Concepts Fondamentaux de la Physique

Introduction to Second Quantization

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Contents

Part of the complexity in the many-body problem - systems involving many particles - comes from the indistinguishability of identical particles, fermions or bosons. Calculations in first quantization thus involve the cumbersome (anti-)symmetrization of wavefunctions.

Second quantization is an efficient technical tool that describes many-body systems in a compact and intuitive way.

1 Preliminaries

Before entering the details of second quantization, it is worth drawing a clear distinction between the single-particle and the many-particle Hilbert spaces.

1.1 Single-particle Hilbert space

Consider a single particle described by the hamiltonian $\hat{h}$ acting on the Hilbert space $\mathcal{H}_1$. $\mathcal{H}_1$ is generated by the complete set of eigenfunctions $|\lambda\rangle$ $(\lambda = \mathbf{k}, \sigma, \nu, \ldots)$

$$\hat{h}|\lambda\rangle = \varepsilon_\lambda |\lambda\rangle,$$

with the eigenvalues ε_λ. The identity operator in $\mathcal{H}_1$ is given by the completeness relation $\mathbb{1} = \sum_\lambda |\lambda\rangle\langle\lambda|$.

Examples:

1. single particle in free space, $\hat{h} = -\hbar^2\nabla^2/(2m)$. The eigenfunctions are labeled by the wavevectors $\mathbf{k}$ with $\psi_k(\mathbf{r}) = \langle \mathbf{r}|\mathbf{k}\rangle = \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{V}}$ and the energies $\varepsilon_k = \hbar^2 k^2/2m$.

2. spin 1/2 in a magnetic field, $\hat{h} = -BS^z$. The Hilbert space has dimension 2, generated by the eigenstates $|\uparrow\rangle$ and $|\downarrow\rangle$ of the spin operator S^z.

The basis of two-particle states, given by the set of (anti-)symmetrized functions, + for bosons and − for fermions,

$$\psi_{\lambda,\nu}(1,2) = \frac{1}{\sqrt{2}}\left[\varphi_\lambda(1)\,\varphi_\nu(2) \pm \varphi_\lambda(2)\,\varphi_\nu(1)\right],$$

is built out of the single-particle states $\varphi_\lambda(1) = \langle 1|\lambda\rangle$. The corresponding Hilbert space[1] is denoted $\mathcal{F}_2$.

1.2 Many-particle Hilbert space

We first discuss fermions. Following the two-particle case, the set of antisymmetrized Slater determinants

$$\psi_{\lambda_1,\ldots,\lambda_N}(1,\ldots,N) = \frac{1}{\sqrt{N!}}\sum_{P\in S_N}(-1)^P\varphi_{\lambda_1}(P_1)\ldots\varphi_{\lambda_N}(P_N), \tag{1}$$

where the summation runs over all permutations of $\{1,\ldots,N\}$, forms the basis[2] of the Hilbert space $\mathcal{F}_N$. In the bosonic case, the basis is obtained from symmetrized states, *i.e.* Eq. (1) where $(-1)^P$ is replaced by 1.

The hamiltonian may describe independent particles in which case

$$\hat{H} = \sum_{i=1}^{N}\hat{h}^{(i)},$$

where each piece $\hat{h}^{(i)}$ acts only on the particle i.

Examples:

1. for particles in free space, $\hat{H} = \sum_i \mathbf{p}_i^2/(2m)$.
2. for an assembly of N distinguishable spins in a magnetic field, $\hat{H} = -B\sum_{i=1}^{N} S_i^z$. The Hilbert space has dimension 2^N and symmetrization is not required.

Interactions between particles can be added, $\hat{H} = \sum_i \hat{h}^{(i)} + \hat{V}$, where $\hat{V}$ includes all multi-particle interactions. For example, Coulomb interactions read

$$\hat{V}_{\text{Coulomb}} = \sum_{i=1}^{N}\sum_{j>i}^{N}\frac{e^2}{4\pi\varepsilon_0}\frac{1}{|\mathbf{r}_i-\mathbf{r}_j|}. \tag{2}$$

2 Basics of second quantization

So far, we have introduced and discussed the many-body problem in the language of first quantization. Second quantization corresponds to a different labelling of the basis of states Eq. (1) together with the introduction of creation and annihilation operators that connect spaces with different numbers of particles.

[1] Restricted to (anti-)symmetrized wavefunctions, $\mathcal{F}_2$ is a subset of the larger space $\mathcal{H}_1\otimes\mathcal{H}_1$.

[2] A different choice for the set of single-particle states $|\lambda\rangle$ gives, using Eq. (1), a different many-particle basis that nevertheless spans the same Hilbert space $\mathcal{F}_N$.

2.1 Occupation number representation

Since identical particles are indistinguishable, it is not possible, for a state of the form Eq. (1), to ascribe a definite single-particle state to a given particle. Therefore, instead of focusing on the wavefunction of each particle individually, one can reverse the perspective and characterize the states of Eq. (1) by the set of single-particle states $\{\lambda_1, \dots, \lambda_N\}$ that are occupied by particles, all other single-particle states being empty.

In terms of notations, $|\{n_\lambda\}\rangle$ represents $|\psi_{\lambda_1,\dots,\lambda_N}\rangle$[3] with, for fermions, $n_\lambda = 1$ for $\lambda = \lambda_i$, $i = 1 \dots N$, and $n_\lambda = 0$ otherwise. The state can be written schematically as

$$|\{n_\lambda\}\rangle = |0 \dots \overset{\lambda_1}{1} \dots 0 \dots \overset{\lambda_2}{1} \dots 0 \dots (\dots) \overset{\lambda_N}{1} \rangle, \tag{3}$$

where it is explicitly specified on the right-hand-side which states are occupied and which state are empty.

Bosonic states have similar expressions although the occupation numbers n_λ can take values larger than 1, for example

$$|\{n_\lambda\}\rangle = |0 \dots \overset{\lambda_1}{5} \dots 0 \dots \overset{\lambda_2}{1} \dots 0 \dots (\dots) \overset{\lambda_N}{7} \rangle, \tag{4}$$

for $n_{\lambda_1} = 5$, $n_{\lambda_2} = 1$, ..., $n_{\lambda_N} = 7$.

2.2 Creation and annihilation operators

The constraint on the number of particles, $\sum_\lambda n_\lambda = N$, can be released by working in the extended Hilbert space

$$\mathcal{F} = \bigoplus_{N=0}^{+\infty} \mathcal{F}_N,$$

called the Fock space. Here, $\mathcal{F}_1 = \mathcal{H}_1$ is the single-particle Hilbert space, $\mathcal{F}_0$ contains a unique vacuum state, often noted $|0\rangle$, in which no particle is present.

In the Fock space, creation operators are introduced that raise the number of particles in a given single-particle state by 1. For fermions, it reads

$$c^\dagger_{\lambda_1}|0 \dots \overset{\lambda_1}{0} \dots 0 \dots \overset{\lambda_2}{1} \dots 0 \dots (\dots) \overset{\lambda_N}{1} \rangle = |0 \dots \overset{\lambda_1}{1} \dots 0 \dots \overset{\lambda_2}{1} \dots 0 \dots (\dots) \overset{\lambda_N}{1} \rangle,$$

while particle creation in a single-particle state that is already occupied gives zero,

$$c^\dagger_{\lambda_2}|0 \dots \overset{\lambda_1}{1} \dots 0 \dots \overset{\lambda_2}{1} \dots 0 \dots (\dots) \overset{\lambda_N}{1} \rangle = 0.$$

The annihilation operator c_λ, lowering the number by 1, is the hermitian conjugate of $c^\dagger_\lambda$. The full basis of the Fock space $\mathcal{F}$ is in fact generated by creation operators applied on the vacuum state, namely $|n_{\lambda_1} = 1, \dots, n_{\lambda_N} = 1\rangle = c^\dagger_{\lambda_1} \dots c^\dagger_{\lambda_N}|0 >$.

The antisymmetric properties of the basis states (Slater determinants) $|n_{\lambda_1} \dots n_{\lambda_N}\rangle$ are ensured by the anticommutation relations

$$\{c_\alpha, c_\beta\} = c_\alpha c_\beta + c_\beta c_\alpha = 0, \qquad \{c_\alpha, c^\dagger_\beta\} = \delta_{\alpha,\beta}. \tag{5}$$

The product $\hat{n}_\lambda = c^\dagger_\lambda c_\lambda$ gives the number of fermions occupying the state $|\lambda\rangle$,

$$c^\dagger_\lambda c_\lambda |\{n_\alpha\}\rangle = n_\lambda |\{n_\alpha\}\rangle$$

where $n_\lambda = 0$ or 1.

[3] $\psi_{\lambda_1,\dots,\lambda_N}(1, \dots, N) = \langle 1, \dots, N|\psi_{\lambda_1,\dots,\lambda_N}\rangle$.

2.3 Bosons

There are only slight differences in the way second quantization works for fermions and for bosons. In the case of bosons, the basis states are symmetrized functions and the number of bosons in a given single-particle state is not restricted. These properties are ensured by the commutation relations

$$[b_\alpha, b_\beta] = b_\alpha b_\beta - b_\beta b_\alpha = 0, \qquad [b_\alpha, b_\beta^\dagger] = \delta_{\alpha,\beta}, \tag{6}$$

with the (annihilation) creation operators (b_α) $b_\alpha^\dagger$. From Eq. (6), one can prove[4] that

$$\begin{aligned} b_\lambda^\dagger |n_\lambda\rangle &= \sqrt{n_\lambda + 1}|n_\lambda + 1\rangle \\ b_\lambda |n_\lambda\rangle &= \sqrt{n_\lambda}|n_\lambda - 1\rangle \end{aligned} \tag{7}$$

such that $\hat{n}_\lambda = b_\lambda^\dagger b_\lambda$ is indeed the number operator, $\hat{n}_\lambda|n_\lambda\rangle = n_\lambda|n_\lambda\rangle$.

