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1 Quantum Many-Body Systems

1.1 Introduction

In this chapter, we will give a brief overview of the mathematical formalism for describing quantum many-body systems. The types of systems that we will consider in this book will typically involve a large number of identical particles forming a composite quantum state. Such systems are best described using the formalism of second quantized operators. We describe how such operators can be defined starting from single-particle wavefunctions, and how they can be used to build up the full Hilbert space of the composite system. We also introduce the way that interactions between atoms can be described using the formalism, illustrating this with the example of s-wave scattering, a fundamental type of interaction between neutral atoms.

1.2 Second Quantization

First, consider the familiar case that you should already be well acquainted with from elementary quantum mechanics – a single particle trapped in a potential $V(\boldsymbol{x})$. The stationary states $\psi_k(\boldsymbol{x})$ are the solutions of the Schrodinger equation

$$H_0(\boldsymbol{x})\psi_k(\boldsymbol{x}) = E_k\psi_k(\boldsymbol{x}), \tag{1.1}$$

where

$$H_0(\boldsymbol{x}) = -\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{x}). \tag{1.2}$$

Here, m is the mass of the particle, E_k are the energies of the stationary states labeled n, and ∇^2 is the Laplacian. As quantum mechanics teaches us, the wavefunction tells us everything about the system that we would like to know (assuming we are working with pure states). This approach is fine if we want to describe a single particle, but what if we have many particles, all possibly interacting with each other as we have in a quantum many-body system?

One way is, of course, to simply increase the number of labels in the wavefunction and write this as $\psi(\boldsymbol{x}_1, \boldsymbol{x}_2, \dots, \boldsymbol{x}_N)$. Each particle has its own label; in this case, we have N particles. Then, if we are dealing with bosonic particles, we must impose that the wavefunction is symmetric under particle interchange, or antisymmetric in the case of fermions. While this approach is certainly one way and mathematically

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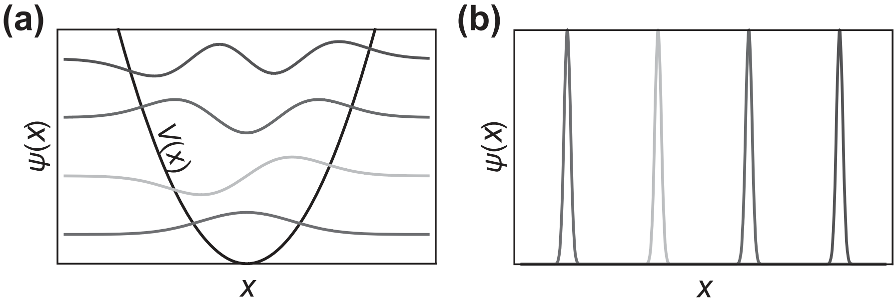

Fig. 1.1 Basis wavefunctions. (a) Wavefunctions $\psi_k(\boldsymbol{x})$ of a quantum harmonic oscillator. (b) Position-basis wavefunctions take the form of delta functions. Color version of this figure available at cambridge.org/quantumatomoptics.

equivalent, using the language of second quantized notation tends to be much more powerful and the method of choice in modern contexts.

In the second quantized approach, one defines an operator that creates or destroys a single particle with an implicit wavefunction. The most intuitive way to define this is in the position basis. The operator corresponding to the creation of one boson at the position $\boldsymbol{x}$ is written $a^\dagger(\boldsymbol{x})$, where the † is Hermitian conjugation. The reverse process of destroying the boson at the position $\boldsymbol{x}$ is written $a(\boldsymbol{x})$. These obey bosonic commutation relations according to

$$[a(\boldsymbol{x}), a^\dagger(\boldsymbol{x}')] = \delta(\boldsymbol{x} - \boldsymbol{x}') \tag{1.3}$$

and

$$[a(\boldsymbol{x}), a(\boldsymbol{x}')] = [a^\dagger(\boldsymbol{x}), a^\dagger(\boldsymbol{x}')] = 0. \tag{1.4}$$

