2 Quantum field theory on the lattice

2.1 Fundamentals

- Quantum field theory (QFT) can be defined using *Feynman's path integral* [R. Feynman, Rev. Mod. Phys. 20, 1948]:

$$Z = \int \Big[\prod_x d\phi(x)\Big] \exp[iS(\phi)]$$
$$S = \int d^4x \mathcal{L}(\phi, \partial_t\phi)$$

  Here $x = (x_0, x_1, x_2, x_3)$, and $g_{\mu\nu} =$ diag(+,-,-,-)

- Physical observables can be evaluated if we add a source $S \to S + J_x\phi_x$. For example, 1- and connected 2-point functions are:

$$\langle\phi_x\rangle = \frac{\partial}{i\partial J_x}\Big|_{J=0} \log Z = \frac{1}{Z}\int [d\phi]\phi_x \exp[iS]$$

$$\langle\phi_x\phi_y\rangle = \frac{\partial}{i\partial J_x}\frac{\partial}{i\partial J_y} \log Z = \frac{1}{Z}\int [d\phi]\phi_x\phi_y \exp[iS] - \langle\phi_x\rangle^2$$

- These can be computed using perturbation theory, if the coupling constants in S are small (see any of the oodles of QFT textbooks).

- How $\prod_x d\phi(x)$ is defined? Needs regularization.

- *However:* if

  – 4-volume is *finite*, and

  – 4-coordinate x is *discrete* ($x \in aZ^4$, a lattice spacing),

  the integral in (1) has finite dimensionality and can, in principle, be evaluated e.g. by brute force (= computers)

  $\mapsto$ gives fully *non-perturbative* results.

- Need to extrapolate: $V \to \infty$, $a \to 0$ in order to recover continuum physics.

- But:
  - the dimensionality of the integral is (typically) huge
  - $\exp iS$ is complex+unimodular: every configuration $\{\phi\}$ contributes with equal magnitude

  $\mapsto$ extremely slow convergence in numerical computations (useless in practice).
- This is (largely) solved by using *imaginary time formalism* (Euclidean spacetime).
- Imaginary time also admits non-zero temperature T.

2.2 Units:

Standard HEP units, where

$$c = \hbar = k_B = 1,$$

and thus

$$[length]^{-1} = [time]^{-1} = [mass] = [temperature] = [energy] = \text{GeV}.$$

Mass m = rest energy mc^2 = (Compton wavelength)$^{-1}$ $mc/\hbar$.

$$(1\,\text{GeV})^{-1} \approx 0.2\,\text{fm}$$

2.3 Path integral in imaginary time

Consider *scalar field theory* in Minkowski spacetime:

$$S = \int d^3x\,dt\,\mathcal{L}(\phi, \partial_t\phi) = \int d^3x\,dt\,\left[\tfrac{1}{2}\partial_\mu\phi\,\partial^\mu\phi - V(\phi)\right]$$

We obtain the (classical) *Hamiltonian* by Legendre transformation:

$$\begin{aligned} H &= \int d^3x\,dt\,\left[\pi\dot{\phi} - \mathcal{L}\right] \\ &= \int d^3x\,dt\,\left[\tfrac{1}{2}\pi^2 + \tfrac{1}{2}(\partial_i\phi)^2 + V(\phi)\right] \end{aligned}$$

Here π is canonical momentum for ϕ: $\pi = \delta\mathcal{L}/\delta\dot{\phi}$.
Quantum field theory: consider Hilbert space of states $|\phi\rangle$, $|\pi\rangle$, and *field operators* ($\phi \to \hat{\phi}$, $\pi \to \hat{\pi}$, $H \to \hat{H}$), with the usual properties:

