

## P7. Statistical Many-Particle System

- For a many-particle quantum system, the knowledge of the exact quantum state,  $\{c_i\}$ , or the specification of the full density operator,  $\{g_{ij}\}$ , contains way too much information to handle.

The information we shall need can be packed into a much more compact object, called the reduced density operator, which contains information about the distribution of particles into one-particle states. It contains also some information about the correlations between the particles, but much less than the full density operator. As an introduction, consider first classical probability distributions in  $N$ -body and 1-body phase space.

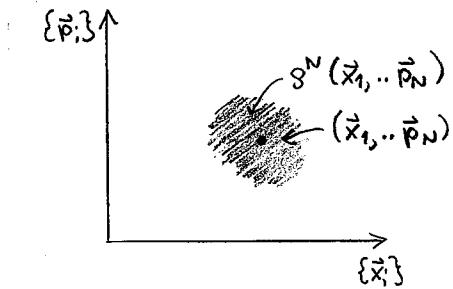
### P7.1 Classical N-body and 1-body Phase Space

- Consider a classical system of  $N$  particles. The state of the system is specified completely by specifying the coordinates  $\vec{x}_i$  and momenta  $\vec{p}_i$  of the  $N$  particles. For 3 dimensions, this is  $6N$  real numbers. Thus the state of the system is represented by a point in the  $6N$ -dimensional  $N$ -body phase space
- $$\{(\vec{x}_1, \vec{p}_1, \dots, \vec{x}_N, \vec{p}_N)\}$$
- More generally, the  $\vec{x}_i, \vec{p}_i$  can be generalized coordinates describing the system, and their conjugate momenta. For example, if the particles are not pointlike, but can be thought of as rigid bodies; in addition to the locations  $\vec{x}_i$  of their centers-of-mass, we also need three angles specifying their orientations, and their angular momenta. For simplicity, we discuss here the point-particle case.
  - If we don't know the exact state of the system, but have just statistical information, it can be represented as a probability density  $g^N$  in the  $N$ -particle phase space:

$$g^N(\vec{x}_1, \vec{p}_1, \dots, \vec{x}_N, \vec{p}_N)$$

As the system evolves according to laws of physics, the probability density also evolves in time, so it is also a function of time,

$$g^N(\vec{x}_1, \dots, \vec{p}_N, t).$$



- Normalization  $\int d^3x_1 d^3p_1 \dots d^3x_N d^3p_N g^N(\vec{x}_1, \dots \vec{p}_N, t) = 1$  (1)
- We get the 1-body probability density  $g_i(\vec{x}_i, \vec{p}_i)$  by integrating over all the other N-1 particles,

$$\underline{g_i(\vec{x}_i, \vec{p}_i, t) = \int d^3x_1 \dots \cancel{d^3x_i} d^3p_i \dots d^3p_N g^N(\vec{x}_1, \dots \vec{x}_i, \vec{p}_i, \dots \vec{p}_N, t)}$$
 (2)

The set of 1-body probability densities  $\{g_i\}$  contains less information than the full N-body probability density  $g^N$ , since it does not contain informations about correlations between particles. For example, if particles 1 and 2 tend to stay close to each other, but the pair can be anywhere w equal probability, then  $g_1$  and  $g_2$  contains only the information that each of the two particles can be anywhere w equal probability.

The information provided by  $\{g_i\}$  is enough, if we only need to know quantities which are "1-body functions".

- We call a function  $G$  of the state of the system a 1-body function, if

$$\underline{G(\vec{x}, \dots \vec{p}_N) = \sum_{i=1}^N G_i(\vec{x}_i, \vec{p}_i)}$$
 (3)

An example is the total energy of the system, in the case it is given only by the kinetic energies of the particles, and possibly their potential energies in an external potential

$$\underline{E(\vec{x}, \dots \vec{p}_N) = \sum_{i=1}^N \left[ \frac{\vec{p}_i^2}{2m_i} + V_i(\vec{x}_i) \right]},$$

but there are no interaction energies between the particles, or such energies, which typically are of the form  $V_{ij}(|\vec{x}_i - \vec{x}_j|)$ , are small enough to be ignored (for example a gas at particles in Earth's gravitational field). If such interaction energies need to be included,  $E$  becomes a "2-body function", and we need to know the "2-body probability densities"; but we shall not go into that.

