

From Gordon Baym, Lectures on Quantum Mechanics

Chapter 19 SECOND QUANTIZATION

When dealing with systems of just a few identical particles, it is easy to construct explicitly symmetric or antisymmetric wave functions. This can prove however to be a rather cumbersome task when studying systems with enormous numbers of identical particles, such as the electrons in a metal, or liquid He⁴. I would like therefore to describe a very elegant way of accounting for the symmetry of the states and the operators of systems of many identical particles, and illustrate its use in a few simple calculations.

CREATION AND ANNIHILATION OPERATORS

In studying the harmonic oscillator we introduced operators a and a^\dagger that annihilated and created one quantum of excitation of the oscillator. We can introduce similar operators in identical particle systems that remove *particles* from and add particles to the system. The photon creation and annihilation operators that we studied in Chapter 13 are examples of such operators. Suppose that we have a potential well $V(\mathbf{r})$ with single particle energy eigenstates, $\varphi_0(\mathbf{r})$, $\varphi_1(\mathbf{r})$, etc. Consider, for the moment the state of an n boson system in which all n particles sit in the lowest level, $\varphi_0(\mathbf{r})$, of the well. Let us denote this state by $|n\rangle$. Since the particles are bosons n can be any nonnegative integer. For completeness, let $|0\rangle$ denote the state with no particles present.

We can now introduce operators a_0 and a_0^\dagger defined formally by

$$a_0 |n\rangle = \sqrt{n} |n-1\rangle$$

$$a_0^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle. \quad (19-1)$$

These operators relate states of an n particle system with all particles in φ_0 with those of an $n \pm 1$ particle system with all particles in φ_0 . a_0 may be thought of as a *particle annihilation operator*, since acting on a state with n particles in the single particle state, φ_0 , it produces the state with only $n - 1$ particles in φ_0 . Similarly a_0^\dagger is a *particle creation operator*; it adds a particle to the state φ_0 .

The operators a_0 and a_0^\dagger have properties identical to the harmonic oscillator operators. For example, a_0 and a_0^\dagger obey the commutation relation

$$[a_0, a_0^\dagger] = 1, \quad (19-2)$$

since acting on any state $|n\rangle$

$$(a_0 a_0^\dagger - a_0^\dagger a_0) |n\rangle = [(n+1) - n] |n\rangle.$$

It follows immediately from (19-1) that we can write

$$|n\rangle = \frac{(a_0^\dagger)^n}{\sqrt{n!}} |0\rangle. \quad (19-3)$$

The state with n particles in the lowest level can be produced by adding n particles, in φ_0 , to the "vacuum," $|0\rangle$.

Also a_0^\dagger is the Hermitian conjugate of a_0 . Note carefully that when a_0^\dagger acts to the left it *removes* a particle, since from (19-1),

$$\langle n | a_0^\dagger = \sqrt{n} \langle n-1 |; \quad (19-4)$$

similarly a_0 acts as a *creation* operator to the left,

$$\langle n | a_0 = \sqrt{n+1} \langle n+1 |. \quad (19-5)$$

The operator $N_0 = a_0^\dagger a_0$ measures the number of particles in a state; $a_0^\dagger a_0 |n\rangle = a_0^\dagger \sqrt{n} |n-1\rangle = n |n\rangle$.

Suppose now that the particles are fermions, and that we only consider states $|n\rangle$ in which all the particles are in the lowest level of the well with spin up. The only such states are $|1\rangle$, the state with one particle, and $|0\rangle$, the state with no particles, since we can't put two fermions in the same state. Again we can introduce creation and annihilation operators a_0^\dagger and a_0 by the definitions

$$a_0 |0\rangle = 0, \quad a_0 |1\rangle = |0\rangle$$

$$a_0^\dagger |0\rangle = |1\rangle, \quad a_0^\dagger |1\rangle = 0. \quad (19-6)$$

Explicitly, in the $|0\rangle, |1\rangle$ basis

$$a_0 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad a_0^\dagger = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \quad (19-7)$$

The condition $a_0^\dagger |1\rangle = 0$ guarantees that we can't put two fermions in the same state. The fermion operators a_0 and a_0^\dagger obey an anti-commutation relation:

$$\{a_0, a_0^\dagger\} \equiv a_0 a_0^\dagger + a_0^\dagger a_0 = 1, \quad (19-8)$$

since

$$(a_0 a_0^\dagger + a_0^\dagger a_0) |1\rangle = (0+1)|1\rangle = |1\rangle$$

$$(a_0 a_0^\dagger + a_0^\dagger a_0) |0\rangle = (1+0)|0\rangle = |0\rangle.$$

Also

$$a_0^2 = 0, \quad (a_0^\dagger)^2 = 0 \quad (19-9)$$

since

$$a_0 a_0 |1\rangle = a_0 |0\rangle = 0$$

$$a_0^\dagger a_0^\dagger |0\rangle = a_0^\dagger |1\rangle = 0.$$

The equation $a_0^2 = 0$ says that it is impossible to remove two fermions from the same state. As before, the operator $N_0 = a_0^\dagger a_0$ measures the number of particles in the state φ_0 since $a_0^\dagger a_0 |0\rangle = 0$ and $a_0^\dagger a_0 |1\rangle = a_0^\dagger |0\rangle = |1\rangle$.

