"Second quantization" (the occupation-number representation)

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1 Systems of identical particles

1.1 Particle statistics

In physics we are often interested in systems consisting of many identical particles. By "identical" we mean that all intrinsic physical properties of the particles are the same. For example, all electrons are identical since they have the same mass, electric charge, and spin ($S = 1/2$). In classical physics one can (at least in principle) follow the trajectories of individual particles, so identical particles are therefore distinguishable in classical physics. In quantum physics, however, identical particles which are in the same region of space can not be distinguished from each other. This puts certain constraints on the many-particle wavefunctions of such systems. If the wavefunction of a system of N identical particles is $\Psi(x_1, x_2, \ldots, x_N)$, where $x_i = (\boldsymbol{r}_i, s_i)$ denotes the position ($\boldsymbol{r}_i$) and spin (s_i) coordinates[1] of particle i, then the quantum indistinguishability implies that

$$|\Psi(x_1, \ldots, x_j, \ldots, x_k, \ldots, x_N)|^2 = |\Psi(x_1, \ldots, x_k, \ldots, x_j, \ldots, x_N)|^2 \tag{1}$$

i.e. the probability (density) is the same for two configurations that differ in the exchange of the coordinates of any two particles (particles j and k in the equation above). [Note that exchanging coordinates for particles with spin means exchanging both spatial and spin coordinates.] In 3 spatial dimensions this can be shown to lead to only two different possibilities

[1] For example, for electrons, which have spin $S = 1/2$, s_i has the possible values $\pm 1/2$ (the eigenvalues of the electron spin operator along some chosen axis).

under exchange of the coordinates of two particles:[2]

$$\Psi \to +\Psi, \quad \text{i.e. the wavefunction is } \textit{symmetric} \text{ under such exchange, or} \tag{2}$$

$$\Psi \to -\Psi, \quad \text{i.e. the wavefunction is } \textit{anti-symmetric}. \tag{3}$$

Particles with a symmetric wavefunction are called **bosons**, particles with an antisymmetric wavefunction are called **fermions**. Using relativistic quantum field theory, it can be shown that bosons have integer spin, and fermions have half-integer spin; this is called the spin-statistics theorem. (We will mostly focus on fermions in this course but will also discuss bosons.) The symmetry properties of the wavefunction has profound implications for the statistics of the particles, and lead to significant differences in the low-temperature behaviour of systems of bosons and fermions, which in the noninteracting case is described in terms of the Bose-Einstein and Fermi-Dirac distribution, respectively.

In this course our main example of fermions will be electrons, which are of great interest in condensed matter physics. Another class of systems that have received a lot of attention in recent years is dilute atomic gases. These consist of neutral atoms, which are composite objects that, under conditions when anything else than exchanging the coordinates of the atoms as a whole (i.e. all their constituent fermions) has a negligible probability amplitude, are effectively bosons or fermions: Atoms consisting of an even number of fermions (electrons + protons + neutrons) behave as bosons, while atoms consisting of an odd number of fermions behave as fermions.

1.2 Many-particle wavefunctions

Next, let us discuss how to construct many-particle wavefunctions. The main part of the job is to construct a *basis set* of many-particle wavefunctions having the appropriate symmetry (symmetric under particle exchange for bosonic particles, antisymmetric for fermionic

[2]For particles restricted to move in 2 spatial dimensions there also turns out to be more exotic possibilities than just bosons and fermions, namely so-called anyons, the simplest versions of which have statistics that are intermediate between bosons and fermions, in the following sense: exchanging two particles causes the wavefunction to change by a phase factor $e^{i\theta}$, where θ is called the statistics angle. Bosons and fermions correspond to the special cases $\theta = 0$ and $\theta = \pi$, respectively, while for intermediate θ the particles are called (abelian) anyons. Here we will not go into the derivation of these results, which were not conceived until the late 1970's in a seminal paper by Jon Magne Leinaas and Jan Myrheim. Note however that many textbooks simply argue, without further justification, that exchanging the particle coordinates twice should be equivalent to no exchange at all, so that if η is the phase factor for one exchange, two exchanges give $\eta^2 = 1$, which thus only gives the solutions $\eta = \pm 1$ corresponding to bosons and fermions. This approach turns out to be incorrect, the problem with it being that it views particle exchange to be merely the abstract mathematical operation of *permuting* coordinates in the wavefunction, while one really needs to consider *physically* exchanging the two particles by *moving* them in continuous paths around each other, and it is the topological properties of these paths (in the properly defined configuration space, which depends on the spatial dimension) that determine the statistics. [For an introduction to these ideas, see e.g. the review by G. S. Canright and S. M. Girvin, Science 247, 1197 (1990).] Also note that anyons are not theoretical abstractions; they are in fact known to exist in experimentally realized systems exhibiting the fractional quantum Hall effect, and research into systems having (quasi-)particles with possible fractional statistics (which is the generic name for particle statistics that's different from that of bosons and fermions) is a very hot topic in modern condensed matter physics. However, in these notes we will not consider such systems any further.

particles). An arbitrary many-particle wavefunction expanded in this basis will then automatically satisfy the appropriate symmetry.

We consider a system with Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{H}_I. \tag{4}$$

Here

$$\hat{H}_0 = \sum_{i=1}^{N} \hat{h}(x_i) \quad \text{where} \quad \hat{h}(x_i) = -\frac{\hbar^2}{2m}\nabla_i^2 + U(x_i). \tag{5}$$

Note that $\hat{H}_0$ is a sum of terms, each involving the coordinates of only one particle. $\hat{H}_0$ is thus called a single-particle operator and represents the noninteracting part of the Hamiltonian. The term $-(\hbar^2/2m)\nabla^2$ is the kinetic energy operator of a particle while U is a potential energy due to some "external" potential. On the other hand, $\hat{H}_I$ will be a sum of terms each involving the coordinates of more than one particle. It is thus called a many-particle operator and represents interactions between the particles. In this course we will limit ourselves to two-particle interactions, but in some systems (such as atomic gases) interactions involving more than two particles may also be important.