3 Representation of operators

The complexity associated with wavefunction (anti)symmetrization has been reduced, in the formalism of second quantization, to the surprisingly simple commutation relations, Eq. (5) for fermions and Eq. (6) for bosons. Had the usual operators of the theory complicated expressions in terms of creation/annihilation operators, this would not be very useful. However, as we shall see below, the hamiltonian as well as standard operators do have simple expressions in second quantization.

3.1 Change of basis and the field operator

Starting with the expression $|\lambda\rangle = c_\lambda^\dagger|0\rangle$, one can insert the closure relation $\mathbb{1} = \sum_\lambda |\lambda\rangle\langle\lambda|$ to derive the transformation law for the creation/annihilation operators

$$c_\alpha^\dagger = \sum_\lambda \langle\lambda|\alpha\rangle\, c_\lambda^\dagger, \qquad c_\alpha = \sum_\lambda \langle\alpha|\lambda\rangle\, c_\lambda, \tag{8}$$

from one basis to another. Hence, the change of basis only requires the calculation of matrix elements $\langle\alpha|\lambda\rangle$ involving single-particle states.

By convention, the field operator $\Psi(\mathbf{r})$ in a continuous problem is associated to the basis of position states $|\mathbf{r}\rangle$,

$$\Psi(\mathbf{r}) = \sum_\lambda \langle\mathbf{r}|\lambda\rangle\, c_\lambda. \tag{9}$$

Using Eq. (5) and Eq. (6), one finds the commutation relation

$$\begin{aligned} &\{\Psi(\mathbf{r}), \Psi(\mathbf{r}')\} = 0, && \{\Psi(\mathbf{r}), \Psi^\dagger(\mathbf{r}')\} = \delta(\mathbf{r} - \mathbf{r}'), && \text{fermions,} \\ &[\Psi(\mathbf{r}), \Psi(\mathbf{r}')] = 0, && [\Psi(\mathbf{r}), \Psi^\dagger(\mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}'), && \text{bosons.} \end{aligned} \tag{10}$$

The total number of particles (fermions or bosons) is then given by

$$\hat{N} = \sum_\lambda c_\lambda^\dagger c_\lambda = \int d^d r\, \hat{\rho}(\mathbf{r}) \tag{11}$$

[4] The states $|n_\lambda\rangle$ are chosen to be normalized to 1.

where the local density operator $\hat{\rho}(\mathbf{r}) = \Psi^\dagger(\mathbf{r})\Psi(\mathbf{r})$ has been introduced.

Example: The transformation to the Fourier momentum representation reads

$$\Psi(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}\, c_{\mathbf{k}}, \tag{12}$$

where $c_{\mathbf{k}}$ destroys a particle with momentum $\mathbf{k}$. The total number of particle is given by $\hat{N} = \sum_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}}$.

3.2 Representation of one-body and two-body operators

Single-particle or one-body operators have the form $\hat{O}^{(1)} = \sum_{i=1}^{N} \hat{o}^{(1)}[i]$ in first quantization, where $\hat{o}^{(1)}[i]$ is a single-particle operator acting on the ith particle. In the language of second quantization, they take the form

$$\hat{O}^{(1)} = \sum_{\alpha,\beta} \langle\alpha|\hat{o}^{(1)}|\beta\rangle\, c_\alpha^\dagger c_\beta, \tag{13}$$

with the matrix elements $\langle\alpha|\hat{o}^{(1)}|\beta\rangle = \int d1\, d2\; \varphi_\alpha^*(1)\langle 1|\hat{o}^{(1)}|2\rangle\varphi_\beta(2)$.

Examples:

1. The kinetic energy operator $\hat{T} = \sum_i \mathbf{p}_i^2/(2m)$, describing independent particles, reads in second quantization

$$\hat{T} = \sum_{\mathbf{k}} \frac{\hbar^2 k^2}{2m}\, c_{\mathbf{k}}^\dagger c_{\mathbf{k}}, \tag{14}$$

   i.e. it is diagonal in the momentum basis. An alternative expression involving the field operator is

$$\hat{T} = \int d^d r\, \Psi^\dagger(\mathbf{r})\, \frac{(\hbar\nabla/i)^2}{2m}\, \Psi(\mathbf{r}) = \int d^d r\, \frac{\hbar^2}{2m}\, \nabla\Psi^\dagger(\mathbf{r}) \cdot \nabla\Psi(\mathbf{r}). \tag{15}$$

2. Tight-binding models are simplified band models for electrons in solids where only neighboring sites hybridize. A particularly simple example is given by the hamiltonian

$$\hat{H} = -t \sum_{\langle i,j\rangle} \left(c_i^\dagger\, c_j + c_j^\dagger\, c_i \right), \tag{16}$$

   where $c_i^\dagger$ creates an electron on site i and $\langle i,j\rangle$ denotes neighboring sites. The product $c_i^\dagger\, c_j$ describes intuitively the hopping of an electron from site j to site i: one electron is annihilated on site j while a novel electron appears on site i. The hamiltonian Eq. (16) is diagonalized by going to the Fourier space $c_{\mathbf{k}} = \frac{1}{\sqrt{N_s}} \sum_i e^{-i\mathbf{k}\cdot\mathbf{r}_i}\, c_i$ (N_s is the number of sites of the lattice), with the result $\hat{H} = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}}$. In one dimension, $\varepsilon_k = -2t\cos(ka)$, a being the lattice spacing.

We now consider a two-body operator such as the Coulomb interaction of Eq. (2). In first quantization, it has the form

$$\hat{O}^{(2)} = \frac{1}{2} \sum_{i\neq j} \hat{o}^{(2)}[i,j], \tag{17}$$

where $\hat{o}^{(2)}[i,j]$ accounts for pair interactions. In second quantization, it reads[5]

$$\hat{O}^{(2)} = \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} \langle \alpha\, \beta | \hat{o}^{(2)} | \gamma \delta \rangle c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma, \tag{18}$$

with the matrix elements

$$\langle \alpha\, \beta | \hat{o}^{(2)} | \gamma \delta \rangle = \int d1\, d2\, \varphi_\alpha^*(1) \varphi_\beta^*(2) \hat{o}^{(2)}[1,2] \varphi_\gamma(1) \varphi_\delta(2). \tag{19}$$

Example: Electron-electron Coulomb interaction is given in second quantization by

$$\hat{V}_{\text{Coulomb}} = \frac{1}{2} \sum_{\sigma_1,\sigma_2} \int d\mathbf{r}_1\, d\mathbf{r}_2\, \frac{e^2}{4\pi\varepsilon_0 |\mathbf{r}_1 - \mathbf{r}_2|}\, \Psi_{\sigma_1}^\dagger(\mathbf{r}_1) \Psi_{\sigma_2}^\dagger(\mathbf{r}_2) \Psi_{\sigma_2}(\mathbf{r}_2) \Psi_{\sigma_1}(\mathbf{r}_1), \tag{20}$$

in terms of the field operator $\Psi_\sigma(\mathbf{r})$. Here the spin σ of electrons has been included. After going to the Fourier momentum representation of Eq. (12), one obtains the alternative expression

$$\hat{V}_{\text{Coulomb}} = \frac{1}{2V} \sum_{\sigma_1,\sigma_2} \sum_{\mathbf{q},\mathbf{k}_1,\mathbf{k}_2} v(q)\, c_{\mathbf{k}_1+\mathbf{q},\sigma_1}^\dagger c_{\mathbf{k}_2-\mathbf{q},\sigma_2}^\dagger c_{\mathbf{k}_2,\sigma_2} c_{\mathbf{k}_1,\sigma_1}$$

with the Fourier transform of the Coulomb pair potential $v(q) = e^2/(\varepsilon_0\, q^2)$.

References

[1] H. Bruus and K. Flensberg, *Many-Body Quantum Theory in Condensed Matter Physics* (Oxford University Press, Oxford, 2004).

[2] A. Altland and B. Simons, *Condensed Matter Field Theory* (Cambridge University Press, Cambridge, 2010).

[5]Note the ordering of indices which, in the product of annihilation operators, is reversed with respect to the ordering in the matrix element.

