phi(\mathbf{x}) \ . \end{aligned} \tag{7.50}$$

The covariant derivative transforms covariantly, i.e. as a group element like $\phi(\boldsymbol{x})$. Hence the kinetic term $(D_i\phi)^*\,D_i\phi$ *is* invariant even under local U(1) transformations.

The kinetic part of the gauge field ($\sim \partial^2A^2$) should also be invariant and, of course, we know it is just the Maxwell action of electrodynamics

$$\sum_{i,j}^{3} F_{ij}^2 = \sum_{i,j=1}^{3}\frac{1}{4}(\partial_iA_j - \partial_jA_i)(\partial_iA_j - \partial_jA_i) \equiv \frac{1}{2}\boldsymbol{B}^2, \tag{7.51}$$

where, in 3 dimensions, we only need the magnetic field

$$B_1 = \partial_2A_3 - \partial_3A_2\ldots, \quad \boldsymbol{B} = \boldsymbol{\nabla}\times\boldsymbol{A}. \tag{7.52}$$

Thus we have been led to a theory defined by the functional integral

$$Z \equiv e^{-Vf} = \int \mathcal{D}A_i(\boldsymbol{x})\,\mathcal{D}\phi(\boldsymbol{x})\,e^{-S[A_i(\mathbf{x}),\phi(\mathbf{x})]} \ , \tag{7.53}$$

where

$$\begin{aligned} S[A_i(\mathbf{x}),\phi(\mathbf{x})] &\equiv \frac{1}{T}F[A_i(\mathbf{x}),\phi(\mathbf{x})] = \\ &= \frac{1}{T}\int d^3x\Big[\frac{\tilde{K}}{4}(\partial_iA_j - \partial_jA_i)^2 + K|(\partial_i + ie_3A_i)\phi|^2 + a|\phi|^2 + b|\phi|^4\Big] \end{aligned} \tag{7.54}$$

In general, this is 3d scalar electrodynamics; i.e., 3d gauge + scalar field theory. It is a superrenormalisable field theory (only two divergent diagrams, the tadpole and the sunset diagrams). In terms of this general formulation, all physics is contained in the expectation values of correlators of gauge invariant operators:

$$\langle O_1(\mathbf{x}_1)...O_n(\mathbf{x}_n)\rangle = \frac{1}{Z}\int \mathcal{D}A_i(\boldsymbol{x})\,\mathcal{D}\phi(\boldsymbol{x})\,O_1(\mathbf{x}_1)...O_n(\mathbf{x}_n)e^{-S[A_i(\mathbf{x}),\phi(\mathbf{x})]}, \tag{7.55}$$

where the O_i are local gauge invariant operators of the type

$$O(\mathbf{x}) = F_{ij}^2(\mathbf{x}), \quad |\phi(\mathbf{x})|^2, \quad \phi^*(\mathbf{x})D_i\phi(\mathbf{x}),\ldots. \tag{7.56}$$

For the time being we shall discuss this theory only in the mean field approximation, i.e., study the minima of the free energy in Eq. (7.54). This approximation is appropriate for superconductivity.

For the Ginzburg-Landau theory of superconductivity the parameters in Eq. (7.54) are given by

$$\widetilde{K} = \frac{1}{\mu_0}, \quad e_3 = \frac{e}{\hbar}, \quad K = \frac{\hbar^2}{2m} \tag{7.57}$$

and further also $e \to 2e$ and $m \to 2m_e^*$, the charge and mass of Cooper pairs, respectively. In the Ginzburg-Landau theory the complex scalar field $\phi(\boldsymbol{x})$ is interpreted as a "condensate wave function" and its absolute value squared, $|\phi(\boldsymbol{x})|^2$ as the "density of Cooper pairs", pairs of e^- near Fermi surface. If $a < 0$, the U(1) symmetry is broken and an expectation value of $\phi^*\phi$ appears. As a consequence, the system goes over into a superconducting (SC) phase (note: there is so far no mention of persistent electric currents!).

For bulk superconductivity again the gradient terms are $= 0$ (if nothing forces A_i, ϕ to vary, they remain constant). For inhomogenous situations (boundaries, external B) they are essential, and then, for dimensional reasons, two distance scales appear in the broken (SC) phase:

- For ϕ:

$$K\partial^2\phi^2 + a\phi^2 \quad \Rightarrow \xi = \sqrt{\frac{K}{-a}} \tag{7.58}$$

  which as before is the coherence length for the "kink" $= \sqrt{2}/m_{\text{Higgs}}$.

- For A_i:

$$\begin{aligned}\widetilde{K}\partial^2A^2 + \overbrace{K\,e_3^2\,\phi^2}^{\text{"photon mass"}}\;A^2 \Rightarrow \delta &= \sqrt{\frac{\widetilde{K}}{K}}\frac{1}{e_3 < |\phi|\sqrt{2} >}\\ &= \sqrt{\frac{\widetilde{K}}{K}}\frac{1}{e_3\sqrt{\frac{-a}{b}}} = \frac{\hbar}{m_\gamma c}\end{aligned} \tag{7.59}$$

  which is the penetration depth of $\boldsymbol{A}$ and $\boldsymbol{B}$.

The ratio of the two scales, κ, is an important parameter:

$$\kappa^2 = \frac{\delta^2}{\xi^2} = \frac{\widetilde{K}}{K}\frac{b}{e_3^2} \ . \tag{7.60}$$

The value $\kappa^2 = 1/2$ separates type I and type II superconductors, with significantly different properties.

7.6 London equation

The classical field configuration ϕ, A_k again has to satisfy the equations of motion. For ϕ one varies F with respect to ϕ^* and obtains the EOM

$$-KD_kD_k\phi + a\phi + 2b|\phi|^2\phi = 0. \tag{7.61}$$

This is just (7.28) with $\partial_i \to D_i$.

For A_k we have

$$\frac{\delta F}{\delta A_k} = 0 \Rightarrow \frac{\partial L}{\partial A_k} - \partial_i \frac{\partial L}{\partial \partial_i A_k} = 0 \ , \tag{7.62}$$

which leads to

$$-\widetilde{K}\partial_i[\partial_i A_k - \partial_k A_i] - iKe_3\left[\phi^* D_k\phi - (D_k\phi)^*\phi\right] = 0 \ , \tag{7.63}$$

where $-\widetilde{K}\partial_i[\partial_i A_k - \partial_k A_i] = \widetilde{K}(\boldsymbol{\nabla}\times\boldsymbol{B})_k$ This, of course, is just Maxwell's equation ($\widetilde{K} \to \mu_0$) $\boldsymbol{\nabla}\times\boldsymbol{B} = \mu_0\mathbf{J}$ without the electric field term and with a derived current satisfying current conservation:

$$\begin{aligned} J_k &= +iKe_3\big[\phi^*(\partial_k\phi + ie_3A_k\phi) - (\partial_k\phi^* - ie_3A_k\phi^*)\phi\big], \\ \partial_k J_k &= \boldsymbol{\nabla}\cdot\boldsymbol{J} = 0 \ . \end{aligned} \tag{7.64}$$

This is just the current (7.45) with the derivative ∂_i replaced by the covariant derivative D_i. Inserting here $\phi = |\phi|e^{iS}$, one obtains the "London equation" (1935)

$$\boldsymbol{J} = -2Ke_3|\phi|^2\boldsymbol{\nabla}S - 2e_3^2K|\phi|^2\boldsymbol{A} = \text{electric current} = \frac{1}{\mu_0}\boldsymbol{\nabla}\times\boldsymbol{B} \ , \tag{7.65}$$

where $\boldsymbol{\nabla}S$ is the gradient of phase. The current $\mathbf{J}$ is, by construction, locally gauge invariant. Gauge invariance requires both the phase S and $\boldsymbol{A}$; a change in S is compensated for by a change in $\mathbf{A}$. For a simply connected region one can "gauge away" the phase, just do the gauge transformation $\phi \to e^{-iS(\boldsymbol{x})}\phi$. To see the reason for this limitation, take S to be the azimuthal angle around the z axis, $\tan S = y/x$. Then $\boldsymbol{\nabla}\times\boldsymbol{\nabla}S = 2\pi\delta^2(\mathbf{r})$, $\mathbf{r} = (x, y, 0)$ (cf. the discussion of superfluid rotational flow) and ($d\mathbf{A}$ is here the surface element)

$$\oint \nabla S\cdot d\mathbf{l} = \int \nabla\times\nabla S\cdot d\mathbf{A} = 2\pi.$$

Thus the existence of the vortex line prevents one from gauging away S.

So where is the magic supercurrent, current without ΔV? The key is symmetry breaking, we have

$$|\phi|^2 = \begin{cases} 0 \text{ in symmetrical normal phase.} \\ \frac{-a}{2b} \text{ in broken SC phase.} \end{cases} \tag{7.66}$$

so that the current vanishes in the normal symmetric phase but it is non-zero in the broken phase. Introducing the penetration length by

$$\frac{1}{\delta^2} = \frac{2Ke_3^2|\phi|^2}{\widetilde{K}} \tag{7.67}$$

and assuming that $|\phi|$ = constant, we can as well write the London equation (7.65) in the form

$$\delta^2 \boldsymbol{\nabla} \times \boldsymbol{B} + \boldsymbol{A} = -\frac{2\pi}{e_3}\frac{\boldsymbol{\nabla} S}{2\pi} \ , \tag{7.68}$$

where

$$\frac{2\pi}{e_3} = \frac{2\pi\hbar}{e} = \frac{h}{e} = 4.13 \cdot 10^{-15}\text{Vs} \tag{7.69}$$

is the flux quantum. Taking again S to be the azimuthal angle and applying $\boldsymbol{\nabla}\times$ once more leads to

$$\delta^2 \boldsymbol{\nabla} \times (\boldsymbol{\nabla} \times \boldsymbol{B}) + \boldsymbol{B} = -\delta^2 \nabla^2 \boldsymbol{B} + \boldsymbol{B} = -\frac{2\pi}{e_3}\delta^2(\mathbf{r}). \tag{7.70}$$

To see the meaning of δ, choose a gauge in which $S = 0$ and the geometry $\boldsymbol{A} = (0,\ A(x),\ 0) \Rightarrow \boldsymbol{B} = (0,\ 0,\ A'(x)) \Rightarrow \boldsymbol{\nabla} \times \boldsymbol{B} = (0, -A''(x), 0)$. Then

$$-\delta^2 A''(x) + A(x) = 0 \quad \Rightarrow A(x) = e^{-x/\delta} A(0) \ . \tag{7.71}$$

Thus the supercurrent is located near the surface, together with the magnetic field B. This is the Meissner effect. We shall study this with more realistic approximations in Section 7.8.

7.7 Ginzburg-Landau as 3d field theory

The three-dimensional U(1)+Higgs theory is a locally gauge invariant 3-dimensional continuum U(1) + complex scalar field theory defined by the functional integral

$$Z = \int \mathcal{D}A_i \mathcal{D}\phi \, \exp\big[-S(A_i,\phi)\big] = \exp\big[-Ve_3^6 f(y,x)\big], \tag{7.72}$$

$$S = \int d^3x \left[\frac{1}{4}(\partial_i A_j - \partial_j A_i)^2 + |(\partial_i + ie_3 A_i)\phi|^2 + m_3^2 \phi^*\phi + \lambda_3 \left(\phi^*\phi\right)^2\right]. \tag{7.73}$$

The parameters m_3, e_3^2, λ_3 of the Lagrangian have the dimension GeV and the fields have dimension $\text{GeV}^{1/2}$. Since the theory in eq. (7.73) is a continuum field theory, one has to carry out ultraviolet renormalization. In 3d the couplings e_3^2 and λ_3 are not renormalised in the ultraviolet, but there is a linear 1-loop and a logarithmic 2-loop divergence for the mass parameter m_3^2. In the $\overline{\text{MS}}$ dimensional regularization scheme in $3 - 2\epsilon$ dimensions the renormalized mass parameter becomes

$$m_3^2(\mu) = \frac{-4e_3^4 + 8\lambda_3 e_3^2 - 8\lambda_3^2}{16\pi^2} \log\frac{\Lambda_m}{\mu}, \tag{7.74}$$

where μ is the running scale and Λ_m is a scale independent physical mass parameter of the theory. Instead of it it is more convenient to use $m_3(e_3^2)$. Choosing e_3^2 to set the scale, the physics of the theory will depend on the two dimensionless ratios

$$y = \frac{m_3^2(e_3^2)}{e_3^4}, \quad x = \frac{\lambda_3}{e_3^2}. \tag{7.75}$$

The standard tree-level symmetry breaking analysis starts by inserting to the action $\phi = (v + \phi_1 + i\phi_2)/\sqrt{2}$ (leave out the subscript 3):

$$\begin{aligned} S \;\; = \;\; & \int d^3x \Big[\tfrac{1}{4}(\partial_i A_j - \partial_j A_i)^2 + \tfrac{1}{2}e^2(v^2 + 2v\phi_1 + \phi_1^2 + \phi_2^2)A_iA_i + evA_i\partial_i\phi_2 + eA_i(\phi_1\partial_i\phi_2 - \phi 2\partial_i\phi_1) \\ & + \tfrac{1}{2}m^2v^2 + \tfrac{1}{4}\lambda v^4 + \tfrac{1}{2}(\partial_i\phi_1\partial_i\phi_1 + \partial_i\phi_2\partial_i\phi_2) + \tfrac{1}{2}(m^2 + 3\lambda v^2)\phi_1^2 + \tfrac{1}{2}(m^2 + \lambda v^2)\phi_2^2 \\ & + (m^2 + \lambda v^2)v\phi_1 + \tfrac{1}{4}\lambda(\phi_1^2 + \phi_2^2)^2 + \lambda v\phi_1((\phi_1^2 + \phi_2^2) \Big], \end{aligned} \tag{7.76}$$

from which one reads the usual tree-level ground state values

$$v = \sqrt{\frac{-m^2}{\lambda}}, \quad m_1 = m_{\text{Higgs}} = \sqrt{-2m^2} = \sqrt{2\lambda}v, \quad m_2 = m_{\text{Goldstone}} = 0, \quad m_A = ev. \tag{7.77}$$

Earlier $\xi = \sqrt{2}/m_{\text{Higgs}}$ was the correlation length and $\delta = 1/m_A$ was the penetration length. There are many different names and notations for these two quantities. On the tree level

$$\frac{m_H^2}{m_A^2} = \frac{2\lambda}{e^2} = 2\kappa^2 = 2x;$$

large Higgs mass correponds to large λ (as also in the Standard Model) and the tree level boundary between type I and II is at $x = \kappa^2 = 1/2$.