Summing up then, for one single particle level of the well, the boson creation and annihilation operators obey the commutation relations

$$[a_0, a_0^\dagger] = 1, \quad [a_0, a_0] = [a_0^\dagger, a_0^\dagger] = 0 \quad (19-10)$$

while the fermion operators obey the anticommutation relations

$$\{a_0, a_0^\dagger\} = 1, \quad \{a_0, a_0\} = \{a_0^\dagger, a_0^\dagger\} = 0. \quad (19-11)$$

Let's consider the situation where we now allow the particles to occupy two levels of the well, say φ_0 and φ_1 . A many boson state will have n_0 particles in the state φ_0 and n_1 particles in the state φ_1 . Let us denote this state by $|n_0, n_1\rangle$. Again we can introduce creation and annihilation operators defined by

$$a_0 |n_0, n_1\rangle = \sqrt{n_0} |n_0 - 1, n_1\rangle$$

$$a_0^\dagger |n_0, n_1\rangle = \sqrt{n_0+1} |n_0+1, n_1\rangle$$

$$a_1 |n_0, n_1\rangle = \sqrt{n_1} |n_0, n_1-1\rangle$$

$$a_1^\dagger |n_0, n_1\rangle = \sqrt{n_1+1} |n_0, n_1+1\rangle. \quad (19-12)$$

a_0 destroys a particle in the state φ_0 , a_1^\dagger creates a particle in the state φ_1 , etc. It is trivial to show that from (19-12) that

$$[a_0, a_0^\dagger] = 1, \quad [a_1, a_1^\dagger] = 1$$

and furthermore that the "0" operators commute with the "1" operators

$$[a_0, a_1] = 0, \quad [a_0^\dagger, a_1^\dagger] = 0$$

$$[a_0, a_1^\dagger] = 0, \quad [a_0^\dagger, a_1] = 0,$$

since for bosons it makes no difference in what order one performs an operation such as adding a particle to one level and removing one from the other level.

Again, all the states $|n_0, n_1\rangle$ can be constructed from the "vacuum" $|0, 0\rangle$ by acting with a_0^\dagger and a_1^\dagger repeatedly:

$$|n_0, n_1\rangle = \frac{(a_1^\dagger)^{n_1}}{\sqrt{n_1!}} \frac{(a_0^\dagger)^{n_0}}{\sqrt{n_0!}} |0, 0\rangle. \quad (19-13)$$

The operator $a_0^\dagger a_0$ is the operator for the number of particles in the state φ_0 and $a_1^\dagger a_1$ measures the number of particles in the state φ_1 . Then

$$N = a_0^\dagger a_0 + a_1^\dagger a_1 \quad (19-14)$$

is the *total number operator*:

$$N |n_1, n_2\rangle = (n_1 + n_2) |n_1, n_2\rangle. \quad (19-15)$$

For fermions occupying the two levels φ_0 and φ_1 (again with their spins up, say) there are four possible states $|n_0, n_1\rangle$:

$$|0, 0\rangle, \quad |0, 1\rangle, \quad |1, 0\rangle, \quad |1, 1\rangle.$$

We first introduce the creation and annihilation operators a_1^\dagger and a_1 defined by the operations

$$a_1^\dagger |0, 0\rangle = |0, 1\rangle, \quad a_1^\dagger |1, 0\rangle = |1, 1\rangle$$

$$a_1^\dagger |0, 1\rangle = a_1^\dagger |1, 1\rangle = 0 \quad (19-16)$$

$$a_1|0, 0\rangle = a_1|1, 0\rangle = 0$$

$$a_1|0, 1\rangle = |0, 0\rangle, \quad a_1|1, 1\rangle = |1, 0\rangle. \quad (19-17)$$

These operators create or destroy particles with the single particle wave function φ_1 . We also define the action of the creation and annihilation operators a_0 and a_0^\dagger on the states with no particles in the state φ_1 by

$$a_0^\dagger|0, 0\rangle = |1, 0\rangle, \quad a_0^\dagger|1, 0\rangle = 0$$

$$a_0|1, 0\rangle = |0, 0\rangle, \quad a_0|0, 0\rangle = 0. \quad (19-18)$$

Now we must take some care in defining how a_0 and a_0^\dagger act on the states $|0, 1\rangle$ and $|1, 1\rangle$ which already have a particle in φ_1 . The reason is that we want to build into the operator language the concept that if we interchange two fermions in a state, the state changes sign. How do we use the a 's and a^\dagger 's to interchange the two particles in the state $|1, 1\rangle$? First we remove one from the state φ_1 , using a_1 :

$$|1, 1\rangle \rightarrow |1, 0\rangle = a_1|1, 1\rangle,$$

then transfer the remaining particle from φ_0 to φ_1 by applying a_0 followed by a_1^\dagger :

$$|1, 0\rangle \rightarrow |0, 1\rangle = a_1^\dagger a_0|1, 0\rangle,$$

and then put the leftover particle back into φ_0 by using a_0^\dagger . This gives a state

$$a_0^\dagger a_1^\dagger a_0 a_1|1, 1\rangle = a_0^\dagger|0, 1\rangle$$

which we want to have opposite sign from the original state. Thus we must require

$$a_0^\dagger|0, 1\rangle = -|1, 1\rangle, \quad (19-19)$$

in order that we get properly antisymmetrized states.

To complete the definition of a_0 and a_0^\dagger we write

$$a_0^\dagger|1, 1\rangle = 0 = a_0|0, 1\rangle \quad (19-20)$$

and

$$a_0|1, 1\rangle = -|0, 1\rangle. \quad (19-21)$$

This latter equation, which is necessary for a_0 to be the Hermitian conjugate of a_0^\dagger , simply says that a_0 undoes the operation of a_0^\dagger .

