Second Quantization: Notes for PHYS5260, Spring 2019

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(Dated: March 6, 2019)
Before we get started, a point on notation – in these notes, we will usually set Planck’s constant $\hbar = 1$.

I. MANY-BODY QUANTUM MECHANICS AND FIRST QUANTIZATION

Our goal here is to introduce a formalism known as second quantization, which is extremely useful when dealing with interacting systems of many identical particles. The formalism is also commonly used even for non-interacting systems. We discussed systems of identical particles last semester; here we will review the basic facts about these systems that are needed to introduce second quantization.

Let’s start by supposing we have a system of $N$ spinless bosons or fermions with mass $m$. The particles have positions $\mathbf{r}_i$ and momenta $\mathbf{p}_i$ ($i = 1, \ldots, N$). We will see later how to add in spin without any difficulty. Let’s consider the following Hamiltonian:

$$H = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} + \sum_{i=1}^{N} U(\mathbf{r}_i) + \frac{1}{2} \sum_{i \neq j} V(\mathbf{r}_i - \mathbf{r}_j).$$  \hspace{1cm} (1)

This describes particles moving in a background potential $U(\mathbf{r})$, and interacting via a potential $V(\mathbf{r})$. In the last sum, $i$ and $j$ range from 1 to $N$, but terms where $i = j$ are excluded as they are self-interactions that we don’t want to consider (even if we do include them, they just give a constant shift of the energy, although it might be an infinite constant).

The wavefunction satisfies the following symmetry property familiar from last semester:

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = \zeta \Psi(\mathbf{r}_2, \mathbf{r}_1, \ldots, \mathbf{r}_N),$$  \hspace{1cm} (2)

where

$$\zeta = \begin{cases} 1, & \text{bosons} \\ -1, & \text{fermions} \end{cases}.$$  \hspace{1cm} (3)

This is true for any exchange of two position coordinates $\mathbf{r}_i, \mathbf{r}_j$, not just the first two. Moreover, this symmetry property holds in any basis – so it also holds if we work in the momentum basis and consider a wavefunction $\Psi(\mathbf{p}_1, \ldots, \mathbf{p}_N)$.

In bra-ket notation, we would write the $N$-particle state as a ket $|\Psi\rangle$, and the wavefunction is given by

$$\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) = d\langle \mathbf{r}_1, \ldots, \mathbf{r}_N | \Psi \rangle,$$  \hspace{1cm} (4)
where
\[ |r_1, \ldots, r_N \rangle_d = |r_1 \rangle \otimes \cdots \otimes |r_N \rangle. \] (5)
is an unphysical state that lives in the distinguishable-particle Hilbert space. Remember that we defined the identical particle Hilbert space to be a subspace of an unphysical distinguishable-particle Hilbert space, where all states in the subspace are eigenstates of permutation operators, with eigenvalue +1 (−1) for a permutation swapping two particles in the case of bosons (fermions). Here, we put the subscript \( d \) on this state to indicate that it’s a distinguishable-particle state, because later on we will write similar-looking expressions but for states that live in the physical Hilbert space.

The formalism above is sometimes referred to as “first quantization.” It’s usually the setting in which we first learn quantum mechanics, and the setting we have used so far to study quantum mechanics in this course. However, it often turns out that first quantization is extremely cumbersome for dealing with many-body problems (though there are important exceptions). This is connected to the fact that the first-quantized formalism forces us to keep track of unphysical information. We know that, for identical particles, it makes no sense to ask “what is particle number 1 doing?” But the first-quantized wavefunction is expressed in terms of the coordinates of particle 1, particle 2, and so on. “Second quantization” is a different formalism that doesn’t keep track of this unphysical information, and is usually much more convenient for calculations. It can be derived from first quantization and it is an entirely equivalent formulation of the same quantum mechanics problem. Our approach here will not be to present derivations, but to explain what the formalism means and how to use it. If you are interested, it is derived in a number of books, my favorite is *Quantum Many-Particle Systems* by Negele and Orland.

II. SLATER DETERMINANTS AND PERMANENTS

Before we actually introduce second quantization, we’ll stick with first quantization a bit longer and introduce a particularly simple class of wavefunctions. For bosons these are called “permanents,” and for fermions they are called Slater determinants. These wavefunctions are important to make contact with the second-quantized formalism. They are also important because the ground state wavefunction of non-interacting bosons/fermions is a permanent/Slater determinant. Finally, it can be shown that any \( N \)-boson (\( N \)-fermion)
wavefunction can be written as a linear combination of permanents (Slater determinants). So these wavefunctions form a basis for the full many-body Hilbert space of \( N \)-particles.