Symmetry breaking has also produced several new interaction terms in Eq. (7.76). The mixed term $m_A A_i\partial_i\phi_2$ can be disposed of by partially integrating and choosing the Coulomb gauge $\partial_i A_i = 0$. Further perturbative quantisation of the theory Eq. (7.76) by gauge fixing is discussed in particle physics text books[1]. However, perturbation theory has only a limited range of applicability and, fundamentally, all physics lies in expectation values of various operators. Since this is a gauge theory, only gauge invariant operators have non-vanishing expectation values. The most relevant one of these are the local (depending only on one point x) operators of lowest dimensionality:

- Dim = 1: the $J^{PC} = 0^{++}$ scalar $O(\mathbf{x}) = \phi^\star(\mathbf{x})\phi(\mathbf{x})$,
- Dim = 1.5: the $J^{PC} = 1^{+-}$ vector $\tilde{O}_i(\mathbf{x}) \equiv B_i = \epsilon_{ijk}F_{jk}(\mathbf{x})/2$ ($F_{ij} = \partial_i A_j - \partial_j A_i$),
- Dim = 2: the $J^{PC} = 1^{--}$ vector $O_i(\mathbf{x}) = \text{Im}\phi^\star(\mathbf{x})D_i\phi(\mathbf{x})$ ($D_i = \partial_i + ie_3A_i$), the 1^{-+} vector $\text{Re}\phi^\star D_i\phi = \partial_i\phi^\star\phi/2$ and the 0^{++} scalar $(\phi^\star\phi)^2$,
- Dim=3: The 0^{++} scalars $F_{ij}F_{ij}$ and $\phi^\star D_iD_i\phi$, the 1^{+-} vector $\phi^\star B_i\phi$ and the 2^{++} tensor $\phi^\star[\{D_i, D_j\} - 2/d\ \delta_{ij}D_kD_k]\phi$,
- Dim = 3.5: The 0^{--} scalar $B_i\,\partial_i\phi^\star\phi$ and the 0^{-+} scalar $B_i\,\text{Im}\phi^\star D_i\phi$,
- Dim = 4: The 0^{+-} scalar $\partial_i\phi^\star\phi\,\text{Im}\phi^\star D_i\phi$

The quantum numbers here refer to O(3). From these one can further construct bilocal, etc. operators and correlators of the above operators, depending on two points.

The first topic of importance is the phase structure of the theory. The critical curve $y = y_c(x)$ (see Fig. 7.7) divides the plane in two disjoint regions, the symmetric phase at $y > y_c(x)$ and the broken phase at $y < y_c(x)$.

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[1] See e.g. Bailin-Love, Introduction to gauge field theory, section 13.5

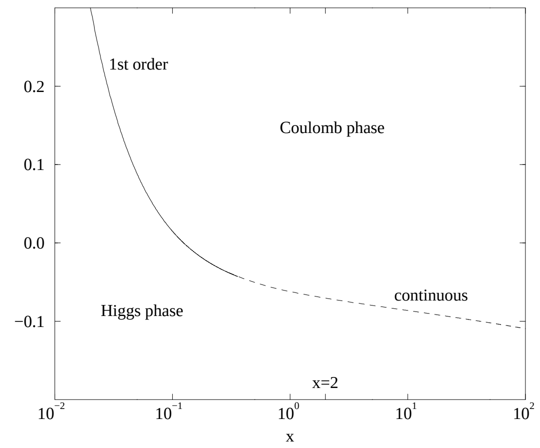

Figure 7.8: The phase diagram of 3d GL theory. Order parameters separating the phases are either the gauge field mass or the vortex tension.

The presence of a critical curve is signalled by singularities in the free energy $Z = \exp\bigl[-Ve_3^6 f(y,x)\bigr]$. On the tree level the critical curve is at $m_3^2 = 0$ (or at $y = 0$). Including fluctuations to one loop, the effective potential becomes

$$V_{1-\mathrm{loop}}/e_3^6 = \frac{1}{4}x\hat{\phi}^2\left[\left(\hat{\phi} - \frac{1}{3\pi x}\right)^2 + \frac{2y}{x}\left(1 - \frac{1}{18\pi^2 xy}\right)\right]. \tag{7.78}$$

Two degenerate states are obtained when the last term vanishes. From this one finds for the critical curve $y_c(x)$, for the upper and lower metastability branches $y_\pm(x)$, the latent heat-like jump $\Delta\ell_3$ of the order parameter-like quantity $\ell_3 \equiv \langle\phi^\dagger\phi(e_3^2)\rangle/e_3^2$ between the broken and symmetric phases at y_c and for the interface tension $\sigma_3 \equiv \sigma/e_3^4$, defined in perturbation theory by

$$\sigma_3 = \int_0^{\phi_b/e_3} d(\phi/e_3)\sqrt{2V(\phi/e_3)/e_3^6}, \tag{7.79}$$

where V is the perturbatively computed effective potential, the following values

$$y_c(x) = \frac{1}{18\pi^2 x}, \quad y_+(x) = \frac{1}{16\pi^2 x}, \quad y_-(x) = 0, \tag{7.80}$$

$$\hat{\phi}_{\mathrm{symm}} = 0, \quad \hat{\phi}_{\mathrm{broken}} = \frac{1}{3\pi x}, \tag{7.81}$$

$$\ell_3 = \frac{1}{18\pi^2 x^2}, \quad \sigma_3 = \frac{2^{3/2}}{648\pi^3 x^{5/2}}. \tag{7.82}$$

Perturbation theory becomes unreliable for large λ_3 or $x > 0.1$ and the transition becomes continuous there. This is also the region of type II superconductors. What is crucial is that there **is** a phase transition there, the phase transition does not first have a first order line which then ends in a second order critical point like the Ising model transition. The point is that there is an order parameter which distinguishes these two phases. This order parameter could, for example, be the gauge field mass. $m_A \equiv m_V \equiv m_\gamma$, which is $= 0$ in the symmetric Coulomb and $\neq 0$ in the broken Higgs phase. Equally, it could be the tension of a vortex line. This can be calculated in the mean-field approximation by solving the field equations numerically. The result can be written in the form

$$T_{\mathrm{MF}} = \frac{\Delta S}{L} = -\frac{y}{x}\pi\mathcal{E}(\sqrt{2x}), \tag{7.83}$$

where the function $\mathcal{E}$, with the value $\mathcal{E}(1) = 1$, has been calculated numerically in, e.g., Ref. [?]. Of course, one must also be able to compute it quite generally as an operator expectation value. Much work on this has been done in Helsinki. **Referenssit**

If one extends the above from U(1)+Higgs gauge theory to SU(2)+fundamental representation Higgs gauge theory, one obtains a theory which describes the thermodynamics of the electroweak theory. Then the phase diagram looks much like that in Fig. 7.7 but with the qualitatively crucial difference: there the 1st order line really ends in a critical point, for larger x or self-coupling λ or the Higgs mass there is no phase transition, only a "cross-over". When all numbers are put carefully together, the endpoint corresponds to Higgs masses of the order of 77 GeV. This is far below the present (2006) lower limit of m_H so that in the physical minimal standard model there is no electroweak phase transition.

7.8 Normal-superconducting interface tension

See the classic work by Ginzburg-Landau from 1950, reprinted in Landau's collected works or Landau & Lifshitz Stat Phys vol. 2 §46 for motivation of separating type I ($\sigma > 0$) and type II ($\sigma < 0$) SC.

Consider now a physical situation in which one forces a magnetic field through a superconductor. Superconductivity then must be at least locally lost and superconductors differ in how this happens. For type I B penetrates through a thick rope while for type II B penetrates through a lattice of vortices. Effectively, in type I the vortices attract each other so that it is more favourable to join them in a rope. In type II they repel and want to be as far from each other as possible, i.e., they form a lattice. Quantitatively, an elegant way to see this difference is to compute the interface tension σ of a planar interface between normal and superconducting phases. For positive σ it pays to reduce the number of interfaces so that the vortices attract each other.

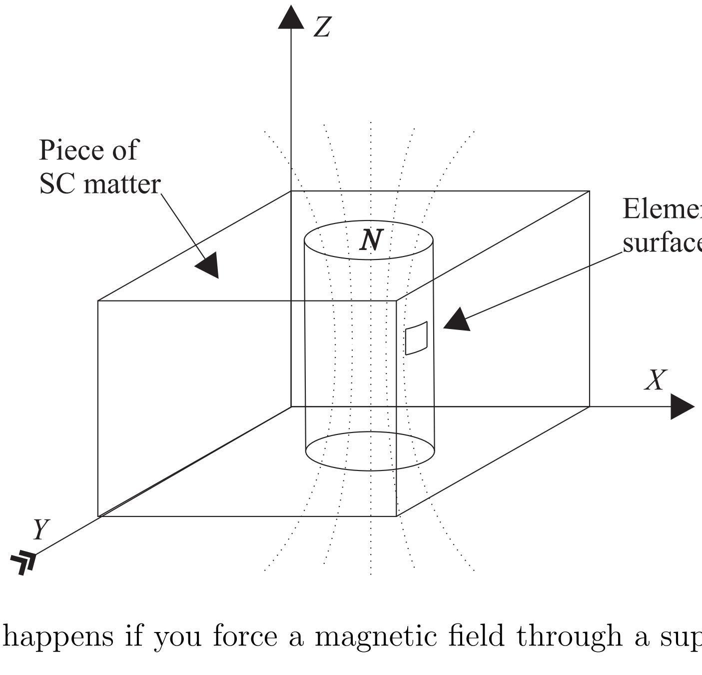

Figure 7.9: What happens if you force a magnetic field through a superconductor? For type I a rope is formed.