- $\hat{\phi}(\bar{x})|\phi\rangle = \phi(\bar{x})|\phi\rangle$
- $\int [\prod_x d\phi(\bar{x})]|\phi\rangle\langle\phi| = 1 \qquad \int [\prod_x d\pi(\bar{x})/(2\pi)]|\pi\rangle\langle\pi| = 1$
- $[\hat{\phi}(\bar{x}), \hat{\phi}(\bar{x}')] = -i\delta^3(\bar{x} - \bar{x}')$
- $\langle\phi|\pi\rangle = \exp\left[i\int d^3x\pi(\bar{x})\phi(\bar{x})\right]$

Time evolution operator is $U(t) = e^{-i\hat{H}t}$

Feynman showed that the quantum theory defined by $\hat{H}$ and the Hilbert space is equivalent to the path integral (1). We shall now do this in imaginary time.

Let us now consider the quantum system in *imaginary time:*

$$t \to \tau = it\,, \qquad \exp[-i\hat{H}t] \to \exp[-\tau\hat{H}]$$

This makes the spacetime *Euclidean*: $g = (+\,-\,-\,-) \to (+\,+\,+\,+)$.
We shall keep the Hamiltonian $\hat{H}$ as-is, and also the Hilbert space.
Let us also discretize space (convenient for us but not necessary at this stage), and use finite volume:

$$\begin{aligned} \bar{x} &= a\bar{n}, \qquad n_i = 0\ldots N_s \\ \int d^3x &\to a^3\sum_x \\ \partial_i\phi &\to \frac{1}{a}[\phi(\bar{x}+\bar{e}_i a) - \phi(\bar{x})] \equiv \Delta_i\phi(\bar{x}) \end{aligned}$$

Thus, the Hamiltonian is:

$$\hat{H} = a^3\sum_x\left[\tfrac{1}{2}[\hat{\pi}(x)]^2 + \tfrac{1}{2}[\Delta_i\hat{\phi}(\bar{x})]^2 + V[\hat{\phi}(\bar{x})]\right]$$

Let us now consider the amplitude $\langle\phi_B|e^{-(\tau_B-\tau_A)\hat{H}}|\phi_A\rangle$:
1) divide time in small intervals: $\tau_B - \tau_A = N_\tau a_\tau$. Obviously

$$\langle\phi_B|e^{-(\tau_B-\tau_A)\hat{H}}|\phi_A\rangle = \langle\phi_B|(e^{-a_\tau\hat{H}})^{N_\tau}|\phi_A\rangle.$$

2) insert 1-operators $\int [\prod_x d\phi_i] |\phi_i\rangle\langle\phi_i|$, $\int [\prod_x d\pi_i] |\pi_i\rangle\langle\pi_i|$

$$
\begin{aligned}
&\langle\phi_B|e^{-\tau\hat{H}}|\phi_A\rangle = \\
&\int \left[\prod_{i=2}^{N_\tau}\prod_x d\phi_i(x)\right]\left[\prod_{i=1}^{N_\tau}\prod_x d\pi_i(x)\right]\langle\phi_B|\pi_{N_\tau}\rangle\langle\pi_{N_\tau}|e^{-a_\tau\hat{H}}|\phi_{N_\tau}\rangle \\
&\times\langle\phi_{N_\tau}|\pi_{N_\tau-1}\rangle\langle\pi_{N_\tau-1}|e^{-a_\tau\hat{H}}|\phi_{N_\tau-1}\rangle\ldots\times\langle\phi_2|\pi_1\rangle\langle\pi_1|e^{-a_\tau\hat{H}}|\phi_A\rangle
\end{aligned}
$$

