1 Lecture 3. Second Quantization, Bosons

In this lecture we discuss second quantization, a formalism that is commonly used to analyze many-body problems. The key ideas of this method were developed, starting from the initial work of Dirac, most notably, by Fock and Jordan. In this approach, one thinks of multi-particle states of bosons or fermions as single particle states each filled with a certain number of identical particles. The language of second quantization often allows to reduce the many-body problem to a single particle problem defined in terms of 'quasiparticles,' i.e. particles 'dressed' by interactions.

1.1 The Fock space

The many-body problem is defined for N particles (here, bosons) described by the sum of single-particle Hamiltonians and the two-body interaction Hamiltonian:

$$\mathcal{H} = \sum_{a=1}^{N} \mathcal{H}^{(1)}(x_a) + \sum_{a\neq b} \mathcal{H}^{(2)}(x_a, x_b) \tag{1}$$

$$\mathcal{H}^{(1)}(x) = -\frac{\hbar^2}{2m}\nabla_x^2 + U(x)\,, \quad \mathcal{H}^{(2)}(x,x') = U^{(2)}(x-x') \tag{2}$$

where x_a are particle coordinates. In some rare cases (e.g. for nuclear particles) one also has to include the three-particle, and higher order multiparticle interactions, such as $\sum_{a,b,c} \mathcal{H}^{(3)}(x_a, x_b, x_c)$, etc.

The system is described by the many-body wavefunction $\Phi(x_1, x_2, ..., x_N)$, symmetric with respect to the permutations of coordinates x_a. The symmetry requirement follows from pareticles indestinguishability and Bose statistics (i.e., the wavefunction invariance under permutations of the particles). The wavefunction $\Phi(x_1, x_2, ..., x_N)$ obeys the Schrödinger equation $i\hbar\partial_t\Phi = \mathcal{H}\Phi$. Since the number of particles in typical situations of interest is extremely large, solving this equation directly presents a very hard problem. There are several approaches, however, that allow to gain insight. The method of second quatization, historically the first many-body technique developed in the 30's, will be discussed here.

We shall start with defining the Fock space, sometimes also called the 'big' many-particle space,

$$\mathcal{V} = \bigoplus_N \Big\{ \bigotimes_{symm}^{N} \mathcal{V}^{(1)} \Big\} \tag{3}$$

— the sum of the N-th symmetric powers of the single particle Hilbert space $\mathcal{V}^{(1)}$. It describes the states of a system containing any number of particles $N = 0, 1, 2, 3, ...$

One can choose the basis in the 'big' space $\mathcal{V}$ in the form of symmetrized products of single particle wavefunctions $\varphi_p(x)$ drawn from an orthonormal complete set of states in $\mathcal{V}^{(1)}$,

$$\Phi_{m_1,m_2,...}(x_1,x_2,...,x_N)=\left(\frac{m_1!m_2!...}{N!}\right)^{1/2}\sum_P\varphi_{p_1}(x_1)\varphi_{p_2}(x_2)...\varphi_{p_N}(x_N) \tag{4}$$

with the sum taken over all permutations of the states $\varphi_p(x)$. The numbers m_p indicate how many times the function $\varphi_p(x)$ appears in the product. The number of permutations in the sum $\sum_P$ is equal to the number of ways to combine N elements into groups containg m_1, m_2, etc., elements each ($m_1+m_2+...=N$). This combinatorial factor, equal to $N!/m_1!m_2!...$, defines the normalization factor in Eq.(4). One can check that the states (4) are orthogonal and form a complete set in $\mathcal{V}$.

As an *example*, consider free Bose particles in a box $L\times L\times L$, in which case the single particle states can be chosen as eigenstates of the single particle problem $E\varphi(x)=-\frac{\hbar^2}{2m}\nabla^2\varphi$. Assuming periodic boundary conditions, we have eigenstates of a plane wave form

$$\varphi_{\mathbf{n}}(\mathbf{r})=\frac{1}{\sqrt{V}}\exp\left(i\mathbf{k_n}\mathbf{r}\right),\quad \mathbf{k_n}=\frac{2\pi}{L}\mathbf{n},\quad \mathbf{n}=(n_1,n_2,n_3) \tag{5}$$

with integer $n_{1,2,3}$ and $V=L^3$. The energies of these states are $E_{\mathbf{n}}=\frac{\hbar^2}{2m}\mathbf{k}_{\mathbf{n}}^2$. The space $\mathcal{V}$ is then spanned by the functions