For fermions, one can similarly define creation and destruction operators $c^\dagger(\boldsymbol{x})$ and $c(\boldsymbol{x})$, but this time obeying anticommutation relations

$$\{c(\boldsymbol{x}), c^\dagger(\boldsymbol{x}')\} = \delta(\boldsymbol{x} - \boldsymbol{x}') \tag{1.5}$$

and

$$\{c(\boldsymbol{x}), c(\boldsymbol{x}')\} = \{c^\dagger(\boldsymbol{x}), c^\dagger(\boldsymbol{x}')\} = 0. \tag{1.6}$$

The bosonic operator $a(\boldsymbol{x})$ (and also the fermion operator $c(\boldsymbol{x})$) is only one of an infinity of ways this can be defined. The reason for this is the same as why there are an infinity of ways of defining a basis. The position basis is just the most intuitive way of defining a basis, where the particle is located at the position $\boldsymbol{x}$. We could equally have used a Fourier basis or the complete set of states $\psi_k(\boldsymbol{x})$ (see Fig. 1.1). This can be written explicitly in the following way:

$$a_k = \int d\boldsymbol{x} \psi_k^*(\boldsymbol{x}) a(\boldsymbol{x}) \tag{1.7}$$

and

$$a_k^\dagger = \int d\boldsymbol{x} \psi_k(\boldsymbol{x}) a^\dagger(\boldsymbol{x}). \tag{1.8}$$

The very neat property of these newly defined operators is that they still have the same commutation relations of bosons that we are familiar with:

$$[a_k, a_l^\dagger] = \delta_{kl} \tag{1.9}$$

and

$$[a_k, a_l] = [a_k^\dagger, a_l^\dagger] = 0. \tag{1.10}$$

We see that, regardless of the basis, bosons always have the same properties. This is one of the reasons why the labels $\boldsymbol{x}$ or n, m are omitted and sometimes even fail to precisely say what the implicit wavefunction of the boson is. It is, however, worth remembering that there is always an implicit wavefunction when defining bosons.

Exercise 1.2.1 Verify (1.9) and (1.10).

Exercise 1.2.2 Show that the fermion version of (1.7),

$$c_k = \int d\boldsymbol{x} \psi_k^*(\boldsymbol{x}) c(\boldsymbol{x}), \tag{1.11}$$

satisfies fermion anticommutation relations

$$\begin{aligned} \{c_k, c_l^\dagger\} &= \delta_{kl}, \\ \{c_k, c_l\} &= \{c_k^\dagger, c_l^\dagger\} = 0. \end{aligned} \tag{1.12}$$

1.3 Fock States

We now have the right mathematical tools to write down a state involving any number of particles. Let's first start with the example that we began the discussion in the previous section – a single particle in a particular stationary state of the Schrodinger equation (1.1). Our starting point is the *vacuum* state, which has absolutely no particles in it at all and which is denoted $|0\rangle$. The vacuum state is defined as the state such that destroying a particle from it gives

$$a_k|0\rangle = 0. \tag{1.13}$$

Then, one particle with wavefunction $\psi_k(\boldsymbol{x})$ is written

$$\begin{aligned} |\psi_k\rangle &= a_k^\dagger|0\rangle \\ &= \int d\boldsymbol{x} \psi_k(\boldsymbol{x}) a^\dagger(\boldsymbol{x})|0\rangle \\ &= \int d\boldsymbol{x} \psi_k(\boldsymbol{x})|\boldsymbol{x}\rangle. \end{aligned} \tag{1.14}$$

In the second line above, we see how the wavefunction explicitly comes into the definition of the state, where we used (1.8). In the third line, we defined delta-function localized position eigenstates as

$$|\boldsymbol{x}\rangle = a^\dagger(\boldsymbol{x})|0\rangle. \tag{1.15}$$

We see that the states can be expanded according to any basis, in the usual way that quantum mechanics allows us to.