Assume now that the interface is in the y, z plane and that the magnetic and the order parameter fields only depend on x and are

$$\phi = \phi(x) = \text{real} \quad \text{(gauge choice)}, \tag{7.84}$$
$$\boldsymbol{A} = (0,\, A(x),\, 0), \tag{7.85}$$
$$\boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A} = (0,\, 0,\, A'(x)). \tag{7.86}$$

The gauge has been fixed by transforming away the phase of ϕ. We also change the notation to the particle physics one, $a \to m^2$, $b \to \lambda$, $K = \widetilde{K} = 1$. Note that $\mathbf{B}$ lies in the interface. The interface tension is F/Area, where

$$F = \int \underbrace{dy\,dz}_{=\text{area}}\, dx \left[\frac{1}{4}F_{ij}^2 + (D_i\phi)^* D_i\phi + m^2\phi^*\phi + \lambda(\phi^*\phi)^2\right].$$

For the present interface geometry

$$\begin{aligned}\frac{1}{4}F_{ij}^2 &= \frac{1}{2}B_z^2 = \frac{1}{2}\big[A'(x)\big]^2\\ |D_i\phi|^2 &= (\partial_i\phi - ie_3A_i\phi)(\partial_i\phi + ie_3A_i\phi) \qquad (\phi^* = \phi!)\\ &= [\phi'(x)]^2 + e_3^2A^2\phi^2\end{aligned}$$

so that

$$\frac{F}{\text{Area}} = \int_{-\infty}^{\infty} dx\Big[\frac{1}{2}(A'(x))^2 + (\phi'(x))^2 + (e_3^2A^2(x) + m^2)\phi^2(x) + \lambda\phi^4(x)\Big] \equiv \int_{-\infty}^{\infty} dx f(x). \tag{7.87}$$

The equations of motion extremising this are

$$\begin{aligned}\tfrac{\partial L}{\partial A} - \partial_x\tfrac{\partial L}{\partial A'} = 0 \qquad &\Rightarrow \qquad A''(x) = 2e_3^2A(x)\phi^2(x)\\ \tfrac{\partial L}{\partial \phi} - \partial_x\tfrac{\partial L}{\partial \phi'} = 0 \qquad &\Rightarrow \qquad \phi''(x) = \big[e_3^2A^2(x) + m^2\big]\phi(x) + 2\lambda\phi^3(x)\ .\end{aligned} \tag{7.88}$$

To solve these equations of motion we also need boundary conditions. We fix them so that the SC phase is at $x > 0$ and the normal phase at $x < 0$. Then, for $x \to \infty$, $\phi(x) \to \langle\phi\rangle = \sqrt{-m^2/2\lambda}$, $A \to 0$, $f(x) \to -m^4/(4\lambda)$. For $x \to -\infty$ $B = A' \to H_c$, $\phi \to 0$, $f(x) \to \frac{1}{2}H_c^2$, where the limiting value H_c is determined in a moment. To isolate $f_{\text{interface}}(x)$ we must demand that $f_{\text{interface}}(x) \to 0$ for $x \to \pm\infty$. This is solved for $x \to +\infty$ by modifying $f(x)$ by $(A')^2 \to (A' - H_c)^2$:

$$\frac{F_{\text{interface}}}{\text{Area}} = \sigma = \int_{-\infty}^{\infty} dx\Big[\frac{1}{2}(A' - H_c)^2 + (\phi')^2 + (e_3^2A^2 + m^2)\phi^2 + \lambda\phi^4\Big]. \tag{7.89}$$

so that

$$f_{\text{interface}}(x \to +\infty) = \frac{1}{2}H_c^2 - \frac{m^4}{4\lambda} = 0. \tag{7.90}$$

Thus one has determined

$$\frac{1}{2}H_c^2 = \frac{m^4}{4\lambda}, \tag{7.91}$$

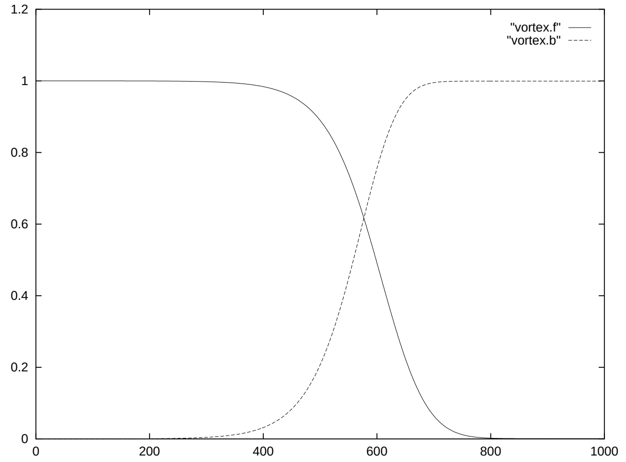

Figure 7.10: Configurations of $\phi(x)$ (grows to the left) and $B(x)$ (grows to the right) for zero interface tension, $\lambda = \frac{1}{2}e_3^2$. Here the SC broken phase is to the left, $x < 0$.

which just expresses the fact that the magnetic energy density on the normal side should equal the condensate energy density on the broken side.

Multiplying the first of the EOMs (7.88) by A' and the second by ϕ' one derives a first integral

$$\frac{1}{2}A'^2 - (e_3^2A^2 + m^2)\phi^2 + \phi'^2 - \lambda\phi^4 = \frac{m^4}{4\lambda}, \tag{7.92}$$

where the constant is determined from boundary conditions. With this one can further write the interface tension in equivalent forms

$$\sigma = \int_{-\infty}^{\infty} dx \left(A'^2 - H_cA' + 2\phi'^2\right) = \int_{-\infty}^{\infty} dx \left[\frac{1}{2}(A' - H_c)^2 - \lambda\phi^4\right]. \tag{7.93}$$

From this we can analytically compute that

- For small $\lambda \ll e_3^2$ the coherence length $\xi = 1/\sqrt{-m^2}$ is much larger than the penetration length $\delta = \sqrt{\lambda/e_3^2(-m^2)}$. The magnetic field then drops suddenly at the interface at $x = 0$ to zero and we can focus only on ϕ. Eq. (7.92) then becomes $\phi' = \sqrt{\lambda}(\langle\phi\rangle^2 - \phi^2)$ which is solved by $\phi = \langle\phi\rangle\tanh(x/\sqrt{2}\xi)$. Inserting this to the first of (7.93) then gives, integrating over $x > 0$,
$$\sigma = \frac{\sqrt{2}}{3}\frac{(-m^2)^{3/2}}{\lambda}. \tag{7.94}$$

- The tension decreases with increasing λ and, remarkably, it vanishes, according to the second of (7.93), if
$$A' - H_c = -\sqrt{2\lambda}\phi^2. \tag{7.95}$$
A closer inspection of the EOMs shows that this happens when $\lambda = \frac{1}{2}e_3^2$ or $\kappa^2 = \frac{\delta^2}{\xi^2} = \frac{\widetilde{K}}{K}\frac{b}{e_3^2} = \frac{1}{2}$. This is shown in detail in Eqs.(46.15-46.18) of Landau & Lifshiz, Stat Phys, part 2, §46. The corresponding numerically computed field configurations are shown in Fig. 7.8.

- For $\lambda > \frac{1}{2}e_3^2$ $\sigma < 0$ and one minimises free energy by maximising the amount of interface, i.e., it pays to distribute the total amount of flux among a number of vortex lines, each carrying a flux quantum h/e.

We thus have two types of superconductors, which differ in how they react to an imposed flux of magnetic field:
$$\Phi_B = B \cdot \text{Area}. \tag{7.96}$$

- Type I has $\sigma > 0$ and the imposed flux forms a rope parallel to $\mathbf{B}$ to minimize the area (perpendicular to $\mathbf{B}$).

- Type II has $\sigma < 0$ and the imposed flux penetrates the plasma through a lattice of (Abrikosov) vortices parallel to $\mathbf{B}$.

Thermodynamically, B is a "canonical" variable (or actually its extensive volume integral $VB = L_z \cdot \Phi_B$), which can be spatially inhomogeneous. Its analogue is N, the particle number. For B we can write $VB = L_z(2\pi/e_3)N$, where N now is the number of flux quanta. The conjugate intensive "grand canonical" (it lets $\Phi_B = BA$ or the number of flux quanta fluctuate) variable is H, which is homogeneous, like the chemical potential μ. Thus we can write $F(T, V, N, B) = E - TS = -pV + \mu N + H \cdot VB$, taking account of the vector nature of $\mathbf{B}$ in a suitable way.

Chapter 8

Physics in 1 + 2 dimensions

8.1 Landau states

Many novel physical phenomena take place in 1+2 dimensions that are not possible in 1+3 dimensions. Experimentally, a two dimensional system is realised either by having an independence of the third spatial dimension or by confining the system effectively to two dimensions by having the thickness of the system in the third dimension much smaller than the relevant dynamical length scale, e.g. correlation length, in two dimensions.

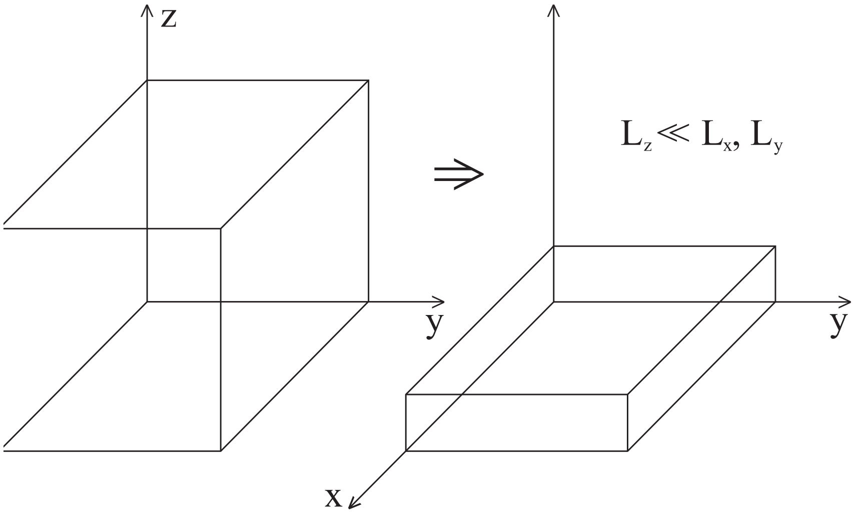

Figure 8.1: 2d means $L_z \ll$ transverse dynamical scales $\ll L_x, L_y$.

Hall effect. The classical two dimensional example is a thin strip of wire in a magnetic field and dates back to E. H. Hall in 1879. Let the wire be in the (x, y)-plane with a current j_x while the constant magnetic field B points to the z-direction, as depicted in Fig.8.1. The ensuing Lorentz force displaces the current electrons into the y-direction:

$$\mathbf{F} = -e(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \propto \hat{e}_y \ . \tag{8.1}$$

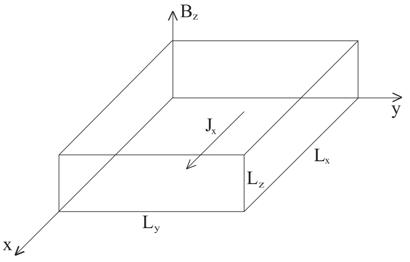

Figure 8.2: The Hall effect.

In addition, the electrons may collide with a collision time τ. As a consequence, the average momentum flow after time Δt reads $\mathbf{p}(t+\Delta t) = (1-\Delta t/\tau)\mathbf{p}(t) + \mathbf{F}\Delta t$ so that

$$\frac{d\mathbf{p}}{dt} = -\frac{\mathbf{p}}{\tau} - e\mathbf{E} - \frac{\mathbf{p}}{m} \times \mathbf{B} \ . \tag{8.2}$$

The steady state is achived when $dp_k/dt = 0$ for $k = x, y$. Thus, multiplying Eq. (8.2) by $-ne\tau/m$ we arrive at

$$\begin{aligned} \sigma E_x &= \frac{eB\tau}{m} j_y + j_x \\ \sigma E_y &= -\frac{eB\tau}{m} j_x + j_y \end{aligned} \tag{8.3}$$

where $\sigma = ne^2\tau/m$ and $\mathbf{j} = ne\mathbf{p}/m$. Balancing now the Lorentz force out so that $j_y = 0$ we find that at equilibrium

$$E_y = -\frac{B}{ne} j_x \ . \tag{8.4}$$

The combination

$$R_H \equiv \frac{E_y}{j_x B_z} = \frac{1}{en} \tag{8.5}$$

is the Hall coefficient that can be measured experimentally. It does not depend on the material of the conducting strip but depends on the sign of e.