$$1,\quad \varphi_{\mathbf{n}}(\mathbf{r}),\quad \frac{1}{\sqrt{2}}\left(\varphi_{\mathbf{n}}(\mathbf{r})\varphi_{\mathbf{m}}(\mathbf{r}')+\varphi_{\mathbf{m}}(\mathbf{r})\varphi_{\mathbf{n}}(\mathbf{r}')\right),\quad \varphi_{\mathbf{n}}(\mathbf{r})\varphi_{\mathbf{n}}(\mathbf{r}'),\quad ... \tag{6}$$

corresponding to the no-particle state, one particle, two particles, etc. The energies of these states are

$$0,\quad E_{\mathbf{n}},\quad E_{\mathbf{n}}+E_{\mathbf{m}},\quad 2E_{\mathbf{n}},\quad ... \tag{7}$$

Note that the structure of the two-particle functions depends on whether the participating single-particle states are different or the same.

To make progress, one can introduce the so-called number representation. Allow any total particle number N and focus on the dependence of the state on the *occupation numbers* m_i. This dependence is captured most vividly by the representation in which an auxiliary oscillator, along with the creation and annihilation operators, is associated with each single particle state. The occupation numbers are interpreted in this representation as number of quanta in eachy oscillator. The corresponing *Fock states*, in the number representation, have the form

$$|m_1,m_2,...\rangle=\prod_{i=1}^{\infty}\frac{1}{\sqrt{m_i!}}\left(a_i^+\right)^{m_i}|0\rangle \tag{8}$$

where $|0\rangle$ is the no-particle state, and $\sum m_i=N$. This representation accounts correctly for the symmetry properties of the states (4) due to Bose statistics.

1.2 Second-quantized operators

In the number representation, the many-body Hamiltonian (1) is represented by a polynomial in the operators a_i, a_i^+:

$$\mathcal{H} = \sum_{ij} H_{ij}^{(1)} a_i^+ a_j + \frac{1}{2} \sum_{ijkm} H^{(2)}{}_{km}^{ij} a_i^+ a_j^+ a_k a_m \tag{9}$$

with the quantities $H_{ij}^{(1)}$, $H_{km}^{(2)\,ij}$ being the one- and two-particle matrix elements,

$$H_{ij}^{(1)} = \langle \varphi_i(x) | \mathcal{H}^{(1)}(x) | \varphi_j(x) \rangle = \int \bar{\varphi}_i(x) \mathcal{H}^{(1)}(x) \varphi_j(x) dx \tag{10}$$
$$H^{(2)}{}_{km}^{ij} = \langle \varphi_i(x)\varphi_j(x') | \mathcal{H}^{(2)}(x,x') | \varphi_k(x)\varphi_m(x') \rangle = \iint \bar{\varphi}_i(x)\bar{\varphi}_j(x') \mathcal{H}^{(2)}(x,x') \varphi_k(x)\varphi_m(x') dx dx'$$

One can prove the equivalence of this representation to the original many-body problem (1) formulated in terms of many-particle wavefunction $\Phi(x_1, x_2, ..., x_N)$ by directly evaluating the matric elements of the Hamiltonian between all pairs of many body states, and showing that in both representations the results agree. The combinatorics involved in this proof is combersom, albeit completely straightforward. Instead of reviewing it here, we refer to the book by J. R. Schrieffer, "The Theory of Superconductivity" that contains an Appendix describing the analysis in some detail. Another proof can be devised using functional integral, and we shall talk about it later on.

The expressions (9),(10) are true for any orthogonal set of functions $\varphi_i(x)$. In the case when these functions are chosen to be the eigenstates of the single-particle problem, the matrix elements of $\mathcal{H}^{(1)}$ vanish between different states,

$$\langle \varphi_i(x) | \mathcal{H}^{(1)}(x) | \varphi_j(x) \rangle = E_i \delta_{ij} \tag{11}$$

and the one-particle part of the Hamiltonian simplifies to

$$\mathcal{H}^{(1)} = \sum_i E_i a_i^+ a_i \tag{12}$$

Since $\hat{n}_i = a_i^+ a_i$ is nothing but the number operator, the eigenvalues of the one-particle Hamiltonian corresponding to the number states (8) are

$$E_{n_1\, n_2\, ...} = \langle n_1, n_2, ... | \mathcal{H}^{(1)} | n_1, n_2, ... \rangle = \sum_i E_i\, n_i \tag{13}$$