Start by considering just a single particle, and let \( \phi_\alpha(r) \) be an orthonormal basis of single particle wavefunctions. So we are saying that \( \alpha \) labels the states of some orthonormal basis. It could, for example, be the energy eigenstates of a single-particle Hamiltonian – but it doesn’t have to be, and could be some other basis.

Let’s write down the permanent/Slater determinant for just two particles, and then generalize it. The basic idea in constructing these states is to “fill up” the single-particle basis states. So let’s suppose that we put one particle in state \( \alpha_1 \) and one particle in state \( \alpha_2 \). If we have bosons, the permanent wavefunction obtained by filling these two states is

\[
\Psi_P(r_1, r_2) = \frac{1}{\sqrt{2}} \left[ \phi_{\alpha_1}(r_1) \phi_{\alpha_2}(r_2) + \phi_{\alpha_1}(r_2) \phi_{\alpha_2}(r_1) \right].
\] (6)

For fermions, the Slater determinant obtained by filling these two states is

\[
\Psi_{SD}(r_1, r_2) = \frac{1}{\sqrt{2}} \left[ \phi_{\alpha_1}(r_1) \phi_{\alpha_2}(r_2) - \phi_{\alpha_1}(r_2) \phi_{\alpha_2}(r_1) \right].
\] (7)

One nice way to think about these wavefunctions is that we start with the state \( \phi_{\alpha_1}(r_1) \phi_{\alpha_2}(r_2) \) – that is, we fill one particle in state \( \alpha_1 \), and another particle in state \( \alpha_2 \). This wavefunction is illegal, because it doesn’t satisfy our symmetry property, but we can fix that. To make a permanent out of it, we symmetrize the particle coordinates and obtain Eq. (6). Or, if we have fermions, to make a Slater determinant we start with the same wavefunction but we antisymmetrize to obtain Eq. (7). The factor of \( 1/\sqrt{2} \) there by convention, but these states are not normalized in general – \( \Psi_{SD} \) is always normalized, and \( \Psi_P \) is normalized unless \( \alpha_1 = \alpha_2 \). Also note that \( \Psi_{SD} \) vanishes if \( \alpha_1 = \alpha_2 \) – this is the Pauli exclusion principle at work, preventing us from filling the same state with two fermions.

To write down a permanent/Slater determinant for \( N \) particles, start by imagining we fill up the states \( \alpha_1, \alpha_2, \ldots, \alpha_N \). This corresponds to the (illegal) wavefunction \( \phi_{\alpha_1}(r_1) \phi_{\alpha_2}(r_2) \cdots \phi_{\alpha_N}(r_N) \). The expression for the permanent/Slater determinant obtained from this wavefunction is:

\[
\Psi_{\alpha_1, \ldots, \alpha_N}(r_1, \ldots, r_N) = \frac{1}{\sqrt{N!}} \sum_P \zeta^{|P|} \phi_{\alpha_1}(r_{P(1)}) \phi_{\alpha_2}(r_{P(2)}) \cdots \phi_{\alpha_N}(r_{P(N)}). \] (8)

Here \( \zeta = 1 \) for bosons and \( \zeta = -1 \) for fermions. The sum is over all permutations \( P \) of the integers \( i = 1, \ldots, N \) – a permutation \( P \) is just a rearrangement of the ordered list
of numbers \((1,\ldots,N)\), and we are summing over all such rearrangements (there are \(N!\) of them). More formally, a permutation is a function \(P(i)\), so that \((P(1), P(2), \ldots, P(N))\) gives the corresponding rearrangement. Any permutation can be obtained by starting with \((1, \ldots, N)\) and repeatedly exchanging pairs of numbers. If this is done an even number of times, the permutation is called even, and it’s done an odd number of times, the permutation is called odd. We define \(|P| = 0\) for even permutations and \(|P| = 1\) for odd permutations. We define the ket corresponding to this state by writing

\[
d\langle r_1, \ldots, r_N | \alpha_1, \ldots, \alpha_N \rangle = \Psi_{\alpha_1,\ldots,\alpha_N}(r_1, \ldots, r_N). \
\]

(9)

It can be shown (exercise) that

\[
|\alpha_1, \alpha_2, \ldots, \alpha_N \rangle = \zeta |\alpha_2, \alpha_1, \ldots, \alpha_N \rangle. \
\]

(10)

So, for fermions, the order of the \(\alpha_i\) matters in writing down this ket.