Classically a charged particle in a constant magnetic field $\mathbf{B} = (0,0,B)$ moves under the effect of the Lorentz force in a circular path with the Larmor frequency and the Larmor radius given by

$$\omega_L = \frac{eB}{m}, \qquad r_L = \frac{v}{\omega} = \frac{mv}{eB}. \tag{8.6}$$

Quantum mechanically one writes down the Schrödinger equation with $\mathbf{p} \to \mathbf{p} - e\mathbf{A}$. There are various gauge choices, such as

$$\left\{ \begin{array}{l} \mathbf{A} = \frac{1}{2}B(-y, x, 0) \\ \mathbf{A} = B(-y, 0, 0) \end{array} \right. \Rightarrow \mathbf{B} = (0,0,B)$$

and and choosing the latter one (the "Landau gauge"; the former is the "symmetric gauge") one obtains the Schrödinger equation for the transverse coordinates x, y:

$$-\frac{\hbar^2}{2m}[(\partial_x - i\frac{y}{l_B^2})^2 + {\partial_y}^2]\psi(x,y) = E\psi(x,y), \tag{8.7}$$

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[0] Landau, born 1908, ZfP 64(1930)629, Kittel Quantum theory of solids, p.217

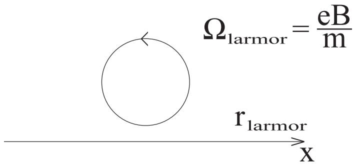

Figure 8.3: Classical motion in a magnetic field

where $l_B = \sqrt{\frac{\hbar}{eB}} = 260\text{Å}1/\sqrt{B/\text{T}}$. Since the z-dependence is trivial, one obviously has

$$\psi(x, y, z) \sim e^{ik_z \cdot z}\psi(x, y), \tag{8.8}$$

and since there is no coordinate dependence on x, the x dependence is $\sim e^{ik_x x}$ and, comparing with the harmonic oscillator Schrödinger equation with the wave functions

$$\psi(x) = \frac{1}{\sqrt{2^n n! x_0 \sqrt{\pi}}} e^{-\frac{1}{2}(\frac{x}{x_0})^2} H_n(\frac{x}{x_0}), \quad x_0^2 \equiv \frac{\hbar}{m\omega}, \tag{8.9}$$

$(H_0 = 1, H_1 = 2x, H_2 = -2 + 4x^2, \dots)$ one finds that Eq. (8.7) is solved by

$$\psi_N(x, y) = N_0 e^{ik_x x} \exp\left[-\frac{1}{2}(\frac{y}{l_B} - l_B k_x)^2\right] H_N(\frac{y}{l_B} - l_B k_x), \tag{8.10}$$

with the energy eigenvalues, called the *Landau levels*,

$$E_N = \frac{p_z^2}{2m} + (N + \frac{1}{2})\hbar\omega_L. \tag{8.11}$$

In the last term

$$\hbar\omega_L = \frac{\hbar^2}{m l_B^2} \tag{8.12}$$

is a quantum Larmor energy. The result is only superficially asymmetric under $x \leftrightarrow y$. The exponential $\exp[-\frac{1}{2}(\frac{y}{l_B} - l_B k_x)^2]$ in Eq. (8.10) has its maximum at

$$y = y_0 = l_B^2 k_x = \frac{\hbar k_x}{eB} = \frac{m v_x}{eB} = r_L \tag{8.13}$$

It is now quite interesting to see how the classical motion is reflected in the quantum mechanical solution.

The key fact here is that E_N does not depend on k_x; in fact, the degeneracy of a state is

$$\frac{e}{h} B L_x L_y.$$

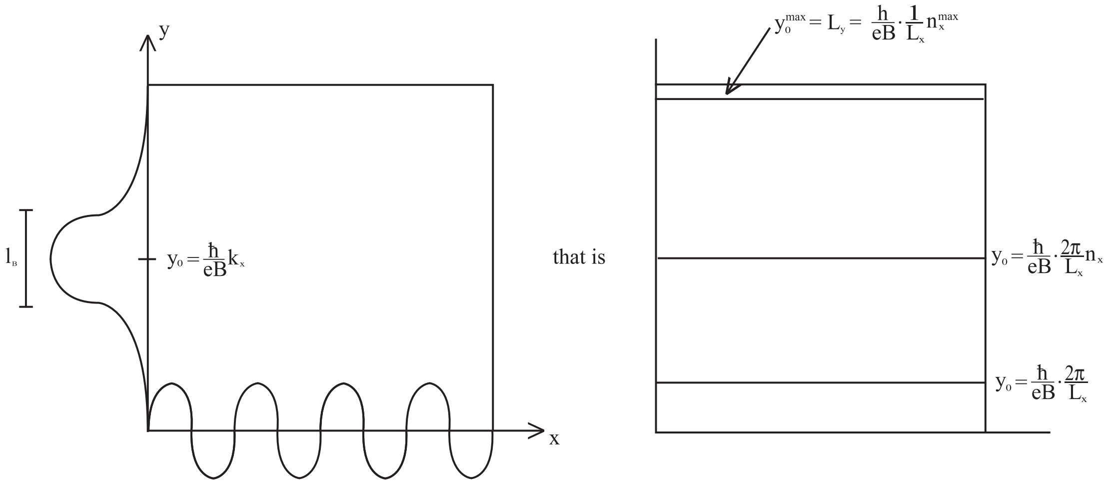

Figure 8.4: Counting the surface density of states

To derive this, note that the x-dependence of the states is $e^{ik_x x}$, where $k_x = 2\pi/L_x n_x,\ n_x = 1, 2, ...$ (periodic boundary conditions). Thus the values of y_0 are $\hbar/(eB) \cdot 2\pi n_x/L_x$, but this has the maximum value L_y so that

$$n_x^{max} = \frac{eB}{h} L_x L_y. \tag{8.14}$$

Since $L_x L_y =$ Area, one finds that the surface density of states is

$$\frac{eB}{h} = \frac{B}{\Phi_0} = \frac{1}{2\pi l_B^2} \frac{\text{states}}{\text{m}^2}. \tag{8.15}$$

Here $h/e \equiv \Phi_0$ =flux quantum $=4.14 \times 10^{-15}$Vs. As a quantitative example, if $B = 1$ T and $L_x = L_y = 1$ cm, then $N_{\text{states}} = \frac{1}{4 \cdot 10^{-15}} (10^{-2})^2 = 10^{10}$ and

$$2\pi l_B^2 = \frac{h}{eB} = \frac{4,14 \cdot 10^{-15} \text{m}^2}{B/\text{T}} \Rightarrow l_B = \frac{2,6 \cdot 10^{-8} m}{\sqrt{B/\text{T}}} = \frac{250\text{Å}}{\sqrt{B/\text{T}}}.$$

To summarize:

- The motion in the z direction, parallel to $\mathbf{B}$, is unaffected by $(0, 0, B) \Rightarrow E = p_z^2/2m$.

- The energy of the motion $\perp$ $\mathbf{B}$ is quantised in steps of $\hbar\omega_{\text{classical}} = \hbar\frac{eB}{m}$.

- Classically the particle can spin around any axis at fixed energy, quantally there are only a finite number of states at any E_N and their number is $\sim L_x L_y =$ Area:

  $$\text{Number of states} = \frac{e}{h} \cdot B L_x L_y = \frac{B \cdot \text{Area}}{h/e} = \frac{\Phi_B}{\Phi_0}$$

  (times 2 for spin). The flux of B is quantised in units of $h/e = 4.14 \cdot 10^{-15}$ Vs.

Flux quantisation also follows from the phase change of a wave function ψ in a vector potential $\mathbf{A}$ along a path from $\mathbf{x}_0$ to $\mathbf{x}$:

$$\psi(\mathbf{x}) = \exp\big[i\frac{e}{\hbar}\int_{\mathbf{x}_0}^{\mathbf{x}} d\mathbf{x}' \cdot \mathbf{A}(\mathbf{x}')\big]\psi_0(\mathbf{x}), \tag{8.16}$$

where ψ_0 is the wave function when $\mathbf{A} = 0$. Taking a closed path then gives a phase change $e/\hbar \cdot \Phi_B$ which has to be $= 2\pi n$ for the wave function to be unique.

8.2 The Quantum Hall effect

When discussing the Landau states, $\psi(\mathbf{x})$ is just the wave function of a quantum mechanical system in general. In practical applications the properties of the system bring in much new physics, as is the case in the classical Hall Effect. This is also true for the Quantum Hall Effect (S. Girvin, cond-mat/9907002).

To see where quantum mechanical effects can appear, we massage the classical relation Eq. (8.4) so that the 2d density $n_{(2)} = N/(L_x L_y)$, $\mathbf{B}$ parallel to the z axis, appears. To this end, let us introduce a potential V_y and the current I_x by

$$E_y = \frac{V_y}{L_y} \qquad J_x = \frac{I_x}{L_y L_z} \tag{8.17}$$

so that

$$\frac{V_y}{L_y \cdot \frac{I_x}{L_y L_z}} = \frac{B}{e\frac{N}{L_x L_y L_z}}, \qquad B \equiv B_z, \tag{8.18}$$

and

$$\rho_{xy} \equiv \frac{V_y}{I_x} = \frac{B}{e\frac{N}{L_x L_y}} \equiv \frac{B}{en_{(2)}} = \frac{1}{\nu}\frac{h}{e^2} = \frac{1}{\nu}25813\frac{V}{A} \tag{8.19}$$

where we used the fact that, in quantum theory, if ν lowest Landau states are filled, the surface density of electrons is

$$\frac{N}{L_x L_y} = \nu\,\frac{eB}{h}. \tag{8.20}$$

This is, qualitatively, the *integer quantum Hall effect.* Note that even here we have said nothing about the electronic structure of the matter, just a place where macroscopic quantum effects could arise has been identified. And, in fact, when measuring ρ_{xy} as a function of B and $n_{(2)}$ one sees an overall decrease with decreasing B and superposed on this plateaus at integer ν.

Understanding the plateaus requires a more detailed discussion of the behavior of Landau states in solids, i.e., here the detailed properties of solids have an effect. This goes even further with the observation (in 1982) that there are plateaus also at fractional values of ν, which is called the *fractional quantum Hall effect.* To explain this one has to include the effects due to the Coulomb forces between electrons. As a consequence, there arises quasiparticles with a fractional charge together with a novel form of a many-body ground state.

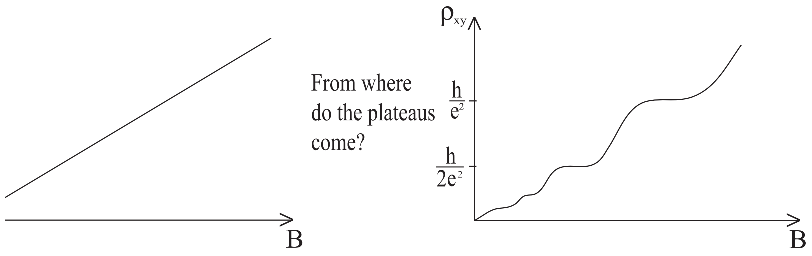

Figure 8.5: ρ_{xy} as a function of B

Consider relevant scales quantitatively. We have

$$l_B = \frac{260\text{Å}}{\sqrt{B/T}} \qquad \hbar\Omega = \hbar\frac{eB}{m_e^*} = 19\text{K}\cdot(B/\text{T}), \tag{8.21}$$

wher $m_e^* = 0.07m_e$ (the effective m_e in matter). To occupy the lowest Landau state we thus must have $T \ll 19\text{K}\cdot\frac{B}{\text{T}}$; in practice $T \sim 0.1$K. The average Coulomb interaction is

$$\begin{aligned}\frac{e^2}{4\pi\epsilon\epsilon_0 l_B} &= \frac{e^2}{\epsilon\cdot 4\pi\epsilon_0\hbar c}\cdot\frac{\hbar c}{l_B} \\ &= \frac{1}{\epsilon}\cdot\frac{1}{137}\cdot\frac{0.229K\cdot 10^8\text{Å}}{2.6\cdot 10^2\text{Å}}\sqrt{B/\text{T}} \\ &= \frac{1}{\epsilon}\cdot 643K\cdot\sqrt{B/T}. \end{aligned}\tag{8.22}$$

In matter $\epsilon \approx 10$ so that the interaction term is quite large in comparison with $\hbar\Omega$.

[Part 3: "Attached Text"]

8.3 Topology in two dimensions

Physics in two dimensions can be different from physics in three dimensions because of topology. Even the statistics of particles can, on general grounds, deviate from the usual Fermi-Dirac or Bose-Einstein of three dimensional world. This is related to the fact that in 2d one may define a winding number that does not exist in 3d.

Consider two 2d quantum states $|x_1\rangle$ and $|x_2\rangle$ as depicted in Fig. XXXX. The amplitude for moving from x_1 to x_2 is given by

$$A = \langle x_1|x_2\rangle = e^{i\delta\theta} = e^{\theta_0 + iN\phi/\pi} \tag{8.23}$$

where $\delta\theta$ is the total path, θ_0 the single-valued amplitude and the winding number N counts how many times the path goes around the origin. In contrast, in 3d the angle ϕ cannot be defined unambiguously as the path can always be "lifted" from the 2d plane; the path does not matter. Thus in 3d we must require that

$$e^{iN\phi/\pi} = e^{iN\phi'/\pi} \tag{8.24}$$

if $\phi' = \phi + 2n\pi$. It then follows that we must also require that $e^{2inN} = 1$ or that only the windings

$$N = 0,\ \pi \tag{8.25}$$

are allowed. It then follows that changing the labels in a two-particle wave function (by reflecting $x_1 \leftrightarrow x_2$ or setting $\phi \rightarrow \pi$) in 3d means that

$$\psi_{21} = e^{iN\phi/\pi}\psi_{12} = e^{iN}\psi_{12} = \pm\psi_{12}\ . \tag{8.26}$$

Hence only the completely symmetric (Bose-Einstein) or completely antisymmetric (Fermi-Dirac) statistics are possible in 3d.