It is convenient to construct a basis set in which the basis many-particle wavefunctions are eigenfunctions of a single-particle operator. It is furthermore often convenient to take this single-particle operator to be $\hat{H}_0$, the noninteracting part of the Hamiltonian, so let us for concreteness do this in the following (but any other hermitian single-particle operator could have been used). So let us assume that we have found the eigenfunctions $\phi_\nu(x)$ and associated eigenvalues ϵ_ν for the single-particle problem defined by $\hat{h}$, i.e.

$$\hat{h}(x)\phi_\nu(x) = \epsilon_\nu \phi_\nu(x). \tag{6}$$

Here ν is a set of quantum numbers (assumed discrete in the following) which completely characterize the single-particle eigenstates ϕ_ν.[3] These states form an orthonormal and complete set for expanding single-particle wavefunctions. Orthonormality means

$$\int dx\ \phi_\nu^*(x)\phi_{\nu'}(x) = \delta_{\nu,\nu'} \tag{7}$$

and completeness means

$$\sum_\nu \phi_\nu^*(x)\phi_\nu(x') = \delta(x - x'), \tag{8}$$

where we introduced the notation[4]

$$\int dx \equiv \sum_s \int d^3r \quad \text{and } \delta(x - x') = \delta(\boldsymbol{r} - \boldsymbol{r}')\delta_{s,s'}. \tag{9}$$

[3]For example, if $\hat{H}_0$ describes free electrons, i.e. electrons not subject to any external potential, $\nu = (\boldsymbol{k}, \sigma)$ where $\boldsymbol{k}$ is a wavevector and $\sigma = \pm 1/2$ is the spin projection.

[4]Here $\delta(\boldsymbol{r})$ is the Dirac delta function, while $\delta_{a,b}$ (often written δ_{ab} for short) is the Kronecker delta function, defined for discrete arguments a, b as $\delta_{a,b} = 1$ if $a = b$ and 0 if $a \neq b$.

From these single-particle wavefunctions we can then construct many-particle wavefunctions, which are eigenfunctions of the noninteracting Hamiltonian H_0, and have the correct symmetry. For bosons the wavefunction must be symmetric and can be written on the form (the superscript S stands for "symmetric")

$$\Phi^{(S)}(x_1,\ldots,x_N) = \frac{1}{\sqrt{N!}\sqrt{\prod_\nu n_\nu!}} \sum_{P\in S_N} P\ \phi_{\nu_1}(x_1)\phi_{\nu_2}(x_2)\cdots\phi_{\nu_N}(x_N). \tag{10}$$

Here the sum is over all permutations P of the N coordinates $x_1,\ldots,x_N$. S_N is the set of all these permutations; there are $N!$ permutations in all. The prefactor has been chosen to make the state normalized to 1. The product $\prod_\nu n_\nu!$ (which means $\prod_\nu (n_\nu!)$ where ! indicates the factorial function, i.e. $m! = 1\cdot 2\cdot 3\cdots(m-1)\cdot m$) is over all states in the single-particle basis set; here n_ν is the number of bosons in the single-particle state ν. Note that for bosons there is no restriction in how many particles can be in the same single-particle state. Hence in this expression different indices ν_j can be identical. For example, if $\nu_3 = \nu_5$ (and all other indices are different from ν_3) the many-particle state would have two particles in the single-particle state ν_3, hence $n_{\nu_3} = 2$.

For fermions the wavefunction must be antisymmetric and can be written (the superscript A stands for "antisymmetric")

$$\Phi^{(A)}(x_1,\ldots,x_N) = \frac{1}{\sqrt{N!}} \sum_{P\in S_N} \mathrm{sgn}(P)\cdot P\ \phi_{\nu_1}(x_1)\phi_{\nu_2}(x_2)\cdots\phi_{\nu_N}(x_N). \tag{11}$$

Compared to the bosonic case, there are two differences: (1) The product over occupation numbers $n_\nu!$ in the prefactor is not there (this is because, as we will shortly see, for fermions n_ν can only be 0 or 1 (otherwise the wavefunction will vanish), in which case $n_\nu! = 1$ and thus this product doesn't have to be explicitly included), and (2) there is a factor $\mathrm{sgn}(P)$ inside the sum. This is the sign of the permutation P. A permutation has a *positive* (*negative*) sign if it can be arrived at by an *even* (*odd*) number of two-particle permutations (transpositions). For example, suppose we had 3 fermions. Let us consider the permutation $(123) \to (231)$. Any permutation can be written as a product of transpositions P_{jk}, each of which interchanges the numbers at position j and k. For example, we have $P_{13}(123) = (321)$ and $P_{12}(321) = (231)$. Hence we can write $(231) = P_{12}P_{13}(123)$. Thus this permutation can be written in terms of an even number of transpositions, and the sign of the permutation is therefore positive. Although the way to express a permutation in terms of transpositions is not unique, the evenness/oddness is unique, and hence the sign is also unique. In the example just considered, we could have written (check!) $(231) = P_{23}P_{13}P_{12}P_{23}(123)$, which involves four transpositions, again an even number.

The fermionic wavefunction in (11) can be written as a determinant (which in this context is often referred to as a *Slater* determinant):

$$\Phi^{(A)} = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_{\nu_1}(x_1) & \cdots & \phi_{\nu_1}(x_N) \\ \vdots & & \vdots \\ \phi_{\nu_N}(x_1) & \cdots & \phi_{\nu_N}(x_N) \end{vmatrix}. \tag{12}$$

Note that the determinant of a matrix vanishes if it contains identical rows and/or identical columns. Therefore the determinant (12) will vanish if $\nu_i = \nu_j$ for some $i \neq j$, i.e. it is not possible to put more than one fermion into a given single-particle state. The determinant will also vanish if $x_i = x_j$ for some $i \neq j$, i.e. it is not possible to bring two fermions with the same spin projection to the same point. These properties are known as the *Pauli exclusion principle*.

Given some collection of N (singly) occupied single-particle states, the fermionic many-particle wavefunction (12) constructed from them is defined only up to an overall sign. For example, consider a two-particle state, with single-particle states ν_1 and ν_2 occupied. Then we could define the wavefunction either as

$$\Phi^{(A1)} = \frac{1}{\sqrt{2}}(\phi_{\nu_1}(x_1)\phi_{\nu_2}(x_2) - \phi_{\nu_1}(x_2)\phi_{\nu_2}(x_1), \tag{13}$$

or as

$$\Phi^{(A2)} = \frac{1}{\sqrt{2}}(\phi_{\nu_2}(x_1)\phi_{\nu_1}(x_2) - \phi_{\nu_2}(x_2)\phi_{\nu_1}(x_1)) = -\Phi^{(A1)}. \tag{14}$$

In order to avoid this kind of sign ambiguity (which could lead to errors in some calculations if we are not sufficiently careful) we should define the overall sign for any such fermionic many-particle wavefunction in a unique way. To do this we first decide on an ordering (that we subsequently stick to) of the states ν_i in the complete set of single-particle states. Then, when constructing the many-particle wavefunction out of N such states we use that ordering in the determinant.

