8.08 Statistical Physics II — Spring 2019
Recitation Note 9

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Contents

1 Second Quantization of Bosons

The field operator of bosons are $\hat{\psi}(\mathbf{r})$ and $\hat{\psi}^\dagger(\mathbf{r})$, which obey commutation relations

$$[\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}'), \tag{1}$$

$$[\hat{\psi}(\mathbf{r}), \hat{\psi}(\mathbf{r}')] = [\hat{\psi}^\dagger(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')] = 0. \tag{2}$$

In the following, we will drop the hat for simplicity, but we should keep in mind they are operators not functions. In other words, they are (infinite-dimensional) matrices not vectors or numbers. They do not have values by themselves but they can produce expectation values when evaluated on states.

We now define several operators from field operators, whose physical meaning will be clear shortly:

$$\hat{\rho}(\mathbf{r}) \equiv \psi^\dagger(\mathbf{r})\psi(\mathbf{r}), \tag{3}$$

$$\hat{N} \equiv \int d\mathbf{r}\hat{\rho}(\mathbf{r}), \tag{4}$$

$$\hat{T} \equiv \int d\mathbf{r}\psi^\dagger(\mathbf{r}) \left(-\frac{\hbar^2\nabla^2}{2m}\right) \psi(\mathbf{r}) = \frac{\hbar^2}{2m} \int d\mathbf{r}\nabla\psi^\dagger(\mathbf{r})\nabla\psi(\mathbf{r}), \tag{5}$$

$$\hat{U} \equiv \int d\mathbf{r}U(\mathbf{r})\hat{\rho}(\mathbf{r}), \tag{6}$$

$$\hat{V} \equiv \int d\mathbf{r}d\mathbf{r}'\psi^\dagger(\mathbf{r})\psi^\dagger(\mathbf{r}')V(\mathbf{r} - \mathbf{r}')\psi(\mathbf{r}')\psi(\mathbf{r}), \tag{7}$$

$$\hat{H} \equiv \hat{T} + \hat{U} + \hat{V}. \tag{8}$$

In Eq. (5), we integrated by parts.

Boson Number Operator We first study the operator $\hat{N}$, which is obviously Hermitian. Thus there exists a complete set of orthonormal basis that are eigenstates of $\hat{N}$:

$$\hat{N} |\Psi_N\rangle = N |\Psi_N\rangle , \ \langle\Psi_N|\Psi_N\rangle = 1. \tag{9}$$

It is often assumed that there exists a unique ground state called "vacuum" state $|0\rangle \equiv |\Psi_0\rangle$[1]:

$$\hat{N} |0\rangle = 0, \ \langle 0|0\rangle = 1. \tag{10}$$

Using the commutation relation Eq. (1), it is not hard to verify

$$\hat{N}\psi(\mathbf{r}) |\Psi_N\rangle = (N-1)\psi(\mathbf{r}) |\Psi_N\rangle , \tag{11}$$

$$\hat{N}\psi^\dagger(\mathbf{r}) |\Psi_N\rangle = (N+1)\psi^\dagger(\mathbf{r}) |\Psi_N\rangle , \tag{12}$$

which means $\psi(\mathbf{r}) |\Psi_N\rangle$ and $\psi^\dagger(\mathbf{r}) |\Psi_N\rangle$ are also eigenstates of $\hat{N}$ with eigenvalues $N-1$ and $N+1$ respectively. In this way, $\hat{N}$ has eigenvalues $0, 1, 2, \ldots$. Physically, $\hat{N}$ is the total boson number, $\hat{\rho}(\mathbf{r})$ is the local boson density, and $\hat{\psi}(\mathbf{r})$ and $\hat{\psi}^\dagger(\mathbf{r})$ annihilates and creates a boson at position $\mathbf{r}$ respectively.

Representing states using the occupation number is usually called "second quantization". The occupation number is called the "Fock state basis". It is more convenient to describe many-body quantum states under the Fock state basis.

Wavefunction We now define a function in the normal sense:

$$\Psi_N(\mathbf{r}_1, \ldots, \mathbf{r}_N) \equiv (N!)^{-1/2} \langle 0|\psi(\mathbf{r}_1) \ldots \psi(\mathbf{r}_N)|\Psi_N\rangle . \tag{13}$$

[1]Depending on the Hamiltonian and the boundary condition the ground state may not be unique. The ground state degeneracy has a deep connection to the Hamiltonian topology.

Keep in mind $\Psi_N(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ is a function of N coordinates while $|\Psi_N\rangle$ is a state vector. $\Psi_N(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ is nonzero because boson annihilation operator is applied N times to $|\Psi_N\rangle$.

