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Solid State Physics II

Chapter 4 Second Quantization

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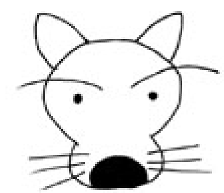


Second Quantization

- What is it?
- Why do we need it? What for?
- How to represent the first-quantization form of observables in terms of second quantization operators?
- How to calculate the expectation values of (a function of) operators in a second-quantization form?
- How do we take account of the statistics: Boson vs. Fermion?

Observables

- Single-Particle Systems: 1st quantization picture

  The observables are position and momentum, i.e., $\{\mathbf{X}, \mathbf{P}\}$.

  According to the uncertainty principle, measurements of a (conjugate) pair of observables (e.g., $\mathbf{X}$ and $\mathbf{P}$) in different sequences give different results:

$$\mathbf{XP}|\psi\rangle \neq \mathbf{PX}|\psi\rangle$$

  Therefore, in general, we can write

$$[\mathbf{X}, \mathbf{P}] = i\hbar \neq 0$$

  (Note that $\mathbf{P}$ and $\mathbf{X}$ are hermitian.)

- Many-Particle Systems: 2nd quantization picture

  $\Rightarrow$ The observables are "amplitudes" in a certain normal mode.

  – What is the **"normal mode"**?

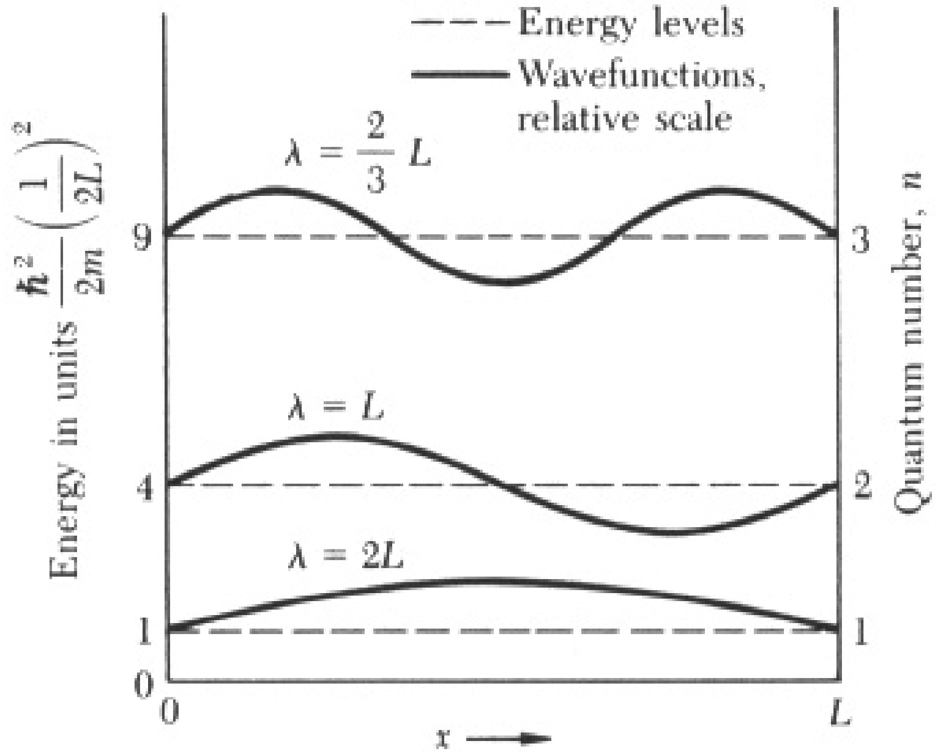
    * eigenstate or eigenmode
    * often described as a decoupled/independent motion with a fixed frequency, e.g.,

$$\eta_k(t) \sim \eta_o e^{i\omega_k t}$$

For examples, such normal modes are determined by the equation-of-motion with boundary conditions:

$$\left(\mathcal{H} - i\frac{\partial}{\partial t}\right)\psi(\mathbf{x}, t) = 0$$

$$\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\mathbf{A}(\mathbf{x}, t) = 0$$