It is trivial to show from the definitions (19-16) - (19-21) that the creation and annihilation operators obey the anticommutation relations

$$\{a_0, a_0^\dagger\} = 1$$

$$\{a_1, a_1^\dagger\} = 1$$

$$\{a_0, a_0\} = \{a_1, a_1\} = 0$$

$$\{a_0^\dagger, a_0^\dagger\} = \{a_1^\dagger, a_1^\dagger\} = 0, \quad (19-22)$$

and furthermore the "0" operators anticommute with the "1" operators:

$$\{a_0, a_1\} = \{a_0^\dagger, a_1^\dagger\} = 0$$

$$\{a_0, a_1^\dagger\} = \{a_0^\dagger, a_1\} = 0. \quad (19-23)$$

These anticommutation relations are a consequence of the antisymmetry of fermion states under the interchange of two particles. The states can all be constructed from the ground state by operating with a_0^\dagger and a_1^\dagger :

$$|n_0, n_1\rangle = (a_1^\dagger)^{n_1} (a_0^\dagger)^{n_0} |0, 0\rangle. \quad (19-24)$$

Note that the a_0^\dagger acts first. There are no factorials in (19-24) since $n! = 1$ for $n = 0$ or 1 .

It is completely straightforward to generalize the above to the situation where we allow the particles to occupy the complete set of states of the well, and to have all spin orientations. We specify the possible states by stating how many particles n_i there are in a given level of the well (and with a given spin orientation, if the particles have spin). The states then look like $|n_0, n_1, n_2, \dots\rangle$. We have a creation and an annihilation operator, a_i^\dagger and a_i , for each different single particle state.

For bosons the a_i and a_i^\dagger obey the commutation relations

$$[a_i, a_j^\dagger] = \delta_{ij}$$

$$[a_i, a_j] = 0 = [a_i^\dagger, a_j^\dagger]. \quad (19-25)$$

We write the state $|n_0, n_1, \dots\rangle$ in terms of the a_i^\dagger 's as

$$|n_0, n_1, n_2, \dots\rangle = \dots \frac{(a_2^\dagger)^{n_2}}{\sqrt{n_2!}} \frac{(a_1^\dagger)^{n_1}}{\sqrt{n_1!}} \frac{(a_0^\dagger)^{n_0}}{\sqrt{n_0!}} |0\rangle, \quad (19-26)$$

where $|0\rangle$ is short for $|0, 0, 0, \dots\rangle$, the vacuum.

The photon annihilation and creation operators that we introduced in studying the interaction of radiation with matter are just like the little a 's except for trivial numerical factors.

For fermions

$$|n_0, n_1, n_2, \dots\rangle = \dots (a_2^\dagger)^{n_2} (a_1^\dagger)^{n_1} (a_0^\dagger)^{n_0} |0\rangle \quad (19-27)$$

and the operators obey anticommutation relations

$$\{a_i, a_j^\dagger\} = \delta_{ij}$$

$$\{a_i, a_j\} = 0 = \{a_i^\dagger, a_j^\dagger\}. \quad (19-28)$$

In either case, the number of particles in the single particle state i is measured by $a_i^\dagger a_i$, and

$$N = \sum_i a_i^\dagger a_i \quad (19-29)$$

measures the total number of particles. For both fermions and bosons

$$[a_i^\dagger a_i, a_j^\dagger a_j] = 0. \quad (19-30)$$

As an example, let the complete set of states be plane waves in a box, using periodic boundary conditions. Then the normalized wave functions are of the form

$$\varphi_{\mathbf{p}}(\mathbf{r}) = \frac{e^{i\mathbf{p} \cdot \mathbf{r}}}{\sqrt{V}}. \quad (19-31)$$

The \mathbf{p} 's are restricted to values

$$\mathbf{p}_{\mathbf{x}} = \frac{2\pi n_{\mathbf{x}}}{L_{\mathbf{x}}}, \quad n_{\mathbf{x}} = 0, \pm 1, \pm 2, \dots, \quad (19-32)$$

etc. The creation operators $a_{\mathbf{p}s}^\dagger$ adds a particle with momentum \mathbf{p} and spin orientation s to the box, while $a_{\mathbf{p}s}$ removes a particle with momentum \mathbf{p} and spin orientation s from the box.

The amplitude at the point \mathbf{r}' for finding the particle added by a $a_{\mathbf{p}s}^\dagger$ is just $e^{i\mathbf{p} \cdot \mathbf{r}'}/\sqrt{V}$. Now the operator

$$\psi_S^\dagger(\mathbf{r}) \equiv \sum_{\mathbf{p}} \frac{e^{-i\mathbf{p} \cdot \mathbf{r}}}{\sqrt{V}} a_{\mathbf{p}S}^\dagger \quad (19-33)$$

adds a particle to the system in a superposition of momentum states with amplitude $e^{-i\mathbf{p} \cdot \mathbf{r}}/\sqrt{V}$; therefore the amplitude at the point \mathbf{r}' for finding the particle added by $\psi_S^\dagger(\mathbf{r})$ is a coherent sum of amplitudes $e^{i\mathbf{p} \cdot \mathbf{r}'}/\sqrt{V}$ with coefficients $e^{-i\mathbf{p} \cdot \mathbf{r}}/\sqrt{V}$. This net amplitude is thus

$$\sum_{\mathbf{p}} \frac{e^{-i\mathbf{p} \cdot \mathbf{r}}}{\sqrt{V}} \frac{e^{i\mathbf{p} \cdot \mathbf{r}'}}{\sqrt{V}} = \delta(\mathbf{r} - \mathbf{r}'). \quad (19-34)$$

[This equation is nothing but the usual statement of Fourier series

$$f(\mathbf{r}') = \frac{1}{V} \sum_{\mathbf{p}} e^{i\mathbf{p} \cdot \mathbf{r}'} \int d^3\mathbf{r}'' e^{-i\mathbf{p} \cdot \mathbf{r}''} f(\mathbf{r}'')$$

applied to the function $f(\mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')$.] In other words, the operator $\psi_S^\dagger(\mathbf{r})$ adds all the amplitude at point \mathbf{r} ; we can say that $\psi_S^\dagger(\mathbf{r})$ adds a particle at point \mathbf{r} (with spin orientation s).