Theory of Condensed Matter

Exercises on second quantization

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1 Starters

1. For $\alpha \neq \beta$, compute the matrix element $\langle 0|c_\alpha c_\beta c_\alpha^\dagger c_\beta^\dagger|0\rangle$ for fermions and for bosons.
2. Consider free fermions with spin 1/2 in a box of volume V. Write the hamiltonian $\hat{H}_0$ in second quantization in the Fourier momentum representation.
   (a) Write the expression of the ground state $|\mathrm{FS}\rangle$.
   (b) Compute the following quantities
   $$\langle \hat{n}_{k\sigma}\rangle = \langle \mathrm{FS}|c_{k\sigma}^\dagger c_{k\sigma}|\mathrm{FS}\rangle, \qquad E_0 = \langle \mathrm{FS}|\hat{H}_0|\mathrm{FS}\rangle, \qquad N_0 = \langle \mathrm{FS}|\hat{N}|\mathrm{FS}\rangle,$$
   in the thermodynamic limit $V \to +\infty$.
3. In the case of fermions, prove that
   $$c_\alpha^\dagger|\{n_\beta\}\rangle = \begin{cases} (-1)^{\sum_{\beta<\alpha} n_\beta}\,|n_1\, n_2 \ldots \overset{\alpha}{1}\; n_{\alpha+1} \ldots n_N\rangle & \text{if } n_\alpha = 0 \\ 0 & \text{if } n_\alpha = 1 \end{cases} \tag{1}$$
   and
   $$c_\alpha|\{n_\beta\}\rangle = \begin{cases} 0 & \text{if } n_\alpha = 0 \\ (-1)^{\sum_{\beta<\alpha} n_\beta}\,|n_1\, n_2 \ldots \overset{\alpha}{0}\; n_{\alpha+1} \ldots n_N\rangle & \text{if } n_\alpha = 1 \end{cases} \tag{2}$$
4. Show that the change of basis
   $$c_\beta^\dagger = \sum_\alpha U_{\beta\alpha} c_\alpha^\dagger,$$
   preserves the canonical commutation relations iff U is a unitary matrix. Is $U_{\beta\alpha} = \langle\beta|\alpha\rangle$ a unitary matrix ? Show that the expression of the number operator $\hat{N} = \sum_\alpha c_\alpha^\dagger c_\alpha$ is not modified by the above transformation.
5. For bosons, show that
   $$|n_1\, n_2 \ldots\rangle = \prod_i \frac{(b_i^\dagger)^{n_i}}{\sqrt{n_i!}}|0\rangle.$$
6. Compute the commutator $[\hat{H}_0, \hat{N}]$ for free fermions. What is the meaning of the result ? Is it modified when interactions are taken into account ?
7. Consider spinless free fermions or free bosons.
   (a) Derive the expression $\hat{H}_0 = \sum_k \varepsilon_k c_k^\dagger c_k$ from $\hat{H}_0 = -(\hbar^2/2m)\int dr\, \psi^\dagger(r)\nabla^2\psi(r)$.
   (b) Derive the expression of the Coulomb pair potential in the momentum representation starting from $\hat{V}_{\text{Coulomb}} = \frac{1}{2}\sum_{\sigma_1,\sigma_2}\int dr_1\, dr_2\, V(r_1 - r_2)\, \Psi_{\sigma_1}^\dagger(r_1)\Psi_{\sigma_2}^\dagger(r_2)\Psi_{\sigma_2}(r_2)\Psi_{\sigma_1}(r_1)$.
8. Consider the one-dimensional tight-binding model ($t > 0$)
   $$\hat{H} = -t\sum_i \left(c_i^\dagger\, c_{i+1} + \text{h.c.}\right), \tag{3}$$
   with periodic boundary conditions $c_{N_s+1} = c_1$, describing the hopping of electrons on a lattice of N_s sites with lattice spacing a. Diagonalize the hamiltonian by going to the Fourier space and show that the eigenenergies are given by
   $$\varepsilon_k = -2t\cos(ka).$$
   What are the admissible values for the wavevector k ?

9. The local density operator is given for a single particle by $\hat{\rho}(\mathbf{r}) = |\mathbf{r}\rangle\langle\mathbf{r}|$. Give the expression of $\hat{\rho}(\mathbf{r})$ in second quantization in a given basis $|\varphi_\lambda\rangle$ of one-particle states. Give $\hat{\rho}(\mathbf{r})$ in the basis of position states $|\mathbf{r}\rangle$. In the basis of momentum states $|\mathbf{k}\rangle$, give $\hat{\rho}(\mathbf{r})$ and then its Fourier transform
$$\hat{\rho}(\mathbf{q}) = \int d\mathbf{r}\, \hat{\rho}(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}}$$

2 Spin operator

We consider fermions with spin 1/2. We denote by $\alpha = \uparrow, \downarrow$ the spin component. The spin operator of the many-body system assumes the form
$$\hat{\mathbf{S}} = \sum_\lambda c^\dagger_{\lambda\alpha'} \frac{\sigma_{\alpha'\alpha}}{2} c_{\lambda\alpha} \tag{4}$$
where $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ is a vector composed by the standard Pauli matrices [1], and λ denotes the set of additional quantum numbers (wavevector, lattice site index, etc).

1. Forget about spin for one moment and consider a finite Hilbert space with N one-particle states. We use the notation $c^\dagger = (c^\dagger_1, c^\dagger_2, \ldots, c^\dagger_N)$ as a vector with N entries. Prove the following identity
$$[c^\dagger A\, c, c^\dagger B\, c] = c^\dagger [A, B]\, c$$
where A and B are $N \times N$ matrices.
2. Use the previous result to show that the spin operator in Eq. (4) satisfies the commutation relations of the Lie group SU(2).
3. Can we say something specific about $\hat{\mathbf{S}}^2$?
4. Give the spin raising and lowering operators $\hat{S}^\pm = \hat{S}_x \pm i\hat{S}_y$ in terms of creation and annihilation operators.

We take the Hubbard model in the atomic limit : a single site governed by the hamiltonian
$$\hat{H} = \varepsilon_d(\hat{n}_\uparrow + \hat{n}_\downarrow) + U\, \hat{n}_\uparrow \hat{n}_\downarrow$$
where $\hat{n}_\sigma = d^\dagger_\sigma d_\sigma$.

5. Give the size of the corresponding Hilbert space.
6. Diagonalize the hamiltonian.
7. Precise the spin for each eigenstate.

3 Hartree-Fock

We consider a gas of N electrons with spin 1/2. The hamiltonian includes kinetic and Coulomb energies, $\hat{H} = \hat{T} + \hat{V}$ or
$$\hat{H} = \sum_{\sigma,\mathbf{k}} \varepsilon_k\, c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{1}{2V} \sum_{\sigma_1,\sigma_2} \sum_{\mathbf{q},\mathbf{k}_1,\mathbf{k}_2} \frac{e^2}{\varepsilon_0\, q^2}\, c^\dagger_{\mathbf{k}_1+\mathbf{q},\sigma_1} c^\dagger_{\mathbf{k}_2-\mathbf{q},\sigma_2} c_{\mathbf{k}_2,\sigma_2} c_{\mathbf{k}_1,\sigma_1}. \tag{5}$$

This hamiltonian can not be diagonalized. We shall therefore treat the Coulomb interaction $\hat{V}$ in perturbation theory.

1. What is the ground state of the system in the absence of $\hat{V}$?

1.
$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

2. Show that the correction to the ground state energy, to leading order in $\hat{V}$, has two contributions : a direct Hartree term, which in this case is infinite, and an exchange Fock term.
3. Compute the Fock term using the identity

$$\mathcal{V}_q = \sum_{\mathbf{k}} \theta[\varepsilon_F - \varepsilon_{\mathbf{k}}]\theta[\varepsilon_F - \varepsilon_{\mathbf{k+q}}] = \frac{4\pi k_F^3}{3}\left[1 - \frac{3}{4}\frac{q}{k_F} + \frac{1}{16}\left(\frac{q}{k_F}\right)^3\right] \qquad \text{for} \quad |\mathbf{q}| < 2k_F$$

and zero for $|\mathbf{q}| \geq 2k_F$. Find the result

$$\frac{\delta E}{V} = -\frac{k_F^4}{4\pi^3}\frac{e^2}{4\pi\varepsilon_0}.$$

4 Finite temperature and thermodynamics

We recall that the partition function Z in the grand canonical ensemble is given by

$$Z = \mathrm{Tr} e^{-\beta(\hat{H}-\mu\hat{N})}$$

where the trace is taken over all states of the many-body Hilbert space. μ denotes here the chemical potential. The mean value of an operator $\hat{O}$ acting in the many-body Hilbert space is then given by

$$\langle\hat{O}\rangle = \frac{1}{Z}\,\mathrm{Tr}\left[\hat{O}\,e^{-\beta(\hat{H}-\mu\hat{N})}\right].$$

1. Suppose that the hamiltonian is diagonal in the occupation number for some particular one-particle basis,
$$\hat{H} = \sum_\lambda \varepsilon_\lambda \hat{n}_\lambda.$$
This implies in passing that particles are independent, *i.e.* not interacting. Show that the partition function factorizes as $Z = \prod_\lambda Z_\lambda$.
2. Give the expression of Z_λ for fermions and for bosons.
3. Compute $\langle\hat{n}_\lambda\rangle$ for fermions and for bosons. Which distributions do we find ?