Thus, we need to calculate

$$
\begin{aligned}
\langle\pi_i|e^{-a_\tau\hat{H}}|\phi_i\rangle &= \exp\left[-a^3a_\tau\sum_x\left(\tfrac{1}{2}\pi_i^2+\tfrac{1}{2}(\Delta_i\phi_i)^2+V[\phi_i]\right)\right] \\
&\times \langle\pi_i|\phi_i\rangle + O(a_\tau^2)
\end{aligned}
$$

and

$$
\begin{aligned}
\langle\phi_{i+1}|\pi_i\rangle\langle\pi_i|\phi_i\rangle &= e^{ia^3\sum_x\pi_i(\bar{x})\phi_{i+1}(\bar{x})}e^{-ia^3\sum_x\pi_i(\bar{x})\phi_i(\bar{x})} \\
&= \exp[ia^3a_\tau\sum_x\pi_i(\bar{x})\Delta_0\phi_i(\bar{x})]
\end{aligned}
$$

where we have defined $\Delta_0\phi_i = \frac{1}{a_\tau}(\phi_{i+1}-\phi_i)$.

We can now integrate over $\pi_i(\bar{x})$:

$$
\begin{aligned}
&\int[\prod_x\pi_i(\bar{x})]\exp[a^3a_\tau\sum_x -\tfrac{1}{2}\pi_i^2+(i\Delta_0\phi_i)\pi_i] \\
&= \left[\frac{2\pi}{a^3a_\tau}\right]^{N_S^3/2}\times\exp[-a^3a_\tau\sum_x\tfrac{1}{2}(\Delta_0\phi_i(\bar{x}))^2]
\end{aligned}
$$

Repeating this for $i = 1\ldots N_\tau$, and identifying the time coordinate $x_0 = \tau = a_\tau i$, we finally obtain the path integral

$$
\langle\phi_B|e^{-\tau\hat{H}}|\phi_A\rangle \propto \int[\prod_x d\phi]e^{-S_E}
$$

where S_E is the *Euclidean* (imaginary time) action

$$
\begin{aligned}
S_E &= a^3a_\tau\sum_x(\tfrac{1}{2}(\Delta_\mu\phi)^2+V[\phi]) \\
&\to \int d^4x(\tfrac{1}{2}(\partial_\mu\phi)^2+V[\phi])
\end{aligned}
$$

and we have the boundary conditions $\phi(\tau_A) = \phi_A$, $\phi(\tau_B) = \phi_B$.

The path integral is precisely in the form of a *partition function* for a 4-dimensional *classical* statistical system, with the identification $S_E \leftrightarrow H/(k_B T)$.
For convenience, we make the system *periodic* in time by identifying $\phi_A = \phi_B$ and integrating over ϕ_A.
In summary:

$$\begin{array}{rcl} \text{Minkowski} & \to & \text{Euclidean} \\ \mathcal{L}_M & \to & \mathcal{L}_E = -\mathcal{L}_M(x_0 \to ix_0; \partial_0 \to -i\partial_0) \\ g = (1,-1,-1,-1) & \to & g = (1,1,1,1) \end{array}$$

We can now make a connection between the correlation functions of the "statistical" theory and the Green's functions of the quantum field theory.
First, note that we can interpret $T_{\phi_{i+1},\phi_i} = \langle \phi_{i+1}|e^{-a_\tau \hat{H}}|\phi_i\rangle$ as a *transfer matrix*. In terms of T the partition function is

$$Z = \int [d\phi] e^{-S_E} = \text{Tr}\,(T^{N_\tau})$$

Let us label the eigenvalues of T by $\lambda_0, \lambda_1 \ldots$, so that $\lambda_0 > \lambda_1 \geq \ldots$. Note that $\lambda_i = \exp -E_i$, where E_i are eigenvalues of $\hat{H}$. Thus, λ_0 corresponds to the state of lowest energy, *vacuum* $|0\rangle$. If we now take N_τ to be very large (while keeping a_τ constant; i.e. take $\Delta\tau$ to be large),

$$Z = \sum_i \lambda_i^{N_\tau} = \lambda_0^{N_\tau}[1 + O((\lambda_1/\lambda_0)^{N_\tau})]$$

For example, a 2-point function can be written as (let $i - j > 0$)

$$\langle \phi_i \phi_j \rangle = \frac{1}{Z}\int [d\phi]\phi_i\phi_j e^{-S_E} = \frac{1}{Z}\text{Tr}\,(T^{N_\tau - i + j}\hat{\phi}T^{i-j}\hat{\phi}).$$

