1 Review: stat mech and single-particle qmech

1.1 Wave Function

Max Born interpretation: probability density of finding a particle at a point $\vec{r}$ is

$$P(\vec{r},t) = |\psi(\vec{r},t)|^2$$

1.2 Single-particle Schrödinger equation.

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{\mathcal{H}}\psi\ , \qquad \hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + V(\hat{\vec{r}})$$

In coordinate representation: $\vec{p} = -i\hbar$; $\hat{\mathcal{H}} = -\frac{\hbar^2}{2m}(\vec{\nabla}^2) + V(\vec{r})$

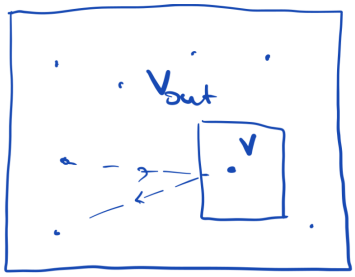
1.3 Linear superposition of waves

If $\psi_a(\vec{r},t)$, $\psi_b(\vec{r},t)$ are solutions of SE, then $\psi_c = a\psi_a + b\psi_b$ is also a solution.

1.3.1 Stationary states, eigenstates

$$\psi_n(\vec{r},t) = e^{-i\varepsilon_n t/\hbar}\varphi_n(\vec{r}) \ \Rightarrow\ \hat{\mathcal{H}}\varphi_n(\vec{r}) = \varepsilon_n\varphi_n(\vec{r})$$
$$\psi(\vec{r},t) = \sum_n \alpha_n e^{-i\varepsilon_n t/\hbar}\varphi_n(\vec{r})$$

1.4 Quantum Gibbs distribution



- System wavefunction: $\psi(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N)$
- Density matrix (coordinate representation:)

$$\rho(\vec{r}_1, \vec{r}_1') \equiv \left(\Pi_{i=2}^N\right)\psi^*(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N)\psi(\vec{r}_1', \vec{r}_2', ..., \vec{r}_N')$$

- Probability density: $P(\vec{r}_1) = \rho(\vec{r}_1, \vec{r}_1)$

We may expand $\rho(\vec{r},\vec{r}')$ in eigenfunctions $\psi_n(\vec{r})$ of a single-particle Hamiltonian (describing an isolated particle)

$$\rho(\vec{r},\vec{r}') = \sum_{nm} w_{mn}\psi_n^*(\vec{r})\psi_m(\vec{r}'); \qquad \hat{\rho} = \underbrace{\sum_{nm} |m\rangle\, w_{mn}\, \langle n|}_{\text{density matrix (Dirac notation)}}$$

Quantum Gibbs distribution (equilibrium distribution): $\boxed{w_{mn} = \frac{1}{Z}e^{-\beta\varepsilon_n}\delta_{mn}}$, where $\beta = 1/k_{\mathrm{B}}T$ (we will mostly stick to $k_{\mathrm{B}} \to 1$)

Quantum Gibbs distribution, statistical operator:

$$\hat{\rho}_G = \frac{1}{Z}\sum_n |n\rangle\, e^{-\beta\varepsilon_n}\, \langle n| = \frac{1}{Z}e^{-\beta\hat{\mathcal{H}}}$$

Partition function: $Z = \sum_n e^{\beta\varepsilon_n}$ (so that $\sum_n w_{nn} = 1.$)

$$Z = \sum_n e^{-\beta\varepsilon_n} = \sum_n \langle n|\, e^{-\beta\hat{\mathcal{H}}}\, |n\rangle = \mathrm{Tr}\left\{e^{-\beta\hat{\mathcal{H}}}\right\}$$

The traditional point of view at microcanonical (fixed energy) and thermal (Gibbs) distributions is based on the motion of statistical ensemble, see Huang, Stat. Mech. Ch. 8 and also employs the notion of ergodicity in evolution of a classical system.

A modern point of view is based on the eigenstate thermalization hypothesis (ETH), see Mark Srednicki Chaos and Quantum Thermalization, Phys. Rev. E, 50, 888(1994)

1.5 Classical limit in statistical mechanics:

$$Z_{cl} = \frac{1}{(2\pi\hbar)^d}\int d^d\vec{p}\int d^d\vec{x}e^{-\beta\mathcal{H}(\vec{p},\vec{x})} \qquad \text{v.s.} \qquad Z = \mathrm{Tr}\left\{e^{-\beta\hat{\mathcal{H}}}\right\}$$

Example: *1D Harmonic Oscillator:* $\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + \frac{m\omega_0^2}{2}x^2$ (1D)

$$\varepsilon = (n + \frac{1}{2r\omega_0}) \qquad Z = \sum_{n=0}^{\infty} e^{-\beta\hbar\omega_0(n+\frac{1}{2})} = \frac{e^{-\beta\hbar\omega_0/2}}{1-e^{-\beta\hbar\omega}} = \frac{1}{2\sinh(\beta\hbar\omega_0/2)}$$

Classical limit: $\beta\hbar\omega_0 \ll 1 \Rightarrow Z \simeq \frac{1}{\beta\hbar\omega_0}$

$$Z_{cl} = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}dp\int_{-\infty}^{\infty}dx e^{-\beta\left(\frac{p^2}{2m}+\frac{m\omega_0^2}{2}x^2\right)} = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}dp e^{-\frac{\beta p^2}{2m}}\int_{-\infty}^{\infty}dx e^{-\frac{\beta m\omega_0^2}{2}x^2} = \frac{1}{\beta\hbar\omega_0}$$

$\frac{1}{2\pi\hbar}$ in Z_{cl} gives the correct state counting ($\Delta p\Delta x = 2\pi\hbar$ per state).

1.6 Free energy

$$F = -T\ln Z$$

Classical description of harmonic oscillator:

$$F_{cl} = -T\ln Z = -T\ln\left(\frac{T}{\hbar\omega_0}\right) \qquad S = -\frac{\partial F}{\partial T} \quad \text{(entropy, as defined in thermodynamics)}$$

$$S_{cl} = -\frac{\partial F_{cl}}{\partial T} \underbrace{=}_{\text{for oscillator}} 1 + \ln\left(\frac{T}{\hbar\omega_0}\right) \qquad \textit{problem at } T = 0!$$

full quantum result for oscillator (with $Z = \sum_n e^{-\beta\varepsilon_n}$):

$$F = \frac{1}{2}\hbar\omega_0 + T\ln\left(1-e^{\beta\hbar\omega_0}\right)$$
$$S = -\ln\left(1-e^{-\hbar\omega_0/T}\right) + \frac{\hbar\omega/T}{e^{\frac{\hbar\omega_0}{T}}-1}$$
$$S \propto \frac{\hbar\omega_0}{T}e^{-\hbar\omega_0/T} \text{ at } T\to 0$$

Entropy (the density matrix definition):

$$S = \ln[\text{number of available states}] = -\sum_n w_n \ln w_n; \quad w_n \text{ is the probability of state } n \text{ occupation}$$

Yields the thermodynamic definition of S for Gibbs distribution ω_n.

1.7 Expectation values

$\hat{O}$: operator of a (measurable) quantity. Expectation value for a given pure state: $\langle\psi|\hat{O}|\psi\rangle$, e.i., average of $\hat{O}$ over a state $|\psi\rangle$.

In the eigenstates of a Hamiltonian representation: $\psi = \sum_n \alpha_n|n\rangle$:

$$\langle\psi|\hat{O}|\psi\rangle = \sum_{mn}\alpha_m^*\alpha_n\langle m|\hat{O}|n\rangle \equiv \sum_{mn}\alpha_m^*\alpha_n O_{mn}$$

$$\langle m|\hat{O}|n\rangle = O_{mn} = \text{matrix element of } \hat{O} \text{ in the eigenstates basis}$$

Time-averaged expectation value for a pure state:

$$\psi = \sum_n \alpha_n|n\rangle \Rightarrow \psi(t) = \sum_n \alpha_n e^{-\varepsilon_n t/\hbar}|n\rangle$$

$$\langle\psi(t)|\hat{O}|\psi(t)\rangle = \sum_{nm}\alpha_m^*\alpha_n e^{i\frac{\varepsilon_m-\varepsilon_n}{\hbar}t}O_{mn}$$

time-averages value: $\overline{A} \equiv \lim_{t_0\to\infty}\int_0^{t_0} dtA(t)$

$$\overline{\langle\psi(t)|\,\hat{O}\,|\psi(t)\rangle} = \sum_{nm}\alpha_m^*\alpha_n\overline{e^{i\frac{\varepsilon_m-\varepsilon_n}{\hbar}t}}O_{mn} = \sum_n |\alpha_n|^2 O_{nn}$$

In general, depends on the initial state (via α_n). ETH states that for a large (infinite in the limit) system and a local quantity $\hat{O}$, $|\alpha_n|^2$ depend only on the state's energy E_n.