With the notation explained, we can now make some statements about the wavefunctions Eq. (8). For bosons, where \(\zeta = 1\), we simply sum over all permutations with positive coefficients (since always \(\zeta|P| = 1\)). On the other hand, for fermions, the odd permutations come with a minus sign, while the even permutations come with a plus sign – it can be shown that this gives the needed antisymmetry property (exercise). The permanent wavefunctions are not normalized if any of the \(\alpha_i\) are the same, while the Slater determinant wavefunctions are always normalized.

III. NON-INTERACTING BOSE AND FERMI GAS – FIRST QUANTIZATION

Let’s recall some basic facts about non-interacting gases of bosons and fermions, and write down the ground state wavefunctions. The Hamiltonian is

\[
H = \sum_{i=1}^{N} \frac{p_i^2}{2m}. \
\]

(11)

We consider the system in a cubic box of volume \(V = L^3\) with periodic boundary conditions. In this case the single-particle energy eigenstates are plane waves given by

\[
\psi_k(r) = \frac{1}{\sqrt{V}} e^{ik\cdot r}. \
\]

(12)
This state has momentum $\mathbf{p} = \mathbf{k}$ (remember $\hbar = 1$), and energy $\epsilon_k = k^2/2m$. Owing to the finite volume, the wavevector takes on the discrete values

$$k = \frac{2\pi}{L} (n_x x + n_y y + n_z z), \quad (13)$$

where $n_x, n_y, n_z$ are arbitrary integers. The wavevector $k$ labels the single-particle states and plays the same role as the abstract index $\alpha$ above.

For bosons, we know that the ground state is obtained by putting all the particles in to the lowest-energy state, which is that with $k = 0$. So the many-particle ground state wavefunction for bosons is

$$\Psi_0(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \psi_0(\mathbf{r}_1) \psi_0(\mathbf{r}_2) \cdots \psi_0(\mathbf{r}_N). \quad (14)$$

This is indeed symmetric under exchanges of $\mathbf{r}_i$ and $\mathbf{r}_j$, and is proportional to the permanent wavefunction obtained when all the $\alpha_i$ are the same, and are equal to $k = 0$.

For fermions, we know that we obtain the ground state by filling up the $N$ lowest-energy states. Suppose that these states have wavevectors $k_1, k_2, \ldots, k_N$, where no two of these wavevectors are the same. Then the many-fermion ground state is just the Slater determinant $\Psi_{k_1, k_2, \ldots, k_N}(\mathbf{r}_1, \ldots, \mathbf{r}_N)$.

**IV. CREATION AND ANNIHILATION OPERATORS**

Here we actually start developing the second quantization formalism.

Let’s return to the notation of Sec. II. The first thing we do in second quantization is extend the Hilbert space to allow for all possible numbers of particles, not just $N$ particles. Of course we don’t need to do this, because the Hamiltonian conserves the number of particles, and all its matrix elements connecting states with, say $N$ particles to states with $N+1$ particles will be zero. Moreover, this is a bit weird, because if we have a closed system it is clearly unphysical to have a state which is a linear superposition of different particle number states – this would violate conservation of particle number. So this extension of the Hilbert space is primarily just a formal trick, but it will be useful. In the language of the states introduced above, we consider a Hilbert space which includes the states $|\alpha_1\rangle$ (one particle), $|\alpha_1, \alpha_2\rangle$ (two particles), $|\alpha_1, \alpha_2, \alpha_3\rangle$ (three particles), and so on.

The basic object of second quantization is the creation operator $a_{\alpha}^\dagger$. Acting on some state in our extended Hilbert space, this operator adds a particle to the system, in the state $\alpha$. 
So, if $|\psi_N\rangle$ is a state with $N$-particles, then $a_\alpha^\dagger |\psi_N\rangle$ is a state with $N + 1$ particles. The Hermitian conjugate of the creation operator is $a_\alpha = (a_\alpha^\dagger)^\dagger$, and is called an annihilation operator. To see why, suppose $|\psi_{N+1}\rangle$ is a state with $N + 1$ particles, and $\langle \psi_{N+1} | a_\alpha^\dagger |\psi_N\rangle \neq 0$. Then we have

$$\langle \psi_{N+1} | a_\alpha^\dagger |\psi_N\rangle^* = \langle \psi_N | a_\alpha |\psi_{N+1}\rangle \neq 0.$$  \hspace{1cm} (15)

For this to be nonzero, it must be the case that $a_\alpha |\psi_{N+1}\rangle$ is a state with $N$ particles, implying that acting with $a_\alpha$ removes (or annihilates) a particle from the system. Moreover, it will turn out that $a_\alpha$ removes a particle from the state $\alpha$ (if there isn’t already a particle occupying that state, then we will see that $a_\alpha |\psi\rangle = 0$).