Exercises on second quantization : solutions

1 - Starters

1. $\langle 0| c_\alpha c_\beta c_\alpha^\dagger c_\beta^\dagger |0\rangle$ $\qquad \alpha \neq \beta$

1st method: $\langle 0| c_\alpha c_\beta c_\alpha^\dagger c_\beta^\dagger |0\rangle = \underset{F}{\overset{B}{\pm}} \langle 0| c_\beta c_\alpha \left(c_\alpha^\dagger c_\beta^\dagger |0\rangle \right)$

$|\psi\rangle = c_\alpha^\dagger c_\beta^\dagger |0\rangle$

$\langle 0| c_\alpha c_\beta c_\alpha^\dagger c_\beta^\dagger |0\rangle = \pm \langle \psi|\psi\rangle = \underset{F}{\overset{B}{\pm}} 1$ ($|\psi\rangle$ is normalized)

→ 2nd method:

F: $\langle 0| c_\alpha c_\beta c_\alpha^\dagger c_\beta^\dagger |0\rangle = -\langle 0| c_\alpha c_\alpha^\dagger c_\beta c_\beta^\dagger |0\rangle$, for $\{c_\beta, c_\alpha^\dagger\} = 0$ if $\alpha \neq \beta$

$= -\langle 0| c_\alpha c_\alpha^\dagger (\mathbb{1} - \underbrace{c_\beta^\dagger c_\beta)|0\rangle}_{= 0 \text{ (null vector)}}$, for $\{c_\alpha, c_\alpha^\dagger\} = \mathbb{1}$

$= -\langle 0| c_\alpha c_\alpha^\dagger |0\rangle$

$= -\langle 0| \mathbb{1} - \underbrace{c_\alpha^\dagger c_\alpha |0\rangle}_{=0} = -1$

B: same thing with + signs. : $+1$

2. $\hat{h} = \sum_{\vec{k},\sigma} \varepsilon_{\vec{k}} |\vec{k},\sigma\rangle\langle\vec{k},\sigma|$, $k_\nu = \frac{2\pi}{L_\nu} n_\nu$, $n_\nu \in \mathbb{Z}$, $\nu = x,y,z$

$\varepsilon_{\vec{k}} = \frac{\hbar^2 \vec{k}^2}{2m}$, $\langle \vec{r}|\vec{k}\rangle = \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}}$ $\qquad \sigma = \uparrow, \downarrow$ (spin)

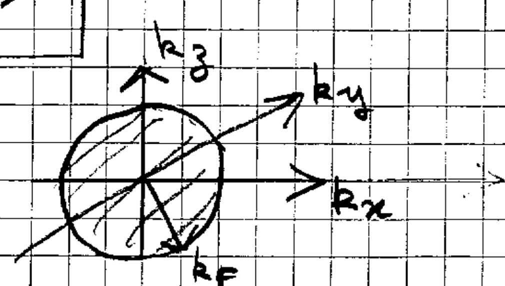
$V = L_x L_y L_z$

Lecture ⇒ $\boxed{\hat{H}_0 = \sum_{\vec{k},\sigma} \varepsilon_{\vec{k}} c_{\vec{k},\sigma}^\dagger c_{\vec{k},\sigma}}$

(a) Fermi Sea (or Fermi Sphere!) : Fill all the 1-particle states with increasing 1-particle energy $\varepsilon_{\vec{k}}$:

$$\boxed{|FS\rangle = \prod_{|\vec{k}|<k_F} c_{\vec{k}\uparrow}^\dagger c_{\vec{k}\downarrow}^\dagger |0\rangle}$$

The wave-vectors of the occupied 1-part. states lie inside a sphere of radius k_F, the Fermi wave-vector



(b) $\langle \hat{n}_{\vec{k}\sigma} \rangle = \langle FS | c^+_{\vec{k}\sigma} c_{\vec{k}\sigma} | FS \rangle$ ②

1st case: $|\vec{k}| > k_F$; the 1-particle state $|\vec{k},\sigma\rangle$ is unoccupied in $|FS\rangle$, therefore $c_{\vec{k}\sigma}|FS\rangle = 0$

hence $\langle FS | c^+_{\vec{k}\sigma} \underbrace{c_{\vec{k}\sigma}|F\rangle}_{=0} = 0 = \langle \hat{n}_{\vec{k}\sigma} \rangle$

2nd case: $|\vec{k}| < k_F$. We have

$$|FS\rangle = c^+_{\vec{k}_1\uparrow} c^+_{\vec{k}_1\downarrow} \cdots c^+_{\vec{k}_i\uparrow} c^+_{\vec{k}_i\downarrow} \; c^+_{\vec{k}\uparrow} c^+_{\vec{k}\downarrow} \; c^+_{\vec{k}_{i+1}\uparrow} c^+_{\vec{k}_{i+1}\downarrow} \cdots |0\rangle$$

$\hat{n}_{\vec{k}\uparrow} = c^+_{\vec{k}\uparrow} c_{\vec{k}\uparrow}$ commute with all the first ith pairs (why?), so we have:

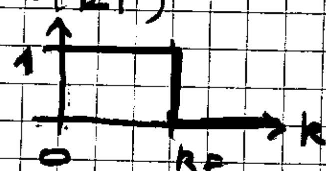
$$\hat{n}_{\vec{k}\uparrow}|FS\rangle = c^+_{\vec{k}_1\uparrow} c^+_{\vec{k}_1\downarrow} \cdots c^+_{\vec{k}_i\uparrow} c^+_{\vec{k}_i\downarrow} \underbrace{\left(c^+_{\vec{k}\uparrow} c_{\vec{k}\uparrow} c^+_{\vec{k}\uparrow} \right)}_{= c^+_{\vec{k}\uparrow} - \underbrace{(c^+_{\vec{k}\uparrow})^2}_{=0} c_{\vec{k}\uparrow}} \cdots |0\rangle$$

$$= |FS\rangle$$

Same thing for $\sigma = \downarrow$.

Therefore: $\langle FS | \hat{n}_{\vec{k}\sigma} | FS \rangle = 1$ if $|\vec{k}| < k_F$

Conclusion: $\langle FS | \hat{n}_{\vec{k}\sigma} | FS \rangle = \Theta(k_F - |\vec{k}|)$



$$E_0 = \langle FS | \hat{H}_0 | FS \rangle = \sum_{k\sigma} \varepsilon_k \langle FS | \hat{n}_{k\sigma} | FS \rangle$$

$$= \sum_{k\sigma} \varepsilon_k \, \Theta(k_F - |\vec{k}|)$$

$V \to \infty$: $\displaystyle \sum_k \to V \int \frac{d^3\vec{k}}{(2\pi)^3}$ (3D)

$$\frac{E_0}{V} = \underset{\text{spin}}{2} \int_{|\vec{k}| < k_F} \frac{d^3\vec{k}}{(2\pi)^3} \frac{\hbar^2 k^2}{2m}$$

$$= 2 \frac{(4\pi)^{\leftarrow \text{angles}}}{(2\pi)^3} \frac{\hbar^2}{2m} \int_0^{k_F} dk \, k^4$$

$$\boxed{\frac{E_0}{V} = \frac{1}{10\pi^2} \frac{\hbar^2}{m} k_F^5}$$

$$N = \sum_{|\vec{k}| < k_F} 1 \underset{V \to \infty}{=} 2^{\swarrow \text{spin}} V \int_{k < k_F} \frac{d^3 \vec{k}}{(2\pi)^3}$$

$$= 2V \frac{(4\pi)^{\swarrow \text{angles}}}{(2\pi)^3} \int_0^{k_F} dk\, k^2$$

$$\boxed{\frac{N}{V} = \frac{k_F^3}{3\pi^2}}$$

3. $$c^+_\alpha |\{n_\beta\}\rangle = c^+_\alpha | n_1\, n_2 \,-\,-\,-\, n_\alpha \,-\,-\,-\, n_N \rangle$$

$$n_\beta = 0 \text{ or } 1$$

By convention, we order the creation operators in the definition of a Fock state $|n_1 n_2 - - n_\alpha - n_N\rangle$, from left to right. For example if the 1-part states $|1\rangle$ and $|2\rangle$ are occupied, we write $|\overset{1}{1}\ \overset{2}{1}\rangle \equiv c^+_1\, c^+_2\, |0\rangle$.

If by <u>definition</u>, we write $(c^+)^0 \equiv \mathbb{1}$, we can write:

$$|n_1 n_2 - - n_N\rangle = (\underset{\uparrow \text{operator}}{c^+_1})^{n_1 \leftarrow \text{occupation \underline{number}}} (c^+_2)^{n_2} \,-\,-\, (c^+_N)^{n_N} |0\rangle$$

Hence we have:

$$c^+_\alpha |\{n_\beta\}\rangle = c^+_\alpha \ (c^+_1)^{n_1} (c^+_2)^{n_2} \cdots (c^+_\alpha)^{n_\alpha} - (c^+_N)^{n_N} |0\rangle$$

It is easy to see that c^+_α <u>anticommute</u> with $(c^+_\beta)^{n_\beta}$ if $n_\beta = 1$ and commute ($(c^+_\beta)^{n_\beta} = \mathbb{1}$!) if $n_\beta = 0$

Therefore $$c^+_\alpha\, (c^+_\beta)^{n_\beta} = (-1)^{n_\beta} (c^+_\beta)^{n_\beta}\, c^+_\alpha$$

Thus we have:

$$c^+_\alpha |\{n_\beta\}\rangle = (-1)^{n_1 + n_2 - - n_{\alpha-1}} (c^+_1)^{n_1} - - - c^+_\alpha (c^+_\alpha)^{n_\alpha} - - - |0\rangle$$

if $n_\alpha = 1$: $c^+_\alpha\, c^+_\alpha = 0$

if $n_\alpha = 0$: we recover the Fock state with $n_\alpha = 1$

$$\boxed{\underline{\text{Conclusion}}:\ c^+_\alpha |\{n_\beta\}\rangle = \begin{cases} (-1)^{\sum_{\beta<\alpha} n_\beta} |n_1 - - \overset{\alpha}{1}\ n_N\rangle, & n_\alpha = 0 \\ 0, & n_\alpha = 1 \end{cases}}$$

In the same way, we find:

$$\boxed{c_\alpha|\{n_\beta\}\rangle = \begin{cases} 0 & \text{if } n_\alpha = 0 \\ (-1)^{\left(\sum_{\beta<\alpha} n_\beta\right)} |n_1 n_2 \cdots \overset{\alpha}{0} \cdots n_N\rangle, & \text{if } n_\alpha = 1 \end{cases}}$$

4. $c^+_\beta = \sum_\alpha U_{\beta\alpha} c^+_\alpha$, hence $c_\beta = \sum_\alpha (U_{\beta\alpha})^* c_\alpha$

F. $\{c_\beta, c_{\beta'}\} = \sum_{\alpha\alpha'} U_{\beta\alpha} U_{\beta'\alpha'} \{c_\alpha, c_{\alpha'}\}$ (1)

$\{c_\beta, c^+_{\beta'}\} = \sum_{\alpha\alpha'} U_{\beta\alpha} (U_{\beta'\alpha'})^* \{c_\alpha, c^+_{\alpha'}\}$ (2)

- If $\{c_\beta, c^+_{\beta'}\} = \delta_{\beta\beta'}$ and $\{c_\alpha, c^+_{\alpha'}\} = \delta_{\alpha\alpha'}$,

from (2): $\delta_{\beta\beta'} = \sum_{\alpha\alpha'} U_{\beta\alpha} (U_{\beta'\alpha'})^* \delta_{\alpha\alpha'}$

$$= \sum_\alpha U_{\beta\alpha} \underbrace{(U_{\beta'\alpha})^*}_{\equiv U^+_{\alpha\beta'}} = \sum_\alpha U_{\beta\alpha} U^+_{\alpha\beta'}$$

$$= (UU^+)_{\beta\beta'}$$

Therefore $UU^+ = \mathbb{1}$.

