Lesson 9 - Second Quantization of Matter
Unit 9.2 Statistical mechanics of non-interacting bosons and fermions

Luca Salasnich

Dipartimento di Fisica e Astronomia "Galileo Galilei", Università di Padova

Structure of Matter - MSc in Physics

Hamiltonian in second quantization (I)

By using the number operators $\hat{N}_\alpha = \hat{c}_\alpha^+ \hat{c}_\alpha$, the quantum Hamiltonian of the matter field can be written as

$$\hat{H} = \sum_\alpha \epsilon_\alpha \, \hat{N}_\alpha \ , \tag{1}$$

after removing the puzzling zero-point energy. This is the second-quantization Hamiltonian of non-interacting matter.
The same Hamiltonian can also be written in the elegant form

$$\hat{H} = \int d^3\mathbf{r} \ \hat{\psi}^+(\mathbf{r},t) \left[-\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{r}) \right] \hat{\psi}(\mathbf{r},t) \ . \tag{2}$$

This quantum Hamiltonian can be directly obtained from the classical Schrödinger energy by promoting the complex classical field $\psi(\mathbf{r},t)$ and $\hat{\psi}(\mathbf{r},t)$ to quantum field operators:

$$\psi(\mathbf{r},t) \quad \to \quad \hat{\psi}(\mathbf{r},t) \ , \tag{3}$$

$$\psi^*(\mathbf{r},t) \quad \to \quad \hat{\psi}^+(\mathbf{r},t) \ , \tag{4}$$

satisfying the commutation relations of bosons or the anti-commutation relations of fermions.

Hamiltonian in second quantization (II)

It is straightforward to show that the bosonic field operator satisfies the following equal-time commutation rules

$$[\hat{\psi}(\mathbf{r}, t), \hat{\psi}^{+}(\mathbf{r}', t)] = \delta(\mathbf{r} - \mathbf{r}') \ , \tag{5}$$

while for the fermionic field operator one gets

$$\{\hat{\psi}(\mathbf{r}, t), \hat{\psi}^{+}(\mathbf{r}', t)\} = \delta(\mathbf{r} - \mathbf{r}') \ . \tag{6}$$

A remarkable property of the field operator $\hat{\psi}^{+}(\mathbf{r}, t)$, which works for bosons and fermions, is the following:

$$\hat{\psi}^{+}(\mathbf{r}, t)|0\rangle = |\mathbf{r}, t\rangle \tag{7}$$

that is the operator $\hat{\psi}^{+}(\mathbf{r}, t)$ creates a particle in the state $|\mathbf{r}, t\rangle$ from the vacuum state $|0\rangle$.

Second quantization at finite temperature (I)

Let us consider the non-interacting matter field in thermal equilibrium with a bath at the temperature T. The relevant quantity to calculate all the thermodynamical properties of the system is the grand-canonical partition function $\mathcal{Z}$, given by

$$\mathcal{Z} = Tr[e^{-\beta(\hat{H}-\mu\hat{N})}] \tag{8}$$

where $\beta = 1/(k_B T)$ with k_B the Boltzmann constant,

$$\hat{H} = \sum_{\alpha} \epsilon_{\alpha} \, \hat{N}_{\alpha} \ , \tag{9}$$

is the quantum Hamiltonian,

$$\hat{N} = \sum_{\alpha} \hat{N}_{\alpha} \tag{10}$$

is total number operator, and μ is the chemical potential, fixed by the conservation of the average particle number.