We still have to fully specify the properties of the creation and annihilation operators. For bosons, they satisfy commutation relations (recall $[A, B] \equiv AB - BA$):

$$[a_\alpha, a_\beta^\dagger] = \delta_{\alpha\beta}$$  \hspace{1cm} (16)

$$[a_\alpha, a_\beta] = [a_\alpha^\dagger, a_\beta^\dagger] = 0.$$  \hspace{1cm} (17)

Even if you haven’t studied second quantization, these commutation relations are familiar – except for the index $\alpha$, they are identical to the commutation relations for the raising and lowering operators used in the solution of the quantum harmonic oscillator. Indeed, a problem of many bosons is mathematically identical to a problem of many quantum harmonic oscillators, one for each basis state $\alpha$. We’ll see below that this analogy goes quite far. On the other hand, for fermions, these operators satisfy anti-commutation relations. We define the anti-commutator $\{A, B\} = AB + BA$, and we have

$$\{a_\alpha, a_\beta^\dagger\} = \delta_{\alpha\beta}$$  \hspace{1cm} (18)

$$\{a_\alpha, a_\beta\} = \{a_\alpha^\dagger, a_\beta^\dagger\} = 0.$$  \hspace{1cm} (19)

For fermions, there is not an analogy like that between bosons and harmonic oscillators.

The next thing we need to do is to specify what the Slater determinant / permanent states are in terms of the creation and annihilation operators. First we define a special state $|0\rangle$ called the vacuum state – this is the unique state containing no particles. Any annihilation operator acting on the vacuum state is defined to give zero:

$$a_\alpha |0\rangle = 0.$$  \hspace{1cm} (20)
This makes sense – you can’t remove the particle and get a physical state, if the particle isn’t there in the first place. We can now write down the expression for our permanent / Slater determinant states:

\[ |\alpha_1, \alpha_2, \ldots, \alpha_N\rangle = a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \cdots a_{\alpha_N}^\dagger |0\rangle. \] (21)

It can be shown that Eq. (10) follows directly from the commutation / anti-commutation relations. This is a very intuitive way to represent the state \(|\alpha_1, \ldots, \alpha_N\rangle\) – we start with the vacuum, and then fill up particles in the desired single-particle states.

All the properties of these states follow from the commutation / anti-commutation relations. For example, let’s compute

\[ \langle \alpha_1|\alpha_2 \rangle = \langle 0| a_{\alpha_1} a_{\alpha_2}^\dagger |0\rangle \] (22)

\[ = \langle 0| \zeta a_{\alpha_2}^\dagger a_{\alpha_1} + \delta_{\alpha_1, \alpha_2} |0\rangle \] (23)

\[ = \delta_{\alpha_1, \alpha_2}. \] (24)

The crucial step is the second line, where we used the commutation / anti-commutation relations – the first term in the second line vanishes because \(a_{\alpha_1}|0\rangle = 0\). This is just a restatement of the fact that our single-particle basis is orthonormal. Let’s now consider the normalization of a 2-particle state with \(\alpha_1 \neq \alpha_2\):

\[ \langle \alpha_1, \alpha_2|\alpha_1, \alpha_2 \rangle = \langle 0| a_{\alpha_2} a_{\alpha_1} a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger |0\rangle \] (25)

\[ = \langle 0| a_{\alpha_2} a_{\alpha_1}^\dagger |0\rangle + \zeta \langle 0| a_{\alpha_2} a_{\alpha_1}^\dagger a_{\alpha_1} a_{\alpha_2}^\dagger |0\rangle \] (26)

\[ = \langle 0| a_{\alpha_2} a_{\alpha_1}^\dagger |0\rangle + \zeta^2 \langle 0| a_{\alpha_2} a_{\alpha_1}^\dagger a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger |0\rangle \] (27)

\[ = \langle 0| a_{\alpha_2} a_{\alpha_2}^\dagger |0\rangle = 1. \] (28)

(Going from the 2nd to the 3rd line is where we used the fact that \(\alpha_1 \neq \alpha_2\).) So this state is normalized. It’s not too hard to show that the state \(|\alpha_1, \ldots, \alpha_N\rangle\) is also normalized, provided that the \(\alpha_i\) are all different – of course, this is automatically true for fermions, so our Slater determinant states are normalized. However, for bosons, if some of the \(\alpha_i\) are the same, then the states are not normalized. For example, I leave it as an exercise to show that \(\langle \alpha_1, \alpha_1|\alpha_1, \alpha_1 \rangle = 2\).
V. NUMBER OPERATORS