Expectation value of $\hat{O}$ for a mixed state described by a density matrix

Return for a minute to the definition of expectation values for a one-particle system and write it out using the real-space coordinate representation:

$$\langle\psi|\,\hat{O}\,|\psi\rangle = \int d\vec{r}\psi^*(\vec{r})\hat{O}(\vec{r},\vec{p})\psi(\vec{r})$$

Now suppose we have a may-particle system in a purse state, $\psi(\vec{r}_1,\vec{r}_2,...,\vec{r}_N)$, but still are interested in the expectation value of an observable associated with one specific particle, namely particle 1: $\hat{O}(\vec{r}_1,\hat{\vec{p}}_1)$.
We will start now from the already introduced definition of the expectation value, $\langle\psi|\,\hat{O}\,|\psi\rangle$, and see how to abbreviate it using the notion of the density matrix $\rho(\vec{r},\vec{r}')$, defined earlier

$$\rho(\vec{r}_1',\vec{r}_1) \equiv \left(\prod_{i=2}^N\int d\vec{r}_i\right)\psi^*(\vec{r}_1',\vec{r}_2,..,\vec{r}_n)\psi(\vec{r}_1,\vec{r}_2,...,\vec{r}_N$$

Indeed,

$$\begin{aligned}
\langle\Psi|\,\hat{O}\,|\Psi\rangle &= \int d\vec{r}_1\int\prod_{i=2}^N d\vec{r}_i\psi^*(\vec{r}_1,\vec{r}_2,...,\vec{r}_N)\hat{O}(\vec{r}_1,\hat{\vec{p}}_1)\psi(\vec{r}_1,\vec{r}_2,...,\vec{r}_N)\\
&= \int d\vec{r}_1\int\prod_{i=2}^N d\vec{r}_i\psi^*(\vec{r}_1,\vec{r}_2,...,\vec{r}_N)\hat{O}(\vec{r}_1,\hat{\vec{p}}_1)\int d\vec{r}_1'\delta(\vec{r}_1-\vec{r}_1')\psi(\vec{r}_1',\vec{r}_2,...,\vec{r}_N)\\
&= \int d\vec{r}_1'\int d\vec{r}_1\int\prod_{i=2}^N d\vec{r}_i\psi^*(\vec{r}_1,\vec{r}_2,...,\vec{r}_N)\hat{O}(\vec{r}_1,\hat{\vec{p}}_1)\delta(\vec{r}_1-\vec{r}_1')\psi(\vec{r}_1',\vec{r}_2,...,\vec{r}_N)\\
&= \int d\vec{r}_1'\int d\vec{r}_1\rho(\vec{r}_1,\vec{r}_1')\hat{O}(\vec{r}_1,\hat{\vec{p}}_1)\delta(\vec{r}_1-\vec{r}_1')
\end{aligned}$$

Now we can use a suitable complete basis of single-particle wave functions:

$$\rho(\vec{r},\vec{r}') = \sum_{nm} w_{nm}\psi_n^*(\vec{r})\psi_m(\vec{r}');\ \hat{\rho} = \sum_{nm}|m\rangle\, w_{mn}\,\langle n|$$

Substitution of $\rho(\vec{r},\vec{r}')$ in this form to the last line above yields

$$\langle\Psi|\,\hat{O}\,|\Psi\rangle = \int d\vec{r}_1'\int dr_1\sum_{nm}w_{mn}\psi_n^*(\vec{r}_1)\psi_m(\vec{r}')\hat{O}(\vec{r}_1,\hat{\vec{p}}_1)\delta(\vec{r}_1-\vec{r}_1')$$

Noting that $\hat{\vec{p}}_1$ acts on $\vec{r}_1$ but not on $\vec{r}_1'$, we may re-write

$$\begin{aligned}
\langle\Psi|\,\hat{O}\,|\Psi\rangle &= \int d\vec{r}_1\sum_{nm}w_{mn}\psi_n^*(\vec{r}_1)\hat{O}(\vec{r}_1,\hat{\vec{p}}_1)\int d\vec{r}_1'\delta(\vec{r}_1-\vec{r}_1')\psi_m(\vec{r}_1')\\
&= \sum_{nm}w_{mn}\underbrace{\int d\vec{r}_1\psi_n^*(\vec{r}_1)\hat{O}(\vec{r}_1,\hat{\vec{p}}_1)\psi_m(\vec{r}_1)}_{O_{mn}} = \sum_{nm}\omega_{mn}O_{nm}
\end{aligned}$$

$$\boxed{\langle\langle\hat{O}\rangle\rangle = \sum_{nm}w_{mn}O_{nm} = \sum_m\sum_n\omega_{mn}O_{nm} = \mathrm{Tr}\Big\{\hat{\rho}\hat{O}\Big\}}$$

Unless the function $\psi(\vec{r}_1,\vec{r}_2,...,\vec{r}_N)$ is factorizable, $\psi(\vec{r}_1,\vec{r}_2,...,\vec{r}_N) = \psi(\vec{r}_1)\cdot\psi(\vec{r}_2,....,\vec{r}_N)$, the density matrix $\hat{\rho}$ corresponds to a mixed state of particle 1. The density matrix definition of the expectation value of $\hat{O}(-\vec{r}_1,\hat{\vec{p}}_1)$ is agnostic wrt states

of other particles.

Within ETH, a thermal ensemble average of a local quantity can be obtained as an expectation value over a pure state with energy $\propto T \cdot N$ of a large system ($N \gg 1$). Assuming that particle 1 interacts with the other particles, but that

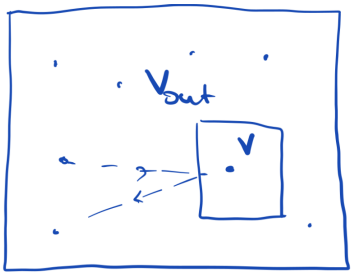


Figure 1: We may consider a system with particle 1 confined to volume V, while other $N-1$ particles reside in volume V_{out}.

interaction is weak compared to single-particle energies ε_m and assuming the ETH is valid, we may use $w_{mn} = \frac{1}{Z} e^{-\beta \varepsilon_m \delta_{mn}}$ (Gibbs distribution) to evaluate $\langle\langle \hat{O} \rangle\rangle$:

$$\langle\langle \hat{O} \rangle\rangle = \frac{1}{Z} \sum_m e^{-\beta \varepsilon_m} O_m = \frac{1}{Z} \mathrm{Tr}\left\{ e^{-\beta \hat{\mathcal{H}}} \hat{O} \right\}$$

In the conventional language, this is operator $\hat{O}$ averaged over the Gibbs (i.e. thermal) ensemble,

$$\hat{\rho}_G = \frac{1}{Z} \sum_m |m\rangle \, e^{-\beta \varepsilon_m} \, \langle m|$$

2 Identical Particles

2.1 Many-body wave function and particle density

$$P(\vec{R}, t) = \left| \psi(\vec{R}, t) \right|^2 ; \qquad P(\vec{R}, t) = \int d\vec{r} \psi^*(\vec{r}, t) \delta(\vec{R} - \vec{r}) \psi(\vec{r}, t)$$

$$\hat{n}(\vec{R}) = \delta(\vec{R} - \hat{\vec{r}})$$

Joint probability density with finding particle 1 at $\vec{r}_1$, particle 2 at point $\vec{r}_2$, ..., particle N at point $\vec{r}_N$:

$$P(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N) = |\psi(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N)|^2$$

Particle density operator: $\hat{n}(\vec{R}) = \sum_{j=1}^N \delta(\vec{R} - \hat{\vec{r}}_j)$

Expectation value of $\hat{n}(\vec{R})$:

$$\hat{n}(\vec{R}) = \int d\vec{r}_1 d\vec{r}_2 ... d\vec{r}_N \psi^*(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) \hat{n}(\vec{R}) \psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) = \int d\vec{r}_1 d\vec{r}_2 ... d\vec{r}_N |\psi(\vec{r}_1, \ldots, \vec{r}_N)|^2 \sum_{j=1}^N \delta(\vec{R} - \vec{r}_j)$$

Consider identical particles: $P(\vec{r}_1, \ldots, \vec{r}_N)$ is invariant with respect to coordinates permutation:

$$|\psi(\vec{r}_1, \ldots, \vec{r}_i, \ldots, \vec{r}_j, \ldots, \vec{r}_N)|^2 = |\psi(\vec{r}_1, \ldots, \vec{r}_j, \ldots, \vec{r}_i, \ldots, \vec{r}_N)|^2$$