It is straightforward to check that the many-particle wavefunctions $\Phi^{(S/A)}$ constructed here are eigenfunctions of the non-interacting part $\hat{H}_0$ of the Hamiltonian, with eigenvalues given by $E = \sum_\nu \epsilon_\nu n_\nu$. The symmetric wavefunctions $\Phi^{(S)}$ (antisymmetric wavefunctions $\Phi^{(A)}$) form a complete orthonormal basis set for the bosonic (fermionic) problem), satisfying

$$\int d^N x \; \Phi_a^* \Phi_b = \delta_{a,b} \quad (\text{where } \int d^N x \equiv \int dx_1 dx_2 \ldots dx_N) \tag{15}$$

so that any many-particle wavefunction Ψ can be expanded in them:

$$\Psi(x_1, \ldots, x_N) = \sum_a f_a \Phi_a(x_1, \ldots, x_N), \tag{16}$$

where the f_a's are the expansion coefficients.

2 Second quantization (the occupation-number formalism)

The many-particle basis wavefunctions considered in the previous section [Eq. (10) for bosons, Eq. (11) or equivalently Eq. (12) for fermions] are rather cumbersome to work with in practice. Fortunately, there exists an alternative and equivalent formalism, called

"second quantization" or the occupation-number representation, that is much more convenient. In this formalism the essential information of many-body states is incorporated in a very succinct way. This essential information consists of (i) the occupation number for each single-particle state (for fermions these numbers can only be 0 or 1), and (ii) the symmetry/anti-symmetry of the state under particle exchange. Note that the wavefunction formalism discussed in the previous section is often referred to as "first quantization" when it is compared and contrasted with the "second quantization" formalism.

In the following we will discuss the second quantization formalism for both fermions and bosons. We start with the fermionic case.

2.1 Second quantization for fermions

2.1.1 Creation and annihilation operators

The second quantization method involves the use of so-called creation and annihilation operators. These operators respectively create and annihilate particles in specified single-particle states. We will see that the anti-symmetry property of fermions manifests itself in characteristic anti-commutation relations obeyed by these operators. Many-particle basis states with the correct anti-symmetry are constructed as products of creation operators acting on the "vacuum state" (the state containing no fermions). These many-particle basis states should be thought of as analogous to the Slater determinants we constructed earlier; they contain exactly the same information.

To make this more concrete, let's consider a 3-particle state with the single-particle states 2, 4, and 6 occupied and all others empty.[5] To this state there corresponds a unique Slater determinant as explained in the previous section. The analogue of this Slater determinant in the **occupation number representation** is written

$$|0_1, 1_2, 0_3, 1_4, 0_5, 1_6, 0_7, 0_8, 0_9, \ldots\rangle \quad \text{or just} \quad |0, 1, 0, 1, 0, 1, 0, 0, 0, \ldots\rangle. \tag{17}$$

This says that there are 0 particles in (single-particle) state 1, 1 in state 2, 0 in state 3, 1 in state 4 etc (note the ascending ordering of the states, in accordance with our ordering convention for Slater determinants discussed previously). The reason for the name "occupation number representation" should be obvious, as the state (17) is specified by giving the occupation number for each single-particle state.

An arbitrary many-particle basis state with n_1 particles in single-particle state 1, n_2 particles in state 2, n_3 particles in state 3 etc. (note that n_i can only take the values 0 or 1) is therefore written as

$$|n_1, n_2, n_3, n_4, n_5, \ldots\rangle. \tag{18}$$

Now we define the **creation operator** $c_\nu^\dagger$ (here ν labels a single-particle state in the single-particle basis set) by how it acts on (18):

$$c_\nu^\dagger |n_1, n_2, \ldots, n_\nu, \ldots\rangle = (-1)^{\sum_{\mu<\nu} n_\mu}(1 - n_\nu)|n_1, n_2, \ldots, 1_\nu, \ldots\rangle, \tag{19}$$

[5] We here use integers to label the single-particle states. The integers correspond to the ordering of single-particle states discussed in the previous section.

where $(-1)^{\sum_{\mu<\nu} n_\mu}$ is a phase factor, equal to $+1$ or -1. Note that if $n_\nu = 1$, i.e. if there is already a fermion in state ν, the result of acting with $c_\nu^\dagger$ is 0, i.e. it's not possible to put another fermion in that state. This is the Pauli principle. On the other hand, if $n_\nu = 0$, i.e. if there was no fermion in state ν, then after the creation operator $c_\nu^\dagger$ has acted, there is a fermion in state ν. Hence the name creation operator is appropriate. The phase factor $(-1)^{\sum_{\mu<\nu} n_\mu}$ depends on whether the total number of fermions in the single-particle states with labels less than ν is even or odd. The role of this phase factor is related to the anti-symmetry property of the fermions. For example, suppose we start with the **vacuum state**, denoted $|0\rangle$, which by definition has no particles in any single-particle state:

$$|0\rangle = |0_1, 0_2, 0_3, \ldots\rangle. \tag{20}$$

First we create a fermion in state 1, which gives

$$c_1^\dagger|0\rangle = |1_1, 0_2, 0_3, \ldots\rangle. \tag{21}$$

and then a fermion in state 2, giving the final state

$$c_2^\dagger c_1^\dagger|0\rangle = c_2^\dagger|1_1, 0_2, 0_3, \ldots\rangle = -|1_1, 1_2, 0_3, \ldots\rangle. \tag{22}$$

If we had created the fermions in the opposite order (i.e. first state 2, then state 1) we would instead have gotten the state

$$c_1^\dagger c_2^\dagger|0\rangle = |1_1, 1_2, 0_3, \ldots\rangle \tag{23}$$

which differs from (22) by a minus sign. This sign difference reflects the anti-symmetry property of fermions. It follows from repeated use of the definition of $c_\nu^\dagger$ that we can write

$$|n_1, n_2, n_3, \ldots\rangle = (c_1^\dagger)^{n_1}(c_2^\dagger)^{n_2}(c_3^\dagger)^{n_3}\cdots|0\rangle. \tag{24}$$

That is, any many-particle basis state can be created by acting on the vacuum state with the appropriate set of creation operators in an appropriate order.