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Extending this to more than one particle in the way that you can probably already guess: For each particle in the state $\psi_k(\boldsymbol{x})$, we apply a creation operator $a_k^\dagger$. There is one small complication, which is how the normalization factors are defined. Suppose that there are n particles that occupy, say, the ground state. Since we are only talking about the ground state here, let's temporarily drop the k-label, which specifies the state, and write

$$a \equiv a_0. \tag{1.16}$$

Such a state with a particular number of atoms in a state is called a Fock (or number) state, which we would write as

$$|n\rangle = \frac{1}{\sqrt{\mathcal{N}_n}}(a^\dagger)^n|0\rangle. \tag{1.17}$$

Working out the normalization factor is an example of a very routine type of calculation when working with bosonic operators, so it is recommended if you haven't done it before. The essential steps can be done by repeatedly applying the commutation relations (1.9). Since $\langle n|n\rangle = 1$, the normalization factor must be

$$\mathcal{N}_n = \langle 0|\underbrace{aa\ldots a}_{n \text{ of these}}\underbrace{a^\dagger a^\dagger \ldots a^\dagger}_{n \text{ of these}}|0\rangle. \tag{1.18}$$

The aim is then to take advantage of (1.13) by commuting all the a's to hit the vacuum state ket on the right. Similarly, we can equally commute all the $a^\dagger$'s to the left to hit the vacuum state bra on the left and use the Hermitian conjugate of (1.13):

$$\langle 0|a_k^\dagger = 0. \tag{1.19}$$

For example, taking one of the a's all the way to the right gives

$$\mathcal{N}_n = n\langle 0|\underbrace{aa\ldots a}_{n-1 \text{ of these}}\ \underbrace{a^\dagger a^\dagger \ldots a^\dagger}_{n-1 \text{ of these}}|0\rangle. \tag{1.20}$$

Repeating this process, we find that $\mathcal{N}_n = n!$, and so the properly normalized Fock state is

$$|n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n|0\rangle. \tag{1.21}$$

From the commutation relations, it follows that the Fock states are orthonormal:

$$\langle n'|n\rangle = \delta_{nn'}. \tag{1.22}$$

Taking account of this normalization factor, we can use similar methods to work out that applying a creation or destruction operator gives numerical coefficients in addition to increasing or decreasing the number of bosons:

$$a|n\rangle = \sqrt{n}|n-1\rangle \tag{1.23}$$

and

$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle. \tag{1.24}$$

For fermions, it is simpler. We can perform the same logic for fermion operators. Define

$$c \equiv c_0, \tag{1.25}$$

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where we have a fermion in the ground state of the states as defined in (1.11). Then, the only Fock states we can define are the vacuum state $|0\rangle$, which satisfies

$$c_k|0\rangle = 0 \tag{1.26}$$

and the one-particle fermion Fock state,

$$|1\rangle_{\mathrm{f}} = c^\dagger|0\rangle, \tag{1.27}$$

where we have labeled the fermion Fock states by a subscript f. We could try to write down a fermion version of (1.21), but from (1.12) we would find that any state with $n \geq 2$ gives zero. This is the Pauli exclusion principle at work – no two fermions can occupy the same state. The creation and destruction operator then simply shifts between these two states:

$$\begin{aligned} c|1\rangle_{\mathrm{f}} &= |0\rangle, \\ c^\dagger|0\rangle &= |1\rangle_{\mathrm{f}}. \end{aligned} \tag{1.28}$$

Exercise 1.3.1 Work through the steps to verify (1.21) and (1.22).

Exercise 1.3.2 Verify (1.23) and (1.24).

Exercise 1.3.3 (a) Show explicitly that the only fermion Fock states are (1.27) and the vacuum. (b) Verify (1.28) using the fermion anticommutation relations (1.12).

1.4 Multimode Fock States

The Fock states that we have written in Section 1.3 are fine if all the particles are in the ground state. This might be the case at zero temperature, or indeed the situation in a Bose–Einstein condensate (BEC), as we will be discussing in later chapters. But more typically, particles will occupy all energy levels, so we need to take into account more than just the ground state. In this case, we can simply just do the same thing as above, for each of the eigenstates labeled by k. The generalized Fock state for bosons is then

$$|n_0, n_1, \ldots, n_k, \ldots\rangle = \prod_k \frac{(a_k^\dagger)^{n_k}}{\sqrt{n_k!}}|0\rangle, \tag{1.29}$$

and similarly, for fermions it is

$$|n_0, n_1, \ldots, n_k, \ldots\rangle_{\mathrm{f}} = \prod_k (c_k^\dagger)^{n_k}|0\rangle. \tag{1.30}$$

Notice we don't need the normalization factors for the fermions because we only ever have $n_k \in \{0, 1\}$.