2.2 Operator of permutation

$$\hat{P}_{ij} \psi(\vec{r}_1, \ldots, \vec{r}_i, \ldots, \vec{r}_j, \ldots, \vec{r}_N) = \psi(\vec{r}_1, \ldots, \vec{r}_j, \ldots, \vec{r}_i, \ldots, \vec{r}_N)$$

$|\psi(\vec{r}_1, \ldots, \vec{r}_N)|^2$ is invariant with respect to $\hat{P}_{ij}$. For a system of identical particles, operators of observable Classical limit! $Z_N = \frac{1}{N!} (Z_1)^N$. Note that the full QM result, $Z = \mathrm{Tr}\left\{ e^{-\beta \hat{\mathcal{H}}} \right\}$, differentiates between statistics, as the complete bases functions are different between Bose and Fermi statistics. Huang, Stat. Mech., 2nd edition, Sec. 6.6 and 9.2

2.3 Exchange Energy

Consider the example of 2 particles $\hat{\mathcal{H}}_0 = \hat{h}(\vec{p}_1, \vec{r}_1) + \hat{h}(\vec{p}_2, \vec{r}_2)$, with $\hat{h} = \frac{p^2}{2M} + U(\vec{r})$. The normalized eigenfunctions are $\hat{h}\psi_n = \varepsilon\psi_n$, $n = 0, 1, \ldots$, and $\|\psi_n\| = 1$.

$$\psi^{\pm}_{m,n}(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}}[\psi_m(\vec{r}_1)\psi_n(\vec{r}_2) \pm \psi_m(\vec{r}_2)\psi_n(\vec{r}_1)]$$

$$\langle \psi^{\pm}_{m,n} | \psi^{\pm}_{mn} \rangle = 1 \text{ if } \|\psi_n\| = 1, \text{ and } m \neq n$$

$m = n$:

Fermions: $\psi^{-}_{m,m} = 0$ (Pauli principle)

Bosons: $\psi^{+}_{m,m} = \sqrt{2}\psi_m(\vec{r}_1)\psi_m(\vec{r}_2)$; to normalize: $\psi_m = \frac{1}{\sqrt{2!}}\psi^{+}_{m,m}$

Ground state energy for 2 particles::

Fermions: $\psi_g = \psi^{-}_{0,1}$; $\varepsilon_g = \varepsilon_0 + \varepsilon_1$

Bosons: $\psi_g = \frac{1}{\sqrt{2!}}\psi^{+}_{0,0} = \psi_0(\vec{r}_1)\psi_0(\vec{r}_2)$; $\varepsilon_g = 2\varepsilon_0$

$$\mathcal{H}_0\psi_{m,n} = (\varepsilon_n + \varepsilon_m)\psi_{m,n} \; m \neq n; \qquad \varepsilon^{(0)}_{m,n} = \varepsilon_m + \varepsilon_n$$
$$\mathcal{H}_0\psi_{m,m} = 2\varepsilon_m\psi_{m,m}; \varepsilon m, m^{(0)} = 2\varepsilon_m \text{ (bosons)}$$

Introduce a weak interaction $V(\vec{r}_1 - \vec{r}_2)$ between articles. We want to find correction to $\varepsilon_m, n^{(0)}$ due to interaction. 1^{st} order correction $\delta\varepsilon$ to $\varepsilon^{(0)}_{m,n}$:

$$\begin{aligned}
\delta\varepsilon &= \langle \psi^{\pm}_{m,n} | \hat{V} | \psi^{\pm}_{m,n} \rangle \\
&= \frac{1}{2}\int d\vec{r}_1 d\vec{r}_2 |\psi_m(\vec{r}_1)\psi_n(\vec{r}_2) \pm \psi_m(\vec{r}_2)\psi_n(\vec{r}_1)|^2 V(\vec{r}_1 - \vec{r}_2) \\
&= \frac{1}{2}\int d\vec{r}_1 d\vec{r}_2 (\psi_m(\vec{r}_1)\psi_n(\vec{r}_2) \pm \psi_m(\vec{r}_2)\psi_n(\vec{r}_1))^* (\psi_m(\vec{r}_1)\psi_n(\vec{r}_2) \pm \psi_m(\vec{r}_2)\psi_n(\vec{r}_1)) V(\vec{r}_1 - \vec{r}_2) \\
&= \frac{1}{2}\int d\vec{r}_1 d\vec{r}_2 \Big(|\psi_m(\vec{r}_1)|^2 |\psi_n(\vec{r}_2)|^2 + |\psi_m(\vec{r}_2)|^2 |\psi_n(\vec{r}_1)|^2 \Big) V(\vec{r}_1 - \vec{r}_2) \\
&\qquad \pm \frac{1}{2}\int d\vec{r}_1 d\vec{r}_2 \left\{ \psi^*_m(\vec{r}_1)\psi_n(\vec{r}_1)\psi^*_n(\vec{r}_2)\psi_m(\vec{r}_2) + \psi_m(\vec{r}_1)\psi^*_n(\vec{r}_1)\psi_n(\vec{r}_2)\psi^*_m(\vec{r}_2) \right\} V(\vec{r}_1 - \vec{r}_2) \\
&= \int d\vec{r}_1 d\vec{r}_2 \overbrace{|\psi_m(\vec{r}_1)|^2 |\psi_n(\vec{r}_2)|^2 V(\vec{r}_1 - \vec{r}_2)}^{\text{density-density interaction}} \pm \underbrace{\int d\vec{r}_1 d\vec{r}_2 \, \mathrm{Re}\left\{ (\psi^*_m(\vec{r}_1)\psi_n(\vec{r}_1))(\psi^*_n(\vec{r}_2)\psi_m(\vec{r}_2)) \right\} V(\vec{r}_1 - \vec{r}_2)}_{\text{exchange energy}}
\end{aligned}$$

2.4 N-particle generalizations

2.4.1 Fermions

$$\hat{P}_{nm}\psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_n, \ldots, \vec{r}_m, \ldots, \vec{r}_N) = \hat{P}_{nm}\psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_m, \ldots, \vec{r}_n, \ldots, \vec{r}_N)$$

Fermion wave function satisfies:

$$\hat{P}_{nm}\psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_n, \ldots, \vec{r}_m, \ldots, \vec{r}_N) = (-1) \cdot \hat{P}_{nm}\psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_n, \ldots, \vec{r}_m, \ldots, \vec{r}_N)$$

To construct a convenient basis for N fermions, consider an orthonormal set of single-particle states $\psi_j(\vec{r}_i)$ and form an antisymmetric combination:

$$\psi = \frac{1}{\sqrt{N!}}\hat{A}\psi_{j_1}(\vec{r}_1)\psi_{j_2}(\vec{r}_2)\ldots\psi_{j_N}(\vec{r}_N)$$

with $\hat{A}$ being the antisymmetrization operator acting on $\{\vec{r}_i\}$. Introduce operator of permutation

$$P\{1, 2, 3, \ldots, N\} = \{P_1, P_2, P_3, \ldots, P_N\} \qquad P_k = P(k) \text{ is an image of integer } k$$

- **Even permutation** P: involves an even number of pairwise permutations to achieve

$$\{P_1, P_2, P_3, \dots, P_N\};\ (-1)^P = 1$$

- **Odd permutation** P: involves an odd number of pairwise permutations to achieve

$$\{P_1, P_2, P_3, \dots, P_N\};\ (-1)^P = -1$$

Example:

$$\{1,2,3\}$$
$$\overbrace{\{3,2,1\}}\ \text{odd}$$
$$\overbrace{\{2,3,1\}}\ \text{even}$$

$$\psi = \frac{1}{\sqrt{N!}}\hat{A}\psi_{j_1}(\vec{r}_1)\psi_{j_2}(\vec{r}_2)\dots\psi_{j_N}(\vec{r}_N) = \frac{1}{\sqrt{N!}}\sum_{\{P\}}(-1)^P\psi_{j_1}(\vec{r}_{P_1})\psi_{j_2}(\vec{r}_{P_2})\dots\psi_{j_N}(\vec{r}_{P_N}) = \frac{1}{\sqrt{N!}}\det M$$

Matrix elements of M: $M_{ij} = \psi_i(\vec{r}_j)$

$$\psi = \frac{1}{\sqrt{N!}}\begin{vmatrix} \psi_{j_1}(\vec{r}_1) & \dots & \psi_{j_1}(\vec{r}_N) \\ \vdots & & \vdots \\ \psi_{j_N}(\vec{r}_1) & \dots & \psi_{j_N}(\vec{r}_N) \end{vmatrix} \qquad \text{Slater determinant}$$