First, because of the commutation relation Eq. (2), $\Psi_N(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ is a symmetric function, i.e. invariant under the permutation of $\mathbf{r}_1,\ldots,\mathbf{r}_N$. Second, $\Psi_N(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ is normalized:

$$\int d\mathbf{r}_1\ldots d\mathbf{r}_N \Psi_N^*(\mathbf{r}_1,\ldots,\mathbf{r}_N)\Psi_N(\mathbf{r}_1,\ldots,\mathbf{r}_N) \tag{14}$$

$$=(N!)^{-1}\int d\mathbf{r}_1\ldots d\mathbf{r}_N \langle\Psi_N|\psi^\dagger(\mathbf{r}_N)\ldots\psi^\dagger(\mathbf{r}_1)|0\rangle\langle 0|\psi(\mathbf{r}_1)\ldots\psi(\mathbf{r}_N)|\Psi_N\rangle \tag{15}$$

$$=(N!)^{-1}\int d\mathbf{r}_1\ldots d\mathbf{r}_N \sum_n \langle\Psi_N|\psi^\dagger(\mathbf{r}_N)\ldots\psi^\dagger(\mathbf{r}_1)|\Phi_n\rangle\langle\Phi_n|\psi(\mathbf{r}_1)\ldots\psi(\mathbf{r}_N)|\Psi_N\rangle \tag{16}$$

$$=(N!)^{-1}\int d\mathbf{r}_1\ldots d\mathbf{r}_N \langle\Psi_N|\psi^\dagger(\mathbf{r}_N)\ldots\psi^\dagger(\mathbf{r}_1)\psi(\mathbf{r}_1)\ldots\psi(\mathbf{r}_N)|\Psi_N\rangle\,. \tag{17}$$

Here $\sum_n |\Phi_n\rangle\langle\Phi_n| = I$ is a complete set of eigenstates of $\hat{N}$. Due to the unique vacuum assumption, unless $|\Phi_n\rangle = |0\rangle$, we have $\langle\Phi_n|\psi(\mathbf{r}_1)\ldots\psi(\mathbf{r}_N)|\Psi_N\rangle = 0$. Therefore, one is free to add zero to the expression and can replace the $|0\rangle\langle 0|$ with identity particularly for the expression above (not true in general!). We then switch the order of taking expectation and integration, and performs the integral one by one. For example, the first two integrals are:

$$\int d\mathbf{r}_1\psi^\dagger(\mathbf{r}_1)\psi(\mathbf{r}_1) = \hat{N}, \tag{18}$$

$$\int d\mathbf{r}_2\psi^\dagger(\mathbf{r}_2)\hat{N}\psi(\mathbf{r}_2) = \int d\mathbf{r}_2\psi^\dagger(\mathbf{r}_2)\psi(\mathbf{r}_2)(\hat{N}-1) = \hat{N}(\hat{N}-1). \tag{19}$$

In this way,

$$\int d\mathbf{r}_1\ldots d\mathbf{r}_N \Psi_N^*(\mathbf{r}_1,\ldots,\mathbf{r}_N)\Psi_N(\mathbf{r}_1,\ldots,\mathbf{r}_N) \tag{20}$$

$$=(N!)^{-1}\langle\Psi_N|\int d\mathbf{r}_1\ldots d\mathbf{r}_N\psi^\dagger(\mathbf{r}_N)\ldots\psi^\dagger(\mathbf{r}_1)\psi(\mathbf{r}_1)\ldots\psi(\mathbf{r}_N)|\Psi_N\rangle \tag{21}$$

$$=(N!)^{-1}\langle\Psi_N|\hat{N}(\hat{N}-1)(\hat{N}-2)\ldots|\Psi_N\rangle \tag{22}$$

$$=1. \tag{23}$$

Hamiltonian Operator It is not hard to check $[\hat{N},\hat{H}]=0$. Mathematically, this means one can find a complete set of orthonormal basis that are eigenstates of $\hat{N}$ and $\hat{H}$ simultaneously. Therefore, we will replace $|\Psi_N\rangle$ with $|\Psi_{N,E}\rangle$.

$$\hat{N}|\Psi_{N,E}\rangle = N|\Psi_{N,E}\rangle,\ \hat{H}|\Psi_{N,E}\rangle = E|\Psi_{N,E}\rangle,\ \langle\Psi_{N,E}|\Psi_{N,E}\rangle = 1. \tag{24}$$