For a single-particle state, obviously the energy of the state is simply given by the eigenvalue of the Schrodinger equation, E_k. If there are multiple particles involved, how do we write the total energy of a Fock state such as that written above? First, we should generalize the single-particle Schrodinger equation to a multiparticle one, which can be done by simply writing

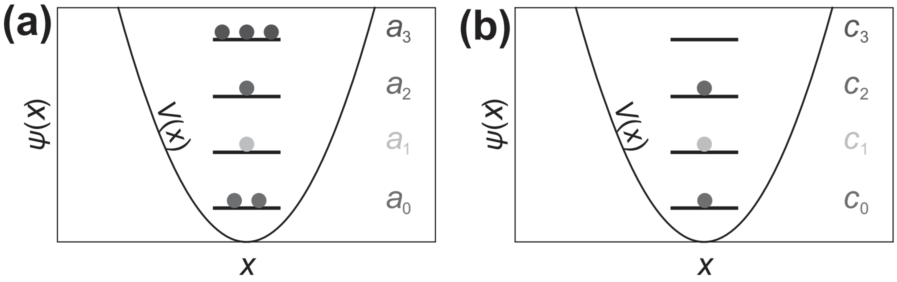

Fig. 1.2 Generalized Fock states for (a) bosons and (b) fermions. The case shown in (b) corresponds to the lowest energy configuration possible for three fermions (Fermi sea). The lowest energy configuration for bosons would correspond to all the particles in the ground state, hence (a) is an excited state for the multiparticle system. Color version of this figure available at cambridge.org/quantumatomoptics.

$$\mathcal{H}_0 = \int d\boldsymbol{x}\, a^\dagger(\boldsymbol{x}) H_0(\boldsymbol{x}) a(\boldsymbol{x}), \tag{1.31}$$

where $H_0(\boldsymbol{x})$ is given by (1.2). For fermions, this takes the same form, except that the bosonic operators are changed to fermionic ones. We now need the inverse relations of (1.7) and (1.8), given by

$$a(\boldsymbol{x}) = \sum_k \psi_k(\boldsymbol{x}) a_k \tag{1.32}$$

and

$$a^\dagger(\boldsymbol{x}) = \sum_k \psi_k^*(\boldsymbol{x}) a_k^\dagger. \tag{1.33}$$

Substituting this into (1.31), we obtain

$$\mathcal{H}_0 = \sum_k E_k N_k, \tag{1.34}$$

where

$$N_k \equiv a_k^\dagger a_k. \tag{1.35}$$

The operators (1.35) are *number operators* that have Fock states as their eigenstates:

$$N_k |n_0, n_1, \dots, n_k, \dots\rangle = n_k |n_0, n_1, \dots, n_k, \dots\rangle. \tag{1.36}$$

The multiparticle Fock state is thus an eigenstate of the Hamiltonian (1.34):

$$\mathcal{H}_0 |n_0, n_1, \dots, n_k, \dots\rangle = E_{\text{tot}} |n_0, n_1, \dots, n_k, \dots\rangle, \tag{1.37}$$

where the total energy is

$$E_{\text{tot}} = \sum_k E_k n_k. \tag{1.38}$$

We thus have the intuitive result that the total energy of the multiparticle Hamiltonian is the sum of the energies of each particle.