The expectation value of a n-body function can be calculated as

$$\begin{aligned} \underline{\langle G(t) \rangle} &= \int d^3x_1 \dots d^3p_N G(\vec{x}_1, \dots \vec{p}_N) g^N(\vec{x}_1, \dots \vec{p}_N, t) \\ &= \int d^3x_1 \dots d^3p_N \sum_{i=1}^N G_i(\vec{x}_i, \vec{p}_i) g^N(\vec{x}_1, \dots \vec{p}_N, t) \\ &= \sum_{i=1}^N \int d^3x_i d^3p_i G_i(\vec{x}_i, \vec{p}_i) g_i(\vec{x}_i, \vec{p}_i, t) \end{aligned}$$
 (4)

since for each term we can move  $G_i(\vec{x}_i, \vec{p}_i)$  outside all the other integrations except  $\int d^3x_i d^3p_i$ , and those other integrations produce  $g_i$  from  $g^N$  according to (2).

## Identical Particles

- For identical particles, we can make no distinction whether it is, say, particle 1 or particle 2 who has the coordinates and momentum  $\vec{x}, \vec{p}$ . To take this into account, the probability density  $\mathcal{S}^N$  must be symmetric under exchange of particle labels  $\Rightarrow$  all  $\mathcal{S}_i$  are identical

$$\mathcal{S}_i(\vec{x}, \vec{p}, t) = \mathcal{S}^{(1)}(\vec{x}, \vec{p}, t) \quad (5)$$

$\therefore$  We have a single 1-particle probability density  $\mathcal{S}^{(1)}$  in 1-particle phase space.

For identical particles, also all  $\mathcal{O}_i$  are the same,  $\mathcal{O}_i(\vec{x}, \vec{p}) = \mathcal{O}^{(1)}(\vec{x}, \vec{p})$

$$\Rightarrow \mathcal{O}(\vec{x}_1, \dots, \vec{p}_N) = \sum_{i=1}^N \mathcal{O}^{(1)}(\vec{x}_i, \vec{p}_i) \quad (6)$$

- From (4), we now get that the expectation value of a one-body function can be calculated as

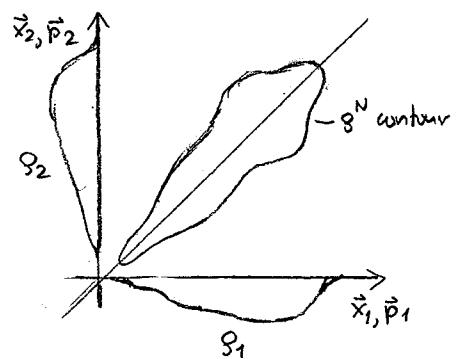
$$\langle \mathcal{O}(t) \rangle = N \int d^3x d^3p \mathcal{O}^{(1)}(\vec{x}, \vec{p}) \mathcal{S}^{(1)}(\vec{x}, \vec{p}, t) \quad (7)$$

- The 1-particle probability density  $\mathcal{S}^{(1)}$  has a close relation to the distribution function, if the distribution function  $f(\vec{x}, \vec{p}, t)$  is understood as the expectation value of the number density in 1-particle phase space,

$$f(\vec{x}, \vec{p}, t) = N \mathcal{S}^{(1)}(\vec{x}, \vec{p}, t). \quad (8)$$

Thus

$$\langle \mathcal{O}(t) \rangle = \int d^3x d^3p \mathcal{O}^{(1)}(\vec{x}, \vec{p}) f(\vec{x}, \vec{p}, t). \quad (9)$$



## D7.2 Quantum Many-Particle System and Reduced Density Operator

- For a many-particle system the density operator  $\hat{\rho}$  is an operator in the Fock space (many-particle space). The normalization is

$$\text{Tr } \hat{\rho} = \sum_{\{n_k\}} \langle n_1, \dots, n_k, \dots | \hat{\rho} | n_1, \dots, n_k, \dots \rangle = 1 \quad (10)$$

Thus the trace in Fock space is analogous to integration over the classical N-particle phase space, Eq. (1).