In 2d any winding number, and therefore *any statistics*, is possible. Hence the name *any*on, which is a particle that can obey a statistics that interpolates between Fermi-Dirac and Bose-Einstein.

Aharonov-Bohm effect. A well-known quantum mechanical example of the fact that in 2d path matters is the Aharonov-Bohm effect. Let there be a magnetic flux $\Phi = \int \mathbf{B} \cdot d\mathbf{A}$ pointing to the z-direction and confined to a small domain in the (x, y)-plane. Then

$$\Phi = \int B_z dA = \int \epsilon^{ij}\partial_i A_j\ dA = \oint d\mathbf{x} \cdot \mathbf{A}\ , \tag{8.27}$$

where ϵ^{ij} is the totally antisymmetric tensor. Let us choose a gauge

$$A_k = \frac{\Phi}{2\pi}\partial_k\theta(\mathbf{x}) = \frac{\Phi}{2\pi}\epsilon_k\dot{j}\frac{x_j}{r^2}\ , \tag{8.28}$$

where θ is the angle around the flux. Taking

$$B_z = \left\{ \begin{array}{ll} B & r < R_0 \\ 0 & r > R_0 \end{array} \right. \rightarrow A_\theta = \left\{ \begin{array}{ll} \frac{1}{2\pi} & r < R_0 \\ \frac{\Phi}{2\pi} & r > R_0 \end{array} \right. . \tag{8.29}$$

Let us now consider a particle moving in 2d in a circle round the flux with a Hamiltonian

$$H = \frac{1}{2m}(\mathbf{p} + e\mathbf{A})^2 + V(r)\ , \tag{8.30}$$

where the potential V generates the circular orbit at $r > R_0$. A gauge transform $\mathbf{A} \rightarrow \mathbf{A} + \nabla\theta(\mathbf{x})$ changes the wave function of the particle by $\psi \rightarrow e^{ie\theta(\mathbf{x})/h}$ so that going around once produces a total phase

$$\theta_{\text{tot}} = \int \theta(\mathbf{x})dl = \int_0^{2\pi} \frac{\Phi}{2\pi r} r d\phi = \Phi\ . \tag{8.31}$$

8.4 Anyons

The Aharonov-Bohm effect provides a natural starting point for modelling anyons. We may consider 2d particles moving under the influence of a hypothetical gauge field which is pure gauge and called the *Chern-Simons gauge field*:

$$\mathbf{A} = \frac{\alpha\phi_0}{2\pi}\nabla\theta = \frac{\alpha\phi_0}{2\pi}\frac{\hat{e}_\theta}{r}\ . \tag{8.32}$$

Here α and ϕ_0 are parameters and are chosen for the convenience of the presentation. Since the Chern-Simons (CS) gauge field is pure gauge, it can be gauged away by $\mathbf{A} \rightarrow \mathbf{A} + \nabla\xi$

except at $r = 0$, where it is singular. The corresponding magnetic field is zero except at $r = 0$, where $\mathbf{B} = \alpha\phi_0\delta^{(2)}(\mathbf{r})$. As in the Aharonov-Bohm case, there is always a non-zero magnetic fluc $\Phi = \alpha\phi_0$. In the presence of the CS gauge field particles will achieve a phase factor which effectively changes the statistics they obey; hence they are anyons.

Let us consider two generic anyons. Their relative angular momentum is

$$\mathbf{L} = \mathbf{r} \times (\mathbf{p} - \mathbf{A}) = \mathbf{r} \times (i\nabla + \frac{\alpha\phi_0}{2\pi}\hat{e}_\theta r) = -i\partial_\theta + i\frac{\alpha\phi_0}{2\pi} \ , \tag{8.33}$$

where we have chosen the CS charge $e = 1$ for convenience.

The wave function should be single-valued under $\mathbf{r} \to -\mathbf{r}$ so that the operator $i\partial_\theta$ has integer eigenvalues. Thus the total angular momentum is fractional:

$$L = n + \frac{\alpha\phi_0}{2\pi} \ . \tag{8.34}$$

Let us now take a specific example by considering two electrons and a CS gauge field with $\alpha\phi_0 = (2n+1)2\pi$. Such anyons are in fact bosons:

$$\psi_{12} = -e^{i\alpha\phi/2}\psi_{21} = -e^{(2n+1)\pi i}\psi_{21} = \psi_{21} \ . \tag{8.35}$$

There is a mean CS magnetic field $B_{\text{CS}} = \alpha\phi_0 n$ (n sums over the electrons). Recall that in the quantum Hall effect $E \propto B$ so that energy is minimized when the real magnetic field eB is cancelled against the CS field B_{CS}. Then one obtains

$$n = \frac{eB}{\alpha\phi_0} = \frac{eB}{2\pi}\frac{1}{2n+1} \tag{8.36}$$

giving rise to a fractional guantum Hall effect. Here the filling factor $\nu = 1/(2n+1)$ is odd as observed.

We may also consider the quantum mechanics of two anyons in more detail. The Hamiltonian is

$$H = \frac{1}{2M}[(\mathbf{p_1} + e\mathbf{A}(x_1))^2 + (\mathbf{p_2} + e\mathbf{A}(x_2))^2] + V(r) \tag{8.37}$$

where $r = |\mathbf{x_1} - \mathbf{x_2}|$ and $e \equiv e^*$ is the effective charge. $\mathbf{A}(x_1) = \frac{\alpha\hbar}{e^*}\nabla\theta(\mathbf{x_1} - \mathbf{x_2})$ is the Chern-Simons field with $\mathbf{A}(x_2) = -\mathbf{A}(x_1)$.

Let us write $H = H_{CM} + H_r$, where H_{CM} is the center-of-mass motion and H_r is the relative motion with

$$\begin{cases} H_{CM} = \frac{p_{CM}^2}{2m_{CM}} & m_{CM} = 2M \\ H_r = \frac{1}{2m_r}(\mathbf{p_r} - e^*\mathbf{A}(r))^2 + V(r) & m_r = \frac{M}{2} \end{cases} \tag{8.38}$$

H_{CM} simply yields a free plane wave while for the relative motion we should solve the Schrödinger equation with

$$H_r = -\frac{\hbar^2}{2m}\left[\frac{1}{r}\frac{d}{dr}(r\frac{d}{dr}) + \frac{1}{r^2}(\frac{d}{d\theta} + i\alpha)^2\right] + V(r) \ . \tag{8.39}$$

If we choose a harmonic potential, $V = \frac{1}{4}m_r\omega^2r^2$, one finds that the energy levels are given by

$$E = \hbar\omega[2n + 1 + |l + \alpha|], \tag{8.40}$$

where $l + \alpha$ is the fractional angular momentum.

One could also consider a gas of anyons. For N anyons

$$H = \sum_{i=1}^{N} \frac{1}{2m}[\mathbf{p_i} + \frac{e}{c}\mathbf{a_i}(\mathbf{x_i})]^2 + \frac{1}{2}m\omega^2\mathbf{x_i}^2 \ . \tag{8.41}$$

The last term is an external harmonic potential for the interacting anyons, and the CS gauge field reads now

$$\mathbf{a_i} = \frac{\alpha\Phi_0}{2\pi}\sum_{j\neq i}\frac{\hat{\mathbf{e}}|\mathbf{x_i} - \mathbf{x_j}|}{|\mathbf{x_i} - \mathbf{x_j}|^2} \ . \tag{8.42}$$

Again one may separate the center-of-mass motion and the relative motion to write the partition function as

$$Z_N = Z_{CM}Z_{RM} \tag{8.43}$$

where the CMS part is trivially

$$Z_{CM} = \frac{u}{u-1}, \qquad u = e^{-\beta\hbar\omega} \ . \tag{8.44}$$

However, Z_{RM} is a complicated story and depends e.g. on whether $[\alpha] = \text{Int}\,\alpha$ is even or odd. Defining $\delta \equiv [\alpha] - \alpha$ one finds for odd $[\alpha]$:

$$Z_N(\omega) = \frac{1}{N!}\cosh[\frac{\beta\hbar\omega N(N-1)\delta}{2}] \times \prod_{l=1}^{N}[\frac{l}{2\sinh(\beta\hbar\omega\frac{l}{2})}]^2 \tag{8.45}$$

and likewise for even $[\alpha]$; for details, see Phys.Rev.Lett. 68(1992)1621.

Appendix A

Units, conventions

We shall use units in which always $k_B = 1$ (unit of temperature is the same as energy) and mostly $\hbar = c = 1$. The gravitational constant G we keep. For completeness, we shall unsystematically in various places insert proper factors of $c, \hbar$.

Conceptually, what is happening here is that these constants of nature are conversion factors:

$$
\begin{aligned}
k_B &= \frac{\text{energy}}{\text{temperature}}, \\
c &= \frac{\text{distance}}{\text{time}}, \\
\hbar &= \frac{\text{energy}}{\text{frequency}}, \\
\frac{G}{\mathrm{c}^4} &= \frac{\text{curvature} = 1/\mathrm{m}^2}{\text{energy density}}.
\end{aligned}
$$

Physics teaches us that temperature is energy, distance and time are related (special relativity), energy and frequency are related (quantum mechanics) and curvature and energy density are related (general relativity) and it is clearly possible to use the same units in measuring either of the pairs.

Numbers:

$$
\begin{aligned}
\hbar &= 1.054573 \cdot 10^{-34}\mathrm{Js} = 6.58212 \cdot 10^{-22}\mathrm{MeV\,s} = 7.64 \cdot 10^{-12}\,\mathrm{Ks} = 1 \\
\hbar c &= 197.327\,\mathrm{MeV\,fm} = 0.229\,\mathrm{K\,cm} = 1973\mathrm{eV}\,\mathrm{\mathring{A}} \\
\alpha &= \frac{e^2}{4\pi\epsilon_0\hbar c} = \frac{1}{137.03599} \quad \text{at scale 0} \\
r_{\mathrm{Bohr}} &= \frac{1}{\alpha}\frac{\hbar}{m_e c} = 0.5291772 \cdot 10^{-10}\mathrm{m} \\
\frac{h}{e} &= 4.14 \cdot 10^{-15}\,\mathrm{Vs} \quad \text{flux quantum} \\
\frac{h}{e^2} &= 25813\,\frac{\mathrm{V}}{\mathrm{A}}
\end{aligned}
$$

Planck units:

$$\begin{aligned} \text{mass} &= \sqrt{\hbar c/G} = 2.177 \cdot 10^{-8}\,\text{kg} \\ \text{length} &= \sqrt{\hbar G/c^3} = 1.616 \cdot 10^{-35}\,\text{m} \\ \text{time} &= \sqrt{\hbar G/c^5} = 5.391 \cdot 10^{-44}\,\text{s} \\ \text{power} &= c^5/G = 3.63 \cdot 10^{52}\,\text{W} \end{aligned}$$

Energy ↔ circular or linear frequency, momentum ↔ wave number or wave length:

$$\begin{aligned} E &= \hbar\omega = h\nu (= \hbar c k = \frac{hc}{\lambda} = \hbar c \frac{2\pi}{\lambda}, \quad \text{for photons}), \\ p &= \hbar k = \frac{h}{\lambda}. \end{aligned}$$

Appendix B

Exercises

Many-body Phenomena. MoKa SL04

Exercise 1

1. Refresh your thermodynamical skills by showing that

$$C_p - C_V = \frac{TV\alpha^2}{\kappa_T},$$

where the heat capacities, the coefficient of thermal expansion α and the isothermal compressibility κ_T are defined by

$$C_p = T\left(\frac{\partial S}{\partial T}\right)_p, \quad C_V = T\left(\frac{\partial S}{\partial T}\right)_V,$$
$$\alpha = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_p, \quad \kappa_T = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_T.$$

2. Calculate the Gaussian integral

$$\int_{-\infty}^{\infty} \mathrm{d}\boldsymbol{x} \exp\left(-\frac{1}{2}\boldsymbol{x}^{\mathrm{T}}A\boldsymbol{x} - \boldsymbol{b}^{\mathrm{T}}\boldsymbol{x}\right),$$

where $\boldsymbol{x}$ and $\boldsymbol{b}$ are n-dimensional vectors and A is a diagonalizable, positive definite $n \times n$-matrix.