We may define ψ by allowing P to act on $\{j_l\}$ instead of $\{\vec{r}_i\}$:

$$\psi = \frac{1}{\sqrt{N!}}\hat{A}\psi_{j_1}(\vec{r}_1)\psi_{j_2}(\vec{r}_2)\dots\psi_{j_N}(\vec{r}_N) = \frac{1}{\sqrt{N!}}\sum_{\{P\}}(-1)^P\psi_{j_{P_1}}(\vec{r}_1)\psi_{j_{P_2}}(\vec{r}_2)\dots\psi_{j_{P_N}}(\vec{r}_N) = \frac{1}{\sqrt{N!}}\det M^\top$$

Matrix elements of $M^\top$: $M^\top_{ij} = \psi_j(\vec{r}_i)$

$$\psi = \frac{1}{\sqrt{N!}}\begin{vmatrix} \psi_{j_1}(\vec{r}_1) & \dots & \psi_{j_N}(\vec{r}_1) \\ \vdots & & \vdots \\ \psi_{j_1}(\vec{r}_N) & \dots & \psi_{j_N}(\vec{r}_N) \end{vmatrix}$$

The introduced many-body function is normalized:

$$\langle\psi|\psi\rangle = \frac{1}{N!}\sum_{\{P\}}\sum_{\{P'\}}(-1)^{P+P'}\prod_{k=1}^{N}\left\langle\psi_{j_{P_k}}\middle|\psi_{j_{P'_k}}\right\rangle = \frac{1}{N!}\sum_{\{P\}}\sum_{\{P'\}}(-1)^{P+P'}\delta_{PP'} = \frac{1}{N!}\sum_{\{P\}}\sum_{\{P'\}}\delta_{PP'} = \frac{1}{N!}\sum_{\{P\}}1 = 1$$

Consider a free-fermion system (no interactions)

$$\mathcal{H} = \sum_j h(\hat{p}_j, \hat{r}_j)\ \text{(symmetric in } (i,j) \text{ for all } (i,j)$$

Pick $\psi_i(\vec{r}_j)$ in ψ as eigenfunctions of $h(\hat{p}_j, \hat{r}_j)$. Suppose ψ is constructed out of states $j_1, j_2, \dots, j_N$. The eigenvalue of energy for ψ is $E = \sum_{k=1}^N \varepsilon_{j_k}$
Introduce occupation numbers of single-particle states n_k
(fermions: $n_k = 0$ or 1 depending on wither j_k is present or absent in $\sum\dots$, respectively). We re-write

$$E = \sum_{k=1}^\infty n_k\varepsilon_k,\ \sum_{k=1}^\infty n_k = N$$

2.4.2 Bosons

$$\psi \propto \sum_{\{P\}}\psi_{P_1}(\vec{r}_1)\dots\psi_{P_N}(\vec{r}_N)$$

We should symmetrize with respect to different one-particle states. Introduce here too the occupation number n_i of state i (it is the number of coinciding indices in the above ψ)
The properly normalized function:

$$\psi = \sqrt{\frac{n_1!n_2!\dots}{N!}}\sum_{\{P\}}\psi_{P_1}(\vec{r}_1)\dots\psi_{P_N}(\vec{r}_N)$$

$\{P\}$: all permutations of different indices. The number of indices $P_1, \ldots, P_N$ is $\leq N$. Free-boson system: $E = \sum_{i=1}^{\infty} n_i \varepsilon_i$; $N = \sum_{i=1}^{\infty} n_i$ (n_i may take values $0, 1, \ldots$)

More: Landau and Lifschitz v. 3, §(you may like also §62, 63) + Negele-Orland, Sec. 1.2 and 1.3

3 Second Quantization

3.1 Boson Statistics

Let $\psi_1(r), \psi_2(r), \ldots$ be a compete orthonormal set of single-particle states (e.g. eigenfunctions of a single-particle Hamiltonian $h(p, r)$).

Introduce occupation number $n_1, n_2, \ldots$ for states $1, 2, \ldots$. We want to construct a formalism operating with $\{n_i\}$ instead of $\{r, \sigma\}_i$.

Use Dirac notations:

$$|n_1, n_2, \ldots\rangle \equiv \sqrt{\frac{\prod_k n_k!}{N!}} \sum_{P'} \psi_{P'_1}(r_1) \ldots \psi_{P'_N}(r_N) \tag{1}$$

(representation by occupation numbers: Fock space)

Our goal is to evaluate matrix elements of operators of observables in the basis $|n_2, n_2, \ldots\rangle$. We start with single-coordinate (single-body) observables:

$$\hat{F}^{(1)} = \sum_a \hat{f}_a^{(1)} = \sum_a f^{(1)}(\hat{r}_a, \hat{p}_a) \qquad a\text{: particle number } a$$

Example: density operator $\hat{n}(R) = \sum_a \hat{n}^{(a)}(R) = \sum_a \delta(R - \hat{r}_a)$ $\qquad \hat{n}^{(a)}(R) = \delta(R - \hat{r}_a)$

We are interested in relating matrix element $\langle n_1, \ldots | F^{(1)} | n'_1, \ldots \rangle$ to the matrix elements $\langle i | f^{(a)} | k \rangle$

$$\langle i | f^{(a)} | k \rangle = \int dr_a \psi_i^*(r_a) f^{(a)}(\hat{r}_a, \hat{p}_a) \psi_k(r_a)$$

Example: $n^{(a)}(R) = \delta(R - r_a) \;\Rightarrow\; \langle i | n^{(a)}(R) | k \rangle = \int dr_a \psi_i^*(r_a) \delta(R - r_a) \psi_k(r_a) = \psi_i^*(R) \psi_k(R)$

Only one single-partticle wave function, each from $\langle \ldots |$ and $| \ldots \rangle$ is involved non-trivially in the integration, once one uses eq. 1 to evaluate $\langle \ldots | F | \ldots \rangle$. This is why at most one particle "moves" from one state (k) to another (i).

The only non-zero matrix elements:

$$n'_k = n_k - 1, \; n_i + 1, \; n'_l = n_l \text{ for } l \neq i, k \text{ or } n'_l = n_l \; \forall l$$

Consider first the matrix elements with two of the occupations numbers changing:

$$\langle n_1, \ldots, n_i, \ldots, n_k - 1, \ldots | \hat{F}^{(1)} | n_1, \ldots, n_i - 1, \ldots, n_k, \ldots \rangle = \sqrt{n_i n_k} f_{ik}$$

$$\text{where } \langle i | f^{(a)} | k \rangle = \int f r_a \psi_i^*(r_a) f^{(a)}(\hat{r}_a, \hat{p}_a) \psi_k(r_a)$$

An **example** of $\hat{n}(R)$ to see the origin of $\sqrt{n_i n_k}$ factor:

$$\hat{n}(R) = \sum_a \hat{n}^{(a)}(R) \qquad \hat{n}^{(a)}(R) = \delta(R - r_a); \qquad f_{ik} = \psi_i^*(R) \psi_k(R) \; .$$

$$\langle n_1, \ldots, n_i, \ldots, n_k = 1, \ldots | \hat{n}(R) | n_1, \ldots, n_i - 1, \ldots, n_k, \ldots \rangle$$

$$= \frac{1}{N!} \prod_{l \neq i,k} n_l! \times \underbrace{N}_{\text{from } \sum_a \ldots} \times \overbrace{\sqrt{n_i!(n_k - 1)! \sqrt{(n_i - 1)! n_k!}}}^{(1)} \psi_i^*(R) \psi_k(R) \underbrace{\overbrace{\prod_{l \neq i,k} n_l!(n_k - 1)!(n_i - 1)!}^{(N-1)!} \sum_{\{P'\}_{\text{bra}}} \sum_{\{P''\}_{\text{ket}}}}_{\text{over } N-1 \text{ parity}} \delta_{\text{bra,ket}}$$

(1) : $\qquad \sqrt{n_i!(n_k - 1)!} \sqrt{(n_i - 1)! n_k!} = \sqrt{n_i n_k} (n_k - 1)! (n_i - 1)!$

$$\frac{1}{N!}\times\prod_{l\neq i,k}n_k!\times N\times\sqrt{n_i!(n_k-1)!}\sqrt{(n_i-1)!n_k!}=\prod_{l\neq i,k}n_l!\times\frac{(n_k-1)!(n_i-1)!}{(N-1)!}\times\sqrt{n_in_k}$$

$$\prod_{l\neq i,k}n_l!\frac{(n_k-1)!(n_i-1)!}{(N-1)!}\underbrace{\sum_{\{P'\}_{\text{bra}}}\sum_{\{P''\}_{\text{ket}}}}_{\text{over }N-1\text{ parity}}\delta_{\text{bra,ket}}=\prod_{l\neq i,k}n_l!\times\frac{(n_k-1)!(n_i-1)!}{(N-1)!}\times\frac{(N-1)!}{\prod_{l\neq i,k}n_l!(n_k-1)!(n_i-1)!}=1$$