Similarly, the operator

$$\psi_S(\mathbf{r}) \equiv \sum_{\mathbf{p}} \frac{e^{i\mathbf{p} \cdot \mathbf{r}}}{\sqrt{V}} a_{\mathbf{p}S}, \quad (19-35)$$

which is the Hermitian adjoint of $\psi_S^\dagger(\mathbf{r})$, removes a particle from the point \mathbf{r} . The ψ 's and ψ^\dagger 's are called *field operators*.

The commutation relations of the ψ 's and ψ^\dagger 's are easy to compute from those of the $a_{\mathbf{p}S}$'s and $a_{\mathbf{p}S}^\dagger$'s. Since $a_{\mathbf{p}S} a_{\mathbf{p}'S'} \mp a_{\mathbf{p}'S'} a_{\mathbf{p}S} = 0$ (the upper sign refers to bosons and the lower to fermions) we find

$$\psi_S(\mathbf{r}) \psi_{S'}^\dagger(\mathbf{r}') \mp \psi_{S'}^\dagger(\mathbf{r}') \psi_S(\mathbf{r}) = 0, \quad (19-36)$$

and similarly

$$\psi_S^\dagger(\mathbf{r}) \psi_{S'}^\dagger(\mathbf{r}') \mp \psi_{S'}^\dagger(\mathbf{r}') \psi_S^\dagger(\mathbf{r}) = 0. \quad (19-37)$$

For bosons, adding a particle at \mathbf{r} is an operation that commutes with adding a particle at \mathbf{r}' ; for fermions these operations commute except for a change of sign of the state. Finally

$$\begin{aligned} \psi_S(\mathbf{r}) \psi_{S'}^\dagger(\mathbf{r}') \mp \psi_{S'}^\dagger(\mathbf{r}') \psi_S(\mathbf{r}) &= \sum_{\mathbf{p}\mathbf{p}'} \frac{e^{i\mathbf{p} \cdot \mathbf{r}} e^{-i\mathbf{p}' \cdot \mathbf{r}'}}{V} (a_{\mathbf{p}S} a_{\mathbf{p}'S'}^\dagger \mp a_{\mathbf{p}'S'}^\dagger a_{\mathbf{p}S}) \\ &= \sum_{\mathbf{p}\mathbf{p}'} \frac{e^{i\mathbf{p} \cdot \mathbf{r}} e^{-i\mathbf{p}' \cdot \mathbf{r}'}}{V} \delta_{\mathbf{p}\mathbf{p}'} \delta_{SS'} = \delta(\mathbf{r} - \mathbf{r}') \delta_{SS'}, \end{aligned}$$

so that

$$\psi_S(\mathbf{r})\psi_S^\dagger(\mathbf{r}') \mp \psi_S^\dagger(\mathbf{r}')\psi_S(\mathbf{r}) = \delta(\mathbf{r} - \mathbf{r}')\delta_{SS'} \quad (19-38)$$

Adding particles commutes (or anticommutes) with removing particles, unless one happens to do the adding and removing at the same point. Then, for example, if there are no particles at \mathbf{r} , $\psi_S^\dagger(\mathbf{r})\psi_S(\mathbf{r})$ gives zero — one can't remove a particle if there are none — while $\psi_S(\mathbf{r})\psi_S^\dagger(\mathbf{r})$ won't be zero since the $\psi_S^\dagger(\mathbf{r})$ adds a particle for the $\psi_S(\mathbf{r})$ to remove.

The state

$$|\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_n\rangle = \frac{1}{\sqrt{n!}} \psi^\dagger(\mathbf{r}_n) \cdots \psi^\dagger(\mathbf{r}_2) \psi^\dagger(\mathbf{r}_1) |0\rangle \quad (19-39)$$

(let's suppress the spin indices for simplicity) is the state of n particles with one at \mathbf{r}_1 , one at \mathbf{r}_2 , etc. These states form a very convenient basis for systems of many identical particles since as a consequence of the commutation relations of the ψ^\dagger 's, (19-39) has the proper symmetry under interchanges of the \mathbf{r}_i . For example, for fermions

$$|\mathbf{r}_2, \mathbf{r}_1, \mathbf{r}_3, \dots, \mathbf{r}_n\rangle = -|\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \dots, \mathbf{r}_n\rangle$$

since

$$\psi^\dagger(\mathbf{r}_2)\psi^\dagger(\mathbf{r}_1) = -\psi^\dagger(\mathbf{r}_1)\psi^\dagger(\mathbf{r}_2).$$

Furthermore

$$\psi^\dagger(\mathbf{r})|\mathbf{r}_1, \dots, \mathbf{r}_n\rangle = \sqrt{n+1}|\mathbf{r}_1, \dots, \mathbf{r}_n, \mathbf{r}\rangle \quad (19-40)$$

so that adding a particle by using a creation operator automatically produces a correctly symmetrized state. This property is really the great advantage of the creation and annihilation operators.