- If U is unitary and $\{c_\alpha, c_{\alpha'}\} = 0$, $\{c_\alpha, c^+_{\alpha'}\} = \delta_{\alpha\alpha'}$

From (1): $\{c_\beta, c_{\beta'}\} = \sum_{\alpha\alpha'} U\,U \times 0 = 0$

From (2): $\{c_\beta, c^+_{\beta'}\} = \sum_{\alpha\alpha'} U_{\beta\alpha} (U_{\beta'\alpha'})^* \delta_{\alpha\alpha'}$

$$= \sum_\alpha U_{\beta\alpha} \underbrace{(U_{\beta'\alpha})^*}_{\equiv U^+_{\alpha\beta'}} = (UU^+)_{\beta\beta'}$$

$$= \delta_{\beta\beta'}$$

Therefore we recover the canonical commutation relation for the operators in the new basis.

B. same thing

- $U_{\beta\alpha} = \langle\beta|\alpha\rangle$, $(U^+)_{\alpha\beta} \equiv (U_{\beta\alpha})^* = (\langle\beta|\alpha\rangle)^*$
$= \langle\alpha|\beta\rangle$

$(U^+U)_{\alpha\alpha'} = \sum_\beta (U^+)_{\alpha\beta} U_{\beta\alpha'}$

$$= \sum_\beta \langle \alpha|\beta\rangle\langle\beta|\alpha'\rangle = \langle\alpha|\underbrace{\left(\sum_\beta |\beta\rangle\langle\beta|\right)}_{=\mathbb{1}}|\alpha'\rangle$$
$$= \langle\alpha|\alpha'\rangle = \delta_{\alpha\alpha'}$$

Therefore U is unitary.

$$\sum_\beta c^+_\beta c_\beta = \sum_\beta \left(\sum_{\alpha_1} U_{\beta\alpha_1} c^+_{\alpha_1}\right)\left(\sum_{\alpha_2} (U_{\beta\alpha_2})^* c_{\alpha_2}\right)$$
$$= \sum_{\alpha_1\alpha_2} c^+_{\alpha_1}\left(\sum_\beta U_{\beta\alpha_1}\underbrace{(U_{\beta\alpha_2})^*}_{U^+_{\alpha_2\beta}}\right) c_{\alpha_2}$$
$$= \sum_{\alpha_1\alpha_2} c^+_{\alpha_1}\underbrace{\left(\sum_\beta U^+_{\alpha_2\beta} U_{\beta\alpha_1}\right)}_{(U^+U)_{\alpha_2\alpha_1} = \delta_{\alpha_1\alpha_2}} c_{\alpha_2}$$
$$= \sum_{\alpha_1} c^+_{\alpha_1} c_{\alpha_1}.$$

N has the same expression in the two basis.

5. We check that, if $|n_1 n_2 \dots\rangle = \prod_i \frac{(b^+_i)^{n_i}}{\sqrt{n_i!}}|0\rangle$, we have:

i) $b^+_i|\dots n_i \dots\rangle = \sqrt{n_i+1}\,|\dots n_i+1\dots\rangle$

ii) $b_i|\dots n_i\dots\rangle = \sqrt{n_i}\,|\dots n_i-1\dots\rangle$

<u>i)</u> $b^+_i|n_1 n_2\dots\rangle$: b^+_i <u>commutes</u> with the $(b^+_j)^{n_j}$. Hence:

$$b^+_i|n_1 n_2\dots\rangle = \frac{(b^+_1)^{n_1}}{\sqrt{n_1!}}\cdots \underbrace{b^+_i\frac{(b^+_i)^{n_i}}{\sqrt{n_i!}}}\frac{(b^+_{i+1})^{n_{i+1}}}{\sqrt{\ }}\cdots|0\rangle$$
$$= \frac{(b^+_i)^{n_i+1}}{\sqrt{(n_i+1)!}}\times\sqrt{n_i+1}$$
$$= \sqrt{n_i+1}\,|n_1 n_2\dots\rangle$$

ii) b_i <u>commutes</u> with all the $(b^+_j)^{n_j}$ if $j\neq i$.
Moreover, all the $(b^+_j)^{n_j}$'s commute, and we place $(b^+_i)^{n_i}$ at the rightmost place.

$$b_i|n_1 n_2\dots\rangle = \frac{(b^+_1)^{n_1}}{\sqrt{n_1!}}\cdots b_i\frac{(b^+_i)^{n_i}}{\sqrt{n_i!}}|0\rangle$$

using : $bb^+ = 1 + b^+b$, we easily find: (6)

$$b\,(b^+)^n = \underbrace{b\,b^+}_{1+b^+b}(b^+)^{n-1} = (b^+)^{n-1} + b^+\underbrace{b\,(b^+)^{n-1}}_{(b^+)^{n-2}+b^+b(b^+)^{n-2}}$$

$$= 2(b^+)^{n-1} + (b^+)^2\, b\,(b^+)^{n-2}$$

$$\vdots$$

$$= n\,(b^+)^{n-1} + (b^+)^n\, b$$

Therefore: $b_i\, |n_1 n_2 \ldots\rangle = \frac{(b_1^+)^{n_1}}{\sqrt{n_1!}} \cdots \frac{1}{\sqrt{n_i!}}\left(n_i\,(b_i^+)^{n_i-1} + (b_i^+)^{n_i}\underbrace{b_i)|0\rangle}_{=0}\right.$

$$= \sqrt{n_i}\;\frac{(b_1^+)^{n_1}}{\sqrt{n_1!}} \cdots \frac{(b_i^+)^{n_i-1}}{\sqrt{(n_i-1)!}}\,|0\rangle$$

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

6. $[\hat H_0, \hat N] = \sum_{\substack{k_1 k_2\\ \sigma_1 \sigma_2}} \varepsilon_{k_1}\,[c^+_{k_1\sigma_1} c_{k_1\sigma_1}, c^+_{k_2\sigma_2} c_{k_2\sigma_2}]$

- if $(\underbrace{k_1\sigma_1}_{\equiv 1}) \neq (\underbrace{k_2\sigma_2}_{\equiv 2})$, $[c^+_1 c_1, c^+_2 c_2] = c^+_1 [c_1, c^+_2 c_2] + [c^+_1, c^+_2 c_2]\, c_1$

  $[c_1, c^+_2 c_2] = \underbrace{c_1 c^+_2}_{-c^+_2 c_1} c_2 - c^+_2 c_2 c_1 = (-1)^2 c^+_2 c_2 c_1 - c^+_2 c_2 c_1 = 0$

  and in the same way $[c^+_1, c^+_2 c_2] = 0$

  Therefore $[c^+_1 c_1, c^+_2 c_2] = 0$

- if $(k_1\sigma_1) = (k_2\sigma_2)$, we have obviously $[\hat n_1, \hat n_1] = 0$

Therefore $[\hat H_0, \hat N] = 0$

From Quantum Mechanics, if a system of hamiltonian $\hat H_0$ commutes with an observable $\hat O$, this means $\hat O$ is conserved. Here, we find that for a system of free fermions (hamiltonian H_0), the total particle number is conserved, which is obvious!