Energy levels
Wavefunctions, relative scale
$\lambda = \frac{2}{3}L$
$\lambda = L$
$\lambda = 2L$
Energy in units $\frac{\hbar^2}{2m}\left(\frac{1}{2L}\right)^2$
Quantum number, n
9
4
1
0
3
2
1
0
L
x

- How is the “amplitude” represented in quantum mechanics?
  - Consider a normal mode oscillation in classical mechanics, which is nothing but a simple harmonic oscillator.

$$\frac{\partial^2}{\partial t^2} u_k(t) + \omega_k^2 u_k(t) = 0$$

  - By replacing $u_k(t) \to \hat{X}$ and $m\dot{u}_k(t) \to \hat{P}$, we can write down a quantum mechanical Hamiltonian $\mathcal{H}$

$$\mathcal{H} = \frac{\hat{P}^2}{2m} + \frac{1}{2} m\omega_k^2 \hat{X}^2$$

where the amplitude of oscillator can be measured by the observables $\hat{X}$ and $\hat{P}$.

- Alternatively, the quantum mechanical harmonic oscillator can be represented by the creation and annihilation operators a^+ and a satisfying the relation

$$[a, a^+] = 1$$

so that the Hamiltonian can be rewritten as

$$\mathcal{H} = \hbar\omega_k(a^+a + \frac{1}{2})$$

(Please refer to the quantum mechanics textbook for the detailed descriptions of a and a^+ operators.)

- Thus , the "amplitude" of the k-th normal mode can be measured by the non-hermitian observable a_k. Indeed the *so-called* number operator $\hat{n_k} = a_k^+ a_k$ is a measure of the number of quanta in the k-th normal mode, which corresponds to the number state $|n_k\rangle$.

One may adopt a set of **coherent states** as basis for the representation of many-particle states. The coherent state $|\alpha\rangle$ is defined by

$$a_k|\alpha\rangle = \alpha|\alpha\rangle,$$

i.e., an eigenstate of the annihilation operator a_k.

$$\begin{aligned} |\alpha\rangle &= \exp(\alpha a_k^+)|0\rangle \\ &= \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}|n\rangle \end{aligned}$$

Please note that $|\alpha\rangle$ has a *semi-classical limit* with the classical state $\{X, P\}$:

$$\alpha = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}X + i\frac{1}{\sqrt{m\hbar\omega}}P\right)$$

N-particle quantum states

- Suppose that we have N (non-interacting) particles in a system with a set of available (single-particle) quantum states $\{\psi_n\}$. Then, the N-particle state can be specified by the "amplitudes" of each quantum state, i.e., normal mode $|\psi_n\rangle$ such as

$$|\Psi_N\rangle = |n_{k=1}, n_{k=2}, n_{k=3}, ...\rangle$$

so that the expectation value of $\hat{n}_k$ becomes

$$\langle\Psi_N|\hat{n}_k|\Psi_N\rangle = n_k.$$

In general, an arbitrary N-particle state can be represented by

$$|\Psi\rangle = \sum_{\{n_k\}} c(\{n_k\})|\Psi_N(\{n_k\})\rangle$$

- Therefore all the observables of the N-particle system can be represented by the operators $\{a_k\}$ and $\{a_k^+\}$:

$$\hat{O}_N = O(\{a_k^+, a_k\})$$

- Note: Uncertainty principle in N-particle system can be regarded as an uncertainty in measuring numbers:

$$aa^+|\psi\rangle \neq a^+a|\psi\rangle$$

That is, $[a, a^+] = 1 \neq 0$ (real).

Why do we need it?

$\Rightarrow$ For the sake of convenience. In Fermion systems, for example, each $|\Psi_N\rangle$ basis state corresponds to a Slater's determinant of N-orbital states $\{|\psi_n\rangle | n = 1, 2, ..., N\}$, which contains $N!$-terms in it. Thus, to represent an arbitrary state $|\Psi\rangle$, we have to make a linear combination of such Slater's determinants.

$$|\Psi\rangle = \sum_{\{n_k\}} c(\{n_k\}) |\Psi_N(\{n_k\})\rangle$$

$\Rightarrow$ Too complicated to deal with!