One of the basic physical questions we can ask about a many-body system is “how many particles are occupying the single particle state $\alpha$?” Since we are dealing with a quantum problem, we expect that the number of particles in state $\alpha$ is represented by a Hermitian operator $\hat{n}_\alpha$ – this is called a number operator (or, sometimes, an occupation number operator). This is a very useful object. For example, suppose that we are dealing with a non-interacting problem, and suppose that $\alpha$ labels energy eigenstates for the single-particle Hamiltonian. Then each particle in state $\alpha$ has an energy $\epsilon_\alpha$, and the total energy of the particles in state $\alpha$ is given by the operator $\epsilon_\alpha \hat{n}_\alpha$. So, the total energy of all particles in the system is

$$H = \sum_\alpha \epsilon_\alpha \hat{n}_\alpha. \quad (29)$$

We have thus constructed the Hamiltonian of a non-interacting system in terms of occupation number operators. We shall see soon that other important observables (for example, momentum) can also be expressed in this way. One important example to mention now is that the operator for the total number of particles is

$$\hat{N} = \sum_\alpha \hat{n}_\alpha. \quad (30)$$

This expression is just saying that the total number of particles is given by adding up all particles in all states.

In order to connect with the second quantization formalism we have been developing, we need to find an expression for $\hat{n}_\alpha$ in terms of creation and annihilation operators. We will simply guess the answer, and then we will check that it has the right behavior. This is our guess:

$$\hat{n}_\alpha = a_\alpha^\dagger a_\alpha. \quad (31)$$

Before we check mathematically, is this a reasonable guess? Well, if there are no particles occupying state $\alpha$, then $\hat{n}_\alpha$ will give zero, since $a_\alpha$ to give zero acting on the wavefunction. More generally, what this operator does is to remove a particle from state $\alpha$ and then put it back. If there is more than one particle in state $\alpha$, what we hope is essentially that this operator can do this process in more than one way, so that it counts the number of particles.
To proceed, it will be very useful to note that the following commutation relations hold:

\[
\begin{align*}
[\hat{n}_\alpha, a^\dagger_\beta] &= a^\dagger_\alpha \delta_{\alpha\beta} \\
[\hat{n}_\alpha, a_\beta] &= -a_\alpha \delta_{\alpha\beta}.
\end{align*}
\]

(32) (33)

These can be proven using the commutation / anti-commutation relations for the creation and annihilation operators, with just some straightforward algebra. Also, the second line above follows upon taking the Hermitian conjugate of both sides of the first line.

First, let’s consider states with no particles occupying state \(\alpha\) – formally we consider the state \(|\beta_1, \ldots, \beta_N\rangle\), where \(\beta_i \neq \alpha\) for \(i = 1, \ldots, N\). We have

\[
\hat{n}_\alpha |\beta_1, \ldots, \beta_N\rangle = a^\dagger_\alpha a_\alpha a^\dagger_\beta_1 \cdots a^\dagger_\beta_N |0\rangle
\]

(34)

\[
= a^\dagger_\beta_1 \cdots a^\dagger_\beta_N a^\dagger_\alpha a_\alpha |0\rangle = 0.
\]

(35)

To get from the second to third line above, we used the fact that \([\hat{n}_\alpha, a^\dagger_\beta] = 0\), so we can bring \(\hat{n}_\alpha\) all the way through to the right.

Next, let’s consider a state with a single particle in state \(\alpha\). Let’s suppose that \(\beta_j = \alpha\), and all the other \(\beta_i\) are different from \(\alpha\). Then we have

\[
\hat{n}_\alpha |\beta_1, \ldots, \beta_N\rangle = \hat{n}_\alpha a^\dagger_\beta_1 \cdots a^\dagger_\beta_N |0\rangle
\]

(36)

\[
= a^\dagger_\beta_1 \cdots a^\dagger_\beta_j-1 [\hat{n}_\alpha a^\dagger_\beta_j] a^\dagger_\beta_{j+1} \cdots a^\dagger_\beta_N |0\rangle
\]

(37)

Using the commutator above, the expression in square brackets becomes

\[
\hat{n}_\alpha a^\dagger_\beta_j = a^\dagger_\beta_j \hat{n}_\alpha + a^\dagger_\beta_j,
\]