### 1-particle operators

- Suppose we have an operator  $\hat{G}^{(1)}$  in the 1-particle (quantum state) space, which is spanned by the basis  $\{|k\rangle\}$ . It is defined by its matrix elements

$$\langle k | \hat{G}^{(1)} | k' \rangle \equiv G_{kk'}^{(1)} \quad (11)$$

$$\text{as } \hat{G}^{(1)} = \sum_{kk'} G_{kk'}^{(1)} |k\rangle \langle k'|. \quad (12)$$

We can then define a corresponding operator  $\hat{G}$  in the many-particle space (Fock space) by

$$\hat{G} = \sum_{kk'} \langle k | \hat{G}^{(1)} | k' \rangle a_k^+ a_{k'}^- \quad (13)$$

Such an operator in the many-particle space, which can be defined in terms of an operator in the 1-particle space, is called a 1-particle operator.

Note that, if  $\{|k\rangle\}$  is chosen as an eigenbasis of  $\hat{G}^{(1)}$ , then

$$\hat{G} = \sum_k G_k \hat{n}_k$$

where  $G_k = \langle k | \hat{G}^{(1)} | k \rangle$  is the eigenvalue corresponding to the eigenstate  $|k\rangle$ .

- Examples: 1) Number operator  $\hat{N}$ , which in 1-particle space is just the identity operator  $\hat{N}^{(1)} = \hat{1} = \sum_k |k\rangle \langle k| \Rightarrow \langle k | \hat{N}^{(1)} | k' \rangle = \langle k | k' \rangle = \delta_{kk'}$

$$\Rightarrow \hat{N} = \sum_{kk'} \langle k | k' \rangle a_k^+ a_{k'}^- = \sum_k a_k^+ a_k^- = \sum_k \hat{n}_k \quad (14)$$

- 2) Energy (Hamiltonian) operator  $\hat{H}$ , which, assuming  $\{|k\rangle\}$  is an energy eigenbasis, in 1-particle space is  $\hat{H}^{(1)} = \sum_k E_k |k\rangle \langle k| \Rightarrow \langle k | \hat{H}^{(1)} | k' \rangle = E_k \delta_{kk'}$

$$\Rightarrow \hat{H} = \sum_{kk'} \langle k | \hat{H}^{(1)} | k' \rangle a_k^+ a_{k'}^- = \sum_k E_k \hat{n}_k \quad (15)$$

(Works only, if there are no interaction energies between particles.)

## Reduced Density Operator

- Define the 1-particle reduced density operator  $\hat{g}^{(1)}$ , corresponding to the full density operator  $\hat{g}$ , as an operator in 1-particle space, by defining its matrix elements

$$\boxed{S_{kk'}^{(1)} = \langle k' | \hat{g}^{(1)} | k \rangle = \underbrace{\text{Tr } a_k^+ a_k \hat{g}}_{\langle a_k^+ a_k \rangle} = \sum_{\{n_i\}} \langle \{n_i\} | a_k^+ a_k \hat{g} | \{n_i\} \rangle} \quad (16)$$

(note the order at  $k, k'$ )

Exercise: Show that  $\hat{g}^{(1)}$  is Hermitian and positive semi-definite

- From the definition follows that the normalization of  $\hat{g}^{(1)}$  is

$$\text{Tr } \hat{g}^{(1)} = \sum_k \langle k | \hat{g}^{(1)} | k \rangle \stackrel{(16)}{=} \sum_k \text{Tr } a_k^+ a_k \hat{g} = \sum_k \text{Tr } \hat{n}_k \hat{g} = \sum_k \langle \hat{n}_k \rangle = \langle \hat{N} \rangle,$$

the expectation value of the number of particles in the system.