Taking now $N_\tau \to \infty$, and recalling $a_\tau(i-j) = \tau_i - \tau_j$,

$$\langle \phi_i \phi_j \rangle = \langle 0|\hat{\phi}(T/\lambda_0)^{i-j}\hat{\phi}|0\rangle = \langle 0|\hat{\phi}(\tau_i)\hat{\phi}(\tau_j)|0\rangle,$$

where we have introduced time-dependent operators

$$\hat{\phi}(\tau) = e^{\tau\hat{H}}\hat{\phi}e^{-\tau\hat{H}}.$$

Allowing for both positive and negative time separations of τ_i and τ_j, we can identify

$$\langle\phi(\tau_i)\phi(\tau_j)\rangle = \langle 0|\mathcal{T}[\hat{\phi}(\tau_i)\hat{\phi}(\tau_j)]|0\rangle,$$

where $\mathcal{T}$ is the time ordering operator.

2.4 Mass spectrum:

• Green's functions in time τ:

$$\begin{aligned}
\langle 0|\Gamma(\tau)\Gamma^\dagger(0)|0\rangle &= \frac{1}{Z}\int[d\phi]\Gamma(\tau)\Gamma^\dagger(0)e^{-S} \\
&= \langle 0|e^{\hat{H}\tau}\Gamma(0)e^{-\hat{H}\tau}\Gamma^\dagger(0)|0\rangle \\
&= \langle 0|\Gamma(0)\sum_n|E_n\rangle\langle E_n|e^{-\hat{H}\tau}\Gamma^\dagger(0)|0\rangle \\
&= \sum_n e^{-E_n\tau}|\langle 0|\Gamma(0)|E_n\rangle|^2 \\
&\to e^{-E_0\tau}|\langle 0|\Gamma(0)|E_0\rangle|^2 \qquad \text{as } \tau\to\infty
\end{aligned}$$

where $|E_0\rangle$ is the *lowest* energy state with non-zero matrix element $\langle 0|\Gamma(0)|E_0\rangle$.

$\to$ measure masses (E_0) from the exponential fall-off of correlation functions.

2.5 Finite temperature

Connection *Euclidean QFT* $\leftrightarrow$ *classical statistical mechanics* was derived for zero-temperature quantum system. However, this can be readily generalized to finite temperature:
Quantum thermodynamics w. the Gibbs ensemble:

$$Z = \text{Tr}\, e^{-\hat{H}/T} = \int[d\phi]\,\langle\phi|e^{-\hat{H}/T}|\phi\rangle$$

Expression is of the same form as the one which gave us the Euclidean path integral for $T = 0$ theory! The difference here is

1) Finite + fixed "imaginary time" interval $1/T$
2) Periodic boundary condition: $\phi(1/T) = \phi(0)$.
Repeating the previous derivation, the partition function becomes

$$Z(T) = \int [d\phi]\, e^{-S_E} = \int [d\phi]\, \exp[-\int_0^{1/T} d\tau \int d^3x \mathcal{L}_{\mathcal{E}}]$$

Thus, a connection between:
– Quantum statistics in 3d: $Z = \mathrm{Tr}\, e^{-\hat{H}/T}$
– Classical statistics in 4d: $Z = \int [d\phi] e^{-S}$
Euclidean P.I. is a very common tool for finite T field theory analysis [J. Kapusta, *Finite Temperature Field Theory*, Cambridge University Press]

2.6 Some terminology:

In numerical work, lattice is a finite box with finite lattice spacing a. In order to obtain continuum results, we should take 2 limits:

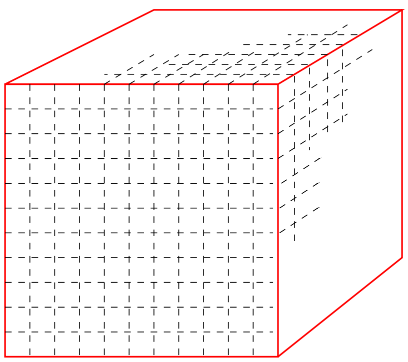
- $V \to \infty$ *thermodynamic limit*
- $a \to 0$ *continuum limit*

Both have to be controlled – expensive!