Next we define the **annihilation operator** c_ν by requiring that

$$c_\nu|n_1, \ldots, n_\nu, \ldots\rangle = (-1)^{\sum_{\mu<\nu} n_\mu} n_\nu|n_1, \ldots, 0_\nu, \ldots\rangle, \tag{25}$$

i.e. the result is nonzero (without a fermion in state ν) only if there already was a fermion in state ν, which makes sense; it shouldn't be possible to annihilate a fermion if it wasn't there to begin with. We see that the vacuum state $|0\rangle$ satisfies

$$c_\nu|0\rangle = 0 \quad \text{for all } \nu. \tag{26}$$

Note that if $|\Psi_N\rangle$ is a state with N fermions, then $c_\nu^\dagger|\Psi_N\rangle$ and $c_\nu|\Psi_N\rangle$ are states with $N+1$ and $N-1$ fermions, respectively (if these expressions do not vanish). Thus c_ν and $c_\nu^\dagger$ are mappings between fixed-particle-number fermionic[6] Hilbert spaces $\mathcal{H}_N$ whose particle numbers differ by 1:

$$c_\nu \;:\; \mathcal{H}_N \to \mathcal{H}_{N-1}, \tag{27}$$

$$c_\nu^\dagger \;:\; \mathcal{H}_N \to \mathcal{H}_{N+1}, \tag{28}$$

[6]By a *fermionic* Hilbert space we mean that the states in the space have the correct fermionic antisymmetry.

where both mappings hold for any value N of the total particle number. The collection[7] of all these fixed-particle-number fermionic Hilbert spaces $\mathcal{H}_N$ for $N = 0, 1, 2, \ldots$ is called the **Fock space** $\mathcal{F}$. For this reason many-particle states are also often called Fock states and are said to live in Fock space. Operators, like c_ν and $c_\nu^\dagger$, are thus mappings between states in the Fock space. Also note that, as suggested by the notation, the definitions of $c_\nu^\dagger$ and c_ν are such that these operators are each other's adjoint in the Fock space, i.e.

$$c_\nu^\dagger = (c_\nu)^\dagger, \quad \text{and equivalently} \quad c_\nu = (c_\nu^\dagger)^\dagger. \tag{29}$$

Let the **anti-commutator** $\{A, B\}$ between two operators A and B be defined as

$$\{A, B\} \equiv AB + BA. \tag{30}$$

By using the definitions (19) and (25) of the creation and annihilation operators one can show that these operators satisfy the following **anti-commutation relations**

$$\{c_\mu, c_\nu\} = 0, \tag{31}$$
$$\{c_\mu^\dagger, c_\nu^\dagger\} = 0, \tag{32}$$
$$\{c_\mu^\dagger, c_\nu\} = \delta_{\mu,\nu}. \tag{33}$$

Let us prove Eq. (31). First consider $\mu \neq \nu$. Since $\{c_\mu, c_\nu\} = \{c_\nu, c_\mu\}$ we can restrict ourselves to $\mu < \nu$ in the proof. For the state $|\ldots, n_\mu, \ldots, n_\nu, \ldots\rangle$, let us define $\theta_\alpha = (-1)^{\sum_{\beta<\alpha} n_\beta}$. Then

$$\begin{aligned} c_\mu c_\nu |\ldots, n_\mu, \ldots, n_\nu, \ldots\rangle &= c_\mu \theta_\nu n_\nu |\ldots, n_\mu, \ldots, 0_\nu, \ldots\rangle \\ &= \theta_\nu n_\nu c_\mu |\ldots, n_\mu, \ldots, 0_\nu, \ldots\rangle \\ &= \theta_\nu n_\nu \theta_\mu n_\mu |\ldots, 0_\mu, \ldots, 0_\nu, \ldots\rangle. \end{aligned} \tag{34}$$

Furthermore,

$$\begin{aligned} c_\nu c_\mu |\ldots, n_\mu, \ldots, n_\nu, \ldots\rangle &= c_\nu \theta_\mu n_\mu |\ldots, 0_\mu, \ldots, n_\nu, \ldots\rangle \\ &= \theta_\mu n_\mu c_\nu |\ldots, 0_\mu, \ldots, n_\nu, \ldots\rangle \\ &= \theta_\mu n_\mu \theta_\nu (-1)^{0-n_\mu} n_\nu |\ldots, 0_\mu, \ldots, 0_\nu, \ldots\rangle \\ &= -\theta_\mu \theta_\nu n_\mu n_\nu |\ldots, 0_\mu, \ldots, 0_\nu, \ldots\rangle. \end{aligned} \tag{35}$$

In the third line the factor $(-1)^{0-n_\mu}$ compensates for a sign $(-1)^{n_\mu}$ too much in θ_ν due to the fact that the ket that c_ν acted on had occupation number 0 instead of n_μ for state μ. In the fourth line we set $n_\mu = 1$ in the exponent. This is ok also if $n_\mu = 0$ since then the result is 0 anyway because of the factor n_μ multiplying the ket. From (34) and (35) it then follows that $(c_\mu c_\nu + c_\nu c_\mu)|\ldots, n_\mu, \ldots, n_\nu, \ldots\rangle = 0$. Similarly, for the case $\mu = \nu$ it is easy to show that $c_\nu^2 |\ldots, n_\nu, \ldots\rangle = 0$. Thus for an arbitrary many-particle basis state $|n\rangle$ we have

$$(c_\mu c_\nu + c_\nu c_\mu)|n\rangle = 0 \quad (\text{for any } \mu, \nu). \tag{36}$$

Any state $|\Psi\rangle$ can be expanded in this basis, i.e. $|\Psi\rangle = \sum_n f_n |n\rangle$. Then

$$(c_\mu c_\nu + c_\nu c_\mu)|\Psi\rangle = \sum_n f_n (c_\mu c_\nu + c_\nu c_\mu)|n\rangle = \sum_n f_n \cdot 0 = 0. \tag{37}$$

Since this holds for all states $|\Psi\rangle$, it follows that $c_\mu c_\nu + c_\nu c_\mu = 0$ is an operator identity. This concludes the proof of Eq. (31). (Note that the case $\mu = \nu$ implies that $c_\mu^2 = 0$ is an operator identity.) Eqs. (32) and

[7] Technically, "collection" should here be replaced by "direct sum".

(33) can be proved in a similar way. Actually, Eq. (32) can be obtained more easily by taking the adjoint of Eq. (31), since

$$\{c_\mu, c_\nu\}^\dagger = (c_\mu c_\nu + c_\nu c_\mu)^\dagger = (c_\mu c_\nu)^\dagger + (c_\nu c_\mu)^\dagger = c_\nu^\dagger c_\mu^\dagger + c_\mu^\dagger c_\nu^\dagger = \{c_\mu^\dagger, c_\nu^\dagger\}, \tag{38}$$

where we used that $(AB)^\dagger = B^\dagger A^\dagger$.