Observables in 2nd Quantization Form

- Consider an operator, e.g., momentum operator $\hat{p} = -i\nabla$, in the 1st quantization picture such that

$$\hat{p}|\phi_k\rangle = k|\phi_k\rangle$$

Then the total momentum P can be found by

$$P = \sum_k k n_k.$$

That is, the total momentum operator $\hat{P}$ in the 2nd quantization form becomes

$$\hat{P} = \sum_k k a_k^+ a_k$$

This is obvious because all we need to do is **just counting** number of particles in the k-th mode and add them up.

- What if we have a set of normal modes which are not the eigenstates of $\hat{p}$?
  - Consider an operator $\hat{\alpha}$ such that

$$\hat{\alpha}|\phi_\alpha\rangle = \alpha|\phi_\alpha\rangle$$

  - One-particle state and the vacuum:

$$|\phi_k\rangle = a_k^+|0\rangle$$

$$|\phi_\alpha\rangle = a_\alpha^+|0\rangle$$

    From the closure relation

$$1 = \sum_k |\phi_k\rangle\langle\phi_k| = \sum_\alpha |\phi_\alpha\rangle\langle\phi_\alpha|,$$

    we know $|\phi_k\rangle = \sum_\alpha |\alpha\rangle\langle\alpha|\phi_k\rangle$, that is,

$$a_k^+ = \sum_\alpha a_\alpha^+\langle\alpha|k\rangle$$

$$a_k = \sum_\alpha \langle k|\alpha\rangle a_\alpha$$

- The total momentum operator $\hat{P}$:

$$\begin{aligned}\hat{P} &= \sum_k k a_k^+ a_k \\ &= \sum_k k \sum_{\alpha\alpha'} a_\alpha^+ \langle\alpha|k\rangle a_{\alpha'} \langle k|\alpha'\rangle \\ &= \sum_{\alpha\alpha'} a_\alpha^+ \langle\alpha|k\rangle k \langle k|\alpha'\rangle a_\alpha \\ &= \sum_{\alpha\alpha'} a_\alpha^+ \langle\alpha|\hat{p}|\alpha'\rangle a_\alpha\end{aligned}$$

- When substituting $\alpha \to \mathbf{x}$,

$$\hat{\psi}(\mathbf{x}) = a_{\mathbf{x}}$$

$$\hat{P} = \int d\mathbf{x} \hat{\psi}^+(\mathbf{x}) \left(\frac{\nabla}{i}\right) \hat{\psi}(\mathbf{x})$$

Note that $\hat{\psi}(\mathbf{x})$ is a so-called field operator:

$$\hat{\psi}(\mathbf{x}) = \sum_k \langle\mathbf{x}|\phi_k\rangle a_k = \sum_k \phi_k(\mathbf{x}) a_k$$

- One-particle operator $\hat{O}_1$: In the 1st quantization representation, we write

$$\hat{O}_1 = \sum_i \hat{o}_i$$

In the 2nd quantization form,

$$\begin{aligned} \hat{O}_1 &= \int d\mathbf{x} \hat{\psi}^+(\mathbf{x}) o(\mathbf{x}) \hat{\psi}(\mathbf{x}) \\ &= \sum_{\alpha\alpha'} \langle \alpha | \hat{o} | \alpha' \rangle a_\alpha^+ a_{\alpha'} \end{aligned}$$

- Two-particle operator $\hat{O}_2$: In the 1st quantization representation,

$$\hat{O}_2 = \frac{1}{2}\sum_{ij}\hat{o}_{ij}$$

In the 2nd quantization form,

$$\begin{aligned}\hat{O}_2 &= \frac{1}{2}\int d\mathbf{x}_1 d\mathbf{x}_2 \hat{\psi}^+(\mathbf{x}_1)\hat{\psi}^+(\mathbf{x}_2) o(\mathbf{x}_1,\mathbf{x}_2)\hat{\psi}(\mathbf{x}_2)\hat{\psi}(\mathbf{x}_1)\\ &= \sum_{\alpha\alpha'\beta\beta'}\langle\alpha\beta|\hat{o}|\alpha'\beta'\rangle a_\alpha^+ a_\beta^+ a_{\beta'} a_{\alpha'}\end{aligned}$$