(38)

and we have

\[
\hat{n}_\alpha |\beta_1, \ldots, \beta_N\rangle = a^\dagger_\beta_1 \cdots a^\dagger_{\beta_{j-1}} [a^\dagger_{\beta_j} \hat{n}_\alpha + a^\dagger_{\beta_j}] a^\dagger_{\beta_{j+1}} \cdots a^\dagger_\beta_N |0\rangle
\]

(39)

\[
= |\beta_1, \ldots, \beta_N\rangle.
\]

(40)

The last equality follows because the first term in the square brackets gives zero – \(\hat{n}_\alpha\) can be brought through all the way to the right as before. The second term in the square brackets just gives the state we started with again, namely \(|\beta_1, \ldots, \beta_N\rangle\).

If we only care about fermions, then at this point we are done, because there can only be one particle in each state – so for fermions we’ve already shown that \(\hat{n}_\alpha\) is indeed the
operator we want. But what about for bosons, in the case that we have multiple particles in a single state? If we consider the case where we have just two particles in a state then it is easy to see how the more general case goes. To make things simpler, let’s consider a state with only two particles in the state \( \alpha \), and no other particles – we’ve already seen above that the other particles don’t really matter, since their creation operators just commute with \( \hat{n}_\alpha \).

So we consider the following expression:

\[
\hat{n}_\alpha |\alpha,\alpha\rangle = \hat{n}_\alpha a_\alpha^\dagger a_\alpha^\dagger |0\rangle = \left[ a_\alpha^\dagger + a_\alpha^\dagger \hat{n}_\alpha \right] a_\alpha^\dagger |0\rangle = a_\alpha^\dagger a_\alpha^\dagger |0\rangle = |\alpha,\alpha\rangle + a_\alpha^\dagger [a_\alpha^\dagger + a_\alpha^\dagger \hat{n}_\alpha ] |0\rangle = |\alpha,\alpha\rangle + a_\alpha^\dagger a_\alpha^\dagger |0\rangle = 2 |\alpha,\alpha\rangle.
\]

So, indeed, this operator correctly counts the two particles in state \( \alpha \). Basically what happened here is that each time \( \hat{n}_\alpha \) “hit” one of the \( a_\alpha^\dagger \), it added an extra term which is just the original state – that’s why it counts the number of particles.

### VI. BASIC PROPERTIES OF NON-INTERACTING HAMILTONIAN

Let’s make a few general statements about the non-interacting Hamiltonian

\[
H = \sum_\alpha \epsilon_\alpha \hat{n}_\alpha.
\]

First, in general, this Hamiltonian has a very large number (in many cases infinite) of constants of the motion. That’s because \([H, \hat{n}_\alpha] = 0\), so the number of particles in any single-particle state \( \alpha \) is a constant of the motion. This why we can construct eigenstates of the non-interacting many body system so easily: we just specify the number of particles occupying each single-particle eigenstate, and we have a many-body eigenstate. The presence of so many constants of the motion is a very special feature of non-interacting problems, and is usually (except in very special cases) not true in the presence of interactions – usually there are just a few constants of the motion, dictated by the symmetries of the system.

Now, let’s understand the many-body ground state, in the cases of \( N \) bosons and \( N \) fermions. First, suppose the single-particle energies are ordered:

\[
\epsilon_1 \leq \epsilon_2 \leq \cdots \leq \epsilon_N \leq \cdots.
\]
For bosons, we put all $N$ particles in the lowest state, and the ground state is

$$|\psi_{gs}^{\text{bosons}}\rangle = \frac{1}{\sqrt{N!}}(a_1^\dagger)^N|0\rangle.$$  \hspace{1cm} (48)

I leave it as an exercise to show that this is the correct normalization factor.

For fermions, we fill the lowest $N$ states, and the ground state is

$$|\psi_{gs}^{\text{fermions}}\rangle = a_1^\dagger a_2^\dagger \cdots a_N^\dagger |0\rangle.$$  \hspace{1cm} (49)

VII. NON-INTERACTING BOSE AND FERMI GAS – SECOND QUANTIZATION

Let’s return to the non-interacting Bose and Fermi gases, but now using second quantization. The single particle eigenstates are labeled by the momentum $\mathbf{k}$. So we can use the non-interacting Hamiltonian above, but with the following changes in notation:

$$\alpha \rightarrow \mathbf{k}$$  \hspace{1cm} (50)

$$a_\alpha \rightarrow \psi(\mathbf{k})$$  \hspace{1cm} (51)

$$a_\alpha^\dagger \rightarrow \psi^\dagger(\mathbf{k})$$  \hspace{1cm} (52)

$$\epsilon_\alpha \rightarrow \epsilon_\mathbf{k} = \frac{k^2}{2m}.$$  \hspace{1cm} (53)