Next consider acting on an arbitrary basis state $|n\rangle$ with the operator $c_\nu^\dagger c_\nu$:

$$c_\nu^\dagger c_\nu |\ldots, n_\nu, \ldots\rangle = \theta_\nu n_\nu c_\nu^\dagger |\ldots, 0_\nu, \ldots\rangle = \theta_\nu^2 n_\nu (1-0) |\ldots, 1_\nu, \ldots\rangle, \tag{39}$$

i.e.,

$$c_\nu^\dagger c_\nu |\ldots, n_\nu, \ldots\rangle = n_\nu |\ldots, n_\nu, \ldots\rangle. \tag{40}$$

Thus a basis state $|n\rangle$ is an eigenstate of $\hat{n}_\nu$ with eigenvalue n_ν. Hence $c_\nu^\dagger c_\nu \equiv \hat{n}_\nu$ counts the number of fermions in single-particle state ν. For this reason $\hat{n}_\nu$ is called a **number operator**. We also define the *total* number operator as

$$\hat{N} = \sum_\nu \hat{n}_\nu. \tag{41}$$

The effect of $\hat{N}$ on a basis state is given by

$$\hat{N}|n\rangle = \sum_\nu \hat{n}_\nu |n\rangle = \sum_\nu n_\nu |n\rangle = N|n\rangle \tag{42}$$

where $N = \sum_\nu n_\nu$ is the total number of particles in $|n\rangle$. Thus $|n\rangle$ is an eigenstate of the total number operator $\hat{N}$ with eigenvalue N. Any linear combination of N-particle basis states is also an eigenstate of $\hat{N}$ with eigenvalue N.

2.1.2 Second-quantization representation of single-particle and two-particle operators

To use the occupation number ("second quantization") formalism, which is formulated in terms of creation and annihilation operators such as the ones just introduced, we need to know how "first-quantized" operators (operators expressed in terms of particle coordinates x_i, like $\hat{H}_0$ in Eq. (5)) can be translated into their second-quantized versions. There are two common types of operators. Single-particle operators (like $\hat{H}_0$) which can be written as a sum of terms, each of which only involve the coordinates of a single particle, and two-particle operators, which can be written as a sum of terms, each of which only involve the coordinates of two particles (an example is the Coulomb interaction between electrons). The "dictionary" for converting from first to second quantization is as follows:

- Single-particle operators:

$$\hat{H}_0 = \sum_{i=1}^{N} \hat{h}(x_i) \quad \Longrightarrow \quad \sum_{\alpha,\beta} \langle\alpha|\hat{h}|\beta\rangle c_\alpha^\dagger c_\beta, \tag{43}$$

  where

$$\langle\alpha|\hat{h}|\beta\rangle = \int dx\ \phi_\alpha^*(x) \hat{h}(x) \phi_\beta(x). \tag{44}$$

- Two-particle operators:

$$\hat{H}_I = \frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}} \hat{v}(x_i, x_j) \quad \Longrightarrow \quad \frac{1}{2}\sum_{\alpha,\beta,\gamma,\delta} \langle\alpha\beta|\hat{v}|\gamma\delta\rangle c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma, \tag{45}$$

where

$$\langle\alpha\beta|\hat{v}|\gamma\delta\rangle = \int\int dx\; dx'\; \phi_\alpha^*(x)\phi_\beta^*(x')\hat{v}(x,x')\phi_\gamma(x)\phi_\delta(x'). \tag{46}$$

To prove this correspondence one can consider the matrix elements $\langle\Phi_a|\hat{O}|\Phi_b\rangle$ of an operator $\hat{O}$ between any two basis states $|\Phi_a\rangle$ and $|\Phi_b\rangle$, and show that the same value is obtained for such a matrix element regardless of which formalism (first or second quantization) is used to calculate it. The basis states in first quantization are Slater determinants (wave functions), the basis states in second quantization are the states $|n\rangle = |n_1, n_2, \ldots\rangle$. (To each Slater determinant there corresponds a unique state of this type.)

It can be seen that the matrix element for single-particle operators is zero if the two Slater determinants differ in the occupation of more than two single-particle states (due to orthogonality of different single-particle states). Therefore the second quantized version of single-particle operators is a sum of terms, each of which only changes (at most) the occupation of two single-particle states (the factor $c_\alpha^\dagger c_\beta$ in Eq. (43) will attempt to transfer an electron from state β to state α). Similarly, the matrix element for two-particle operators is zero if the two Slater determinants differ in the occupation of more than four single-particle states. Therefore the second quantized version of two-particle operators is a sum of terms, each of which only changes (at most) the occupation of four single-particle states (the factor $c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma$ in Eq. (45) will attempt to transfer two fermions in states γ and δ to states α and β).

We will discuss the proofs of (43) and (45) later, after we have developed a bit more of the basic formalism of second quantization.

2.2 Second quantization for bosons

It is assumed here that you have already been exposed to bosonic creation and annihilation operators, through the solution of the single harmonic oscillator problem using creation and annihilation operators $b^\dagger$ and b satisfying $[b, b^\dagger] = 1$ (in that problem, when the system is in the state $|n\rangle$ ($n = 0, 1, 2, \ldots$) one can think of the system as being in the eigenstate with n bosons). The only difference in the many-particle problem considered here is that we have one set of creation and annihilation operators ($b_\nu^\dagger$ and b_ν) for each single-particle state ν. But this is a trivial change since for bosons, creation/annihilation operators belonging to different single-particle states simply commute with each other (as will be seen below). Thus most of the results below can be obtained by trivial generalizations of the results for the single harmonic oscillator. Therefore we will just state the main results without giving derivations.