In the above example of free bosons in a box, the states are labeled by discrete momenta, and the expression (13) becomes

$$E_{n_1\, n_2\, ...} = \sum_{\mathbf{k}} E_{\mathbf{k}}\, n_{\mathbf{k}} \tag{14}$$

If the bosons are interacting via a two-body potential $U^{(2)} = U(\mathbf{r} - \mathbf{r}')$, from Eqs.(9),(10) we obtain the two-particle Hamiltonian of the form

$$\mathcal{H}^{(2)} = \frac{1}{2} \sum_{\mathbf{k}_1\,\mathbf{k}_2\,\mathbf{k}_3\,\mathbf{k}_4} \langle \mathbf{k}_1 \mathbf{k}_2 | U^{(2)} | \mathbf{k}_3 \mathbf{k}_4 \rangle a_{\mathbf{k}_1}^+ a_{\mathbf{k}_2}^+ a_{\mathbf{k}_3} a_{\mathbf{k}_4} \tag{15}$$

where the matrix element in (15), evaluated on the plane wave states (5), has the form

$$\langle \mathbf{k}_1\mathbf{k}_2|U^{(2)}|\mathbf{k}_3\mathbf{k}_4\rangle = \iint \frac{1}{V^2} e^{-i\mathbf{k}_1\mathbf{r}-i\mathbf{k}_2\mathbf{r}'+i\mathbf{k}_3\mathbf{r}+i\mathbf{k}_4\mathbf{r}'} U(\mathbf{r}'-\mathbf{r}) d^3r d^3r' \tag{16}$$

This expression can be simplified and evaluated by choosing $\mathbf{a} = \mathbf{r}' - \mathbf{r}$ as an integration variable instead of $\mathbf{r}'$, after which the integral in (16) factors as

$$\left(\int e^{i(\mathbf{k}_4-\mathbf{k}_2)\mathbf{a}} U(\mathbf{a}) d^3a\right) \times \left(\int e^{-i\mathbf{k}_1\mathbf{r}-i\mathbf{k}_2\mathbf{r}+i\mathbf{k}_3\mathbf{r}+i\mathbf{k}_4\mathbf{r}} d^3r\right) = \tilde{U}(\mathbf{k}_2-\mathbf{k}_4)\, \delta_{\mathbf{k}_1+\mathbf{k}_2=\mathbf{k}_3+\mathbf{k}_4} \tag{17}$$

where $\tilde{U}(\mathbf{k}) = \int e^{-i\mathbf{k}\mathbf{r}} U(\mathbf{r}) d^3r$ is the Fourier transform of the interaction potential, and

$$\delta_{\mathbf{k}_1+\mathbf{k}_2=\mathbf{k}_3+\mathbf{k}_4} = \begin{cases} V, & \mathbf{k}_1+\mathbf{k}_2=\mathbf{k}_3+\mathbf{k}_4 \\ 0, & \mathbf{k}_1+\mathbf{k}_2\neq\mathbf{k}_3+\mathbf{k}_4 \end{cases} \tag{18}$$

Finally, the two-body Hamiltonian takes the form

$$\mathcal{H}^{(2)} = \frac{1}{2V} \sum_{\mathbf{k}_1+\mathbf{k}_2=\mathbf{k}_3+\mathbf{k}_4} \tilde{U}(\mathbf{k}_2-\mathbf{k}_4) a^+_{\mathbf{k}_1} a^+_{\mathbf{k}_2} a_{\mathbf{k}_3} a_{\mathbf{k}_4} \tag{19}$$

where the sum is taken over all integers parameterizing the plane wave states (5) subject to the constraint $\mathbf{k}_1+\mathbf{k}_2 = \mathbf{k}_3+\mathbf{k}_4$. This constraint, as it is clear from the calculation, arises due to translational invariance of the system. Physically, it expresses the conservation of momentum in two particle scattering.

The second-quantized interaction Hamiltonian is written in terms of the operators $a_{\mathbf{k}}$, $a^+_{\mathbf{k}}$ which remove or add particles. One may thus be worried by apparent particle non-conservation. After looking at it closer, however, and taking into account the commutation relations of a, a^+ with the number operator $\hat{n} = a^+a$,

$$\hat{n}a = a(\hat{n}-1)\,, \quad \hat{n}a^+ = a^+(\hat{n}+1) \tag{20}$$

one can show that the total number of particles $\hat{N} = \sum_{\mathbf{k}} a^+_{\mathbf{k}} a_{\mathbf{k}}$ commutes with the Hamiltonian and is thus conserved.