Thus,

$$|n_1,\ldots,n_i,\ldots,n_k-1,\ldots\rangle\,\hat{n}(R)\,|n_1,\ldots,n_i-1,\ldots,n_k\ldots\rangle=\sqrt{n_in_k}\psi_i^*(R)\psi_k(R)$$

$$\langle n_1,\ldots,n_i,\ldots,n_k-1,\ldots|\,\hat{F}^{(1)}\,|n_1,\ldots,n_i-1,\ldots,n_k,\ldots\rangle=\sqrt{n_i,n_k}f_{ik}^{(1)}$$

$$\langle n_1,\ldots,n_i\ldots,n_k,\ldots|\,\hat{F}^{(1)}\,|n_1,\ldots,n_i,\ldots,n_k,\ldots\rangle=\sum_{i=1}^{\infty}n_if_{ii}^{(1)}$$

$$f_{ik}^{(1)}=\int dr\psi_i^*(r)\hat{f}^{(1)}\psi_k(r)\cong\langle i|\,f^{(1)}\,|k\rangle$$

Reading:
Eq. (64.2) in LL v.3 *details:* Fetter & Walecka, Ch .1

Introduce annihilation operator $\hat{a}_i$ acting on $|n_1,n_2,\ldots,n_i,\ldots\rangle$:

$$\hat{a}_i\,|n_1,n_2,\ldots,n_i,\ldots\rangle=\sqrt{n_1}\,|n_1,n_2,\ldots,n_i-1,\ldots\rangle$$

The only non-zero matrix element of $\hat{a}_i$ is

$$\langle n_1,\ldots,n_i-1,\ldots|\,\hat{a}_i\,|n_1,\ldots,n_i,\ldots\rangle=\sqrt{n_i}$$

abbreviate to

$$\begin{cases}\langle n_1-1|\,\hat{a}_i\,|n_i\rangle=\sqrt{n_i}\\ \langle n_i|\,\hat{a}_i^\dagger\,|n_i-1\rangle=\langle n_i-1|\,\hat{a}_i\,|n_1\rangle^*=\sqrt{n_i}\end{cases}$$

$a_i^\dagger$: creation operator (of a particle in state i)

$$a_i^\dagger\,|n_1,n_2,\ldots,n_i,\ldots\rangle=\sqrt{n_i+1}\,|n_1,n_2,\ldots,n_i+1,\ldots\rangle$$

Consider

$$a_i^\dagger a_i\,|n_1,\ldots,n_i,\ldots\rangle=a_i^\dagger\sqrt{n_i}\,|n_1,\ldots,n_i-1,\ldots\rangle=n_i\,|n_1,\ldots,n_i,\ldots\rangle$$

($\hat{a}_i^\dagger\hat{a}_i$: operator of particle # in state i):

$$\hat{a}_i\hat{a}_i^\dagger\,|n_1,\ldots,n_i,\ldots\rangle=(n_i+1)\,|n_1,\ldots,n_i,\ldots\rangle$$

$$\hat{a}_i\hat{a}_i^\dagger-\hat{a}_i^\dagger\hat{a}_i=1\qquad\text{(regardless }n_i\text{)}$$

Generalizing for $i\neq k$:

$$\hat{a}_i\hat{a}_k^\dagger-\hat{a}_k^\dagger a_i=0\qquad(i\neq k)$$

$$\hat{a}_i\hat{a}_k-\hat{a}_k\hat{a}_i=0\qquad(\text{any }i,k)$$

$$[\hat{a}_i,\hat{a}_k^\dagger]=\delta_{ik},\qquad[\hat{a}_i,\hat{a}_k]=0\qquad(\forall\ i,k)$$

Generalization on a "2-particle" operator, such as pair interaction potential ($\hat{f}_{ab}^{(2)}=V(r_a-r_b)$)

$$\hat{F}^{(2)}=\sum_{a>b}\hat{f}_{ab}^{(2)}=\frac{1}{2}\sum_{a,b}\hat{f}_{ab}^{(2)}-\frac{1}{2}\sum_a\hat{f}_{aa}^{(2)}$$

$$\hat{F}^{(2)} = \frac{1}{2}\sum_{i,k,l,m} \langle ik|\, \hat{f}^{(2)}\, |lm\rangle\, a_i^\dagger a_k^\dagger a_m a_l$$
$$\langle ik|\, \hat{f}^{(2)}\, |lm\rangle = \int dr_1 \int dr_2 \psi^*(r_1)\psi^*(r_2)\hat{f}^{(2)}(\hat{r}_1,\hat{p}_1;\hat{r}_2,\hat{p}_2)\psi_l(r_1)\psi_m(r_2)$$

$$\hat{\mathcal{H}} = \sum_a \hat{\mathcal{H}}_a^{(1)} + \sum_{a>b} V(\vec{r}_a,\vec{r}_b), \qquad \text{with } \hat{\mathcal{H}}_a^{(1)} = -\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r}_a)$$

In second quantization:

$$\hat{\mathcal{H}} = \sum_{ik} \langle i|\, \hat{\mathcal{H}}^{(1)}\, |k\rangle\, a_i^\dagger a_k + \frac{1}{2}\sum_{i,k,l,m} \langle ik|\, \hat{V}\, |lm\rangle\, a_i^\dagger a_k^\dagger a_m a_l$$

$$\hat{N} = \sum_i a_i^\dagger a_i; \quad [\hat{N},\hat{\mathcal{H}}] = 0 \text{ (particle \# conservation)}$$

The wave function $|n_1, n_2, \ldots\rangle$ can be represented by action of creation operators on vacuum $|0\rangle$:

$$|n_1, n_2, \ldots\rangle = \frac{1}{\sqrt{n_1! n_2! \ldots}} (a_1^\dagger)^{n_1}(a_2^\dagger)^{n_2} \ldots |0\rangle$$

(recall that $a_i^\dagger\, |n_1, \ldots, n_i, \ldots\rangle = \sqrt{n_i+1}\, |n_1, \ldots, n_i+1, \ldots\rangle$,

$$(a_i^\dagger)^{n_1}\, |0\rangle = (a_i^\dagger)^{n_i-1})a_i^\dagger\, |0\rangle = (a_i^\dagger)^{n_i-1}\sqrt{1}\, |1\rangle = (a_i^\dagger)^{n_i-1}\sqrt{2}\times\sqrt{1}\, |2\rangle = \cdots - \sqrt{n_i!}\, |n_1\rangle)$$

In real space: $\Psi = \psi_0(r_1)\psi_0(r_2)\ldots\psi_0(r_N)$

3.2 Fermions

Order one-particle states once and for all.

Consider a "single-body" operator, $\hat{F}^{(1)} = \sum_a \hat{f}_a^{(1)} = \sum_a f(\hat{r}_a, \hat{p}_a)$. The only non-zero elements of $\hat{F}$ in the basis of Fock states involve $\{n_i'\} = \{n_i\}$ (no change in occupations) or shift one particle from a state (i) to a state (k): $n_i' = n_i \pm 1, n_k' = n_k \mp 1$ (all n'^s are 0 or 1)

Direct calculation shows:

$$\begin{cases} \langle \ldots 1_i, \ldots, 0_k \ldots|\, \hat{F}^{(1)}\, |\ldots, 0_i, \ldots, 1_k, \ldots\rangle = \langle i|\, f^{(1)}\, |k\rangle \times (-1)^{\Sigma(i+1,k-1)} & i<k \\ \langle \ldots, 0_k, \ldots, 1_i, \ldots|\, \hat{F}^{(1)}\, |\ldots, 1_k, \ldots, 0_i, \ldots\rangle = \langle i|\, f^{(1)}\, |k\rangle \times (-1)^{\Sigma(k+1,i-1)} & i>k \end{cases}$$

Here $|\ldots, 0_i, \ldots, 1_k \ldots\rangle = |n_1, n_2, \ldots, n_i = 0, \ldots, n_k = 1, \ldots\rangle$ (One may use properties of det to check the relations, and figure out $\Sigma(m,a)$)

Diagonal elements:

$$\Sigma(m,q) = \begin{cases} \sum_{\lambda=m}^{q} n_\lambda & q \geq m \\ 0 & q < m \end{cases}$$