3. Calculate the density of states of a Maxwell-Boltzmann gas on N non-interacting particles by performing the inverse Laplace transformation of the partition function:

$$g(E,N) = \frac{1}{2\pi i}\int_{-i\infty+\beta_c}^{i\infty+\beta_c} \mathrm{d}\beta\, e^{\beta E} Z(\beta,N),$$

where β_c is the saddle-point of the integrand, and

$$Z(\beta,N) = \frac{1}{N!}\left(\frac{V}{\pi^2\beta^3}\right)^N.$$

4. Calculate the most probable, the mean, and the root mean square absolute velocity in the ideal gas, using the normalized velocity distribution

$$f(\boldsymbol{v}) = \left(\frac{m}{2\pi T}\right)^{3/2} \exp\left[-\frac{m\boldsymbol{v}^2}{2T}\right].$$

Hint: The differential $d^3w(\boldsymbol{v}) = f(\boldsymbol{v})d^3\boldsymbol{v}$ denotes the probability of finding a particle in the ideal gas with the velocity vector $\boldsymbol{v}$ between (v_x, v_y, v_z) and $(v_x + dv_x, v_y + dv_y, v_z + dv_z)$ independent of its position. Use this to first calculate the probability of finding a particle which has an absolute value of velocity between $|\boldsymbol{v}|$ and $|\boldsymbol{v}| + |d\boldsymbol{v}|$.

5. Consider a system of 4 particles and 12 possible states $i = 1, \ldots, 12$ for each of them. The probability to deliver a particle to a state i depends on the distribution of previously delivered particles in the following way. The Pauli exclusion principle forbids two particles to occupy the same state. If a state i is previously unoccupied, the probability for its occupation depends on the occupation number of the neighboring states $i-1$ and $i+1$ such that

$$p(i) \;=\; \begin{cases} p_0 & \text{if } i-1 \text{ and } i+1 \text{ are not occupied} \\ p_0/2 & \text{if either } i-1 \text{ or } i+1 \text{ is occupied} \\ p_0/4 & \text{if both } i-1 \text{ and } i+1 \text{ are occupied} \end{cases}$$

where p_0 is to be normalized in such a way that the particle is delivered to some state for certainty. Periodic boundary conditions are assumed (that is, state $i \equiv$ state $i + 12$)

a) How many possible partitions are there?

b) What is the average distance $\langle |i - j| \rangle$ of particles (distances are not calculated over the boundaries)? You may need to write a short computer code to solve the problem.

Exercise 2

1. Some history on "Physics is where the action is": for Finnish-speaking participants, read the articles **http://www.tieteessatapahtuu.fi/0304/pekonen.pdf** and **http://www.tieteessatapahtuu.fi/0304/maupertuis.pdf** and try to find out how in the latter Maupertuis's formulation is related to today's formulation of the action principle, i.e., that the classical equation of motion for $q(t)$ is the function extremizing $S = \int dt\, L(q, \dot{q})$, $L = T - V$. Remember Snell's law $n_1 \sin\theta_1 = n_2 \sin\theta_2$, velocity of light in matter $= c/n$. Note that Maupertuis had the velocity of light all wrong. Unfortunately Google does not locate Maupertuis's original "Accord de différentes lois de la nature qui avaient jusqu'ici paru incompatibles" but non-Finnish-speaking participants might try to find something in other languages.

2. Solve the diffusion equation

$$\partial_t n(t,x) \;=\; D\partial_x^2 n(t,x), \qquad n(0,x) = \delta(x)$$

by solving for the Fourier transform $n(\omega, k)$ and inverting back to $n(t,x)$. Compare with the matrix element $\langle x_1 | e^{-\epsilon H} | x_2 \rangle$ encountered in the derivation of the path integral form of $\mathrm{Tr} e^{-\beta H}$.

3. Calculate the imaginary time correlator

$$\langle x(\tau) x(0) \rangle \;=\; \mathrm{Tr}\left[e^{-\beta H} x(\tau) x(0) \right]$$

for the harmonic oscillator in one dimension. Put a complete set of states to appropriate places, relate $x(\tau)$ to $x(0)$ with the use of the time-evolution equation and use the known matrix elements of x for the harmonic oscillator.

4. - 5. The following intermediate step was met with in the derivation of the path integral form of the partition function

$$\begin{aligned} Z \;&=\; \mathrm{Tr}\, e^{-\beta H} = \sum_{\text{states}} e^{-\frac{E_n}{T}}, \qquad H = \frac{p^2}{2m} + V(x) \\ &=\; \int \prod_1^N \frac{dx_i}{\sqrt{\frac{2\pi\hbar\epsilon}{m}}} \exp\Big[-\frac{\epsilon}{\hbar} \Big\{ \frac{m}{2} [(\frac{x_1 - x_2}{\epsilon})^2 + \ldots + (\frac{x_N - x_{N-1}}{\epsilon})^2 + (\frac{x_1 - x_N}{\epsilon})^2] \\ &\qquad\qquad + V_1 + V_2 + \ldots + V_N \Big\} \Big] \end{aligned}$$

Take now $V(x) = \frac{1}{2}m\omega^2 x^2$ and evaluate this Gaussian integral for finite N, then take $N \to \infty$ to recover the simple form of the vibrational partition function. To evaluate the finite-N integral you need the determinant

$$\begin{vmatrix} 1 & -a & 0 & 0 & \cdots & 0 & -a \\ -a & 1 & -a & 0 & \cdots & 0 & 0 \\ 0 & -a & 1 & -a & \cdots & 0 & 0 \\ 0 & 0 & -a & 1 & -a & & \vdots \\ \vdots & \vdots & \vdots & & \ddots & & 0 \\ 0 & 0 & 0 & & & & -a \\ -a & 0 & 0 & \cdots & 0 & -a & 1 \end{vmatrix} .$$

The non-zero elements on the upper-right and lower-left corners make the evaluation problematic. It is easier to first calculate the transition element $\langle x_1|\mathrm{e}^{-\beta H}|x_{N+1}\rangle$, for which these corner elements are not there. That can be calculated by recursively relating the $N \times N$ and $N-1 \times N-1$ determinants to $N-1 \times N-1$ and $N-2 \times N-2$ determinants. The recursion relation can be solved by writing it in terms of a 2×2 matrix, and then diagonalizing that matrix. The desired end result is obtained when we equate $x_1 = x_{N+1}$ and perform the integral

$$Z = \int_{-\infty}^{\infty} \mathrm{d}x \, \langle x|\mathrm{e}^{-\beta H}|x\rangle$$

Exercise 3

1. The temperature of the cosmic microwave background (CMB) is today $T = 2.735$ K. What are the average and median photon frequencies and wave lengths in CMB? How many photons are there per cm^3? Imagine that the CMB photons are trapped in a box with a size L_0. If the box size scales in time as $L(t) = L_0(t/t_0)^{2/3}$ (as in our Universe), when did the CMB photon temperature equal the surface temperature of the Sun (= 6000 K)?

2. Compute the following large-T ($T \gg m$) expansion (or as many terms as you can) of the pressure of an ideal gas of bosons:

$$\begin{aligned} p(T) - p(0) &= -T\int \frac{\mathrm{d}^3k}{(2\pi)^3} \ln(1 - e^{-\beta\sqrt{k^2+m^2}}) \\ &= \frac{\pi^2 T^4}{90} - \frac{m^2T^2}{24} + \frac{m^3T}{12\pi} + \frac{m^4}{64\pi^2}\left(\ln\frac{m^2}{T^2} - 2\ln 4\pi + 2\gamma_E - \frac{3}{2}\right) + \mathcal{O}(m^6/T^6). \end{aligned}$$

   (γ_E = Euler gamma)

3. Show that the particle number fluctuations for quantum ideal gases in the grand canonical ensemble are

$$\begin{aligned} \langle (n_k - \bar{n}_k)^2 \rangle &= \bar{n}_k(1 \mp \bar{n}_k)\,, \\ \langle (N - \bar{N})^2 \rangle &= \bar{N} \mp \sum\nolimits_k \bar{n}_k^2\,, \end{aligned}$$

   where $\bar{n}_k = 1/[\exp\beta(E_k - \mu) \pm 1]$ is the equilibrium occupation number, $\bar{N} = \sum_k \bar{n}_k$ and where the upper sign refers to FD gas, the lower to BE one. Note that the distribution in any n_k is an exponential distribution, $P_n \sim e^{-\lambda n}$, $\lambda = \text{const}$. The brave may even compute the third central moment $\langle (n_k - \bar{n}_k)^3 \rangle$.

4. Consider the Euclidean action

$$\int_0^{\beta\hbar} \mathrm{d}\tau \left[\frac{m}{2}\dot{q}^2 + V(q)\right]$$

in the limits β fixed, $\hbar \to 0$ (classical limit) or $\beta \to 0$, $\hbar$ fixed (large T limit). Show that in these limits only the zero mode $q = \text{const.} = q_0$ contributes to the functional integral form of Z so that $Z = e^{-\beta V(q_0)}$. Take $\tau' = \tau/(\beta\hbar)$ as a new variable. Which are the configurations dominating if $\hbar \to 0, \beta\hbar = \text{const}$?

5. Assume we have a 1+1d theory with a linear term in the potential: $L = \frac{1}{2}m\dot{x}^2 + \frac{1}{2}m\omega^2 x^2 + m\omega_0 x$. Calculate the partition function $Z(T)$ and normalize it to the partition function of the harmonic oscillator ($\omega_0 = 0$).

Exercise 4

1. The energy flux from the Sun is 1400 W/m^2 and it comes with a Bose-Einstein energy distribution corresponding to 6000 K. What is the photon flux, number/s/m^2? What is the density of photons, number/m^3, in the radiation? How does is compare with the density of photons in thermal equilibrium at 6000 K? What is the incident energy density in photons and what is the radiation pressure?
2. You know that, for a bosonic system,
$$\Omega = -Vp(T, \mu) = T \sum_k \log[1 - e^{\beta(\mu - E_k)}].$$
Derive from this the entropy S and internal energy E in terms of the average occupation number
$$n_k = \frac{1}{e^{\beta(E_k - \mu)} - 1}$$
of the state k.
3. Compute the integral
$$\int_0^\infty dx\, x^2 \left(\frac{1}{e^{x-y} + 1} - \frac{1}{e^{x+y} + 1} \right)$$
by evaluating its Taylor series around $y = 0$. When computing d/dy, note that this is $\pm d/dx$ and get rid of the d/dx by partial integration.
4. Consider an ideal gas of ^{87}Rb atoms at $T = 0$, confined by the harmonic trap $V(r) = \frac{1}{2}m\omega^2 r^2$ where m is the mass of the atom. A characteristic trap frequency is $\omega/2\pi = 150$ Hz. Determine the ground state density profile and estimate its width. Find the root-mean-square momentum and velocity of a particle. What is the value of the central density when the number of atoms is 10^4?
5. Consider the specific heat $C = \partial E/\partial T$ of a 3-dimensional Bose gas trapped in a harmonic potential. Show that the classical (i.e. Maxwell-Boltzmann) value at high T is $C = 3N$. Show then that at the transition temperature T_c there is a discontinuity in the specific heat given by
$$\Delta C = -9\frac{\zeta(3)}{\zeta(2)}N = -6.58\ N\ . \tag{B.1}$$

Exercise 5

1. Consider a system of N non-interacting bosons in 2 dimensions in a rectangular box of area L^2 at a temperature T. Let $T \to 0$, will the bosons condense to the ground state? Replace the box by a harmonic trap, $V = \frac{1}{2}m\omega^2(x^2 + y^2)$, what happens then? If condensation is possible, determine at what T it takes place.

2. You are given the functional

$$E[\Psi] = \int d^3x \left[\frac{\hbar^2}{2m} |\nabla\Psi(\mathbf{r})|^2 + V(r)|\Psi(\mathbf{r})|^2 + \frac{1}{2} U_0 |\Psi(\mathbf{r})|^4 \right]. \tag{B.2}$$

   for the wave function $\Psi(\mathbf{r})$, $\int d^3x|\Psi|^2 = N$ of an N-boson condensate. $V(r)$ is the trapping potential and U is a parameter (what are its dimensions?). Vary the total energy with respect to ψ^* while keeping the total number of particles fixed and find the equation giving the extremal configurations, the Gross-Pitaevskii equation.

3. Compute $E[\Psi]$ of the previous problem with $V = \frac{1}{2}m\omega^2 r^2$ for the trial wave function (check normalisation!)

$$\Psi(\mathbf{r}) = \frac{\sqrt{N}}{\pi^{3/4} b^{3/2}} e^{-r^2/(2b^2)}. \tag{B.3}$$

   Write the energy in terms of the parameter x defined by

$$b = \sqrt{\frac{\hbar}{m\omega}}\, x; \tag{B.4}$$

   use the characteristic energy defined by

$$U = \frac{NU_0}{2(2\pi)^{3/2}(\hbar/(m\omega))^{3/2}}. \tag{B.5}$$

   Find the equation giving the minimum of $E(x)$ and solve it assuming x to be $\gg 1$. Find the value $E/N = 5/4 \cdot (2U)^{2/5}(\hbar\omega)^{3/5}$ for the contribution to the energy per particle.