1.3 Field operator

A very useful representation of the second-quantized many-body hamiltonian is provided by the *field operator*, first introduced by Jordan,

$$\hat{\varphi}(x) = \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}} \varphi_{\mathbf{k}}(x)\,, \quad \hat{\varphi}^+(x) = \sum_{\mathbf{k}} \hat{a}^+_{\mathbf{k}} \bar{\varphi}_{\mathbf{k}}(x) \tag{21}$$

where x labels configuration space, e.g., $x = \mathbf{r}$ in $D = 3$ The states $\varphi_{\mathbf{k}}(x)$ in Eq.(21) can be the eigenstates of a single-particle problem, such as, e.g., the plane waves of the above section, or any other convenient orthonormal basis set.

The operators (21) obey commutation relations

$$[\hat{\varphi}(x), \hat{\varphi}(x')] = [\hat{\varphi}^+(x), \hat{\varphi}^+(x')] = 0\,, \quad [\hat{\varphi}(x), \hat{\varphi}^+(x')] = \delta(x-x') \tag{22}$$

which can be proven by using the commutation relations of $\hat{a}_{\mathbf{k}}$ and $\hat{a}^+_{\mathbf{k}}$ along with the orthogonality of the states $\varphi_{\mathbf{k}}(x)$. For example,

$$[\hat{\varphi}(x), \hat{\varphi}^+(x')] = \sum_{\mathbf{k},\mathbf{k}'} \varphi_{\mathbf{k}}(x)\bar{\varphi}_{\mathbf{k}'}(x')[\hat{a}_{\mathbf{k}}, \hat{a}^+_{\mathbf{k}'}] = \sum_{\mathbf{k},\mathbf{k}'} \varphi_{\mathbf{k}}(x)\bar{\varphi}_{\mathbf{k}'}(x')\delta_{\mathbf{k},\mathbf{k}'} \tag{23}$$

$$= \sum_{\mathbf{k}} \varphi_{\mathbf{k}}(x)\bar{\varphi}_{\mathbf{k}}(x') = \delta(x-x') \tag{24}$$

We note that, although some particular basis set $\varphi_{\mathbf{k}}(x)$ was employed to contruct the field operators, their properties, such as the commutation relations (22), are invariant with respect to the choice of basis.

Using the field operators, the second-quantized problem (9),(10) can be expressed as a polynomial

$$\mathcal{H} = \int \hat{\varphi}^+(x)\left(-\frac{\hbar^2}{2m}\nabla_x^2 + U(x)\right)\hat{\varphi}(x)dx + \frac{1}{2}\iint \hat{\varphi}^+(x)\hat{\varphi}^+(x')U(x-x')\hat{\varphi}(x)\hat{\varphi}(x')dxdx' \tag{25}$$

in which the quadratic and the quartic parts describe noninteracting particles and their interaction, respectively.

It is sometimes helpful to think of $\hat{\varphi}(x)$ as a "quantized wavefunction." In the field operator representation, the many body problem starts looking very much like a single particle problem. Of course, this simplicity is only apparent, since we still have a quartic term in the Hamiltonian, expressing the interactions and leading to "nonlinear" dynamics.

Not just the Hamiltonian, but many other quantities also take a simple form in terms of the field operator. For example, particle density $n(x) = \sum_a \delta(x-x_a)$ becomes

$$\hat{n}(x) = \sum_{ij} \langle \varphi_i(x')|\delta(x-x')|\varphi_j(x')\rangle a_i^+ a_j = \hat{\varphi}^+(x)\hat{\varphi}(x) \tag{26}$$

due to $\int \bar{\varphi}_i(x')\delta(x-x')\varphi_j(x')dx' = \bar{\varphi}_i(x)\varphi_j(x)$. Similarly, the particle current operator is

$$\hat{j}(x) = \frac{\hbar}{2mi}\left(\varphi^+(x)\nabla_x\varphi(x) - \left(\nabla_x\varphi^+(x)\right)\varphi(x)\right) \tag{27}$$

The density (26) and current (26) obey continuity relation written as an operator equation $\partial_t\hat{n} + \nabla\hat{j} = 0$.