Interactions do not change the total particle number therefore we also have $[\hat H_{int}, \hat N] = 0$

7. Lecture: field operator

$$\Psi(\vec{r}) = \sum_\alpha \underbrace{\varphi_\alpha(\vec{r})}_{\langle \vec{r}|\alpha\rangle} c_\alpha \quad \text{for } \{|\alpha\rangle\} \text{ orthonormal 1-part. bas.}$$

e.g.: $\Psi(\vec{r}) = \sum_{\vec{k}} \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}} c_{\vec{k}}$

Inverse: $c_\alpha = \int d\vec{r}\, (\varphi_\alpha(\vec{r}))^* \Psi(\vec{r})$

e.g.: $c_{\vec{k}} = \int d\vec{r}\, \frac{e^{-i\vec{k}\cdot\vec{r}}}{\sqrt{V}} \Psi(\vec{r})$

(a)

$$\hat{H}_0 = -\frac{\hbar^2}{2m}\int d\vec{r}\, \Psi^+(\vec{r})\, \nabla^2 \underbrace{\Psi(\vec{r})}_{=\sum_{\vec{k}} \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}} c_{\vec{k}}}$$

$$= \left(-\frac{\hbar^2}{2m}\right)\sum_{\vec{k}} \left[\int d\vec{r}\, \Psi^+(\vec{r})\, \underbrace{\nabla^2\left(\frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}}\right)}_{-k^2 \frac{e^{i(\,)}}{\sqrt{V}}}\right] c_{\vec{k}}$$

$$= \sum_{\vec{k}} \frac{\hbar^2 k^2}{2m} \underbrace{\left[\int d\vec{r}\, \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}} \Psi^+(\vec{r})\right]}_{c_k^+} c_k$$

$$\hat{H}_0 = \sum_{\vec{k}} \frac{\hbar^2 k^2}{2m} c_k^+ c_k$$

(b) $\hat{V}_{\text{Coulomb}} = \frac{1}{2}\sum_{\sigma_1\sigma_2} \int dr_1 dr_2\, V(r_1 - r_2)\, \Psi^+_{\sigma_1}(r_1) \Psi^+_{\sigma_2}(r_2) \Psi_{\sigma_2}(r_2) \Psi_{\sigma_1}(r_1)$

$$= \frac{1}{2}\sum_{\sigma_1\sigma_2}\sum_{k_{1,2,3,4}} \left[\int dr_1 dr_2\, V(r_1 - r_2) \frac{e^{i(-k_4\cdot r_1 - k_3\cdot r_2 + k_2\cdot r_2 + k_1\cdot r_1)}}{(\sqrt{V})^4}\right] c^+_{k_4\sigma_1} c^+_{k_3\sigma_2} c_{k_2\sigma_2} c_{k_1\sigma_1}$$

change of variables: $\begin{cases} \rho = r_1 - r_2 \\ R = \frac{1}{2}(r_1 + r_2) \end{cases}$, $dr_1 dr_2 = d\rho\, dR \quad (J = 1)$

$\Leftrightarrow \begin{cases} r_1 = R + \rho/2 \\ r_2 = R - \rho/2 \end{cases}$

$$-k_4 r_1 - k_3 r_2 + k_2 r_2 + k_1 r_1 = (-k_4 + k_1)(R + \tfrac{\rho}{2}) + (-k_3 + k_2)(R - \tfrac{\rho}{2})$$

$$= \left((k_1 + k_2) - (k_3 + k_4)\right)\cdot R + (+k_1 - k_4 - k_2 + k_3)\cdot\frac{\rho}{2}$$

$\cdot \int dR\, e^{i(+(k_1+k_2)-(k_3+k_4))\cdot R} = V\,\delta_{k_1+k_2,\,k_3+k_4}$

$k_3+k_4 = k_1+k_2 \Rightarrow$ 3 indep. vectors $k_1, \ldots, k_4$

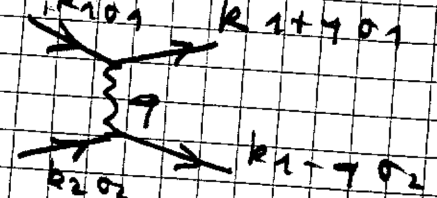
Define $q \equiv k_4 - k_1$; 3 new variables

$= -(k_3 - k_2)$

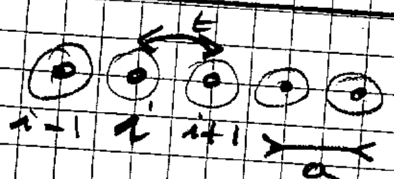
$\cdot\ +k_1 - k_4 - k_2 + k_3 = -2q$

$\int d\rho \quad \int d\rho\, e^{-iq\cdot\rho}\, V(\rho) = \tilde{V}(q)$ (FT of V)

$\underline{\text{el}}$ $\hat{V}_{Coulomb} = \frac{1}{2}\sum_{\sigma_1\sigma_2} \frac{1}{V} \sum_{k_1 k_2 q} \tilde{V}(q)\, c^+_{k_1+q\sigma_1}\, c^+_{k_2-q\sigma_2}\, c_{k_2\sigma_2}\, c_{k_1\sigma_1}$



8.



Atomic orbital (s, p, d ...) located around $\vec{R}_i$. State $|i\rangle$

$i = 1, N_S$

Tight-binding hamiltonian:

$\hat{H} = -t \sum_i c^+_i c_{i+1} + h.c.$; periodic boundary condition

Define $\boxed{c_k = \sum_{n=1}^{N_S} \frac{1}{\sqrt{N_S}} e^{-ikna} c_n}$

Unitary transform $\langle n|k\rangle = \frac{e^{ikna}}{\sqrt{N_S}} \Rightarrow c_k$ is a fermion annihilation operator.

$c_{k+\frac{2\pi}{a}} = \sum e^{-i2\pi n}(\;) = c_k \Rightarrow k \in 1BZ = [-\frac{\pi}{a}, \frac{\pi}{a}]$

$\underline{k}$? $|k\rangle = \sum_{n=1}^{N_S} \frac{e^{ikna}}{\sqrt{N_S}} |n\rangle$

$|k\rangle$: eigenvector of translation operator $\hat{T}_a$: $\hat{T}_a|n\rangle = |n+1\rangle$

$\hat{T}_a|k\rangle = \sum_{n=1}^{N_S} \frac{e^{ikna}}{\sqrt{\;}} |n+1\rangle = \frac{e^{-ika}}{\sqrt{\;}}\Big[e^{2ika}|2\rangle + \ldots e^{ikN_Sa}|N_S\rangle + e^{ikN_Sa}e^{ika}\underbrace{|N_S+1\rangle}_{=1}\Big]$

$|k\rangle$ eigenvector with eigenvalue e^{-ika}

iff $\boxed{e^{ikN_Sa} = 1}$ $\boxed{k = \frac{2\pi}{N_S a} m,\ m \in \mathbb{Z} \text{ and } k \in [-\pi/a, \pi/a]}$ (periodic b.c.)

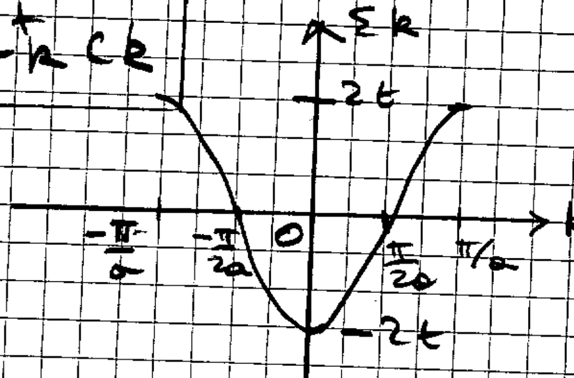
check : $c_n = \sum_{k \in 1BZ} \frac{1}{\sqrt{N_s}} e^{-ikna} c_k$ (9)

$$\hat{H} = -t \sum_n \left(\sum_{k_1} \frac{1}{\sqrt{\ }} e^{ik_1 na} c^\dagger_{k_1} \right) \left(\sum_{k_2} e^{-ik_2(n+1)a} c_{k_2} \right) + h.c.$$

$$= \sum_{k_1 k_2} \frac{1}{(\sqrt{N_s})^2} (-t) \underbrace{\left(\sum_n e^{ina(k_1-k_2)} \right)}_{N_s \delta_{k_1,k_2}} e^{-ik_2 a} c^\dagger_{k_1} c_{k_2} + h.c.$$

$$= \sum_{k_1} -t \left(e^{-ik_1 a} + e^{ik_1 a} \right) c^\dagger_{k_1} c_{k_1}$$

$$\boxed{\hat{H} = \sum_k -2t \cos ka \; c^\dagger_k c_k}$$



9. 1 part. operator :

$\hat{\rho}^{(1)}(\vec{r}) = |\vec{r}\rangle\langle\vec{r}|$

2nd quant^{on} :

$$\hat{\rho}(\vec{r}) = \sum_{\lambda_1 \lambda_2} \langle \lambda_1 | \hat{\rho}^{(1)}(\vec{r}) | \lambda_2 \rangle c^\dagger_{\lambda_1} c_{\lambda_2}$$

$$= \sum_{\lambda_1 \lambda_2} \underbrace{\langle \lambda_1 | \vec{r} \rangle}_{(\varphi_{\lambda_1}(\vec{r}))^*} \underbrace{\langle \vec{r} | \lambda_2 \rangle}_{\varphi_{\lambda_2}(\vec{r})} c^\dagger_{\lambda_1} c_{\lambda_2} = \sum_{\lambda_1 \lambda_2} (\varphi_{\lambda_1}(\vec{r}))^* \varphi_{\lambda_2}(\vec{r}) c^\dagger_{\lambda_1} c_{\lambda_2}$$

- $|\lambda_1\rangle = |\vec{r}_1\rangle$: $\varphi_{\lambda_1}(\vec{r}) = \langle \vec{r}_1 | \vec{r} \rangle = \delta(\vec{r}_1 - \vec{r})$

$c_{\lambda_1} = \psi(\vec{r}_1)$

$$\hat{\rho}(\vec{r}) = \int dr_1 dr_2 \, \delta(\vec{r}_1 - \vec{r}) \, \delta(\vec{r}_2 - \vec{r}) \, \psi^\dagger(\vec{r}_1) \psi(\vec{r}_2)$$

$$\boxed{\hat{\rho}(\vec{r}) = \psi^\dagger(\vec{r}) \, \psi(\vec{r})}$$

- $|\lambda_1\rangle = |k_1\rangle$ $\quad \varphi_{\lambda_1}(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k}_1 \cdot \vec{r}}$

$$\hat{\rho}(\vec{r}) = \sum_{k_1 k_2} \frac{1}{V} e^{-i(k_1-k_2)\cdot\vec{r}} c^\dagger_{k_1} c_{k_2}$$

$$\int d\vec{r} \, e^{-i\vec{q}\cdot\vec{r}} \hat{\rho}(\vec{r}) = \sum_{k_1 k_2} \frac{1}{V} \left[\int d\vec{r} \, e^{-i\vec{r}(q+k_1-k_2)} \right] c^\dagger_{k_1} c_{k_2}$$

$[\ ] = V \delta_{k_2 - k_1, q}$: $k_1 = k_2 - q$

$$\boxed{\hat{\rho}(\vec{q}) = \sum_{k} c^{+}_{\vec{k}-\vec{q}}\, c_{\vec{k}}}$$

2- Spin operator:

$$\vec{S} = \sum_\lambda c^+_{\lambda\alpha'} \frac{\sigma_{\alpha'\alpha}}{2} c_{\lambda\alpha}$$

$\begin{array}{c|cc} & |\uparrow\rangle & |\downarrow\rangle \\ \hline \langle\uparrow| & & \\ \langle\downarrow| & & \end{array}$ $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

Summation on α and α'. Einstein notation (repeated indices).