4. Derive the small-T expansion of an integral over the Fermi-Dirac distribution $n(E) = 1/(\exp(\beta(E - \mu)) + 1)$:

$$\int_0^\infty f(E)n(E)dE = \int_0^\mu f(E)dE + \frac{\pi^2}{6}T^2 f'(\mu) + \frac{7\pi^4}{360}T^4 f'''(\mu) + \mathcal{O}((T/\mu)^6)\,,$$

   where $f(E)$ is some sufficiently regular function.

5. Can you from the result of the previous problem derive the grand potential $\Omega(T,\mu)$ of an ideal massless fermion gas, valid at all T and μ? Remember antiparticles with $\mu \to -\mu$.

Exercise 6

1. Consider ultrarelativistic electron gas, $T,\mu \gg m_e$, the Grand Potential of which is $\Omega(T,V,\mu) = -Vp(T,\mu), p = aT^4 + bT^2\mu^2 + c\mu^4$, a, b, c are known constants. Determine its specific heat C_V, especially near the degenerate limit, $T \ll \mu$. Remember that C_V is defined keeping N constant. How does this compare with the standard computation of the specific heat of electrons in metals, $C_V = N \cdot \pi^2/2 \cdot T/T_F$?

2. As an illustration of Pauli principle effects, consider uds-matter (composed of u,d and s quarks of charges 2/3,-1/3,-1/3, respectively) in comparison with normal udd-matter. Show that the average energies per quark are in the ratio

$$\frac{E_q(\text{uds})}{E_q(\text{udd})} = \left(\frac{3}{1+2^{4/3}}\right)^{3/4} \approx 0.89$$

   if the two systems are kept at the same pressure at $T = 0$. Demand charge neutrality (what is the degeneracy factor for spin and colour?) and neglect quark masses (Witten, PRD30 (1984) 272).

3. Determine the surface temperature T_s of a planet (the earth, in particular) by assuming that the sun radiates as a black body at a temperature 6000 K and that the earth radiates all the energy it gets from the sun as a black body at the temperature T_s. The result will only depend on $T_{\rm sun}$, the radius $R_{\rm sun}$ of the sun and the planet-sun distance R, not on $R_{\rm planet}$ nor on the Stefan-Boltzmann constant σ. Apply to the earth starting from the fact that the observed angular diameter of the sun from the earth is 0.57 degrees.

4. Use the uncertainty principle to estimate the size of a Cooper pair. To get Δp assume that the uncertainty in the energy of the pair is the gap Δ. Compare with the average electron-electron distance.

5. Consider a thermodynamic system in two phases Q and H at $\mu = 0$ with

$$\begin{aligned} p_q(T) &= a_q T^4 - B, \\ p_h(T) &= a_h T^4, \\ a_q &> a_h, \quad B = \text{constant}. \end{aligned}$$

Sketch a plot p_q and p_h as a function of T, find which one of the phases is the equilibrium one and find the temperature T_c at which both phases are in equilibrium. Plot similarly the entropy density $s(T)$ and energy density $\epsilon(T)$ for both phases and compute the latent heat $L \equiv T_c[s_q(T_c) - s_h(T_c)]$. What would be the values of a_q, a_h if this were a model of the quark-hadron phase transition with the Q phase containing gluons and u,d quarks and the hadron phase containing massless pions of charges $\pm, 0$. What would then be B if $T_c = 200$ MeV?

Exercise 7

1. At any T the superconducting gap equation is

$$1 = gT \sum_{n=-\infty}^{\infty} \int \frac{d^3k}{(2\pi)^3} \frac{1}{(\hbar\omega_n)^2 + \xi_k^2 + \Delta^2},$$

where $\hbar\omega_n = (2n+1)\pi T$, g is a four-fermion coupling, and $\xi_k = \hbar^2 k^2/(2m) - E_F \approx v_F(p - p_F)$. Derive from here the equation

$$1 = g \cdot g(E_F) \int_0^\delta \frac{d\xi}{\sqrt{\xi^2 + \Delta^2}} \tanh\left[\frac{1}{2}\beta\sqrt{\xi^2 + \Delta^2}\right]$$

for the T-dependence of the gap $\Delta(T)$; $\delta = \hbar\omega_{\rm Debye}$ and $g(E_F)$ is the density of states on the Fermi surface.

Use:

$$\sum_{n=-\infty}^{\infty} \frac{x}{(2n+1)^2\pi^2 + x^2} = \frac{1}{2} - \frac{1}{e^x + 1}$$

2. In the weak coupling limit $\Delta \ll \delta$, derive that

$$\log \frac{\Delta(0)}{\Delta(T)} = 2I\left(\frac{\Delta(T)}{T}\right),$$

$$I(y) = \int_0^\infty \frac{dx}{\sqrt{x^2 + y^2}} \frac{1}{(\exp\sqrt{x^2 + y^2} + 1)}.$$

Derive the large-y and small-y expansions of $I(y)$ (the latter is $I(y) = \frac{1}{2}\log(\pi/y) - \frac{1}{2}\gamma_{\rm Euler} + 7\zeta(3)/(16\pi^2)y^2 + \ldots$). Find from here T_c in terms of $\Delta(0)$ and study the behavior of $\Delta(T)$ when $T \to 0$ and $T \to T_c$.

3. Show that the dissipative part of the momentum flux density,

$$\Delta\Pi_{ik} = \eta\left(\partial_k v_i + \partial_i v_k - \frac{2}{3}\delta_{ik}\nabla\cdot\boldsymbol{v}\right) + \zeta\delta_{ik}\nabla\cdot\boldsymbol{v}$$

where η and ζ are shear and bulk viscosities, vanishes when the fluid is in constant rotational motion, ($\boldsymbol{v} = \boldsymbol{\omega}\times\boldsymbol{x}$). Show also that if the fluid is expanding in the radial direction, $\Delta\Pi_{ik}$ depends only on ζ.

4. Show that the Euler equations lead to entropy conservation, $\partial s/\partial t + \mathbf{v}\cdot\nabla s = 0$.

5. Show that the energy density satisfies the equation ($U = E/V$ is the internal energy density)

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\rho v^2 + U\right) + \nabla\cdot\left[\left(\frac{1}{2}\rho v^2 + U + p\right)\boldsymbol{v}\right] = 0$$

using the Euler and the continuity equations together with entropy conservation.

Exercise 8

1. Let us assume that we have a one-dimensional ideal gas at rest at pressure p_0 and density ρ_0 in a container extending over $0 \le x < \infty$. The equation of state is

$$p = p_0\left(\frac{\rho}{\rho_0}\right)^{\gamma}, \quad \gamma \ge 1, \quad v_s^2 = \left.\frac{\partial p}{\partial \rho}\right|_S .$$

The plug of the container at $x = 0$ is removed at $t = 0$. How does the gas flow out of the container, i.e., what is the velocity field $v(x,t)$? Plot a figure of what is happening.

To solve this, write down the continuity and Euler equations in $1+1$ dimensions and take into account that $\partial_x p = v_s^2(\rho)\partial_x\rho$. Use the fact that v and ρ depend only on x/t (the flow is a similarity flow) and show that $v + v_s = x/t$ and that $v - \int_0^\rho d\rho v_s(\rho)/\rho = \text{const}$, then solve $v = 2/(\gamma-1)\cdot[x/t - v_s(0)]$.

2. In the previous problem, what are the particle trajectories in the (x,t)-plane, i.e., what is the path followed by a particle when it leaks out of the container?

3. Consider a situation in which there initially is non-relativistic fluid with constant ρ_0, p_0 at rest, $\mathbf{v} = 0$. Then a gravitational field $\mathbf{g}$, $\nabla\cdot\mathbf{g} = -\mathbf{4\pi G}\rho$, is imposed; effects of gravity are neglected for the initial configuration. Add small perturbations $\rho_1, p_1, \mathbf{v}, \mathbf{g}_1$, linearize the continuity and Euler equations and find a dispersion relation

$$\omega^2 = v_s^2\mathbf{k}^2 - 4\pi G\rho_0.$$

Argue that this is an instability and determine the associated length and time scales. In what time would the sun collapse if the gas pressure were turned off?

4. Consider viscous flow, i.e., one in which

$$\Delta\Pi_{ik} = \eta\left(\partial_k v_i + \partial_i v_k - \frac{2}{3}\delta_{ik}\nabla\cdot\boldsymbol{v}\right) + \zeta\delta_{ik}\nabla\cdot\boldsymbol{v}$$

is added to the spatial part of the energy-momentum tensor. Consider small oscillations around the constant configuration $\epsilon_0, p_0, \mathbf{v} = 0$, linearize the equations of motion using Fourier components and show first that there is a transverse (relative to $\mathbf{k}$) mode with the dispersion relation

$$\omega = \frac{-i\eta}{\epsilon_0 + p_0}\mathbf{k}^2.$$

Why is this called a diffusive mode?

5. As in the previous problem, but now for the longitudinal modes. Show that their dispersion relation becomes
$$\omega = \pm v_s|\mathbf{k}| - iL\mathbf{k}^2, \quad L = \frac{4\eta/3 + \zeta}{\epsilon_0 + p_0}.$$
What is the time and space dependence of these sound waves?

Exercise 9

1. In the last problem of the previous exercise it was shown that there is a longitudinal mode with the dispersion relation
$$\omega = \pm v_s|\mathbf{k}| - iL\mathbf{k}^2, \quad L = \frac{4\eta/3 + \zeta}{\epsilon_0 + p_0}.$$
Discuss numerically, using the value of η obtained from kinetic theory ($\zeta = 0$ in this case), whether this would apply to damping of sound waves in air. Show also that the condition of negligible damping is the same as the usual condition for local thermal equilibrium, mean free path $\ll$ wave length.
2. We have a kinetic equation of the type
$$\frac{dN_i}{dt} = -N_i {\sum_j}' u_{ji} + {\sum_j}' u_{ij} N_j,$$
where N_i, ($\sum_i N_i = N$=constant) is the occupation number of state i, u_{ij} is the probability of the transition $j \to i$ per unit time and the prime means that $i \to i$ is excluded. Assume first T = CP invariance, $u_{ij} = u_{ji}$, and show that
$$S = -\sum_i \frac{N_i}{N} \log \frac{N_i}{N}$$
satisfies $dS/dt \geq 0$. Then prove the same by only assuming unitarity, $\sum_j u_{ij} = \sum_j u_{ji}$ for all i.
3. When is $dS/dt = 0$ in the previous problem? Then consider the same problem with the further constraint that $E = \sum_i N_i$ be constant. When is $dS/dt = 0$ in this case?
4. Consider the kinetic equation for only one type of particles, $f(t, \mathbf{x}, \mathbf{v})$. Write down explicitly the collision term $(\partial f/\partial t)_c$ appropriate for 2→2 collisions and show that it conserves energy and momentum, i.e., satisfies
$$\int d^3p\, \boldsymbol{p} \left(\frac{\partial f}{\partial t}\right)_c = \int d^3p\, E_p \left(\frac{\partial f}{\partial t}\right)_c = 0.$$
5. Show that one obtains the Euler equation by taking the first $\mathbf{v}$ moment of the kinetic equation (i.e., $\int d^3v\, v_i \times$ the equation). You have to argue that $\rho\langle v_i v_k\rangle = \rho u_i u_k + p\delta_{ik}$.

Exercise 10

1. Show that the partition function of the 1d Ising model,
$$Z(T, h) = \sum_{s_1} \cdots \sum_{s_N} \exp\{\beta \sum_1^N [J s_k s_{k+1} + h(s_k + s_{k+1})/2]\}$$

where $s_{N+1} = s_1$ and $N \to \infty$ is understood, can be written as $Z(T,h) = \mathrm{Tr}P^N$, where the elements of the 2×2 matrix P are

$$\langle s|P|s'\rangle = \exp\{\beta \sum_1^N [Jss' + h(s+s')/2]\}.$$

Compute from here the partition function as the $N \to \infty$ limit of the trace.

2. Consider the 2d Ising model at temperature T in a region $0 < x < L_0$, $-L_0 < y < L_0$. Assume that the spin is mostly $+1$ when $y > 0$ and mostly -1 when $y < 0$, but that the boundary line, with endpoints fixed at $x = 0, y = 0$ and $x = L_0, y = 0$, is not straight because of fluctuations. The length of the boundary is

$$L = L_0 + \sum_{k=1}^{L_0} |y_k|,$$

where y_k is the length of the k'th vertical boundary line. Argue that the free energy of the boundary line, $F = -T \ln Z$, can be obtained from

$$Z = \sum_{y_1,y_2,\dots,y_{L_0}=-\infty}^{\infty} \delta\left(y_1 + y_2 + \cdots + y_{L_0}\right) e^{-\frac{2JL}{T}},$$

and estimate that $F = \alpha L_0$, where

$$\alpha = 2J + T \ln \tanh \frac{J}{T}$$

is the surface energy of the Ising model. Plot as a function of T and find T_c.