We can picture such Fock states as shown in Fig. 1.2. Each single-particle quantum level is labeled by an index k, and this is occupied by a number n_k, which tells us

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how many particles are occupied in that level. The total energy of the system is just the sum of the energies of the individual particles. For bosons, we are allowed to fill each level more than once, so the minimum energy is if all the particles are in the ground state. In this case, we would have

$$E_{\text{tot}} = NE_0, \qquad \text{(minimum, bosons)} \tag{1.39}$$

where N is the total number of bosons in the system. For fermions, each level cannot be filled more than once, so the minimum energy will be

$$E_{\text{tot}} = \sum_{k=0}^{N-1} E_k. \qquad \text{(minimum, fermions)} \tag{1.40}$$

Exercise 1.4.1 (a) Derive (1.32) by multiplying it by $\psi_k(\boldsymbol{x}')$ and summing (1.7) over k, using the completeness relation. (b) Derive (1.7) by multiplying it by $\psi_l^*(\boldsymbol{x})$ and integrating (1.32) over x.

Exercise 1.4.2 Verify that (1.34) starting from (1.31).

Exercise 1.4.3 Verify that (1.36) starting from the bosonic commutation relations.

1.5 Interactions

Up to this point, we have not included any interactions between the particles. The energy of the whole system was therefore determined entirely by the sum of the single-particle energies, as seen in (1.38). This is usually called the single-particle or *noninteracting limit*. More realistically, there are interactions present between the particles, due to the presence of some forces – naturally occurring or otherwise – that particles feel between each other. Suppose that the energy between two particles can be written as $U(\boldsymbol{x}, \boldsymbol{y})$, where the location of the first particle is $\boldsymbol{x}$ and the second is $\boldsymbol{y}$. The two-particle time-independent Schrodinger equation would be written in this case as

$$[H_0(\boldsymbol{x}) + H_0(\boldsymbol{y})]\,\psi(\boldsymbol{x}, \boldsymbol{y}) + U(\boldsymbol{x}, \boldsymbol{y})\psi(\boldsymbol{x}, \boldsymbol{y}) = E\psi(\boldsymbol{x}, \boldsymbol{y}). \tag{1.41}$$

The first term on the left-hand side is the single-particle Hamiltonian for the two-particle case, as given in (1.31). The second is the interaction term between the particles. There is only one term because the interaction corresponds to a pair of particles.

To generalize this to any number of particles, we write it in the form

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_I, \tag{1.42}$$

where the interaction Hamiltonian is

$$\begin{aligned} \mathcal{H}_I &= \frac{1}{2}\int dxdy a^\dagger(\boldsymbol{x}) a^\dagger(\boldsymbol{y}) U(\boldsymbol{x}, \boldsymbol{y}) a(\boldsymbol{y}) a(\boldsymbol{x}) \\ &= \frac{1}{2}\int dxdy U(\boldsymbol{x}, \boldsymbol{y}) n(\boldsymbol{x})(n(\boldsymbol{y}) - \delta(\boldsymbol{x} - \boldsymbol{y})), \end{aligned} \tag{1.43}$$

where we have used the commutation relations (1.3) and (1.4). Equation (1.43) has the simple interpretation of counting all the pairs of particles between the particles

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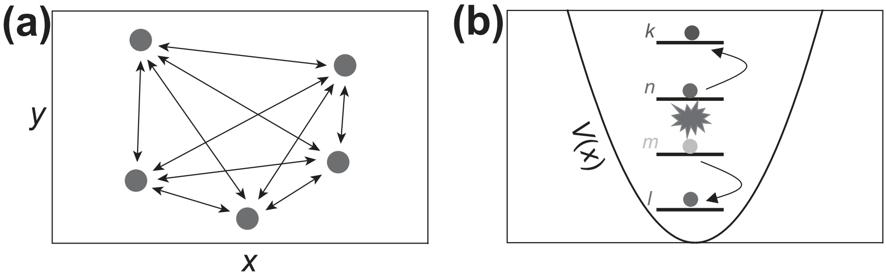

Fig. 1.3 Interactions between particles shown in (a) the position basis and (b) the single-particle eigenstate basis. In (a), for N particles there are $N(N-1)/2$ pairs of interactions. In (b), two particles initially in levels labeled by n and m scatter to other levels k and l. Color version of this figure available at cambridge.org/quantumatomoptics.

(see Fig. 1.3). For an N-particle system, there will be $N(N-1)/2$ pairs of interactions, which are potentially dependent on the positions of the particles $U(\boldsymbol{x}, \boldsymbol{y})$.