In the occupation-number representation, many-particle basis states for bosons take the form

$$|n_1, n_2, n_3, \ldots\rangle \equiv |n\rangle. \tag{47}$$

For bosons the occupation number n_ν of a single-particle state ν is not restricted to 0 or 1, but can be any nonnegative integer. There is a one-to-one correspondence between states of the form (47) and bosonic wavefunctions of the form (10). The bosonic creation and annihilation operators $b_\nu^\dagger$ and b_ν are defined as

$$\begin{aligned} b_\nu^\dagger|\ldots, n_\nu, \ldots\rangle &= \sqrt{n_\nu + 1}|\ldots, n_\nu + 1, \ldots\rangle, & (48)\\ b_\nu|\ldots, n_\nu, \ldots,\rangle &= \sqrt{n_\nu}|\ldots, n_\nu - 1, \ldots\rangle. & (49) \end{aligned}$$

From these definitions it follows that $b_\nu^\dagger b_\nu$ counts the number n_ν of bosons in single-particle state ν:

$$b_\nu^\dagger b_\nu|\ldots, n_\nu, \ldots\rangle = (\sqrt{n_\nu})^2|\ldots, n_\nu, \ldots\rangle = n_\nu|\ldots, n_\nu, \ldots\rangle, \tag{50}$$

and thus $b_\nu^\dagger b_\nu \equiv \hat{n}_\nu$ is called the number operator for this single-particle state. The total number operator is defined as

$$\hat{N} = \sum_\nu \hat{n}_\nu \tag{51}$$

and satisfies

$$\hat{N}|n\rangle = N|n\rangle \tag{52}$$

where $N = \sum_\nu n_\nu$ is the total number of bosons in the state $|n\rangle$.

An arbitrary (properly normalized) basis state can be written as

$$|n_1, n_2, n_3, \ldots\rangle = \prod_\nu \frac{(b_\nu^\dagger)^{n_\nu}}{\sqrt{n_\nu!}}|0\rangle \tag{53}$$

where $|0\rangle$ is the vacuum state containing no bosons. The operators b_ν and $b_\nu^\dagger$ are adjoints of each other, and satisfy the **commutation relations**

$$\begin{aligned} [b_\mu, b_\nu] &= 0, & (54)\\ [b_\mu^\dagger, b_\nu^\dagger] &= 0, & (55)\\ [b_\mu, b_\nu^\dagger] &= \delta_{\mu,\nu}. & (56) \end{aligned}$$

The formulas describing the conversion between the first- and second-quantized versions of single- and two-particle operators for bosons are exactly the same as for fermions, i.e.

$$\begin{aligned} \hat{H}_0 &= \sum_{i=1}^{N} \hat{h}(x_i) \quad \Longrightarrow \quad \sum_{\alpha,\beta} \langle\alpha|\hat{h}|\beta\rangle b_\alpha^\dagger b_\beta, & (57)\\ \hat{H}_I &= \frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}} \hat{v}(x_i, x_j) \quad \Longrightarrow \quad \frac{1}{2}\sum_{\alpha,\beta,\gamma,\delta} \langle\alpha\beta|\hat{v}|\gamma\delta\rangle b_\alpha^\dagger b_\beta^\dagger b_\delta b_\gamma. & (58) \end{aligned}$$

3 Basis transformations

So far in our analysis we have been using one particular basis set $\{\phi_\alpha(x)\}$ of single-particle wavefunctions. Now we will see how to transform to some other single-particle basis set.

Let $|\alpha\rangle$ be the single-particle ket whose overlap with the position-spin eigenstate $|x\rangle$ is the single-particle wavefunction $\phi_\alpha(x)$, i.e.

$$\phi_\alpha(x) \equiv \langle x|\alpha\rangle. \tag{59}$$

For both bosonic and fermionic particles we can write

$$|\alpha\rangle = a_\alpha^\dagger|0\rangle \tag{60}$$

where $a_\alpha^\dagger$ is the creation operator for a particle in single-particle state α. Let us now consider a different single-particle basis set $\{\tilde{\phi}_{\tilde{\alpha}}(x)\}$ whose single-particle kets are denoted $|\tilde{\alpha}\rangle$. That is,

$$\tilde{\phi}_{\tilde{\alpha}}(x) \equiv \langle x|\tilde{\alpha}\rangle \tag{61}$$

with

$$|\tilde{\alpha}\rangle = a_{\tilde{\alpha}}^\dagger|0\rangle, \tag{62}$$

i.e. $a_{\tilde{\alpha}}^\dagger$ is the creation operator for a particle in the single-particle state $\tilde{\alpha}$. As a concrete example, $\{|\alpha\rangle\}$ could be the set of eigenstates of the kinetic-energy operator $\hat{p}^2/(2m)$, while $\{|\tilde{\alpha}\rangle\}$ could be the eigenstates of the operator $\hat{p}^2/(2m) + U(\hat{x})$, where $U(\hat{x})$ is a potential energy term.

To transform between the two single-particle basis sets we use the resolution of the identity I in the single-particle Hilbert space:

$$I = \sum_\alpha |\alpha\rangle\langle\alpha| = \sum_{\tilde{\alpha}} |\tilde{\alpha}\rangle\langle\tilde{\alpha}|. \tag{63}$$

Thus

$$a_\alpha^\dagger|0\rangle = |\alpha\rangle = \sum_{\tilde{\alpha}} |\tilde{\alpha}\rangle\langle\tilde{\alpha}|\alpha\rangle = \sum_{\tilde{\alpha}} \langle\tilde{\alpha}|\alpha\rangle|\tilde{\alpha}\rangle = \sum_{\tilde{\alpha}} \langle\tilde{\alpha}|\alpha\rangle a_{\tilde{\alpha}}^\dagger|0\rangle. \tag{64}$$

We use this to conclude that

$$a_\alpha^\dagger = \sum_{\tilde{\alpha}} \langle\tilde{\alpha}|\alpha\rangle a_{\tilde{\alpha}}^\dagger. \tag{65}$$

Taking the adjoint of this equation gives the transformation rule for the annihilation operators:

$$a_\alpha = \sum_{\tilde{\alpha}} \langle\alpha|\tilde{\alpha}\rangle a_{\tilde{\alpha}}. \tag{66}$$

The inverse transformations can be derived in the same way (or more simply by interchanging α and $\tilde{\alpha}$ in the expressions so far):

$$a_{\tilde{\alpha}}^\dagger = \sum_\alpha \langle\alpha|\tilde{\alpha}\rangle a_\alpha^\dagger, \tag{67}$$

$$a_{\tilde{\alpha}} = \sum_\alpha \langle\tilde{\alpha}|\alpha\rangle a_\alpha. \tag{68}$$

From these results we can also find the transformation rules for the wavefunctions:

$$\phi_\alpha(x) = \langle x|\alpha\rangle = \langle x|\left(\sum_{\tilde{\alpha}}\langle\tilde{\alpha}|\alpha\rangle|\tilde{\alpha}\rangle\right) = \sum_{\tilde{\alpha}}\langle\tilde{\alpha}|\alpha\rangle\langle x|\tilde{\alpha}\rangle = \sum_{\tilde{\alpha}}\langle\tilde{\alpha}|\alpha\rangle\tilde{\phi}_{\tilde{\alpha}}(x), \tag{69}$$

and similarly

$$\tilde{\phi}_{\tilde{\alpha}}(x) = \sum_{\alpha}\langle\alpha|\tilde{\alpha}\rangle\phi_\alpha(x). \tag{70}$$