If we act on $|\mathbf{r}_1, \dots, \mathbf{r}_n\rangle$ with $\psi(\mathbf{r})$ we get

$$\begin{aligned} \psi(\mathbf{r})|\mathbf{r}_1, \dots, \mathbf{r}_n\rangle &= \frac{1}{\sqrt{n!}} \psi(\mathbf{r})\psi^\dagger(\mathbf{r}_n) \cdots \psi^\dagger(\mathbf{r}_1) |0\rangle \\ &= \frac{1}{\sqrt{n!}} [\delta(\mathbf{r} - \mathbf{r}_n) \pm \psi^\dagger(\mathbf{r}_n)\psi(\mathbf{r})] \psi^\dagger(\mathbf{r}_{n-1}) \cdots \psi^\dagger(\mathbf{r}_1) |0\rangle. \end{aligned}$$

If we continue to commute the $\psi(\mathbf{r})$ with the ψ^\dagger 's to its right until it reaches the $|0\rangle$, (and $\psi|0\rangle = 0$) we find

$$\begin{aligned} \psi(\mathbf{r})|\mathbf{r}_1, \dots, \mathbf{r}_n\rangle &= \frac{1}{\sqrt{n}} [\delta(\mathbf{r} - \mathbf{r}_n)|\mathbf{r}_1, \dots, \mathbf{r}_{n-1}\rangle \\ &\pm \delta(\mathbf{r} - \mathbf{r}_{n-1})|\mathbf{r}_1, \dots, \mathbf{r}_{n-2}, \mathbf{r}_n\rangle \\ &+ \dots + (\pm 1)^{n-1} \delta(\mathbf{r} - \mathbf{r}_1)|\mathbf{r}_2, \dots, \mathbf{r}_n\rangle]. \end{aligned} \quad (19-41)$$

Thus removing a particle at \mathbf{r} can work only if $\mathbf{r} = \mathbf{r}_n$, or $\mathbf{r}_n = \mathbf{r}_{n-1}, \dots$, or $\mathbf{r} = \mathbf{r}_1$. What remains is the correctly symmetrized combination of $n - 1$ particle states.

It is very important to notice that ψ^\dagger adds a particle only when it acts to the right. Acting to the left it *removes* a particle, and ψ acting to the left *adds* a particle. For example, the state $\langle \mathbf{r}_1, \dots, \mathbf{r}_n |$, which is the row vector conjugate to the state $|\mathbf{r}_1 \dots \mathbf{r}_n\rangle$, is

$$\langle \mathbf{r}_1 \dots \mathbf{r}_n | = [\psi^\dagger(\mathbf{r}_n) \dots \psi^\dagger(\mathbf{r}_1) | 0 \rangle]^\dagger / \sqrt{n!} = \langle 0 | \psi(\mathbf{r}_1) \dots \psi(\mathbf{r}_n) / \sqrt{n!},$$

since $[\psi^\dagger(\mathbf{r})]^\dagger = \psi(\mathbf{r})$. Thus one builds up the state $\langle \mathbf{r}_1, \dots, \mathbf{r}_n |$ by acting to the left on $\langle 0 |$ with ψ 's. Note also that the order of the ψ 's in $\langle \mathbf{r}_1 \dots \mathbf{r}_n |$ is reversed from that of the ψ^\dagger 's in $|\mathbf{r}_1, \dots, \mathbf{r}_n\rangle$.

By similar repeated commutations one can calculate the normalization condition on the $|\mathbf{r}_1, \dots, \mathbf{r}_n\rangle$ basis states:

$$\begin{aligned} \langle \mathbf{r}_1', \dots, \mathbf{r}_{n'}' | \mathbf{r}_1, \dots, \mathbf{r}_n \rangle \\ = \frac{\delta_{nn'}}{n!} \sum_P (\pm 1)^P P \delta(\mathbf{r}_1 - \mathbf{r}_1') \delta(\mathbf{r}_2 - \mathbf{r}_2') \dots \delta(\mathbf{r}_n - \mathbf{r}_n') \end{aligned} \quad (19-42)$$

where the sum is over all permutations of the coordinates $\mathbf{r}_1', \dots, \mathbf{r}_{n'}'$, and $(\pm 1)^P = 1$ for bosons and equals the sign of the permutation for fermions. n' must equal n since states with different numbers of particles are orthogonal.

Let us now construct the n particle state $|\Phi\rangle$ in which the particles have a wave function $\varphi(\mathbf{r}_1, \dots, \mathbf{r}_n)$. This state is simply the coherent sum of localized states $|\mathbf{r}_1, \dots, \mathbf{r}_n\rangle$ with relative phases $\varphi(\mathbf{r}_1, \dots, \mathbf{r}_n)$. Thus

$$|\Phi\rangle = \int d^3r_1 \dots d^3r_n \varphi(\mathbf{r}_1, \dots, \mathbf{r}_n) |\mathbf{r}_1, \dots, \mathbf{r}_n\rangle. \quad (19-43)$$

The state $|\Phi\rangle$ is correctly symmetrized, even if the wave function $\varphi(\mathbf{r}_1, \dots, \mathbf{r}_n)$ used to construct $|\Phi\rangle$ isn't symmetrized. In fact, we may ask for the amplitude for observing particles at $\mathbf{r}_1', \dots, \mathbf{r}_n'$ if they are in the state $|\Phi\rangle$. This amplitude is

$$\begin{aligned} \langle \mathbf{r}_1', \dots, \mathbf{r}_n' | \Phi \rangle \\ = \int d^3r_1 \dots d^3r_n \varphi(\mathbf{r}_1, \dots, \mathbf{r}_n) \langle \mathbf{r}_1', \dots, \mathbf{r}_n' | \mathbf{r}_1, \dots, \mathbf{r}_n \rangle, \end{aligned}$$

and from (19-42) we then find

$$\langle \mathbf{r}_1', \dots, \mathbf{r}_n' | \Phi \rangle = \frac{1}{n!} \sum_P (\pm 1)^P P \varphi(\mathbf{r}_1', \dots, \mathbf{r}_n'). \quad (19-44)$$