N-electron system

$$\mathcal{H} = \sum_i -\frac{\hbar^2}{2m}\nabla_i^2 + \sum_i v(\mathbf{x}_i) + \frac{1}{2}\sum_{ij}{}' \frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|}$$

$$\mathcal{H} = \sum_{k\sigma} \frac{\hbar^2 k^2}{2m} c^+_{k\sigma} c_{k\sigma} + \sum_{kk'\sigma} v_{kk'} c^+_{k\sigma} c_{k'\sigma} + \frac{1}{2} \sum_{kk'k''k'''\sigma\sigma'} V^C{}_{kk'k''k'''} c^+_{k\sigma} c^+_{k'\sigma'} c_{k'''\sigma'} c_{k''\sigma}$$

$$v_{kk'} = \langle k | v(\mathbf{x}) | k' \rangle$$

$$V^C_{kk'k''k'''} = \langle kk' | \frac{e^2}{|\mathbf{x}_1 - \mathbf{x}_2|} | k''k''' \rangle$$

Statistics

Pauli Exclusion Principle

$$a_k^+ |n_k = 1\rangle = 0$$

Since $|n_k = 1\rangle = a_k^+ |0\rangle$, the Pauli principle states that

$$(a_k^+)^2 = 0$$

Accordingly, we can generalize the commutation rule for Fermions:

$$[a_k, a_{k'}]_+ = 0$$

$$[a_k^+, a_{k'}^+]_+ = 0$$

$$[a_k, a_{k'}^+]_+ = \delta_{kk'}$$

Note that $[A, B] \equiv [A, B]_- = AB - BA$ and $[A, B]_+ = AB + BA$.

An Example: Hartree Fock Theory

Consider an electron gas in a homogeneous, positively charged medium (jellium model).

$$\mathcal{H} = \mathcal{H}_o + \mathcal{H}_1$$

$$\mathcal{H}_o = \sum_i h_i = \sum_i \left[-\frac{\hbar^2}{2m} \nabla_i^2 + v(\mathbf{x}_i) \right]$$

$$\mathcal{H}_1 = \frac{1}{2} \sum_{ij}{}' \frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|}$$

where the external potential $v(\mathbf{x})$ is given by

$$v(\mathbf{x}) = -e^2 \int d\mathbf{x}' \, \frac{n_b}{|\mathbf{x} - \mathbf{x}'|}$$

with n_b is a positive charge density equal to the average electron density.

First Quantization Method: Slater's Determinant

Hartree Approximation

- Solving the one-particle Hamiltonian:

$$\mathbf{H}_o|\Phi\rangle = E_o|\Phi\rangle$$

$$\Phi(\mathbf{x}_1, ..., \mathbf{x}_N) = \varphi_1(\mathbf{x}_1)\ldots\varphi_N(\mathbf{x}_N) = \prod_i \varphi_k(\mathbf{x}_k)$$

$$h_i\varphi_k(\mathbf{x}_i) = \epsilon_k\varphi_k(\mathbf{x}_i)$$

(Note that Φ has no permutation symmetry.)

- With the orthogonality constraint $\langle \varphi_k | \varphi_l \rangle = \delta_{kl}$, obtain a variational equation for φ for the total energy $E = \langle \Phi | \mathcal{H} | \Phi \rangle$:

$$\delta \left[\langle \Phi | \mathcal{H} | \Phi \rangle - \sum_k \lambda_k (\langle \varphi_k | \varphi_k \rangle - 1) \right]$$

$$\left[-\frac{1}{2} \nabla^2 + {\sum_l}' \int d\mathbf{x}' \frac{|\varphi_l(\mathbf{x}')|^2}{|\mathbf{x} - \mathbf{x}'|} - \int d\mathbf{x}' \frac{n_b}{|\mathbf{x} - \mathbf{x}'|} \right] \varphi_k(\mathbf{x}) = \epsilon_k \varphi_k(\mathbf{x})$$