Using the commutation relation, it is straightforward to verify:

$$[\psi(\mathbf{r}_i),\hat{H}] = \left[-\frac{\hbar^2\nabla^2}{2m} + U(\mathbf{r}_i) + \int d\mathbf{r}'\psi^\dagger(\mathbf{r}')V(\mathbf{r}_i-\mathbf{r}')\psi(\mathbf{r}')\right]\psi(\mathbf{r}_i). \tag{25}$$

With this, one can show

$$E\Psi_{N,E}(\mathbf{r}_1,\ldots,\mathbf{r}_N) = (N!)^{-1/2}\langle 0|\psi(\mathbf{r}_1)\ldots\psi(\mathbf{r}_N)\hat{H}|\Psi_N\rangle \tag{26}$$

$$= \left[-\frac{\hbar^2}{2m}\sum_{i=1}^N\nabla_i^2 + \sum_{i=1}^N U(\mathbf{r}_i) + \sum_{i,j=1}^N V(\mathbf{r}_i-\mathbf{r}_j)\right]\Psi_{N,E}(\mathbf{r}_1,\ldots,\mathbf{r}_N), \tag{27}$$

which is exactly the many-body Schrödinger equation. In this way, $\Psi_{N,E}(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ is the many-body wavefunction in the usual "first quantization" sense. As one can see, "first quantization" and "second quantization" descriptions are equivalent, while second quantization is more succinct.

2 Bogoliubov Approximation and Gross-Pitaevskii Equation

At low temperature, a macroscopic number of bosons will condense to the zero-momentum state. We can Fourier transform the field operator:

$$\psi(\mathbf{r}) = \frac{1}{\sqrt{V}} \left(b_0 + \sum_{\mathbf{k}\neq 0} e^{i\mathbf{k}\cdot\mathbf{r}} b_{\mathbf{k}} \right). \tag{28}$$

The Bogoliubov approximation is to replace the zero-momentum operator with numbers:

$$b_0, b_0^\dagger \to \sqrt{N_0}. \tag{29}$$

The rationale behind the approximation is that when there are so many bosons at zero momentum, the expectation value of $\hat{N}_0(\mathbf{r}) \equiv b_0^\dagger b_0$ will be so large that it does not matter whether it is N_0 or $N_0 + 1$. Also, at thermodynamic limit the condensed boson number fluctuation will be zero, so it does not matter whether b_0 or $b_0^\dagger$ change the boson number. Therefore, we simply set them to numbers.

In this way, the field operator is decomposed as

$$\hat{\psi}(\mathbf{r}) = \Phi(\mathbf{r}) + \hat{\psi}'(\mathbf{r}), \tag{30}$$

where $\Phi(\mathbf{r})$ is a classical field often called the "order parameter" of the BEC or the "wavefunction" of the BEC (the latter name is very bad and confusing, as $\Psi_{N,E}(\mathbf{r}_1, \ldots, \mathbf{r}_N)$ is the real many-body wavefunction). The density of condensed bosons is $\rho_0(\mathbf{r}) = |\Phi(\mathbf{r})|^2$.

If we are only interested in the condensation itself but not excitations, we can completely ignore the remaining $\psi'(\mathbf{r})$ term. Consider interacting bosons with delta interactions: $V(\mathbf{r} - \mathbf{r}') = g\delta(\mathbf{r} - \mathbf{r}')$. The interaction potential operator becomes:

$$\hat{V} = g \int d\mathbf{r} \psi^\dagger(\mathbf{r}) \psi^\dagger(\mathbf{r}) \psi(\mathbf{r}) \psi(\mathbf{r}). \tag{31}$$

Using Bogoliubov approximation, the Hamiltonian operator also becomes a number:

$$H = \int d\mathbf{r} \Phi^*(\mathbf{r}) \left(-\frac{\hbar^2 \nabla^2}{2m} + U(\mathbf{r}) + g|\Phi(\mathbf{r})|^2 \right) \Phi(\mathbf{r}). \tag{32}$$

Minimizing the energy with respect to $\delta H / \delta \Psi^*(\mathbf{r}) = 0$, it follows

$$\left(-\frac{\hbar^2 \nabla^2}{2m} + U(\mathbf{r}) + 2g|\Phi(\mathbf{r})|^2 \right) \Phi(\mathbf{r}) = 0. \tag{33}$$

This is the (time-independent) Gross-Pitaevskii (GP) equation. One can also fix the chemical potential instead of the boson number, and minimize the grand potential. The corresponding GP equation is

$$\left[-\frac{\hbar^2 \nabla^2}{2m} + (U(\mathbf{r}) - \mu) + 2g|\Phi(\mathbf{r})|^2 \right] \Phi(\mathbf{r}) = 0. \tag{34}$$