Thus the "true" wave function of the state, $\langle \mathbf{r}_1', \dots, \mathbf{r}_n' | \Phi \rangle$, is always properly symmetrized. If φ is already properly symmetrized, then all $n!$ terms on the right side of (19-44) are equal and

$$\langle \mathbf{r}_1', \dots, \mathbf{r}_n' | \Phi \rangle = \varphi(\mathbf{r}_1', \dots, \mathbf{r}_n').$$

The state $|\Phi\rangle$ is normalized to one if $\varphi(\mathbf{r}_1, \dots)$ is symmetrized and is itself normalized to one. To see this we write

$$\begin{aligned} \langle \Phi | \Phi \rangle &= \int d^3\mathbf{r}_1 \cdots d^3\mathbf{r}_n \varphi^*(\mathbf{r}_1, \dots, \mathbf{r}_n) \\ &\quad \times \langle \mathbf{r}_1, \dots, \mathbf{r}_n | \int d^3\mathbf{r}_1' \cdots d^3\mathbf{r}_n' | \mathbf{r}_1', \dots, \mathbf{r}_n' \rangle \varphi(\mathbf{r}_1', \dots, \mathbf{r}_n') \\ &= \int d^3\mathbf{r}_1 \cdots d^3\mathbf{r}_n d^3\mathbf{r}_1' \cdots d^3\mathbf{r}_n' \varphi^*(\mathbf{r}_1, \dots, \mathbf{r}_n) \\ &\quad \times \varphi(\mathbf{r}_1', \dots, \mathbf{r}_n') \frac{1}{n!} \sum_P (\pm 1)^P P \delta(\mathbf{r}_1 - \mathbf{r}_1') \cdots \delta(\mathbf{r}_n - \mathbf{r}_n') \\ &= \int d^3\mathbf{r}_1 \cdots d^3\mathbf{r}_n |\varphi(\mathbf{r}_1, \dots, \mathbf{r}_n)|^2 = 1. \end{aligned} \quad (19-45)$$

Since $\langle \mathbf{r}_1, \dots, \mathbf{r}_n | \Phi \rangle$ is always the amplitude for observing particles at $\mathbf{r}_1, \dots, \mathbf{r}_n$, we can always write $|\Phi\rangle$, (Eq. 19-43), as

$$|\Phi\rangle = \int d^3\mathbf{r}_1 \cdots d^3\mathbf{r}_n |\mathbf{r}_1, \dots, \mathbf{r}_n\rangle \langle \mathbf{r}_1, \dots, \mathbf{r}_n | \Phi \rangle. \quad (19-46)$$

In other words, the operator

$$1_n = \int d^3\mathbf{r}_1 \cdots d^3\mathbf{r}_n |\mathbf{r}_1, \dots, \mathbf{r}_n\rangle \langle \mathbf{r}_1, \dots, \mathbf{r}_n| \quad (19-47)$$

is the unit operator when operating on properly symmetrized n particle states. If $|\Phi\rangle$ is an n particle state then

$$1_{n'} |\Phi\rangle = \delta_{nn'} |\Phi\rangle. \quad (19-48)$$

Thus

$$1 = \sum_{n=0}^{\infty} 1_n = |0\rangle\langle 0| + \sum_{n=1}^{\infty} 1_n \quad (19-49)$$

is the unit operator when acting on properly symmetrized states of any number of particles.

SECOND QUANTIZED OPERATORS

Let us now learn how to write operators for physical observables in this formalism. As a first example, let us show that

$$\rho(\mathbf{r}) = \psi^\dagger(\mathbf{r})\psi(\mathbf{r}) \quad (19-50)$$

is the operator for the density of particles at \mathbf{r} . To see this we write the matrix element $\langle \Phi' | \rho(\mathbf{r}) | \Phi \rangle$ of $\rho(\mathbf{r})$ between two n particle states in terms of the wave functions of the states:

$$\begin{aligned} \langle \Phi' | \rho(\mathbf{r}) | \Phi \rangle &= \langle \Phi' | \psi^\dagger(\mathbf{r})\psi(\mathbf{r}) | \Phi \rangle = \langle \Phi' | \psi^\dagger(\mathbf{r}) 1 \psi(\mathbf{r}) | \Phi \rangle \\ &= \langle \Phi' | \psi^\dagger(\mathbf{r}) 1_{n-1} \psi(\mathbf{r}) | \Phi \rangle \end{aligned}$$

since ψ acting on an n particle state leaves an $n-1$ particle state. Then using (19-46) and (19-40) we have

$$\begin{aligned} \langle \Phi' | \rho(\mathbf{r}) | \Phi \rangle &= \int d^3\mathbf{r}_1 \cdots d^3\mathbf{r}_{n-1} \langle \Phi' | \psi^\dagger(\mathbf{r}) | \mathbf{r}_1 \cdots \mathbf{r}_{n-1} \rangle \langle \mathbf{r}_1 \cdots \mathbf{r}_{n-1} | \psi(\mathbf{r}) | \Phi \rangle \\ &= n \int d^3\mathbf{r}_1 \cdots d^3\mathbf{r}_{n-1} \langle \Phi' | \mathbf{r}_1, \dots, \mathbf{r}_{n-1}, \mathbf{r} \rangle \langle \mathbf{r}_1, \dots, \mathbf{r}_{n-1}, \mathbf{r} | \Phi \rangle. \end{aligned}$$