1) Perform simulations with fixed a, various V. Extrapolate $V \to \infty$.
2) Repeat 1) using different a's. Extrapolate $a \to 0$.
3) [In QCD, one often has to extrapolate $m_q \to m_{q,\mathrm{phys.}}$.]

$T = 0$:

1) $V \to \infty$:
   $N_\tau, N_s \to \infty$, a constant.
2) continuum:
   $a \to 0$.



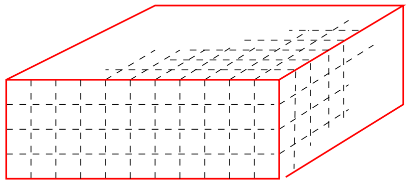
$T > 0$:

1) $V \to \infty$:

   $N_s \to \infty$, N_τ, a constant.

2) continuum:

   $a \to 0$, $\frac{1}{T} = aN_\tau$ constant.



2.7 Scalar field

Free scalar field on a finite d-dimensional lattice with periodic boundary conditions:

$$x_\mu = an_\mu, \quad n_\mu \in Z$$

Action:

$$S = \sum_x a^d \left[\tfrac{1}{2} \sum_\mu \frac{1}{a^2}(\phi_{x+\mu} - \phi_x)^2 + \frac{1}{2} m^2 \phi^2 \right] = a^d \left[\tfrac{1}{2} \phi_x \Box_{x,y} \phi_y + \tfrac{1}{2} m^2 \phi_x^2 \right]$$

(implicit sum over x, y), and we define the lattice d'Alembert operator as

$$\Box_{x,y}\phi_y = -\Delta^2 \phi = \sum_\mu \frac{2\phi_x - \phi_{x+\hat{\mu}} - \phi_{x-\hat{\mu}}}{a^2}$$

The action is of form $S = \frac{1}{2}\phi_x M_{x,y} \phi_y$, and

$$Z = \int [d\phi] e^{-S} = (\mathrm{Det}\, M/2\pi)^{-1/2}$$

2.8 Fourier transforms:

$$\tilde{f}(k) = \sum_x a^d e^{-ikx} f(x)$$

Since $x = an$, $\tilde{f}(ak + 2\pi n) = \tilde{f}(k)$, and we restrict k to *Brillouin zone*: $-\pi < ak_\mu \leq \pi$

Inverse transform:

$$f(x) = \int_{-\pi/a}^{\pi/a} \frac{d^d k}{(2\pi)^d} e^{ikx} \tilde{f}(k)$$

Note: often it is convenient to use dimensionless natural lattice units $x_\mu \in Z$, $-\pi < k_\mu \leq \pi$.

The above inverse transform is for infinite lattice. On a finite lattice $0 \leq x_\mu/a < N$, and for simplicity assuming *periodic boundary conditions*: $x_\mu + aN = x_\mu$, only momenta $ak_\mu = \frac{2\pi}{N} n_\mu - \pi$, where $0 < n_\mu \leq N$ are allowed. Now the inverse transform is:

$$f(x) = \sum_k \frac{1}{(aN)^d} e^{ikx} \tilde{f}(k), \quad k_\mu = \frac{2\pi}{N} n_\mu - \pi.$$

This approaches the previous one when $N \to \infty$.