The basis transformations are unitary transformations. To see this, consider the matrix D defined by the matrix elements entering the transformations: $D_{\tilde{\alpha}\alpha} \equiv \langle\tilde{\alpha}|\alpha\rangle$. D is a unitary matrix, since

$$\begin{aligned}\delta_{\tilde{\alpha},\tilde{\beta}} &= \langle\tilde{\alpha}|\tilde{\beta}\rangle = \sum_\gamma\langle\tilde{\alpha}|\gamma\rangle\langle\gamma|\tilde{\beta}\rangle = \sum_\gamma\langle\tilde{\alpha}|\gamma\rangle\langle\tilde{\beta}|\gamma\rangle^* \\ &= \sum_\gamma D_{\tilde{\alpha}\gamma}D^*_{\tilde{\beta}\gamma} = \sum_\gamma D_{\tilde{\alpha}\gamma}(D^\dagger)_{\gamma\tilde{\beta}} = (DD^\dagger)_{\tilde{\alpha}\tilde{\beta}}, \quad \Rightarrow \quad DD^\dagger = I.\end{aligned} \tag{71}$$

The basis transformations preserve (anti-)commutation relations. In other words, the creation/annihilation operators in the new basis satisfy the same kinds of (anti-)commutation relations as the creation/annihilation operators in the old basis. To see this, let us define

$$[A, B]_\zeta \equiv AB + \zeta BA, \tag{72}$$

where $\zeta = -1$ gives the commutator (appropriate for bosons) and $\zeta = +1$ gives the anti-commutator (appropriate for fermions). Thus, for example, from the fact that $[a_\alpha, a^\dagger_{\alpha'}]_\zeta = \delta_{\alpha\alpha'}$ it follows that

$$[a_{\tilde{\alpha}}, a^\dagger_{\tilde{\alpha}'}]_\zeta = \sum_{\alpha,\alpha'}\langle\tilde{\alpha}|\alpha\rangle\langle\alpha'|\tilde{\alpha}'\rangle\underbrace{[a_\alpha, a^\dagger_{\alpha'}]_\zeta}_{\delta_{\alpha\alpha'}} = \langle\tilde{\alpha}|\tilde{\alpha}'\rangle = \delta_{\tilde{\alpha},\tilde{\alpha}'}. \tag{73}$$

Similarly, it is easily shown that $[a_{\tilde{\alpha}}, a_{\tilde{\alpha}'}]_\zeta = [a^\dagger_{\tilde{\alpha}}, a^\dagger_{\tilde{\alpha}'}]_\zeta = 0$ just like the corresponding (anti-)commutators in the old basis.

3.1 Proof of the second-quantized representation for single-particle operators

We will now give a proof of the second-quantized representation for single-particle operators presented earlier (Eqs. (43) and (57)). Consider an arbitrary single-particle operator

$$\hat{O} = \sum_{i=1}^N \hat{o}_i. \tag{74}$$

Let us choose $\{|\tilde{\alpha}\rangle\}$ to be the single-particle basis of eigenstates of $\hat{o}$, i.e.

$$\hat{o}|\tilde{\alpha}\rangle = o_{\tilde{\alpha}}|\tilde{\alpha}\rangle \tag{75}$$

where $o_{\tilde{\alpha}}$ is the eigenvalue of $\hat{o}$ associated with the eigenstate $|\tilde{\alpha}\rangle$. Then we claim that the second-quantized representation of $\hat{O}$ can be written

$$\hat{O} = \sum_{\tilde{\alpha}} o_{\tilde{\alpha}} \hat{n}_{\tilde{\alpha}} \tag{76}$$

where $\hat{n}_{\tilde{\alpha}} = a^\dagger_{\tilde{\alpha}} a_{\tilde{\alpha}}$ is the number operator for state $|\tilde{\alpha}\rangle$. To prove this, we calculate the matrix elements of $\hat{O}$ in both first and second quantization and show that both formalisms give the same result (here, we use the many-particle basis that is built from the single-particle basis $\{|\tilde{\alpha}\rangle\}$). Consider then the matrix element $\langle\Phi'|\hat{O}|\Phi\rangle$ where $|\Phi\rangle$ and $|\Phi'\rangle$ are two arbitrary basis states in this many-particle basis set. Using second quantization this matrix element is

$$\begin{aligned}
\langle\Phi'|\hat{O}|\Phi\rangle &= \langle n'_{\tilde{\alpha}_1}, n'_{\tilde{\alpha}_2}, \ldots | \sum_{\tilde{\alpha}} o_{\tilde{\alpha}} \hat{n}_{\tilde{\alpha}} | n_{\tilde{\alpha}_1}, n_{\tilde{\alpha}_2}, \ldots \rangle \\
&= \sum_{\tilde{\alpha}} o_{\tilde{\alpha}} n_{\tilde{\alpha}} \langle n'_{\tilde{\alpha}_1}, n'_{\tilde{\alpha}_2}, \ldots | n_{\tilde{\alpha}_1}, n_{\tilde{\alpha}_2}, \ldots \rangle \\
&= \delta_{\Phi,\Phi'} \sum_{\tilde{\alpha}} o_{\tilde{\alpha}} n_{\tilde{\alpha}}.
\end{aligned} \tag{77}$$