- We can now calculate the expectation value of any 1-particle operator in Fock space in terms of the corresponding operator in 1-particle space and the reduced density operator:

$$\begin{aligned} \langle \hat{G} \rangle &= \text{Tr } \hat{G} \hat{g} = \sum_{\{n_i\}} \langle \{n_i\} | \hat{G} \hat{g} | \{n_i\} \rangle \\ &\stackrel{(13)}{=} \sum_{kk'} \langle k | \hat{G}^{(1)} | k' \rangle \sum_{\{n_i\}} \langle \{n_i\} | a_k^+ a_{k'} \hat{g} | \{n_i\} \rangle \\ &\stackrel{(16)}{=} \sum_{kk'} \langle k | \hat{G}^{(1)} | k' \rangle \langle k' | \hat{g}^{(1)} | k \rangle = \sum_k \langle k | \hat{G}^{(1)} \hat{g}^{(1)} | k \rangle = \text{Tr } \hat{G}^{(1)} \hat{g}^{(1)} \\ &= \sum_{kk'} G_{kk'}^{(1)} S_{kk'}^{(1)} \end{aligned} \quad (17)$$

Here  $\hat{G}$  and  $\hat{g}$  are operators in the many-particle (Fock) space

$\hat{G}^{(1)}$  and  $\hat{g}^{(1)}$  are operators in 1-particle space

- The reduced density operator  $\hat{g}^{(1)}$  contains a lot less information about the many-particle system than the full density operator  $\hat{g}$ . However, it contains sufficient information to calculate the expectation values of all 1-particle operators.

The information that was lost, includes information about the correlations between the different particles, that would be needed to calculate expectation values of, e.g., 2-particle operators such as the Hamiltonian operator in the case of interaction energies between the particles.

However, there is some correlation information (off-diagonal elements of  $\hat{g}^{(1)}$ ) which is needed when the 1-particle basis  $\{|k\rangle\}$  is not an eigenbasis of  $\hat{G}^{(1)}$ .

### P7.3 Application to Stokes Parameters

- For simplicity, consider the case where all photons have the same momentum  $\vec{q}$ , and use the  $\{|x\rangle, |y\rangle\}$  basis in the 1-particle space. Now ( $\S P3$ )

$$\begin{aligned}\hat{I}^{(1)} &= |x\rangle\langle x| + |y\rangle\langle y| = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \\ \hat{Q}^{(1)} &= |x\rangle\langle x| - |y\rangle\langle y| = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \\ \hat{U}^{(1)} &= |x\rangle\langle y| + |y\rangle\langle x| = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ \hat{V}^{(1)} &= i|y\rangle\langle x| - i|x\rangle\langle y| = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\end{aligned}\quad (18)$$

Using (13) we get for the many-particle space

$$\begin{aligned}\hat{I} &= \sum_{ij} \langle ii|\hat{I}^{(1)}|jj\rangle a_i^+ a_j = a_x^+ a_x + a_y^+ a_y = \hat{n}_x + \hat{n}_y \\ \hat{Q} &= \sum_{ij} \langle ii|\hat{Q}^{(1)}|jj\rangle a_i^+ a_j = a_x^+ a_x - a_y^+ a_y = \hat{n}_x - \hat{n}_y \\ \hat{U} &= \sum_{ij} \langle ii|\hat{U}^{(1)}|jj\rangle a_i^+ a_j = a_x^+ a_y + a_y^+ a_x \\ \hat{V} &= \sum_{ij} \langle ii|\hat{V}^{(1)}|jj\rangle a_i^+ a_j = i a_y^+ a_x - i a_x^+ a_y\end{aligned}\quad (19)$$

To get the expectation values of these operators, we need to know only the reduced density operator of the system: (compare to  $\S PS$ ):