3. The free energy per site of 2d Ising model is

$$F/N = -T\left[\ln 2 + \frac{2}{(2\pi)^2}\int_0^\pi \int_0^\pi d\xi d\eta \ln\left[\cosh^2\epsilon - \sinh\epsilon\left(\cos\xi + \cos\eta\right)\right]\right],$$

where $\epsilon = \beta J/2$. Show that F degenerates into the free energy per site of $d = 1$ Ising model in the limit $T \to \infty$. Show that the integral is singular when $\sinh\epsilon = 1$ and determine from here T_c.

4. Consider a stochastic differential equation

$$m\ddot{x} + m\gamma\dot{x} = \xi(t), \tag{B.6}$$

where $1/\gamma$ is a relaxation time scale, $\xi(t)$ is a random force with zero average and uncorrelated in time, $\langle\xi(t)\xi(t')\rangle = I\delta(t-t')$, I is to be determined. Integrate first $p(t) = m\dot{x}(t)$ and $x(t)$ with given $x(0) = 0, p(0)$ and compute then the correlators $\langle p(t)p(t+\tau)\rangle$ and $\langle x(t)x(t+\tau) - x^2(t)\rangle$ in the limit $t \gg 1/\gamma$.

5. Argue using the thermalisation condition $\langle p^2(t)/(2m)\rangle = T/2$ that $I = 2\gamma T m$. Determine the diffusion constant using $\langle x^2(t)\rangle$. What is the relation obtained of one inserts γ in terms of viscosity using the Stokes formula? Compare with the formula $\eta = \rho D$ obtained from kinetic theory. How can the formulas be compatible?

Problem 4:

$$p(t) = \int_0^t dt' e^{-\gamma(t-t')}\xi(t') + e^{-\gamma t}p(0)$$

$$mx(t) = \frac{1}{\gamma}p(0)(1 - e^{-\gamma t}) + \frac{1}{\gamma}\int_0^t dt'[1 - e^{-\gamma(t-t')}]\xi(t')$$

$$\langle p(t)p(t+\tau)\rangle = \frac{I}{2\gamma}e^{-\gamma\tau}, \quad \langle x(t)x(t+\tau) - x^2(t)\rangle = \frac{I}{2m^2\gamma^3}(1 - e^{-\gamma\tau})$$

Problem 5:

$$\langle p^2(t)\rangle = T/2\cdot 2m = Tm = \frac{I}{2\gamma} \Rightarrow I = 2\gamma T m$$

$$\langle x^2(t)\rangle = \frac{2T}{m\gamma} = 2Dt \Rightarrow D = \frac{T}{\gamma m} = \frac{T}{6\pi R\eta}$$

(using Stokes: $m\gamma = 6\pi R\eta$). The Einstein relation holds for liquids, the kinetic theory formulas for gases.

Exercise 11

1. The Van der Waals equation of state is

$$\left(p + a\frac{N^2}{V^2}\right)(V - bN) \quad = \quad NT.$$

   Show that close to the critical point the difference between the gas and the liquid densities behaves as

$$n_{\text{gas}} - n_{\text{liquid}} \quad = \quad 4n_c\left(1 - \frac{T}{T_c}\right)^{1/2} + \ldots$$

   What value would you predict for the surface tension of water, knowing that for water $p_c = 2.2\times 10^7$ Pa and $T_c = 647\,\text{K}$. (Experimentally one gets $0.1\,\text{J/m}^2$.)

2. Show that in the mean field approximation the latent heat (discontinuity of $TS(T)$ at T_c per lattice site) of the q-state Potts model is

$$\frac{Kd}{q}\frac{(q-2)^2}{q-1}.$$

3. Consider the $d = 2$, $q = 7$ Potts model in the mean field approximation with the order parameter s defined at the lectures. What is the temperature T_+ at which a non-trivial minimum $s_0 \neq 0$ appears? What is T_c? Plot $s_0(T)$.

4. Consider the free energy density

$$f(\phi, T) \quad = \quad f_0(T) + \frac{1}{2}a_2(T - T_0)\phi^2 + \frac{1}{3}a_3\phi^3 - \phi h,$$

   where ϕ is an order parameter and a_2, a_3, h are constants. The susceptibility is defined by $\chi = (\partial\langle\phi\rangle/\partial h)_T$. Calculate the critical exponents γ, γ' defined by $\chi \sim |t|^{-\gamma}$ for $t \to 0^+$, $\chi \sim |t|^{-\gamma'}$ for $t \to 0^-$, where $t = T - T_c$.

5. Study the phase structure of a system with the free energy density

$$f(\phi, T) = \frac{1}{2}\gamma(T^2 - T_0^2)\phi^2 - \frac{1}{3}\alpha T\phi^3 + \frac{1}{4}\lambda\phi^4,$$

   where α, γ, λ and T_0 are positive parameters. Show that

   (a) The system has a first-order transition with the critical temperature $T_c^2 = T_0^2/[1 - 2\alpha^2/9\lambda\gamma]$.

   (b) The second minimum at $\phi > 0$ exists only when $T^2 \leq T_+^2 = 8T_0^2/[9(T_0/T_c)^2 - 1]$.

   (c) The latent heat $L = 4\gamma\alpha^2 T_0^2 T_c^2/9\lambda^2$.

Exercise 12

1. Consider a system with the free energy

$$f(T,B,M) = -BM + (T - T_c)M^2 + \lambda M^4 + \frac{1}{M_*^2}M^6$$

(M_* is some mass scale) as a function of the order parameter M in the Landau theory.

   (a) Analyse the general behaviour of f and, in particular, its minima in the λ, T plane when $B = 0$.

   (b) Find the first and second order transitions when $B = 0$.

2. An inflationary cosmological phase transition in the background of an expanding universe with radius $R(t)$ may be described by a Landau model with the free energy

$$F = \int \mathrm{d}t \left[\frac{1}{2}\dot{\phi}^2 + V(\phi)\right] R^3(t),$$

where ϕ is a time dependent order parameter and near $\phi \approx 0$ the potential is $V = V_0(1 - \epsilon\phi - \delta\phi^2)$ where $\epsilon, \delta \ll 1$. Initially $\phi = 0$ and $\ddot{\phi}$ is small, $\ddot{\phi} \ll H\dot{\phi}$, $H = \dot{R}/R$. The order parameter is coupled to gravity via the Einstein equation

$$H^2 = \left(\frac{\dot{R}}{R}\right)^2 = \frac{8\pi G}{3}\left(\frac{1}{2}\dot{\phi}^2 + V(\phi)\right).$$

Show that initially R expands exponentially. Study the behaviour of ϕ and estimate the time the exponential expansion ends. What is the value of ϕ at that point?

3. After many years of intensive labour, Theory of Nothing has finally been found. In terms of a complex order parameter M it has the free energy

$$F = \int \mathrm{d}^3x \left[\left(1 - \frac{\kappa}{M_*^2}|M|^2\right)|\nabla M|^2 + \alpha \cdot (T - T_c)|M|^2 + \lambda |M|^4\right],$$

where $\kappa \ll 1$, α is a constant and M_* is some mass scale. Does the theory admit global strings? Study how κ affects $\kappa = 0$ global strings.

4. Liquid crystals are anisotropic fluids formed by lengthy (length/thickness > 10) molecules. The macroscopic state of nematic crystals is described by a unit vector $\mathbf{n}(\mathbf{r})$. According to Landau's theory the equilibrium state of the system can be found by minimising the free energy density, which is a series in the order parameter and its derivatives:

$$f = f_0 + \sum_{ij=1}^{3} a_{ij}\partial_i n_j + \sum_{ikjl} a_{ikjl}\partial_i n_k \partial_j n_l + \ldots.$$

Since the system has to be rotationally invariant, a_{ij} and a_{ikjl} are tensors which have to be formed of n_i ja δ_{ij}. Show that this reduces the expansion to the form

$$f = f_0 + b\mathbf{n}\cdot\nabla\times\mathbf{n} + \tfrac{1}{2}a_1(\nabla\cdot\mathbf{n})^2 + \tfrac{1}{2}a_2(\mathbf{n}\cdot\nabla\times\mathbf{n})^2 + \tfrac{1}{2}a_3[(\mathbf{n}\cdot\nabla)\mathbf{n}]^2 + a_{12}(\mathbf{n}\cdot\nabla\times\mathbf{n})\nabla\cdot\mathbf{n},$$

where the coefficients may depend on the temperature. Separate the symmetric and antisymmetric parts of the tensor $\partial_i n_j$ and relate various terms in the system $\mathbf{n} = (0,0,1)$, in which $\partial_i n_3 = 0$. Argue physically that the coefficients are of the order of $a \approx 10^{-11}$N.

5. Consider superfluid in a cylindrical vessel of radius R and height H.

   (a) Determine the energy and the angular momentum of one vortex parallel to the axis of the cylinder in terms of the superfluid density n_s, mass of the atom m and the quantum of the circulation of the velocity h/m.

(b) Show that the critical angular velocity for the formation of one vortex in the rotation about the axis of the cylinder is

$$\omega_c = \frac{\hbar}{mR^2} \ln \frac{R}{\xi}\,.$$

(c) Show that when the cylinder is rotating at a high angular velocity Ω, the number of vortices per unit area of the surface is

$$N = \frac{2m\Omega}{h}\,.$$

6. A type I superconductor has a 1st order transition at $\mu_0 H_c^2(T)/2 = a^2(T)/4b$, $T < T_c$. Show that there is an entropy jump

$$V\frac{a(T)}{2b}\frac{\mathrm{d}a(T)}{\mathrm{d}T} = V\mu_0 H_c \frac{\mathrm{d}H_c}{\mathrm{d}T}\,,$$

so that the SC phase has a lower entropy. What is the latent heat $L = T\Delta S$, if $H_c = H_{c0}(1 - T^2/T_c^2)$?

7. The following problems collect important general properties of thermal expectation values of operator products. The spatial dependence, $\mathbf{x}, \mathbf{k}$ is suppressed. Assume that $A(t)$ and $B(t)$ are two operators the time dependence of which is given by the evolution operator $\exp(-itH/\hbar)$. The dynamical structure function is defined by

$$J_1(\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t} \langle A(t)B(0)\rangle,$$

where the thermal expectation value is defined by $\langle O\rangle = Z^{-1}\mathrm{Tr}e^{-\beta H}O$. Show that

$$J_2(\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t} \langle B(0)A(t)\rangle = e^{-\beta\omega} J_1(\omega).$$

Insert a complete set of energy eigenstates suitably. Show further that the Fourier transform of the thermal expectation value of the retarded Green's function,

$$G_R(t) = \langle\, i\,[A(t), B(0)]\,\theta(t)\,\rangle$$

is given by

$$G_R(\omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\rho(\omega')}{\omega' - \omega - i\epsilon}, \qquad \rho(\omega) = \tfrac{1}{2}(1 - e^{-\beta\omega})J_1(\omega) = \mathrm{Im}G_R(\omega),$$

where the spectral function $\rho(\omega)$ is the Fourier transform of the commutator $\frac{1}{2}[A(t), B(0)]$. Show finally that the fluctuations of A are obtained from

$$\langle A^2\rangle = \int_0^{\infty} \frac{d\omega}{\pi}\rho(\omega)[1 + n(\omega)], \quad n(\omega) = 1/(e^{\beta\omega} - 1).$$

8. Now continue analytically $G_R(\omega)$ to the imaginary axis by defining

$$G_\beta(\omega_n) = G_R(\omega + i\epsilon \to i\omega_n \equiv i2\pi nT) = \int_0^{\beta} d\tau\, e^{i\omega_n\tau} G_\beta(\tau),$$

where n=integer. Show that $G_\beta(\tau)$ has the representation

$$G_\beta(\tau) = T\sum_{n=-\infty}^{\infty} e^{-i\omega_n\tau} G_\beta(\omega_n) = \int_{-\infty}^{\infty} \frac{d\omega}{\pi}\rho(\omega)\frac{\exp(-\omega\tau)}{1 - \exp(-\beta\omega)}, \quad \tau > 0.$$

To do the sum over n you may have to use Poisson's summation formula.

Finally express the Fourier transform of the thermal expectation value of the usual time ordered product $T(A(t)B(0)) = A(t)B(0)\theta(t) + B(0)A(t)\theta(-t)$ in terms of $\rho(\omega)$. The answer is

$$G_T(\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t} i\langle A(t)B(0)\theta(t) + B(0)A(t)\theta(-t)\rangle = \int_{-\infty}^{\infty} \frac{d\omega'}{\pi}\rho(\omega')\left[\frac{1 + n(\omega')}{\omega' - \omega - i\epsilon} - \frac{n(\omega')}{\omega' - \omega + i\epsilon}\right].$$