So the Hamiltonian is

$$H = \sum_\mathbf{k} \epsilon_\mathbf{k} \psi^\dagger(\mathbf{k})\psi(\mathbf{k}),$$  \hspace{1cm} (54)

where $\psi(\mathbf{k})$ annihilates a particle with momentum $\mathbf{k}$. If we’re dealing with bosons, then $[\psi(\mathbf{k}), \psi^\dagger(\mathbf{k}')] = \delta_{\mathbf{k},\mathbf{k}'}$, or, for fermions $\{\psi(\mathbf{k}), \psi^\dagger(\mathbf{k}')\} = \delta_{\mathbf{k},\mathbf{k}'}$. The operator

$$\hat{n}(\mathbf{k}) = \psi^\dagger(\mathbf{k})\psi(\mathbf{k})$$  \hspace{1cm} (55)

is the number operator counting particles with the momentum $\mathbf{k}$. We can follow the discussion above to write down the ground state wavefunction, for both boson and fermion cases.

An important physical question we can ask about a boson or fermion systems is “what is the particle density at a given position $\mathbf{r}$?” Basically, what we need is a density operator $\hat{n}(\mathbf{r})$, which is like a number operator in position space – so far we only have the number
operator in momentum space. In order to construct the density operator, we need to construct position-space creation and annihilation operators. If these are written $\psi^\dagger(r)$ and $\psi(r)$, respectively, then we can guess that

$$\hat{n}(r) = \psi^\dagger(r)\psi(r).$$

(56)

This is a reasonable guess because it destroys a particle at $r$ and then puts it back again -- just like our number operator. However it has to be a little bit different, because $\hat{n}(r)$ should have units of inverse volume, while our number operator was dimensionless.

We can construct $\psi^\dagger(r)$ by returning to single-particle quantum mechanics. First, note that the single-particle momentum state $|k\rangle$ can be expressed as

$$|k\rangle = \psi^\dagger(k)|0\rangle.$$ 

(57)

Because we’re working in a box, the single-particle momentum states are normalized: $\langle k|k'\rangle = \delta_{kk'}$. We also define single-particle position eigenstates $|r\rangle$, satisfying the usual delta-function normalization $\langle r|r'\rangle = \delta(r - r')$. The single-particle wavefunctions are given by

$$\psi_k(r) = \langle r|k\rangle = \frac{1}{\sqrt{V}} e^{ik\cdot r},$$

(58)

and so we have

$$|k\rangle = \frac{1}{\sqrt{V}} \int d^3r e^{ik\cdot r}|r\rangle,$$

(59)

where the integral is taken over the volume of the box. There is also the inverse relation

$$|r\rangle = \frac{1}{\sqrt{V}} \sum_k e^{-ik\cdot r}|k\rangle.$$ 

(60)

We want the position space creation operator to satisfy

$$\psi^\dagger(r)|0\rangle = |r\rangle.$$ 

(61)

Looking at Eqs. (57, 59, 61), we define

$$\psi^\dagger(k) = \frac{1}{\sqrt{V}} \int d^3r e^{ik\cdot r}\psi^\dagger(r),$$

(62)

and we have the inverse relation (just the inverse Fourier transform),

$$\psi^\dagger(r) = \frac{1}{\sqrt{V}} \sum_k e^{-ik\cdot r}\psi^\dagger(k).$$

(63)
With this definition, we can check that the real-space creation and annihilation operators satisfy the anticommutation relations

$$\{ \psi(\mathbf{r}), \psi^\dagger(\mathbf{r}') \} = \delta(\mathbf{r} - \mathbf{r}') \tag{64}$$

So these operators are just like the creation / annihilation operators we’ve been discussing, with the difference that we replace the Kronecker delta by the Dirac delta function – this makes sense, since \( \mathbf{r} \) is a continuous variable, whereas before we were dealing with discrete variables.

We can now express the Hamiltonian in terms of the real-space creation / annihilation operators. I claim that the right answer is

$$H = \int d^3 \mathbf{r} \psi^\dagger(\mathbf{r}) \left[ -\frac{\nabla^2}{2m} \right] \psi(\mathbf{r}) \tag{65}$$

This can be checked by simply plugging in the expression for \( \psi(\mathbf{r}) \) in terms of \( \psi(\mathbf{k}) \) – after a bit of algebra it can be shown that one gets back the same Hamiltonian we started with in Eq. (54).