$$\begin{aligned}I &\equiv \langle \hat{I} \rangle = \text{Tr } \hat{I}^{(1)} \hat{\rho}^{(1)} = \sum_i \langle ii|\hat{I}^{(1)} \hat{\rho}^{(1)}|ii\rangle = \sum_{ij} I_{ij}^{(1)} S_{ji}^{(1)} = S_{xx}^{(1)} + S_{yy}^{(1)} \\ Q &\equiv \langle \hat{Q} \rangle = \text{Tr } \hat{Q}^{(1)} \hat{\rho}^{(1)} = \sum_{ij} Q_{ij}^{(1)} S_{ji}^{(1)} = S_{xx}^{(1)} - S_{yy}^{(1)} \\ U &\equiv \langle \hat{U} \rangle = \text{Tr } \hat{U}^{(1)} \hat{\rho}^{(1)} = \sum_{ij} U_{ij}^{(1)} S_{ji}^{(1)} = S_{xy}^{(1)} + S_{yx}^{(1)} \\ V &\equiv \langle \hat{V} \rangle = \text{Tr } \hat{V}^{(1)} \hat{\rho}^{(1)} = \sum_i \langle ii|\hat{V}^{(1)} \hat{\rho}^{(1)}|ii\rangle = \sum_{ij} V_{ij}^{(1)} S_{ji}^{(1)} = -i S_{yx}^{(1)} + i S_{xy}^{(1)}\end{aligned}\quad (20)$$

Using that  $\hat{\rho}^{(1)}$  is Hermitian,  $S_{yx}^{(1)*} = S_{xy}^{(1)}$  we get that the reduced density matrix can be written

$$\hat{\rho}^{(1)} = \frac{1}{2} \begin{bmatrix} I+Q & U-iV \\ U+iV & I-Q \end{bmatrix} \quad (21)$$

so that it contains exactly the same information as the (expectation values of) the four Stokes parameters. The result (21) is like Eq. (4) in  $\S PS$  (Statistical One-Photon System), but the difference is that now  $I = \langle \hat{I} \rangle = \text{Tr } \hat{\rho}^{(1)} \hat{I}^{(1)} = \text{Tr } \hat{\rho}^{(1)} = \langle N \rangle$ , since  $\hat{\rho}^{(1)}$  describes a many-photon system.

- We derived the description of the many-photon system in terms of the reduced density operator  $\hat{S}^{(1)}$ , from a statistical description. However,  $\hat{S}^{(1)}$  can also be used to describe a pure many-photon quantum state.

$$|\psi\rangle = C_0|0\rangle + C_{10}|10\rangle + C_{01}|01\rangle + C_{20}|20\rangle + C_{11}|11\rangle + C_{02}|12\rangle + \dots \quad (22)$$

and provides the most compact description of it to fully describe the polarization.

A lot of information contained in the set of  $\{C_{\{\alpha\}}\}$ , which fully describes the quantum state, is thrown away, but all  $\langle \hat{n}_s \rangle$ , where  $s$  is any polarization state, can be obtained from  $\hat{S}^{(1)}$ .

- For a pure 1-photon state, we necessarily had  $Q^2+U^2+V^2 = I^2 (=1)$ , so that a single photon is always fully polarized, but for a pure many-photon state we get just that

$$\underline{0 \leq Q^2+U^2+V^2 \leq I^2} \quad (23)$$

so the system can be fully polarized, unpolarized ( $Q=U=V=0$ ), or partially polarized.

This can be easily seen by considering, e.g., a 2-photon system.

$$|\psi\rangle = a_1 e^{i\alpha_1}|20\rangle + a_2 e^{i\alpha_2}|11\rangle + a_3 e^{i\alpha_3}|02\rangle \quad (24)$$

(exercise).

- The Stokes parameters for pure quantum states such as (22) or (24) can be calculated directly as  $I = \langle \hat{I} \rangle = \langle \psi | \hat{I} | \psi \rangle$   $Q = \langle \hat{Q} \rangle = \langle \psi | \hat{Q} | \psi \rangle$  etc.

and the reduced density matrix is obtained as (16)

$$\underline{S_{ij}^{(1)} = \langle a_j^\dagger a_i \rangle = \langle \psi | a_j^\dagger a_i | \psi \rangle} \quad (26)$$

- In the classical treatment we had to include more than one frequency to get unpolarized or partially polarized radiation. We now see that this is not necessary in the quantum treatment. We can have an unpolarized or partially polarized systems even if all photons have the same momentum  $\vec{q}$ ; we just need to have more than one photon! (A fully polarized case correspond to the situation, where all photons are in the same polarization state  $s$ ).