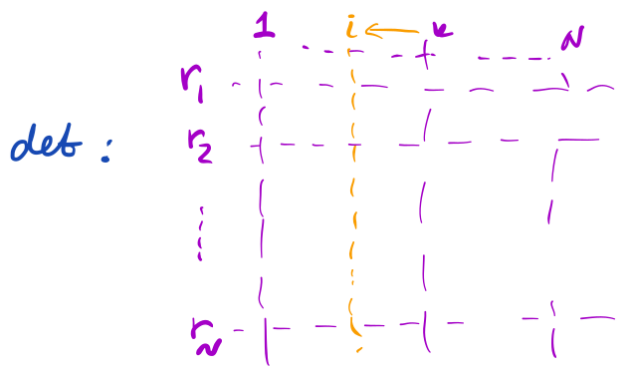


Figure 2: Example Image

$$\overbrace{\underbrace{\langle n_1}_{\text{position of state (ordered once and for all)}}}^{\text{occup. number (0 or 1)}} \ldots |F^{(1)}| \, |n_1, \ldots\rangle = \sum_{i=0}^{\infty} \langle i| \, f^{(1)} \, |i\rangle \, n_i$$

Introduce operators $a^\dagger, a$ as matrices between the basis Fock states with the non-zero matrix elements:

$$\langle 0_i| \, \hat{a}_i \, |1_i\rangle = \langle 1_i| \, \hat{a}_i^\dagger \, |0_i\rangle = (-1)^{\Sigma(1,i-1)))))))))}$$

Use this relation to evaluate

$$\begin{cases} \overbrace{\langle 1_i, 0_k}^{i<k} | \hat{a}_i^\dagger \hat{a}_k^\dagger\rangle = (-1)^{\Sigma(i+1,k-1)} & i < k \\ \langle 1_i 0_k| \, \hat{a}_k \hat{a}_i^\dagger \, |0_i, 1_k\rangle = -(-1)^{\Sigma(i+1,k-1)} & i < k \end{cases}$$

Similarly, at $k < i$ one gets these relations with $\Sigma(i+1, k-1) \to \Sigma(k+1, i-1)$

$$a_i^\dagger a_k + a_k a_i^\dagger = 0, \qquad i \neq k$$

$\langle n_i| \, \hat{a}_i^\dagger \hat{a}_i \, |n_i\rangle = n_i$ $\qquad$ $\langle n_1| \, a_i a_i^\dagger \, |n_i\rangle = 1 - n_i$ (check directly from def. of $a, a^\dagger$) $\qquad$ $\hat{a}_i \hat{a}_i^\dagger + \hat{a}_i^\dagger \hat{a}_i = 1$

Therefore

$$a_i^\dagger a_k + a_k a_i^\dagger = \delta_{ik}, \text{ or } \{a_i^\dagger, a_k\} = \delta_{ik}$$

(Here $\{\hat{A}, \hat{B}\} \equiv \hat{A}\hat{B} + \hat{B}\hat{A}$, anticommutator) Similarly one gets:

$$a_i a_k + a_k a_i = 0, \text{ or } \{a_i, a_k\} = 0 \ (\forall i, k)$$

Using the creation and annihilation operators, we may write $\hat{F}^{(1)}$ in the second-quantization representation:

$$\hat{F}^{(1)} = \sum_{i,k} \langle i| \, f^{(1)} \, |k\rangle \, a_i^\dagger a_k$$

Now we derive for 2-body operators:

$$\hat{F}^{(2)} = \sum_{a>b} f_{ab}^{(2)} \Rightarrow \hat{F}^{(2)} = \frac{1}{2} \sum_{iklm} \langle ik| \, f^{(2)} \, |lm\rangle \, a_i^\dagger a_k^\dagger a_m a_l$$

normal order of operators $a^\dagger, a$

with

$$\langle ik| \, f^{(2)} \, |lm\rangle = \int dr_1 \int dr_2 \psi_i^*(r_1) \psi_k^*(r_2) \hat{f}^{(2)}(\hat{r}_1, \hat{p}_1; \hat{r}_2, \hat{p}_2) \psi_l(r_2) \psi_m(r_2)$$

The "two-body" operator in second quantization:

$$\begin{aligned} \hat{F}^{(2)} &= \sum_{a>b} \hat{f}_{ab}^{(2)} = \frac{1}{2} \sum_{a,b} f^{(2)}(r_a, r_b) - \frac{1}{2} \sum_a f(\hat{r}_a, \hat{r}_a) \\ &= \frac{1}{2} \sum_{a,b} \int dR_1 \int dR_2 \delta(R_1 - r_1) f(R_1, R-2) \delta(R_2 - r_b) - \frac{1}{2} \sum_a \int dR \delta(R - r_a) f(R, R) \\ &= \frac{1}{2} \int dR_1 \int dR_2 f(R_1, R_2) \sum_a \delta(R_1 - r_a) \sum_b \delta(R_2 - r_b) - \frac{1}{2} \int dR f(R, R) \sum_a \delta(R - r_a) \\ &= \tfrac{1}{2} \textstyle\int dR_1 \int dR_2 f(R_1, R_2) \hat{n}(R_1) \hat{n}(R_2) - \tfrac{1}{2} \int dR f(R, R) \hat{n}(R) \end{aligned}$$

Use the "one-body" operators $\hat{n}(R)$ in second-quantized form:

$$\hat{n}(R_1) = \sum_{m,n} \psi_m^*(R_1) \psi_n(R_1) a_m^\dagger a_n \qquad \text{(recall } \langle m| \, \hat{n}(R) \, |n\rangle = \psi_m^*(r) \psi_n(R))$$

$$\hat{n}(R_2) = \sum_{k,l} \psi_k^*(R_2) \psi_l(R_2) a_k^\dagger a_l$$

$$\hat{n}(R_1)\hat{n}(R_2) \longrightarrow a_m^\dagger a_n a_k^\dagger a_l$$

(1) Check that $a_m^\dagger a_n a_k^\dagger a_l = a_m^\dagger a_k^\dagger a_l a_n + \delta_{nk} a_m^\dagger a_l$

(2) use $\sum_{nk}\delta_{nk}\psi_k^*(R_2)\psi_n(R_1)=\delta(R_1-R_2)$

(3) see the cancellation of $\int dR f(R,R)\hat{n}(R)$ upon normal ordering.

$$\hat{\mathcal{H}}=\sum_a \hat{\mathcal{H}}_a^{(1)}+\sum_{a>b}V(\vec{r}_a,\vec{r}_b), \qquad \text{with } \hat{H}_a^{(1)}=-\frac{\hbar^2}{2m}\nabla^2+U(\vec{r}_a)$$

In second quantization:

$$\hat{\mathcal{H}}=\sum_{ik}\langle i|\,\mathcal{H}^{(1)}\,|k\rangle\, a_i^\dagger a_k+\overbrace{\frac{1}{2}\sum_{i,k,l,m}\langle ik|\,\hat{V}\,|lm\rangle\, a_i^\dagger a_k^\dagger a_m a_l}^{\text{order matters!}}$$

$$\langle ik|\,\mathcal{H}^{(1)}\,|k\rangle=\int dr_1\psi_i^*(r_1)\left(-\frac{\hbar^2}{2m}\nabla^2+U(\vec{r}_a)\right)\psi_i(\vec{r}_1)$$

$$\langle ik|\,\hat{V}\,|lm\rangle=\int dr_1\int dr_2\psi_i^*(r_1)\psi_k^*(r_2)V(r_1,r_2)\psi_l(r_1)\psi_m(r_2)$$

$$\hat{N}=\sum_i a_i^\dagger a_k, \qquad [\hat{N},\hat{\mathcal{H}}]=0$$

Ground-state wave function for non-interacting fermions:

$$|\text{GS}\rangle=\underbrace{|1,1,1,\ldots,1,0,0,0\rangle}_{N\text{ total \# ofparticles)}}=\prod_{E_i\le E_\text{F}}a_i^\dagger\,|0\rangle$$

3.3 Field Operators

We may justify the term "second quantization."
Introduce:

$$\hat{\psi}(\vec{r})=\textstyle\sum_i\psi_i(\vec{r})\hat{a}_i \qquad\qquad \hat{\psi}^\dagger(\vec{r})=\textstyle\sum_i\psi_i^*(\vec{r})\hat{a}_i^\dagger$$