- If we look for a homogeneous solution, i.e.,

$$\sum_l |\varphi_l(\mathbf{x}')|^2 = n_b,$$

then the Hartree equation becomes a simple plane wave equation:

$$\left[-\frac{1}{2} \nabla^2 \right] \varphi_k(\mathbf{x}) = \epsilon_k \varphi_k(\mathbf{x})$$

Hartree-Fock Approximation

- Since the electrons are "indistinguishable" particles obeying the Pauli exclusion principle,

$$\Phi = \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_1(\mathbf{x}_1) & \dots & \varphi_N(\mathbf{x}_1) \\ \vdots & & \vdots \\ \varphi_1(\mathbf{x}_N) & \dots & \varphi_N(\mathbf{x}_N) \end{vmatrix}$$

$$= \frac{1}{\sqrt{N!}} \sum_{P(1,\ldots,N)} (-)^P \prod_{i=1}^{N} \varphi_i(\mathbf{x}_{Pi})$$

(Here we assume that all the particles have the same spin!)

- Hartree-Fock equation:

$$-\frac{1}{2}\nabla^2\varphi_k(\mathbf{x}) \quad + \quad \sum_l{}' \int d\mathbf{x}' \frac{(|\varphi_l(\mathbf{x}')|^2 - n_b)}{|\mathbf{x}-\mathbf{x}'|}]\varphi_k(\mathbf{x})$$

$$- \quad \sum_{l(\sigma_l=\sigma_k)} \int d\mathbf{x}' \frac{\varphi_l^*(\mathbf{x}'\varphi_k(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}\varphi_l(\mathbf{x}) = \epsilon_k\varphi_k(\mathbf{x})$$

(It is noted that, when looking for a homogeneous solution, $\varphi_k(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}}$ becomes a solution!)

2nd Quantization Method

$$\mathcal{H} = \mathcal{H}_o + \mathcal{H}_1$$

$$\mathcal{H}_o = \sum_{k\sigma} \epsilon_{ok} c^+_{k\sigma} c_{k\sigma}$$

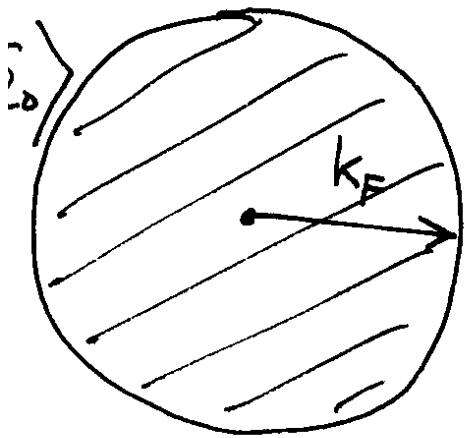
$$\mathcal{H}_1 = \frac{1}{2} \sum_{kp,q\neq 0}{}' \sum_{\sigma\sigma'} V_q c^+_{k+q\sigma} c^+_{p-q\sigma'} c_{p\sigma'} c_{k\sigma}$$

$$\epsilon_{ok} = \frac{k^2}{2}$$

$$V_q = \frac{4\pi e^2}{q^2}$$

From the Hartree-Fock solution of the 1st quantization calculation, we know that $\varphi_k = e^{i\mathbf{k}\cdot\mathbf{x}}$ is a good candidate of normal modes and can assume the ground state:

$$|\Phi_o\rangle = \prod_{k\sigma} \theta(k_F - k) c^{+}_{k\sigma} |0\rangle$$



Note that the cut-off in momentum space is different from the energy cut-off $\theta(\epsilon_F - \epsilon_k)$. This is valid when we assume the translation and rotation symmetry of the ground state.