- Linear polarization in  $\varphi$ -direction and rotation of the  $xy$  ind. system:

A photon linearly polarized in a direction making an angle  $\varphi$  w the  $x$  axis corresponds to the state

$$|\varphi\rangle = e^{i\alpha} (\cos \varphi |x\rangle + \sin \varphi |y\rangle)$$

(see §P3), where  $e^{i\alpha}$  is an irrelevant overall phase factor (only relative phases have significance), which we drop.

In Fock space, this can be written

$$\begin{aligned} |\varphi\rangle &= \cos \varphi |10\rangle + \sin \varphi |01\rangle \\ &= \cos \varphi a_x^+ |0\rangle + \sin \varphi a_y^+ |0\rangle = a_\varphi^+ |0\rangle \end{aligned}$$

where we defined the creation operator that creates a  $\varphi$ -polarized photon

$$\begin{aligned} a_\varphi^+ &\equiv \cos \varphi a_x^+ + \sin \varphi a_y^+ \\ \Rightarrow a_\varphi &= (a_\varphi^+)^+ = \cos \varphi a_x + \sin \varphi a_y \end{aligned} \tag{27}$$

- Note that if  $\varphi = \pi$ ,  $|\varphi\rangle = -|x\rangle$  which represents the same physical situation as  $|x\rangle$  ( $\varphi = 0$ ), since it differs from it only by an overall phase factor  $-1$ .
- From this we get easily the effect of rotating the  $xy$  ind axes by some angle  $\varphi$ , since  $|x'\rangle = |\varphi\rangle$  and  $|y'\rangle = |\varphi + \pi/2\rangle$ , so

$$\begin{aligned} a_{x'}^+ &= \cos \varphi a_x^+ + \sin \varphi a_y^+ & a_{x'} &= \cos \varphi a_x + \sin \varphi a_y \\ a_{y'}^+ &= -\sin \varphi a_x^+ + \cos \varphi a_y^+ & a_{y'} &= -\sin \varphi a_x + \cos \varphi a_y \end{aligned} \tag{28}$$

- Consider finally measurement at polarization. A linear polarimeter oriented in the  $\varphi$  direction detects photons with the linear  $\varphi$  polarization, so its measurement is proportional to  $\langle \hat{n}_\varphi \rangle$ , where

$$\begin{aligned} \hat{n}_\varphi &\equiv a_\varphi^+ a_\varphi = (\cos \varphi a_x^+ + \sin \varphi a_y^+) (\cos \varphi a_x + \sin \varphi a_y) \\ &= \cos^2 \varphi a_x^+ a_x + \cos \varphi \sin \varphi a_x^+ a_y + \sin \varphi \cos \varphi a_y^+ a_x + \sin^2 \varphi a_y^+ a_y \end{aligned} \tag{29}$$

$$\begin{aligned} \Rightarrow \langle \hat{n}_\varphi \rangle &= \underbrace{\cos^2 \varphi \langle a_x^+ a_x \rangle}_{S_{xx}^{(1)} = \frac{1}{2}(I+Q)} + \underbrace{\cos \varphi \sin \varphi \langle a_x^+ a_y \rangle}_{S_{yx}^{(1)} = \frac{1}{2}(U+iV)} + \underbrace{\sin \varphi \cos \varphi \langle a_y^+ a_x \rangle}_{S_{xy}^{(1)} = \frac{1}{2}(U-iV)} + \underbrace{\sin^2 \varphi \langle a_y^+ a_y \rangle}_{S_{yy}^{(1)} = \frac{1}{2}(I-Q)} \\ \text{using (16): } S_{xx}^{(1)} &= \frac{1}{2}(I+Q) & S_{yx}^{(1)} &= \frac{1}{2}(U+iV) & S_{xy}^{(1)} &= \frac{1}{2}(U-iV) & S_{yy}^{(1)} &= \frac{1}{2}(I-Q) \\ &= \frac{1}{2} [(w^2 \varphi + \sin^2 \varphi) I + (w \sin^2 \varphi - \sin^2 \varphi) Q + 2w \sin \varphi \sin \varphi U] \\ &= \frac{1}{2} [I + Q \cos 2\varphi + U \sin 2\varphi] \end{aligned} \tag{30}$$