1. $c^+ = (c^+_1 \dots c^+_N)$ $\quad c = \begin{pmatrix} c_1 \\ \vdots \\ c_N \end{pmatrix}$

$$[c^+ A c, c^+ B c] = [c^+_{\alpha_1} A_{\alpha_1\alpha_2} c_{\alpha_2}, c^+_{\alpha_3} B_{\alpha_3\alpha_4} c_{\alpha_4}]$$

or $[c^+_1 A_{12} c_2, c^+_3 B_{34} c_4]$

$$= A_{\alpha_1\alpha_2} B_{\alpha_3\alpha_4} [c^+_{\alpha_1} c_{\alpha_2}, c^+_{\alpha_3} c_{\alpha_4}]$$

$$[c^+_1 c_2, c^+_3 c_4] = c^+_1 [c_2, c^+_3 c_4] + [c^+_1, c^+_3 c_4] c_2$$
$$= \delta_{2,3} c^+_1 c_4 - \delta_{1,4} c^+_3 c_2$$

$$[\ ,\ ] = A_{\alpha_1\alpha_2} B_{\alpha_3\alpha_4} (\delta_{\alpha_2,\alpha_3} c^+_{\alpha_1} c_{\alpha_4} - \delta_{\alpha_1,\alpha_4} c^+_{\alpha_3} c_{\alpha_2})$$
$$= c^+_{\alpha_1} A_{\alpha_1\alpha_2} B_{\alpha_2\alpha_4} c_{\alpha_4}$$
$$- c^+_{\alpha_3} B_{\alpha_3\alpha_4} A_{\alpha_1\alpha_2} c_{\alpha_2}$$
$$= c^+ A B c - c^+ B A c$$
$$= c^+ \underbrace{[A, B]}_{N\times N \text{ matrix}} c$$

2. $\nu = x, y, z$

$$\hat{S}_\nu = \sum_\lambda c^+_{\lambda\alpha'} \left(\tfrac{1}{2}\sigma_\nu\right)_{\alpha'\alpha} c_{\lambda\alpha}$$

$$[\hat{S}_\nu, \hat{S}_{\nu'}] = \sum_{\lambda,\lambda'} [\ \lambda\ ,\ \lambda'\ ]$$

$[\ ] = 0$ if $\lambda' \neq \lambda$ $\qquad$ 2×2 matrices

$$= \sum_\lambda [c^+_\lambda (\tfrac{1}{2}\sigma_\nu) c_\lambda, c^+_\lambda (\tfrac{1}{2}\sigma_{\nu'}) c_\lambda]$$

$$c^+_\lambda = (c^+_{\lambda\uparrow}\ c^+_{\lambda\downarrow})$$

$$= \sum_\lambda c^+_\lambda \underbrace{[\tfrac{1}{2}\sigma_\nu, \tfrac{1}{2}\sigma_{\nu'}]}_{i\,\varepsilon_{\nu\nu'\nu''} \frac{\sigma_{\nu''}}{2}} c_\lambda$$

$$= i\,\varepsilon_{\nu\nu'\nu''}\ \hat{S}_{\nu''} \qquad (\text{"}\hbar = 1\text{"}) \qquad 12$$

The ~~usual~~ the commutation relations of angular momentum operators (Lie group "$SU(2)$").

3. 1st quantization :

$$\hat{\vec{S}} = \sum_{i=1}^{N} \hat{\vec{s}}^{(i)} \ ; \quad \text{Addition a } N \text{ spins } 1/2.$$

Total spin $\left\{\begin{array}{l} 0 \ N\text{ even} \\ \frac{1}{2} \ N\text{ odd} \end{array}\right. \leq S \leq \frac{N}{2}$

$$\hat{\vec{S}}^2 = \hbar^2 S(S+1).$$

4. $$\hat{S}^+ = S_x + i S_y$$
$$= \frac{1}{2}\sum_{\lambda} c^+_{\lambda\alpha'} (\sigma_x + i\sigma_y)_{\alpha'\alpha}\, c_{\lambda\alpha}$$

$$\frac{1}{2}(\sigma_x + i\sigma_y) = \begin{pmatrix} 0 & \frac{1}{2}(1 - i^2) \\ \frac{1}{2}(1+i^2) & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$ only term $\neq 0$: $\alpha' = \uparrow, \alpha = \downarrow$

$$\boxed{\hat{S}^+ = \sum_{\lambda} c^+_{\lambda\uparrow}\, c_{\lambda\downarrow}} \qquad \hat{S}_z = \frac{1}{2}\sum_{\lambda} c^+_{\lambda\uparrow} c_{\lambda\uparrow} - c^+_{\lambda\downarrow} c_{\lambda\downarrow}$$

$$\hat{S}^- = \sum_{\lambda} c^+_{\lambda\downarrow}\, c_{\lambda\uparrow}$$

5. Single site. Hilbert space : $\{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\}$

Dimension : $\underline{4}$. $\quad |\sigma\rangle = d^+_\sigma |0\rangle$

$|\uparrow\downarrow\rangle = d^+_\uparrow d^+_\downarrow |0\rangle$

6. $\hat{H}|0\rangle = 0$, $\hat{H}|\uparrow\rangle = \varepsilon_d |\uparrow\rangle$, $\hat{H}|\downarrow\rangle = \varepsilon_d |\downarrow\rangle$

$\hat{H}|\uparrow\downarrow\rangle = (2\varepsilon_d + U)|\uparrow\downarrow\rangle$

Matrix $\hat{H} =$

$$\begin{array}{cccc} |0\rangle & |\uparrow\rangle & |\downarrow\rangle & |\uparrow\downarrow\rangle \end{array}$$
$$\begin{pmatrix} 0 & & & \\ & \varepsilon_d & & 0 \\ & & \varepsilon_d & \\ 0 & & & 2\varepsilon_d + U \end{pmatrix}$$

Spin of each eigenstate:

$|0\rangle$: $S=0$

$|\uparrow\rangle$: $S=\frac{1}{2}$, $|\downarrow\rangle$: $S=\frac{1}{2}$

$|\uparrow\downarrow\rangle$: $S=0$

Proof: $\hat{S}^+|\uparrow\downarrow\rangle = d_\uparrow^\dagger d_\downarrow d_\uparrow^\dagger d_\downarrow^\dagger|0\rangle$

$= -\underbrace{d_\uparrow^\dagger d_\uparrow^\dagger}_{=0} d_\downarrow d_\downarrow^\dagger|0\rangle = 0$

$\hat{S}^-|\uparrow\downarrow\rangle = d_\downarrow^\dagger d_\uparrow d_\uparrow^\dagger d_\downarrow^\dagger|0\rangle$

$= (-1)^2 d_\uparrow d_\uparrow^\dagger \underbrace{(d_\downarrow^\dagger)^2}_{=0}|0\rangle = 0$

$\hat{S}_z|\uparrow\downarrow\rangle = \frac{1}{2}(d_\uparrow^\dagger d_\uparrow - d_\downarrow^\dagger d_\downarrow) d_\uparrow^\dagger d_\downarrow^\dagger|0\rangle$

$= (\frac{1}{2} - \frac{1}{2}) d_\uparrow^\dagger d_\downarrow^\dagger|0\rangle = 0$

3. Hartree - Fock: $H = \hat{T} + \hat{V}$ 14

1. Ground state of the non-interacting system.

Fermi - Sea

$$|FS\rangle = \prod_{|\vec{k}|<k_F} c^{+}_{\vec{k}\uparrow} c^{+}_{\vec{k}\downarrow} |0\rangle$$

2. Perturbation theory 1st order in $\hat{V}$.

$$\delta E = \langle FS| \hat{V} |FS\rangle$$

$$= \frac{1}{2V} \sum_{\substack{\sigma_1\sigma_2 \\ q k_1 k_2}} \frac{e^2}{\varepsilon_0 q^2} \langle FS| c^{+}_{k_1+q,\sigma_1} c^{+}_{k_2-q,\sigma_2} c_{k_2,\sigma_2} c_{k_1,\sigma_1} |FS\rangle$$

$$\langle FS| \underbrace{c^{+}_{k_1+q,\sigma_1} c^{+}_{k_2-q,\sigma_2} c_{k_2,\sigma_2} c_{k_1,\sigma_1} |FS\rangle}_{\text{This state must be } |FS\rangle \text{ (with a prefactor)}}$$

Therefore the annihilated particles must be created "later".