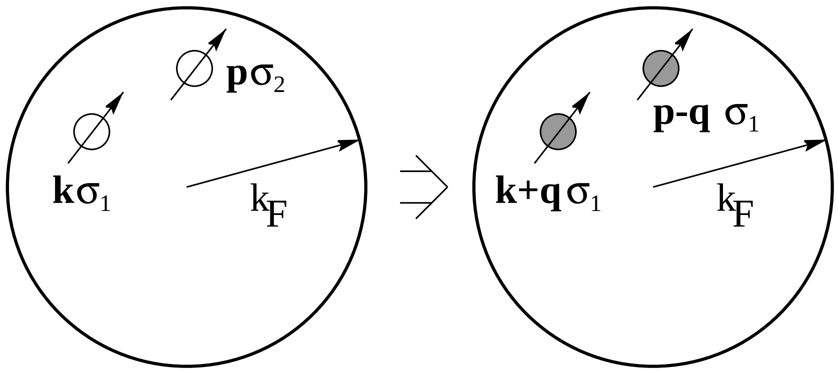
Perturbation Expansion

- 0th order:

$$
\begin{aligned}
E^{(0)} &= \langle \Phi_o | \mathcal{H}_o | \Phi_o \rangle \\
&= \sum_{k\sigma} \epsilon_{ok} \langle \Phi_o | c^{+}_{k\sigma} c_{k\sigma} | \Phi_o \rangle \\
&= \sum_{k\sigma} \epsilon_{ok} \theta(k_F - k)
\end{aligned}
$$

- 1st order correction: (Hartree-Fock term)

$$
\begin{aligned}
E^{(1)} &= \langle \Phi_o | \mathcal{H}_1 | \Phi_o \rangle \\
&= \frac{1}{2} \sum_{kp,q\neq 0} \sum_{\sigma\sigma'}{}' V_q \langle \Phi_o | c^{+}_{k+q\sigma} c^{+}_{p-q\sigma'} c_{p\sigma'} c_{k\sigma} | \Phi_o \rangle \\
&= -\frac{1}{2} \sum_{\sigma} \sum_{kq}{}' V_q \theta(k_F - |\mathbf{k}+\mathbf{q}|) \theta(k_F - |\mathbf{k}|)
\end{aligned}
$$



$$\mathbf{k}+\mathbf{q}\sigma_1 = \mathbf{k}\sigma_1, \quad \mathbf{p}-\mathbf{q}\sigma_2 = \mathbf{p}\sigma_2 \quad (\times)$$

$$\mathbf{k}+\mathbf{q}\sigma_1 = \mathbf{p}\sigma_2, \quad \mathbf{p}-\mathbf{q}\sigma_2 = \mathbf{k}\sigma_1 \quad (\mathrm{O})$$

$$|i\rangle = c_{\mathbf{p}\sigma_2} c_{\mathbf{k}\sigma_1} |\Phi_0\rangle, \quad |f\rangle = c_{\mathbf{p}-\mathbf{q}\sigma_2} c_{\mathbf{k}+\mathbf{q}\sigma_1} |\Phi_0\rangle$$

$$\begin{aligned} \rightarrow \langle f|i\rangle &= \delta_{\mathbf{k}+\mathbf{q},\mathbf{p}} \delta_{\sigma_1,\sigma_2} \langle\Phi_0| c^+_{\mathbf{k}+\mathbf{q}\sigma_1} c^+_{\mathbf{k}\sigma_1} c_{\mathbf{k}+\mathbf{q}\sigma_1} c_{\mathbf{k}\sigma_1} |\Phi_0\rangle \\ &= \delta_{\mathbf{k}+\mathbf{q},\mathbf{p}} \delta_{\sigma_1,\sigma_2} \langle\Phi_0| \hat{n}_{\mathbf{k}+\mathbf{q}\sigma_1} \cdot (-\hat{n}_{\mathbf{k}+\mathbf{q}\sigma_1}) |\Phi_0\rangle \\ &= -\delta_{\mathbf{k}+\mathbf{q},\mathbf{p}} \delta_{\sigma_1,\sigma_2} \Theta(k_F - |\mathbf{k}+\mathbf{q}|)\Theta(k_F - |\mathbf{k}|) \end{aligned}$$