Because the wave functions $\langle \mathbf{r}_1, \dots, \mathbf{r}_n | \Phi \rangle$ and $\langle \mathbf{r}_1, \dots, \mathbf{r}_n | \Phi' \rangle$ are symmetrized (or antisymmetrized), this equation is equivalent to

$$\begin{aligned} \langle \Phi' | \rho(\mathbf{r}) | \Phi \rangle &= \int d^3\mathbf{r}_1 \cdots d^3\mathbf{r}_n \langle \Phi' | \mathbf{r}_1 \cdots \mathbf{r}_n \rangle \sum_i \delta(\mathbf{r} - \mathbf{r}_i) \langle \mathbf{r}_1 \cdots \mathbf{r}_n | \Phi \rangle, \end{aligned} \quad (19-51)$$

which is nothing but the matrix element of the operator $\sum_i \delta(\mathbf{r} - \mathbf{r}_i)$, our old form for the density operator, between the wave functions $\langle \mathbf{r}_1 \cdots \mathbf{r}_n | \Phi' \rangle$ and $\langle \mathbf{r}_1 \cdots \mathbf{r}_n | \Phi \rangle$. Thus the operator $\psi^\dagger(\mathbf{r})\psi(\mathbf{r})$ has the same matrix elements as the usual density operator and therefore it is the representation of the density operator in terms of the field operators.

We can think of $\psi^\dagger(\mathbf{r})\psi(\mathbf{r})$ as examining the density of particles at \mathbf{r} by trying to remove a particle from \mathbf{r} and then putting it back. If the particles have spin, then $\psi_S^\dagger(\mathbf{r})\psi_S(\mathbf{r})$ is the operator for the density of particles at \mathbf{r} with spin orientation s . The total density is

$$\rho(\mathbf{r}) = \sum_{\mathbf{s}} \psi_{\mathbf{s}}^{\dagger}(\mathbf{r}) \psi_{\mathbf{s}}(\mathbf{r}), \quad (19-52)$$

and the operator for the total number of particles in the system is

$$N = \int d^3\mathbf{r} \rho(\mathbf{r}). \quad (19-53)$$

Just as a check, let us substitute for the ψ 's in terms of the a 's. Then (19-53) becomes

$$\begin{aligned} N &= \sum_{\mathbf{s}} \int d^3\mathbf{r} \sum_{\mathbf{p}} \frac{e^{-i\mathbf{p} \cdot \mathbf{r}}}{\sqrt{V}} a_{\mathbf{p}\mathbf{s}}^{\dagger} \sum_{\mathbf{p}'} \frac{e^{i\mathbf{p}' \cdot \mathbf{r}}}{\sqrt{V}} a_{\mathbf{p}'\mathbf{s}} \quad (19-54) \\ &= \sum_{\mathbf{s}} \sum_{\mathbf{p}\mathbf{p}'} a_{\mathbf{p}\mathbf{s}}^{\dagger} a_{\mathbf{p}'\mathbf{s}} \int d^3\mathbf{r} \frac{e^{i(\mathbf{p}' - \mathbf{p}) \cdot \mathbf{r}}}{V}. \end{aligned}$$

However the \mathbf{r} integral vanishes unless $\mathbf{p} = \mathbf{p}'$, when it is equal to one. Thus (19-54) becomes

$$N = \sum_{\mathbf{p}\mathbf{s}} a_{\mathbf{p}\mathbf{s}}^{\dagger} a_{\mathbf{p}\mathbf{s}}, \quad (19-55)$$

which is our previous result.

The operator for the kinetic energy of the particles is most easily written down directly in terms of the $a_{\mathbf{p}}$ and $a_{\mathbf{p}}^{\dagger}$ operators. To measure the kinetic energy of a system we count the number of particles of momentum \mathbf{p} , multiply it by $p^2/2m$, the kinetic energy of a particle of momentum \mathbf{p} , and then sum over all \mathbf{p} . But $a_{\mathbf{p}}^{\dagger} a_{\mathbf{p}}$ is the operator for the number of particles of momentum \mathbf{p} , and therefore the kinetic energy operator is

$$T = \sum_{\mathbf{p}\mathbf{s}} \frac{p^2}{2m} a_{\mathbf{p}\mathbf{s}}^{\dagger} a_{\mathbf{p}\mathbf{s}}. \quad (19-56)$$

To express T in terms of the field operators we first invert (19-33) and (19-35), finding

$$\begin{aligned} a_{\mathbf{p}\mathbf{s}}^{\dagger} &= \int d^3\mathbf{r} \frac{e^{i\mathbf{p} \cdot \mathbf{r}}}{\sqrt{V}} \psi_{\mathbf{s}}^{\dagger}(\mathbf{r}) \\ a_{\mathbf{p}\mathbf{s}} &= \int d^3\mathbf{r} \frac{e^{-i\mathbf{p} \cdot \mathbf{r}}}{\sqrt{V}} \psi_{\mathbf{s}}(\mathbf{r}). \end{aligned} \quad (19-57)$$