As was done in the previous sections, it is possible to write the interaction Hamiltonian $\mathcal{H}_I$ in terms of the eigenstates of the single-particle Hamiltonian. This is done by simply substituting (1.32) and (1.33) into (1.43). This gives

$$\mathcal{H}_I = \sum_{klmn} U_{klmn} a_k^\dagger a_l^\dagger a_m a_n, \tag{1.44}$$

where

$$U_{klmn} = \frac{1}{2} \int d\boldsymbol{x} d\boldsymbol{y} \psi_k^*(\boldsymbol{x}) \psi_l^*(\boldsymbol{y}) U(\boldsymbol{x}, \boldsymbol{y}) \psi_m(\boldsymbol{x}) \psi_n(\boldsymbol{y}). \tag{1.45}$$

In this basis, we find that the interactions are not diagonal. This is in contrast to (1.43), which consists entirely of number operators. This means that for particles that are spatially localized, as shown in Fig. 1.3(a), the interaction Hamiltonian $\mathcal{H}_I$ leaves the state unaffected. In the basis of the eigenstates of the single-particle Hamiltonian, the interaction Hamiltonian $\mathcal{H}_I$ can cause some scattering between states. Specifically, a particle in level n can feel the effect of another particle in level m, and both particles can be scattered to different levels k and l (see Fig. 1.3(b)).

In many cases, it is possible to simplify the form of the interaction. For example, typically we can safely say that the interaction only depends upon the relative position between the particles. This is a reasonable assumption in most experimental situations. The most common type of interaction for BECs is the s-wave interaction, which is a type of contact interaction,

$$U(\boldsymbol{x}, \boldsymbol{y}) = U_0 \delta(\boldsymbol{x} - \boldsymbol{y}), \tag{1.46}$$

where the interaction energy is

$$U_0 = \frac{4\pi\hbar^2 a_s}{m}. \tag{1.47}$$

Here, a_s is the scattering length, an experimentally measured quantity. In this case, the interaction matrix elements take the form (1.45):

$$g_{klmn} = \frac{2\pi\hbar^2 a_s}{m} \int d\boldsymbol{x} \psi_k^*(\boldsymbol{x}) \psi_l^*(\boldsymbol{x}) \psi_m(\boldsymbol{x}) \psi_n(\boldsymbol{x}). \tag{1.48}$$

Specifically, for the atoms in the ground state, the interaction is

$$g_{0000} = \frac{2\pi\hbar^2 a_s}{m} \int d\boldsymbol{x} |\psi_0(\boldsymbol{x})|^4. \tag{1.49}$$

As we will see in Chapter 2, in a BEC many of the atoms occupy the ground state, and this will be the dominant interaction energy.

For the general interaction (1.48), very often some of the matrix elements will be zero automatically. To see an example of this, consider the simple case where $V(\boldsymbol{x}) = 0$. In this case, the eigenstates are simply plane waves,

$$\psi_{\boldsymbol{k}}(\boldsymbol{x}) = \frac{e^{i\boldsymbol{k}\cdot\boldsymbol{x}}}{\sqrt{V}}, \tag{1.50}$$

where V is a suitable normalization factor. Substituting into (1.48), we find that

$$g_{\boldsymbol{klmn}} = \frac{2\pi\hbar^2 a_s}{mV} \delta(\boldsymbol{n} + \boldsymbol{m} - \boldsymbol{k} - \boldsymbol{l}). \tag{1.51}$$

In this case, the labels k, l, m, n have the interpretation of momentum, and the delta function is a statement of the conservation of momentum between the initial states and the final states. This occurs due to the translational invariance of the potential (1.46). While realistic potentials are not exactly $V(\boldsymbol{x}) = 0$, approximate relations for the conservation of momentum are obeyed in practice.

1.6 References and Further Reading

- Section 1.2: For further details about quantum mechanics and second quantization, see the textbooks [407, 9, 94].
- Sections 1.3, 1.4: Fock states and their algebra in a quantum optics setting are further described in [421, 168, 477].
- Section 1.5: Further details about interactions in Bose–Einstein condensates are provided in [369, 375, 497, 286, 169].