Lattice propagator:

The lattice propagator $G(x,y)$ is defined to be the inverse of operator $a^{-d} M = (\Box + m^2)$:

$$\sum_y a^d (\Box_{x,y} + m^2 \delta_{x,y}) G(y,z) = \delta_{x,z}$$

Take Fourier transform ($G(x,y) = G(x-y)$):

$$\left[\sum_\mu \frac{2}{a^2}(1 - \cos k_\mu a) + m^2 \right] \tilde{G}(k) = 1$$

which gives the lattice propagator

$$\tilde{G}(k) = \frac{1}{\hat{k}^2 + m^2}, \quad \text{where} \quad \hat{k}^2 = \sum_\mu \hat{k}_\mu^2 = \sum_\mu \left[\frac{2}{a} \sin \frac{k_\mu a}{2} \right]^2.$$

Continuum limit: when $a \to 0$, $\tilde{G}(k) = 1/(k^2 + m^2) + O(a^2)$.

Generating function for Green's functions:

$$S \to S(J) = \sum_x a^d \left[\tfrac{1}{2} \phi_x (\Box + m^2) \phi_x - J_x \phi_x \right]$$

Now

$$Z(J) = \int [d\phi] e^{-S(J)} = Z(0) \exp[\sum_{x,y} a^{2d} \tfrac{1}{2} J_x G(x,y) J_y]$$

N-point functions

$$\langle \phi_x \dots \phi_y \rangle = Z(0)^{-1} \frac{\delta}{\delta J_x} \dots \frac{\delta}{\delta J_y} Z(J) \Big|_{J=0}$$

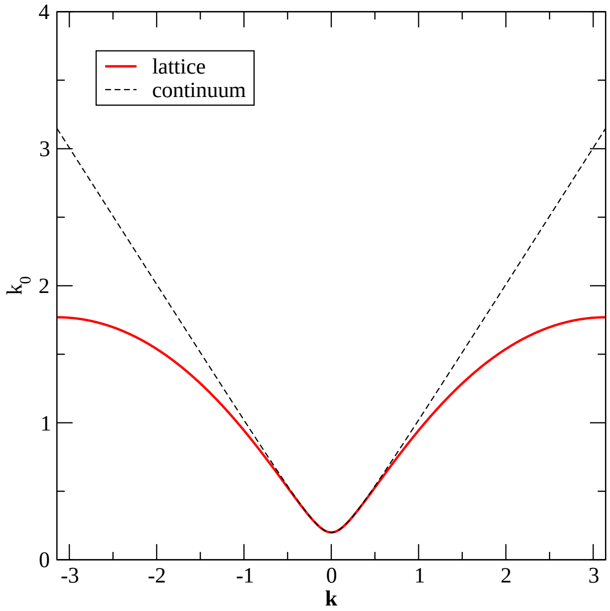
Interactions: just modify (for example)

$$\mathcal{L} = \mathcal{L}_{\text{free}} + \frac{1}{4!} \lambda \phi^4$$

2.9 Pole structure of the propagator

In Minkowski spacetime, the pole of the propagator gives the dispersion relation of the free particle: if $k^2 = m^2$, we have $k_0^2 = \mathbf{k}^2 + m^2$. For the Euclidean propagator the denominator is always positive, and there are no poles.
However, the pole structure can be recovered by performing a Wick rotation back to Minkowski space: $k_0^M \leftrightarrow -ik_0^E$, as will be shown in more detail below. With this substitution we obtain for the pole

$$\begin{aligned}
0 &= \left[\frac{2}{a} \sin \frac{ik_0 a}{2} \right]^2 + \sum_i \hat{k}_i^2 + m^2 \\
&\to \frac{4}{a} \sinh^2 \frac{k_0 a}{2} = \sum_i \hat{k}_i^2 + m^2 \\
&\to k_0 a = 2 \sinh^{-1} \sqrt{\sum_i \sin^2 \frac{k_i a}{2} + \frac{(ma)^2}{4}}
\end{aligned}$$



In figure above the lattice and continuum dispersion relations are shown for $ma = 0.2$-mass particle, with $\mathbf{k} = (k, 0, 0)$.