If we instead use first quantization we get the same result

$$\begin{aligned}
\langle\Phi'|\hat{O}|\Phi\rangle &= \int d^N x \; \Phi'^*(x_1, \ldots, x_N) \sum_{i=1}^{N} \hat{o}(x_i) \Phi(x_1, \ldots, x_N) \\
&= \sum_{\tilde{\alpha}} o_{\tilde{\alpha}} n_{\tilde{\alpha}} \int d^N x \; \Phi'^*(x_1, \ldots, x_N) \Phi(x_1, \ldots, x_N) \\
&= \delta_{\Phi,\Phi'} \sum_{\tilde{\alpha}} o_{\tilde{\alpha}} n_{\tilde{\alpha}},
\end{aligned} \tag{78}$$

which proves (76). Note again that in (76) the single-particle basis used is the one that diagonalizes $\hat{o}$, i.e. this expression for $\hat{O}$ is not valid for an arbitrary basis. However, starting from this expression we can use the basis transformations considered earlier to derive an expression for $\hat{O}$ that *is* valid in an arbitrary basis:

$$\begin{aligned}
\hat{O} &= \sum_{\tilde{\alpha}} o_{\tilde{\alpha}} a^\dagger_{\tilde{\alpha}} a_{\tilde{\alpha}} = \sum_{\tilde{\alpha}} o_{\tilde{\alpha}} \left(\sum_{\alpha} \langle\alpha|\tilde{\alpha}\rangle a^\dagger_\alpha \right) \left(\sum_{\beta} \langle\tilde{\alpha}|\beta\rangle a_\beta \right) \\
&= \sum_{\alpha,\beta} \langle\alpha| \underbrace{\left(\sum_{\tilde{\alpha}} |\tilde{\alpha}\rangle o_{\tilde{\alpha}} \langle\tilde{\alpha}| \right)}_{\hat{o}} |\beta\rangle a^\dagger_\alpha a_\beta = \sum_{\alpha,\beta} \langle\alpha|\hat{o}|\beta\rangle a^\dagger_\alpha a_\beta.
\end{aligned} \tag{79}$$

Here we used that the eigenvalue equation $\hat{o}|\tilde{\alpha}\rangle = o_{\tilde{\alpha}}|\tilde{\alpha}\rangle$ implies that we can write $\hat{o} = \hat{o}I = \hat{o}\sum_{\tilde{\alpha}}|\tilde{\alpha}\rangle\langle\tilde{\alpha}| = \sum_{\tilde{\alpha}} o_{\tilde{\alpha}}|\tilde{\alpha}\rangle\langle\tilde{\alpha}| = \sum_{\tilde{\alpha}}|\tilde{\alpha}\rangle o_{\tilde{\alpha}}\langle\tilde{\alpha}|$. The matrix element $\langle\alpha|\hat{o}|\beta\rangle$ can be written[8]

$$\langle\alpha|\hat{o}|\beta\rangle = \int dx \int dx' \, \langle\alpha|x\rangle \underbrace{\langle x|\hat{o}|x'\rangle}_{\hat{o}(x)\delta(x-x')} \langle x'|\beta\rangle = \int dx \, \langle\alpha|x\rangle\hat{o}(x)\langle x|\beta\rangle = \int dx \, \phi_\alpha^*(x)\hat{o}(x)\phi_\beta(x). \tag{80}$$

As Eqs. (79)-(80) are precisely Eqs. (43) (equivalently (57)) and (44), this concludes the proof of these results.

4 Field operators

In this section we consider the creation and annihilation operators in the single-particle basis consisting of the states $|x\rangle$ where, as before, $x = (\boldsymbol{r}, s)$. The creation and annihilation operators in this basis are called **field operators** and are denoted $\hat{\psi}^\dagger(x)$ and $\hat{\psi}(x)$. Thus, rather than putting the state label as a subscript as usual, it is here instead written as an argument. We also put a hat on the field operators to avoid confusing them with wavefunctions. Using Eqs. (67)-(68), the field operators can be written in terms of the creation/annihilation operators in some other basis $\{|\alpha\rangle\}$ as

$$\hat{\psi}^\dagger(x) = \sum_\alpha \langle\alpha|x\rangle a_\alpha^\dagger = \sum_\alpha \phi_\alpha^*(x) a_\alpha^\dagger, \tag{81}$$

$$\hat{\psi}(x) = \sum_\alpha \langle x|\alpha\rangle a_\alpha = \sum_\alpha \phi_\alpha(x) a_\alpha. \tag{82}$$

These field operators respectively create and annihilate a particle at space-spin coordinate x. The field operators obey the (anti-)commutation relations (again, $\zeta = \mp$ corresponds to bosons/fermions)

$$[\hat{\psi}(x), \hat{\psi}(x')]_\zeta = [\hat{\psi}^\dagger(x), \hat{\psi}^\dagger(x')]_\zeta = 0, \tag{83}$$

$$[\hat{\psi}(x), \hat{\psi}^\dagger(x')]_\zeta = \delta(x - x'). \tag{84}$$

These relations follow directly from the results derived for the (anti-)commutators in the previous section. Note that $\delta(x - x')$ in Eq. (84) comes from $\langle x|x'\rangle$ (see Eq. (73)); we here get a Dirac delta instead of a Kronecker delta because x is a continuous rather than discrete label and so it is not possible to normalize the states $\{|x\rangle\}$ to 1.

[8] Note that $\langle x|\hat{o}|x'\rangle = \hat{o}(x)\delta(x - x')$ is valid also if $\hat{o}$ is not diagonal in the x-basis, for example if $\hat{o}$ is the momentum operator $\hat{p}$ or some power of it. To see this, let's forget about spin for simplicity and take x to mean position only. Then from $[\hat{x}, \hat{p}] = i\hbar$ we get $\langle x|[\hat{x}, \hat{p}]|x'\rangle = i\hbar\delta(x - x')$. On the other hand, $\langle x|[\hat{x}, \hat{p}]|x'\rangle = \langle x|(\hat{x}\hat{p} - \hat{p}\hat{x})|x'\rangle = (x - x')\langle x|\hat{p}|x'\rangle$. Therefore $\langle x|\hat{p}|x'\rangle = i\hbar\delta(x - x')/(x - x')$. Now use $(d/dx)\delta(x - x') = (du/dx)(d/du)\delta(u)$ with $u = x - x'$. Using $(d/du)\delta(u) = -\delta(u)/u$ this gives $(d/dx)\delta(x - x') = -\delta(x - x')/(x - x')$. Thus $\langle x|\hat{p}|x'\rangle = -i\hbar(d/dx)\delta(x - x')$ which is on the claimed form with $\hat{p}(x) = -i\hbar(d/dx)$.

The second-quantization representation of single- and two-particle operators using the $\{|x\rangle\}$ basis reads

$$\hat{H}_0 = \int dx\ \hat{\psi}^\dagger(x)\hat{h}(x)\hat{\psi}(x), \tag{85}$$

$$\hat{H}_I = \frac{1}{2}\int dx \int dx'\ \hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x')\hat{v}(x,x')\hat{\psi}(x')\hat{\psi}(x). \tag{86}$$

The correctness of (85) is easily verified by inserting (81) and (82) which immediately leads back to the general form (43) for single-particle operators which we already proved in Sec. 3.1. Furthermore, in a tutorial you will study so-called *density operators* and use these to prove Eq. (86). Then inserting (81)-(82) leads to the general form (45) for two-particle operators.