($\psi_i(\vec{r})$ form full orthonormal basis)
Commutation relations for $\hat{\psi},\hat{\psi}^\dagger$:

$$\begin{aligned}\hat{\psi}(\vec{r}_1)\hat{\psi}^\dagger(\vec{r}_2)\pm^{\text{fermions}}_{\text{bosons}}\hat{\psi}^\dagger(\vec{r}_2)\hat{\psi}(\vec{r}_1)&=\sum_i\psi_i(\vec{r}_1)\hat{a}_i\sum_j\psi_j^*(\vec{r}_2)\hat{a}_j^\dagger\pm\sum_j\psi_j^*(\vec{r}_2)\hat{a}_j^\dagger\sum_i\hat{\psi}_i(\vec{r}_1)\hat{a}_i\\&=\sum_{ij}\psi_i(\vec{r}_1)\psi_j^*(\vec{r}_2)(\hat{a}_i\hat{a}_j^\dagger\pm a_j^\dagger a_i)\\&=\sum_{ij}\delta_{ij}\psi_i(\vec{r}_1)\psi_j^*(\vec{r}_2)\\&=\sum_i\psi_i(\vec{r}_1)\psi_i^*(\vec{r}_2)\\&=\delta(\vec{r}_1-\vec{r}_2)\end{aligned}$$

$$\begin{cases}\hat{\psi}(\vec{r}_1)\hat{\psi}^\dagger(\vec{r}_2)\overset{f}{\pm}b\hat{\psi}^\dagger(\vec{r}_2)\psi(\vec{r}_2)=\delta(\vec{r}_1-\vec{r}_2)\\ \hat{\psi}(\vec{r}_1)\hat{\psi}(r_2)\overset{f}{\pm}b\hat{\psi}(\vec{r}_2)\hat{\psi}(\vec{r}_1)=0\end{cases}$$

$$\mathcal{H}=\int d\vec{r}\left\{-\frac{\hbar^2}{2m}\hat{\psi}^\dagger(\vec{r})\nabla^2\hat{\psi}(\vec{r})+\hat{\psi}^\dagger(\vec{r})\mathcal{U}(\vec{r})\psi(\vec{r})\right\}+\frac{1}{2}\int d\vec{r}_1\int d\vec{r}_2\hat{\psi}^\dagger(\vec{r}_1)\hat{\psi}^\dagger(\vec{r}_2)V(\vec{r}_1,\vec{r}_2)\hat{\psi}(\vec{r}_2)\psi(\vec{r}_2)$$

$$\hat{n}(\vec{r})=\hat{\psi}^\dagger(\vec{r})\hat{\psi}(\vec{r}); \qquad \hat{N}=\int d\vec{r}\hat{n}(\vec{r})=\int d\vec{r}\hat{\psi}^\dagger(\vec{r})\hat{\psi}(\vec{r})$$

Particles with spin:

$$\hat{\psi}(\vec{r})\longrightarrow\hat{\psi}(\vec{r},\sigma)\equiv\hat{\psi}_\sigma(\vec{r})$$

$$V=\frac{1}{2}\sum_{\sigma_1\sigma_2}\int d\vec{r}_1\int d\vec{r}_2\hat{\psi}_{\sigma_1}^\dagger\hat{\psi}_{\sigma_2}(\vec{r}_2)V(\vec{r}_1,\vec{r}_2)\hat{\psi}_{\sigma_2}(\vec{r}_2)\hat{\psi}_{\sigma_1}(\vec{r}_1)$$

↑
spin-conserving interaction

3.4 Change of the one-particle basis in second quantization

3.5 Momentum representation of field operators

3.6 Time evolution of observables, equations of motion

4 Free fermions

2.16

4.1 Two point correlation function of density in an ideal Fermi gas

4.2 Wick's theorem

4.3 Elementary theory of photoelectric effect and the fermion spectral function

2.21

Definition (Spectral Function)**.** *We consider an incident photon of momentum $\vec{q}$. The spectral function for a hole is defined*

$$A_h(\vec{p},\omega) = \frac{1}{\pi}\,\mathrm{Re}\int_{-\infty}^{0} dt e^{i\omega t+0.t}\int d\vec{r}e^{-i\vec{p}\cdot\vec{r}}\,\langle G|\,\psi^\dagger(0,0)\psi(\vec{r},t)\,|G\rangle$$

In terms of the probability amplitude for a hole to propagate from a point $\vec{r}$ at time t to 0 at time 0 $\langle G|\,\psi^\dagger(0,0)\psi(\vec{r},t)\,|G\rangle$. Then the frequency of transition from an incident photon of momentum $\vec{q}$ to a scattered electron of momentum $|k\rangle$ is

$$\omega_{\vec{q},\vec{k}} = \frac{2\pi}{\hbar^2}|\lambda|^2\int d\omega\delta(\omega+(\omega_{\vec{q}}-\frac{\hbar^2k^2}{2m}))\int d\vec{p}\delta(\vec{p}+\omega_{\vec{q}}-\vec{k}))A_h(\vec{p},\omega))$$

The spectral function for noninteracting fermions is

$$A_h(\vec{p},\omega)) = \theta(\varepsilon_F-\varepsilon(\vec{p}))\delta(\omega-\frac{\varepsilon(\vec{p})}{\hbar}))$$

The spectral function for a particle can be similarly constructed:

$$A_p(\vec{p},\omega) = \sum_n \left|\langle n|\,a^\dagger_{\vec{p}}|G\rangle\right|^2\delta(\omega+\frac{1}{\hbar}(E_g(N+1)-E_n(N)))$$

4.4 Notion of the Fermi Liquid

Lecture: 2.28

We consider the effect of the momentum-conserving interaction Hamiltonian

$$\hat{V} = \frac{1}{2}\sum_{\vec{p}\vec{p}\vec{q}} v(\vec{q})a^\dagger_{\vec{p}-\vec{q}}a^\dagger_{\vec{p}'+\vec{q}}a_{\vec{p}'}a_{\vec{q}}$$

On the lifetime of the single-particle state with energy (momentum) $\xi,\vec{p}$. For the general 3D case, we have $\frac{1}{\tau}\propto\xi^2$. For the Coulomb interaction specifically,

$$\frac{1}{\tau(\xi)}\sim\frac{e^2}{\hbar v_F}\frac{\xi^2}{E_F}$$

For weak interactions, we take $n_p(t)\approx|\,\langle G|\,a_p(t)a^\dagger_p(0)\,|G\rangle\,|^2 = e^{-t/\tau(\chi_p)}$, which leads to the Fermi liquid spectral function (in units with $\hbar=1$),

$$A(\vec{p},\omega) = \mathrm{Im}\,\frac{1}{\omega-\xi_{\vec{p}}-i/2\tau(\xi_{\vec{p}})}$$

5 Linear response, FDT, and the dynamic structure factor

5.1 General Linear Response (Kubo Formula)

Definition (Kubo formula)**.** *We consider an observable $\hat{A}$ and a perturbation $\hat{V}(t) = f(t)\hat{B}$. The change in the expectation of $\hat{A}$ is*

$$\langle \delta \hat{A} \rangle = \frac{1}{i\hbar} \int_{-\infty}^{t} dt' \langle [A^I(t), B^I(t')] \rangle_0 f(t') e^{0.t'}$$

For the case of a time-translation invariant system, this is written

$$\langle \delta A \rangle = \frac{1}{i\hbar} \int_{-\infty}^{\infty} dt' \Pi_R^{AB}(t - t') f(t')$$

Definition (Retarded response function)**.**

$$\Pi_R^{AB}(t) = -\frac{i}{\hbar} \theta(t) \langle [A^I(t), B^I] \rangle_0$$

also called the retarded correlation function.

5.2 Fluctuation-Dissipation Theorem (FDT)

The imaginary part of the response function fourier components for an operator $\hat{A}$ to a perturbation by $\hat{A}$ can be evaluated:

$$\operatorname{Im} \Pi_R(\omega) = \frac{\pi}{\hbar}(e^{-\beta\hbar\omega} - 1) \sum_{mn} \frac{e^{-\beta E_m}}{A} |A_{mn}|^2 \delta(\omega + \omega_m - \omega)$$

Then we define the symmetrized correlation function (not distinguishing between absorption and scattering)

$$\langle A^2 \rangle_\omega \equiv \int_{-\infty}^{\infty} dt \frac{1}{2} \langle \hat{A}(0)\hat{(t)} + \hat{A}(t)\hat{A}(0) \rangle_0 e^{i\omega t - 0.|t|}$$

Expanding, this can be re-written as

$$\langle A^2 \rangle_\omega = \pi(1 + e^{-\beta\hbar\omega}) \sum_{mn} \frac{e^{-\beta E_m}}{Z} |A_{nm}|^2 \delta(\omega + \omega_m - \omega_n)$$

Which in terms of the response function evaluates to

$$\langle A^2 \rangle_\omega = -\coth\left(\frac{\hbar\omega}{2k_{\mathrm{B}}T}\right) \hbar \operatorname{Im} \Pi_R(\omega)$$

using the fact that $\operatorname{Im} \Pi_R(\omega)$ is an odd function of frequency, we have

$$\langle A^2 \rangle_0 = -\hbar \int_0^{\infty} \frac{d\omega}{\pi} \coth\left(\frac{\hbar\omega}{2k_{\mathrm{B}}T}\right) \operatorname{Im} \Pi_R(\omega)$$

