An Introduction to Second Quantization in Statistical Mechanics

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1 Introduction

Second Quantization is the best way to describe the many-body quantum systems. We can use the creation-annihilation operators to get a lot of interesting results by this method. In this article I will follow the formalism of Pathria's book and show how to use second quantization to get the statistical properties of boson liquid and fermi liquid.

2 Second quantization of Bosons and Fermions and free particle system

2.1 Second Quantization Algebra

Actually second quantization is the quantization of fields. So we need to define the creation-annihilation operators of the boson or fermion field:

$$\begin{aligned} [a_i, a_j^\dagger] &= \delta_{ij} && (1) \\ [a_i, a_j] &= 0 && (2) \\ \left[a_i^\dagger, a_j^\dagger\right] &= 0 && (3) \end{aligned}$$

and the vacuum state is needed: $|0\rangle$. We can act the creation operator on the vacuum state to obtain a single-particle state. And the subspace (of the Hilbert space) with different particle numbers are connected by these operators. See the figure below:

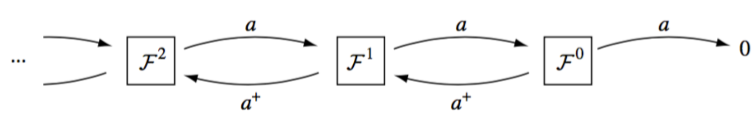

Figure 1: Fock space

In Eq.(1)(2)(3), indexes i, j means some eigenvalue of some operators. For Fermions the commutation relation is altered by anti-commutation relation. Since the commutation relation is just like the upper and lower operators of Harmonic oscillator, we can find that

$$N = \sum_i a_i^\dagger a_i$$

is the operator of particle number. For example we can find that the normalized N particle state can be written as:

$$|\psi\rangle = \prod_i \frac{1}{\sqrt{n_i!}} a_i^\dagger |0\rangle$$

2.2 One-body Operators

Now introduce the **one-body operator**: for any one-body operator $\mathcal{O}_1$, its second-quantized form under its eigenbasis are:

$$\hat{O} = \sum_i o_i a_i^\dagger a_i \tag{4}$$

and o_i is the eigenvalue of first-quantized operator O_1. Now if we do an representation transformation to basis that are not the eigenvectors of O_1, then the operators will change into:

$$a_{i'}^\dagger = \sum_i \langle i|i'\rangle a_i^\dagger \tag{5}$$

then the second quantized operator will be:

$$\hat{O} = \sum_{ij} \langle i|O_1|j\rangle \, a_i^\dagger a_j \tag{6}$$

For example, the second quantized Hamiltonian is

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma} \quad \text{Free particle system}$$

or

$$H = -t \sum_{\langle ij\rangle} a_i^\dagger a_j \quad \text{(Tight-binding approximation)}$$

Now if we transform to the real-space representation, the Hamiltonian will have the following form:

$$H = \int d^3x \, \psi^\dagger(\mathbf{x}) \left(-\frac{\hbar^2}{2m} \nabla^2 \right) \psi(\mathbf{x}) \tag{7}$$

in which $\psi^\dagger(\mathbf{x})$ is the creation operator at position $\mathbf{x}$. This is easily obtained from Eq.(6).

3 Relation between first quantization and second quantization

3.1 Wave Function

So what is the relationship between the formalism with so called “first quantization” we familiar with? Remember that the wave function is the inner product of $\langle \mathbf{r}_i|$ (the eigenvector of the position operator) and the eigenstate of the Hamiltonian $|\psi\rangle$ (with fixed particle number N), we can find that

$$\psi_N(\mathbf{r}_i) = \langle \mathbf{r}_i|\psi_N\rangle = \frac{1}{\sqrt{N!}} \langle 0|\psi(\mathbf{r}_1)\psi(\mathbf{r}_2)\cdots\psi(\mathbf{r}_N)|\psi_N\rangle \tag{8}$$

and it automatically satisfies the exchange symmetry of Boson wave function. We can also find that this wave function is normalized:

$$\begin{aligned}
\int d^{3N}r \, \psi(\mathbf{r}_i)\psi^*(\mathbf{r}_i) &= \frac{1}{N!} \int d^{3N}r \, \langle \psi_N|\psi^\dagger(\mathbf{r}_N)\cdots\psi^\dagger(\mathbf{r}_1)|0\rangle\langle 0|\psi(\mathbf{r}_1)\cdots\psi(\mathbf{r}_N)|\psi\rangle \\
&= \frac{1}{N!} \int d^{3N}r \, \langle \psi_N|\psi^\dagger(\mathbf{r}_N)\cdots\psi^\dagger(\mathbf{r}_1)\psi(\mathbf{r}_1)\cdots\psi(\mathbf{r}_N)|\psi_N\rangle \\
&= \frac{1}{N!} \int d^{3N-3}r \, \langle \psi_N|\psi^\dagger(\mathbf{r}_N)\cdots\psi^\dagger(\mathbf{r}_2)N\psi(\mathbf{r}_2)\cdots\psi^(\mathbf{r}_N)|\psi_N\rangle \\
&= \frac{1}{N!} \int d^{3N-6}r \, \langle \psi_N|\psi^\dagger(\mathbf{r}_N)\cdots\psi^\dagger(\mathbf{r}_3)N(N-1)\psi(\mathbf{r}_3)\cdots\psi^(\mathbf{r}_N)|\psi_N\rangle \\
&= \frac{1}{N!} \langle \psi_N|N(N-1)\cdots|\psi_N\rangle \\
&= 1
\end{aligned} \tag{9}$$

So clearly we see that the wave function is the inner product of a position eigenstate and an quantum state with a fixed particle number.

3.2 Schrödinger Equation

In this part I will show that the wave function we get in the previous section satisfies the Schrödinger equation. Now assume that the quantum state $|\psi_N\rangle$ has fixed particle number and energy, and we calculate the following equation:

$$\begin{aligned}
E_N\psi_N(\mathbf{r}) &= \frac{1}{\sqrt{N!}}\langle 0|\psi(\mathbf{r}_1)\cdots\psi(\mathbf{r}_N)H|\psi_N\rangle \\
&= \frac{1}{\sqrt{N!}}\langle 0|\sum_{i=1}^{N}\int d^3\mathbf{r}\,\psi(\mathbf{r}_1)\cdots\psi(\mathbf{r}_{i-1})\delta(\mathbf{r}-\mathbf{r}_i)\psi(\mathbf{r}_{i+1})\cdots\psi(\mathbf{r}_N)\left(-\frac{\hbar^2\nabla^2}{2m}\right)\psi(\mathbf{r})|\psi_N\rangle \\
&= \frac{1}{\sqrt{N!}}\sum_{i=1}^{N}(-\frac{\hbar^2\nabla_i^2}{2m})\langle 0|\psi(\mathbf{r}_1)\cdots\psi(\mathbf{r}_N)|\psi_N\rangle \\
&= \sum_{i=1}^{N}(-\frac{\hbar^2\nabla_i^2}{2m})\psi_N(\mathbf{r})
\end{aligned} \tag{10}$$

So up till now we have proved that the wave function satisfies the Schrödinger equation. The interacting term is the same, and for simplicity, I won't show it here.

4 Interacting Boson system

4.1 Two-body interaction term

Now we need to add the interaction term into the Hamiltonian. In the momentum representation, the Hamiltonian will be:

$$H = \sum_{\mathbf{k}\sigma}\frac{\mathbf{k}^2}{2m}a^\dagger_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma} + \frac{1}{2L^3}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}}u_{\mathbf{q}}a^\dagger_{\mathbf{k}+\mathbf{q}\sigma}a^\dagger_{\mathbf{k}'-\mathbf{q}\sigma'}a_{\mathbf{k}'\sigma'}a_{\mathbf{k}\sigma} \tag{11}$$

And this can be easily obtained from the Fourier transformation of an interacting system:

$$\hat{u} = \frac{1}{2}\int d^3x d^3x'\,V(\mathbf{x}-\mathbf{x}')\rho(x)\rho(x')\,.$$

and the interacting term can be shown by the following graph:

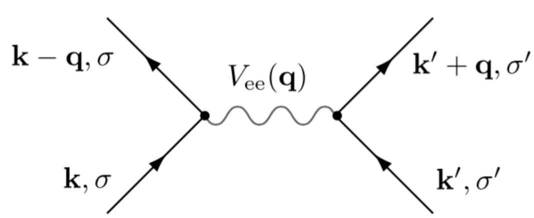

Figure 2: "Feynman Diagram"

Now if we write the interacting term by the scattering length, the Fourier component will be

$$a(\mathbf{q}) =$$

5 Low temperature behavior of imperfect Bose gas

6 Vortex and Topological Excitations