Second quantization at finite temperature (II)

This implies that

$$
\begin{aligned}
\mathcal{Z} &= \sum_{\{n_\alpha\}} \langle \ldots n_\alpha \ldots | e^{-\beta(\hat{H}-\mu\hat{N})} | \ldots n_\alpha \ldots \rangle \\
&= \sum_{\{n_\alpha\}} \langle \ldots n_\alpha \ldots | e^{-\beta \sum_\alpha (\epsilon_\alpha - \mu)\hat{N}_\alpha} | \ldots n_\alpha \ldots \rangle \\
&= \sum_{\{n_\alpha\}} e^{-\beta \sum_\alpha (\epsilon_\alpha - \mu) n_\alpha} = \sum_{\{n_\alpha\}} \prod_\alpha e^{-\beta(\epsilon_\alpha - \mu) n_\alpha} = \prod_\alpha \sum_{n_\alpha} e^{-\beta(\epsilon_\alpha - \mu) n_\alpha} \\
&= \prod_\alpha \sum_{n=0}^{\infty} e^{-\beta(\epsilon_\alpha - \mu)\, n} = \prod_\alpha \frac{1}{1 - e^{-\beta(\epsilon_\alpha - \mu)}} \qquad \text{for bosons} \qquad (11) \\
&= \prod_\alpha \sum_{n=0}^{1} e^{-\beta(\epsilon_\alpha - \mu)\, n} = \prod_\alpha \left(1 + e^{-\beta(\epsilon_\alpha - \mu)}\right) \qquad \text{for fermions} \qquad (12)
\end{aligned}
$$

Second quantization at finite temperature (III)

Quantum statistical mechanics dictates that the thermal average of any operator $\hat{A}$ is obtained as

$$\langle \hat{A} \rangle_T = \frac{1}{\mathcal{Z}} Tr[\hat{A}\, e^{-\beta(\hat{H}-\mu\hat{N})}] \,. \tag{13}$$

Let us suppose that $\hat{A} = \hat{H} - \mu\hat{N}$, it is then quite easy to show that

$$\frac{1}{\mathcal{Z}} Tr[(\hat{H}-\mu\hat{N})\, e^{-\beta(\hat{H}-\mu\hat{N})}] = -\frac{\partial}{\partial\beta} \ln\left(Tr[e^{-\beta(\hat{H}-\mu\hat{N}}]\right) = -\frac{\partial}{\partial\beta}\ln(\mathcal{Z}) \,. \tag{14}$$

By using Eq. (11) or Eq. (12) we immediately obtain

$$\ln(\mathcal{Z}) = \mp \sum_\alpha \ln\left(1 \mp e^{-\beta(\epsilon_\alpha-\mu)}\right) \,, \tag{15}$$

where $-$ is for bosons and $+$ for fermions, and finally from Eq. (14) we get

$$\langle \hat{H} \rangle_T = \sum_\alpha \epsilon_\alpha \langle \hat{N}_\alpha \rangle_T \quad \text{with} \quad \langle \hat{N}_\alpha \rangle_T = \frac{1}{e^{\beta(\epsilon_\alpha-\mu)} \mp 1} \,. \tag{16}$$

Second quantization at finite temperature (IV)

The one-body local density operator is defined as

$$\hat{\rho}(\mathbf{r},t) = \hat{\psi}^{+}(\mathbf{r},t)\,\hat{\psi}(\mathbf{r},t)\ , \tag{17}$$

and it is such that

$$\int d^3\mathbf{r}\,\hat{\rho}(\mathbf{r},t) = \sum_{\alpha} \hat{c}_{\alpha}^{+}(t)\hat{c}_{\alpha}(t) = \sum_{\alpha} \hat{N}_{\alpha} = \hat{N}\ , \tag{18}$$

taking into account the expansion

$$\hat{\psi}(\mathbf{r},t) = \sum_{\alpha} \hat{c}_{\alpha}(t)\ \phi_{\alpha}(\mathbf{r})\ . \tag{19}$$

Moreover, one immediately finds the following thermal average

$$\langle\hat{\rho}(\mathbf{r},t)\rangle_T = \sum_{\alpha} |\phi_{\alpha}(\mathbf{r})|^2 \langle\hat{N}_{\alpha}\rangle_T = \sum_{\alpha} \frac{|\phi_{\alpha}(\mathbf{r})|^2}{e^{\beta(\epsilon_{\alpha}-\mu)} \mp 1}\ , \tag{20}$$

that is the local density at temperature T for identical bosons $(-)$ or identical fermions $(+)$.