2 cases:

i) $(k_1+q, \sigma_1) = (k_1, \sigma_1)$ "Hartree"
$(k_2-q, \sigma_2) = (k_2, \sigma_2)$

ii) $(k_1+q, \sigma_1) = (k_2, \sigma_2)$ "Fock"
$(k_2-q, \sigma_2) = (k_1, \sigma_1)$

i) $q=0$, $\langle\ \rangle = \langle FS| c^{+}_{k_1,\sigma_1} c^{+}_{k_2,\sigma_2} c_{k_2,\sigma_2} c_{k_1,\sigma_1} |FS\rangle$

$\neq 0$ iff $|k_1| < k_F$, $|k_2| < k_F$ $\quad (k_1,\sigma_1) \neq (k_2,\sigma_2)$

$$\langle\ \rangle = (-1)^2 \langle FS| c^{+}_{k_2,\sigma_2} c_{k_2,\sigma_2} \underbrace{c^{+}_{k_1,\sigma_1} c_{k_1,\sigma_1} |FS\rangle}_{\theta(k_F-|k_1|)\,|FS\rangle}$$

$$= \theta(k_F - |k_1|)\,\theta(k_F - |k_2|)$$

NB: $(k_1\sigma_1) = (k_2\sigma_2)$ gives 0, but negligible weight.

Hartree contribution: $\frac{1}{2V} \frac{e^2}{\varepsilon_0 (0)^2} \left(\sum_{k_1} \theta(k_F-|k_1|)\right)\left(\sum_{k_2} \theta(k_F-|k_2|)\right)$

DIVERGENT!

$\longrightarrow$ needs a background of positive ions.
(cf. jellium model)

ii) $\sigma_2 = \sigma_1 \quad k_2 = k_1 + q$ (1)

$\langle FS | c^+_{k_1+q,\sigma_1} c^+_{k_1,\sigma_1} c_{k_1+q,\sigma_1} c_{k_1,\sigma_1} | FS \rangle$

· If $q \neq 0$, $\langle \ \rangle = \ominus \langle FS | c^+_{k_1+q,\sigma_1} c_{k_1+q,\sigma_1} c^+_{k_1,\sigma_1} c_{k_1,\sigma_1} | FS \rangle$

$= \ominus \theta(k_F - |k_1|)\, \theta(k_F - |k_1+q|)$

· If $q = 0$, $\langle (c^+_{k_1+q,\sigma_1})^2 (c_{k_1,\sigma_1})^2 \rangle = 0$

Fock contribution:

$$\ominus \frac{1}{2V} 2 \sum_{q\neq 0}^{\text{spin}} \frac{e^2}{\varepsilon_0 q^2} \left[\sum_{k_1} \theta(k_F - |k_1|)\, \theta(k_F - |k_1+q|) \right]$$

cf text : $[\ ] = V_q = \frac{V}{(2\pi)^3} \frac{4\pi k_F^3}{3} \left[1 - \frac{3}{4}\frac{q}{k_F} + \frac{1}{16}\left(\frac{q}{k_F}\right)^3 \right]$

$\theta(|q| - 2k_F)$

$$\delta E_{Fock} = -\frac{1}{2\cancel{V}} 2 \frac{\cancel{V}}{(2\pi)^3} \frac{4\pi k_F^3}{3} \frac{e^2}{\varepsilon_0} \frac{V}{(2\pi)^3} \int_{|q|<2k_F} d^3\vec{q}\, \frac{1}{q^2} \left[1 - \frac{3}{4}\frac{q}{k_F} + \frac{1}{16}\left(\frac{q}{k_F}\right)^3\right]$$

$\int d^3\vec{q}$: $\int d\Omega \to 4\pi$ (angles)

$$\to 4\pi \int_0^{2k_F} dq\, \cancel{q^2} \frac{1}{\cancel{q^2}} [1 - \dots] \qquad x = q/k_F$$

$$= 4\pi k_F \int_0^2 dx \left[1 - \frac{3}{4}x + \frac{1}{16}x^3\right] = 4\pi k_F \left[x - \frac{3}{8}x^2 + \frac{1}{64}x^4\right]_0^2$$

$$= 4\pi k_F \left[2 - \frac{3}{2} + \frac{1}{4}\right] = 3\pi k_F$$

$$\frac{\delta E_{Fock}}{V} = -\frac{\cancel{2}}{2} \frac{4\pi \cdot 3\pi}{(2\pi)^3 \cdot 3 \cdot (2\pi)^3} \frac{e^2}{\varepsilon_0} k_F^4$$

$$= -\frac{1}{16\pi^4} \frac{e^2}{\varepsilon_0} k_F^4$$

$$\boxed{\frac{\delta E_{Fock}}{V} = -\frac{k_F^4}{4\pi^3} \frac{e^2}{4\pi\varepsilon_0}}$$

4. Finite temperature and thermodynamics: (16)

1. $Z = \mathrm{Tr}\left[e^{-\beta\left(\sum_\lambda (\varepsilon_\lambda - \mu)\hat{n}_\lambda\right)} \right]$

Basis of Fock states:

$|n_{\lambda_1}\; n_{\lambda_2} \;\cdots\rangle$ F: $n_\lambda = 0, 1$
B: $n_\lambda = 0, 1, 2, \ldots \infty$

$$Z = \sum_{n_{\lambda_1}=0,1\ldots} \sum_{n_{\lambda_2}=0,1} \cdots \langle n_{\lambda_1}\, n_{\lambda_2} \cdots | e^{-\beta \sum_\lambda (\varepsilon_\lambda - \mu)\hat{n}_\lambda} | n_{\lambda_1} n_{\lambda_2} \cdots \rangle$$

$$= \qquad e^{-\beta \sum_\lambda (\varepsilon_\lambda - \mu) n_\lambda}$$

n_b!

$$= \left(\sum_{n_{\lambda_1}=0,1\ldots} e^{-\beta(\varepsilon_{\lambda_1} - \mu) n_{\lambda_1}} \right) \left(\sum_{n_{\lambda_2}=} \quad \right) \left(\quad \right)$$

$$Z = Z_{\lambda_1} \cdot Z_{\lambda_2} \cdots = \prod_\lambda Z_\lambda$$

2. $Z_\lambda = \sum_{\substack{n_\lambda = 0,1 \quad F \\ [0,1,\ldots\infty \quad B}} e^{-\beta(\varepsilon_\lambda - \mu) n_\lambda}$

F: $\boxed{Z_\lambda = 1 + e^{-\beta(\varepsilon_\lambda - \mu)}}$

B: $Z_\lambda = 1 + e^{-\beta(\varepsilon_\lambda - \mu)} + e^{-2\beta(\varepsilon_\lambda - \mu)} + \cdots e^{-n\beta(\varepsilon_\lambda - \mu)}$

$$\boxed{Z_\lambda = \frac{1}{\left[1 - e^{-\beta(\varepsilon_\lambda - \mu)}\right]}} \quad (\varepsilon_\lambda - \mu > 0 \,!)$$

3. $\langle \hat{n}_\lambda \rangle = \frac{1}{Z} \sum_{n_{\lambda_1}=0,1\ldots} \sum_{n_{\lambda_2}=0,1\ldots} \cdots \sum_{n_\lambda = 0,1\ldots} n_\lambda e^{-\beta(\varepsilon_\lambda - \mu) n_\lambda}$

$$= \frac{\prod_{\lambda_1 \neq \lambda} Z_{\lambda_1} \left[\sum_{n_\lambda = \ldots} n_\lambda e^{-\beta(\varepsilon_\lambda - \mu) n_\lambda} \right]}{\prod_{\lambda_1 \neq \lambda} Z_{\lambda_1} \left[\sum_{n_\lambda = \ldots} e^{-\beta(\varepsilon_\lambda - \mu) n_\lambda} \right]}$$

$$\langle \hat{n}_\lambda \rangle = \frac{\frac{1}{\beta} \frac{\partial}{\partial\mu} (Z_\lambda)_T}{Z_\lambda} = \frac{1}{\beta} \frac{\partial}{\partial \mu} (\log Z_\lambda)_T$$

$\underline{F}$: $\langle \hat{n}_\lambda \rangle = \frac{1}{\cancel{\beta}} \frac{\cancel{\beta} e^{-\beta(\varepsilon_\lambda - \mu)}}{1 + e^{-\beta(\varepsilon_\lambda - \mu)}}$

$$\boxed{\langle \hat{n}_\lambda \rangle = \frac{1}{\left[1 + e^{\beta(\varepsilon_\lambda - \mu)}\right]}}$$ "Fermi – Dirac"

$\underline{B}$: $\langle \hat{n}_\lambda \rangle = -\frac{1}{\beta} \frac{\partial}{\partial \mu} \left(\log \frac{1}{Z_\lambda}\right) = -\frac{1}{\cancel{\beta}} \frac{\left(-\cancel{\beta} e^{-\beta(\varepsilon_\lambda - \mu)}\right)}{\left(1 - e^{-\beta(\varepsilon_\lambda - \mu)}\right)}$

$$\boxed{\langle \hat{n}_\lambda \rangle = \frac{1}{\left[e^{\beta(\varepsilon_\lambda - \mu)} - 1\right]}}$$ "Bose – Einstein"