5.3 Absorption power

Why care about the imaginary part of $\Pi_R(\omega)$? Consider a time-dependent perturbation to a time-independent Hamiltonian $\hat{V} = V_0 \cos(\omega t)\hat{A}$. Then the absorption power is the time-average of the derivative of the expected energy, which can be expressed

$$W \equiv \overline{\frac{\mathrm{d}H}{\mathrm{d}t}}^t = -\frac{1}{2}\omega V_0^2 \operatorname{Im} \Pi_R(\omega)$$

5.4 Dynamic density structure factor (DSF)

Definition (DSF)**.** *Assuming a translationally invariant system, the density structure is defined as the fourier transform of $\langle n(\vec{r}_1, t) n(\vec{r}_2, 0) \rangle$, which determines the linear response of $\hat{n}(t, t)$ to a field coupled to particle density;*

$$S(\vec{q}, \omega) = \int_{\infty}^{\infty} dt d\vec{r} e^{i\omega t} e^{iq\vec{r}} \langle n(\vec{r}, t) n(0, 0) \rangle = \int_{-\infty}^{\infty} dt e^{i\omega t} \langle \hat{n}_{\vec{q}} n(t) \hat{n}_{-\vec{q}}(0) \rangle_0$$

Now, consider a perturbation of the form

$$\hat{V} = -\int d\vec{r}' r(\vec{r}', t)\hat{n}(\vec{r}', t)e^{-i\omega t} + h.c. = -(\sum_{\vec{q}} v_{\vec{q}}\hat{n}_{-\vec{q}}e^{-i\omega t} + h.c.)$$

Using the Kubo formula and FDT,

$$S(\vec{q}, \omega) = -2\hbar \frac{\mathrm{Im}\,\Pi_R(\vec{q}, \omega)}{1 - e^{-\beta\hbar\omega}}$$

Note that $S(\vec{q}, \omega)$ characterizes the rate of absorption of incoming photons while $\mathrm{Im}\,\Pi_R(\vec{q}, \omega)$ characterizes the absorbed power.

5.5 Free Fermion response fucntion

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$$\Pi_R(\vec{q}, \omega^+) = -\frac{1}{\hbar}\frac{1}{L^3}\sum_{\vec{k}} \frac{n_{\vec{k}} - n_{\vec{k}+\vec{q}}}{\frac{\varepsilon_{\vec{k}+\vec{q}}}{\hbar} - \frac{\varepsilon_{\vec{k}}}{\hbar} - (\omega + i\delta)}$$

$$\mathrm{Im}\,\Pi_R(\vec{q}, \omega) = -\pi \int \frac{d^k}{(2\pi)^d}(n_{\vec{k}} - n_{\vec{k}+\vec{q}})\delta(\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}} - \hbar\omega)$$

The above is only nonzero for the region $k_F \geq \frac{m^*}{\hbar^2 q}\left|\hbar\omega - \frac{\hbar^2 q^2}{2m}\right|$. (check why this is!)
A static potential does not lead to dissipation because $\mathrm{Im}\,\Pi_R(\vec{q}, \omega) \to 0$ as $\omega \to 0$. Limits: fig

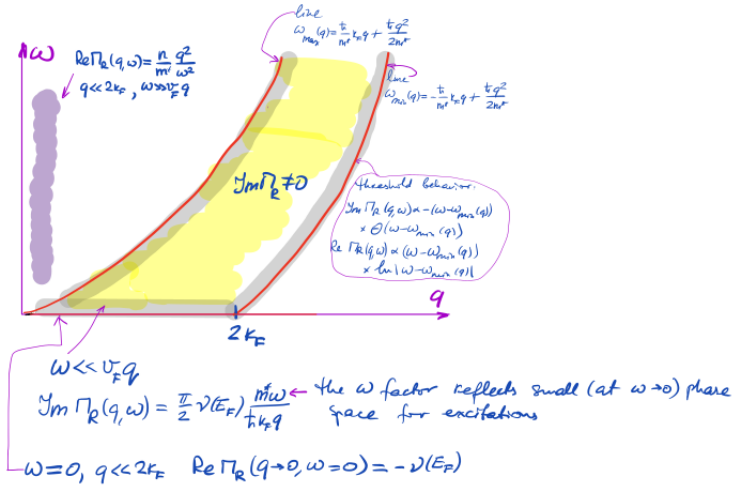

Figure 3: Free fermion response in different limits

6 Random phase approximation

4.04 Consider weakly interacting Fermions and a long-ranged potential produced by an external charge $v_{\vec{q}} = V_q n_q^{ext}$. The response function in RPA is

$$\Pi^{RPA}(\vec{q}, \omega) = \frac{\Pi_0}{1 - \Pi_0 v_{\vec{q}}}$$

where Π_0 is the response function of noninteracting fermions. This approximation is only valid for small q.

6.1 Static limit, screening in RPA approximation

Introduce the screened potential

$$\delta n(\vec{q}, \omega) = \Pi(\vec{q}, \omega)v_{ext}(\vec{q}, \omega) = \Pi_0(\vec{q}, \omega)v_{sc}(\vec{q}, \omega)$$

The dialectric function is defined as

$$\frac{1}{\varepsilon(\vec{q}, \omega)} = \frac{1}{1 - \Pi_0(\vec{q}, \omega)} = 1 + \Pi^{RPA}(\vec{q}, \omega)V_{\vec{q}}$$

Plugging in the coulomb potential, we find

$$V_{sc}(q) = \frac{4\pi e^2}{q^2 + r_{TF}^{-2}}$$

where $r_{TF} = (4\pi e^2 \nu_0)^{-\frac{1}{2}}$ is the Thomas-Fermi radius.

6.2 Plasma Oscillations

7 Mean field theory

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7.1 Variational method

Apply variational method to a trial free energy

$$\Omega_{trial} = \Omega_0 + \langle H - H_0 \rangle$$

With $H = T + V$, $T = \sum_k (\varepsilon(\vec{k}) - \mu) c^\dagger_{\vec{k}} c_{\vec{k}}$ and $V = \frac{1}{2} \sum_{\vec{k}\vec{p}\vec{q}} v_(q) c^\dagger_{\vec{k}+\vec{q}} c^\dagger_{\vec{p}-\vec{q}} c_{\vec{p}} c_{\vec{k}}$, the self-consistency equation is

$$\Sigma(\vec{k}) = v(0) \sum_{\vec{p}} n_F(\varepsilon(\vec{p}) + \Sigma(\vec{p}) - \mu) \pm^B_F \sum_{\vec{q}} v(\vec{q}) n_F(\varepsilon(\vec{k}+\vec{q}) + \Sigma(\vec{k}+\vec{q}) - \mu)$$

The first term is the Hartree term, and the second term is the Fock or exchange term.

7.2 Self-consistent field theory (another formulation of MFT)

Like the homework, replace every $c^\dagger c$ with $\langle N \rangle$.

7.2.1 Fermi liquid theory in Hartree-Fock approximation

Effective mass m^* comes from self-energy:

$$\frac{m}{m^*} \equiv 1 + \frac{\partial \Sigma(k)}{\partial \varepsilon(k)}\Big|_{k=k_F}$$

‘ This comes from the definition of the fermi velocity,

$$v_F = \frac{1}{\hbar} \frac{\mathrm{d}}{\mathrm{d}\vec{k}} \Big(\varepsilon(\vec{k}) + \Sigma(\vec{k}) \Big)$$

The heat capacity of noninteracting fermions is

$$c_0(T) = \frac{\pi^2}{6} k_{\mathrm{B}}^2 \nu_0(E_F) T$$

The Jacobian is renormalized by the interaction:

$$\left| \frac{\partial \varepsilon}{\partial \vec{k}} \right| \to \left| \frac{\partial}{\partial \vec{k}} \Big(\varepsilon(\vec{k}) + \Sigma(\vec{k}) \Big) \right|$$

7.3 Time-Dependent Hartree approximation

8 Weakly-interacting Bose gas

8.1 Uniform gas, Bogoliubov theory

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8.2 Non-uniform interacting Bose gas at $T = 0$

9 Superconductivity, BCS model

9.1 Scatting in Cooper Channel

9.2 The model Hamiltonian for many-body system, mean field solution

9.3 Josephson effect

9.4 Quantum fluctuations of phase, qubits

10 Green functions at $T = 0$

11 Perturbations Theory for Green functions

12 Sources

Huang Stat Mech LL Fetter and Walecka