Now, let’s go back to the density operator \( \hat{n}(\mathbf{r}) = \psi^\dagger(\mathbf{r}) \psi(\mathbf{r}) \). How do we know our guess was correct? We can at least check it is consistent with things we already know. In the non-interacting Bose and Fermi gas, the density is uniform in space, so we expect

$$\langle \psi_{gs} | \hat{n}(\mathbf{r}) | \psi_{gs} \rangle = n = \frac{N}{V}. \tag{66}$$

Now, for both Bose and Fermi gases, the expectation value \( \langle \psi_{gs} | \psi^\dagger(\mathbf{k}) \psi(\mathbf{k}') | \psi_{gs} \rangle \) vanishes unless \( \mathbf{k} = \mathbf{k}' \) – this is because if you start with the ground state, remove a particle in state \( \mathbf{k}' \), and put it back in the different state \( \mathbf{k} \), you will get a new state, orthogonal to the ground state. Therefore we must have

$$\langle \psi_{gs} | \psi^\dagger(\mathbf{k}) \psi(\mathbf{k}') | \psi_{gs} \rangle = \delta_{kk'} \langle \psi_{gs} | \psi^\dagger(\mathbf{k}) \psi(\mathbf{k}) | \psi_{gs} \rangle \tag{67}$$
This implies
\[
\langle \psi_{gs} | \hat{n}(r) | \psi_{gs} \rangle = \frac{1}{V} \sum_k \langle \psi_{gs} | \psi(k) \rangle \langle \psi(k) | \psi_{gs} \rangle = \frac{1}{V} \langle \psi_{gs} | \hat{N} | \psi_{gs} \rangle \leq \frac{n}{V} = n,
\]
the desired result. The last equality follows from the fact that the ground state has a definite number of particles $N$.

**VIII. HAMILTONIAN FOR THE INTERACTING SYSTEM**

We now know enough to write down the Hamiltonian for the interacting system in second quantized form. The crucial point is that we can think about both the motion in the external potential $U(r)$, as well as the interaction potential term, in terms of the density operator. The form is
\[
H = \int d^3r \, \psi^\dagger(r) \left[ -\frac{\nabla^2}{2m} \right] \psi(r) + \int d^3r \, U(r) \hat{n}(r) + \frac{1}{2} \int d^3r \, d^3r' \, V(r - r') \hat{n}(r) \hat{n}(r')\leq \frac{1}{2} \int d^3r \, d^3r' \, V(r - r') \psi^\dagger(r) \psi(r) \psi^\dagger(r') \psi(r').
\]
One simple way to understand why this is true is to look at the last two terms of the first line, Eq. (72). We can plug in the first quantized form of the density operator,
\[
\hat{n}(r) = \sum_{i=1}^N \delta(r - r_i),
\]
and obtain the original first-quantized form of the Hamiltonian (for those two terms). The form Eq. (72) is also quite intuitive on its own – for example, we see that the interaction term can be understood as an interaction between particle density at different points in space.

**IX. ADDING SPIN**

Suppose we are interested in particles with spin. For concreteness, consider the case of fermions with spin-1/2 (namely, electrons). All we need to do to represent spin is to add an
extra index to the creation and annihilation operators:

$$\psi(r) \rightarrow \psi_\sigma(r) \quad \quad \quad (75)$$

$$\psi^\dagger(r) \rightarrow \psi^\dagger_\sigma(r). \quad \quad \quad (76)$$

The index $\sigma$ represents the projection of the spin along the $z$-axis and can can take on two values, $\sigma = \uparrow, \downarrow$. So $\psi^\dagger_\uparrow(r)$, for example, creates a spin-up electron at position $r$. We have the anticommutation relations

$$\{\psi_\sigma(r), \psi_{\sigma'}(r')\} = \{\psi^\dagger_\sigma(r), \psi^\dagger_{\sigma'}(r')\} = 0 \quad \quad \quad (77)$$

$$\{\psi_\sigma(r), \psi^\dagger_{\sigma'}(r')\} = \delta_{\sigma\sigma'}\delta(r-r'). \quad \quad \quad (78)$$

The density of spin-$\sigma$ electrons is $\hat{n}_\sigma(r) = \psi^\dagger_\sigma(r)\psi_\sigma(r)$, so the total density is $\hat{n}(r) = \sum_\sigma \hat{n}_\sigma(r)$.

Everything is essentially the same in the case of bosons with spin, except that we have, of course, commutation relations instead.