The first equation says that to add a particle with momentum \mathbf{p} one

adds a particle at different points \mathbf{r} with relative amplitude $e^{i\mathbf{p}\cdot\mathbf{r}}/\sqrt{V}$. Substituting (19-57) into (19-53) gives

$$T = \frac{1}{2m} \frac{1}{V} \sum_{\mathbf{p}, \mathbf{s}} \int d^3\mathbf{r} d^3\mathbf{r}' (\nabla e^{i\mathbf{p}\cdot\mathbf{r}}) \cdot (\nabla' e^{-i\mathbf{p}\cdot\mathbf{r}'}) \psi_{\mathbf{s}}^\dagger(\mathbf{r}) \psi_{\mathbf{s}}(\mathbf{r}'),$$

where we have written $\mathbf{p}e^{i\mathbf{p}\cdot\mathbf{r}} = -i\nabla e^{i\mathbf{p}\cdot\mathbf{r}}$. Integrating by parts and doing the sum over \mathbf{p} then yields

$$T = \frac{1}{2m} \int d^3\mathbf{r} \nabla \psi^\dagger(\mathbf{r}) \cdot \nabla \psi(\mathbf{r}). \quad (19-58)$$

Notice how this expression for the kinetic energy operator for a many-particle system looks, in form, exactly like the expression $(1/2m) \int d\mathbf{r} \nabla \varphi^*(\mathbf{r}) \cdot \nabla \varphi(\mathbf{r})$ we would write down for the expectation value of the kinetic energy for a single particle in terms of its wave function, $\varphi(\mathbf{r})$. Similarly the density operator $\psi^\dagger(\mathbf{r})\psi(\mathbf{r})$ looks like the usual wave function expression for the probability density $\varphi^*(\mathbf{r})\varphi(\mathbf{r})$ for finding a single particle with wave function φ at point \mathbf{r} . This formal similarity is the reason the creation and annihilation operator formalism is called *second quantization*; one-particle wave functions appear to have become operators which create and annihilate particles, while single particle expectation values appear to have become operators for physical quantities. This is *only* an appearance though; we don't now have a super doubly quantized quantum mechanics — only a new language for the old quantum mechanics.

We can use this similarity to write down other operators. For example, the particle current density operator is

$$\mathbf{j}(\mathbf{r}) = \frac{1}{2im} [\psi^\dagger(\mathbf{r}) \nabla \psi(\mathbf{r}) - \nabla \psi^\dagger(\mathbf{r}) \cdot \psi(\mathbf{r})]; \quad (19-59)$$

this is the same form as the probability current density for a single particle we studied a long time ago. Also for spin $1/2$ particles, the operator for the density of spin at point \mathbf{r} is

$$\mathbf{S}(\mathbf{r}) = \frac{1}{2} \sum_{\mathbf{s}\mathbf{s}'} \psi_{\mathbf{s}}^\dagger(\mathbf{r}) \boldsymbol{\sigma}_{\mathbf{s}\mathbf{s}'} \psi_{\mathbf{s}'}(\mathbf{r}) \quad (19-60)$$

where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the three Pauli spin matrices.

To develop some feeling for this new formalism, let us examine some properties of a gas of noninteracting spin $1/2$ fermions in their ground state. The ground state $|\Phi_0\rangle$ is characterized by all the momentum states being filled up to some momentum p_f , the Fermi momentum. Then

$$n_{\mathbf{p}\uparrow} = \langle \Phi_0 | a_{\mathbf{p}\uparrow}^\dagger a_{\mathbf{p}\uparrow} | \Phi_0 \rangle = \begin{cases} 1, & |\mathbf{p}| \leq p_f \\ 0, & |\mathbf{p}| \geq p_f \end{cases}, \quad (19-61)$$

and $n_{\mathbf{p}\downarrow} = n_{\mathbf{p}\uparrow}$. The Fermi momentum is determined by the condition that the total number of particles is given by

$$N = \sum_{\mathbf{s}, \mathbf{p}} n_{\mathbf{p}\mathbf{s}} = 2 \sum_{|\mathbf{p}| \leq p_f} 1.$$

Converting the sum to an integral gives

$$N = 2V \int_0^{p_f} \frac{d^3p}{(2\pi)^3} = \frac{p_f^3}{3\pi^2} V. \quad (19-62)$$

Thus

$$p_f^3 = \frac{3\pi^2 N}{V} = 3\pi^2 n, \quad (19-63)$$

where n is the average particle density.

Next let us consider $\langle \rho(\mathbf{r}) \rangle = \sum_{\mathbf{S}} \langle \Phi_0 | \psi_{\mathbf{S}}^\dagger(\mathbf{r}) \psi_{\mathbf{S}}(\mathbf{r}) | \Phi_0 \rangle$ in the gas. Expressing the ψ 's in terms of a 's we find

$$\langle \rho(\mathbf{r}) \rangle = \sum_{\mathbf{s}, \mathbf{p}, \mathbf{p}'} \frac{e^{-i\mathbf{p} \cdot \mathbf{r}} e^{i\mathbf{p}' \cdot \mathbf{r}}}{V} \langle \Phi_0 | a_{\mathbf{p}\mathbf{s}}^\dagger a_{\mathbf{p}'\mathbf{s}} | \Phi_0 \rangle.$$

Now the latter expectation value vanishes unless $\mathbf{p} = \mathbf{p}'$, since if we remove a particle of momentum \mathbf{p}' from the ground state, we can only come back to the ground state by adding back a particle of the same momentum \mathbf{p}' . Thus

$$\langle \Phi_0 | a_{\mathbf{p}\mathbf{s}}^\dagger a_{\mathbf{p}'\mathbf{s}} | \Phi_0 \rangle = \delta_{\mathbf{p}\mathbf{p}'} n_{\mathbf{p}\mathbf{s}}, \quad (19-64)$$

whereupon

$$\langle \rho(\mathbf{r}) \rangle = \frac{1}{V} \sum_{\mathbf{s}, \mathbf{p}} n_{\mathbf{p}\mathbf{s}} = n; \quad (19-65)$$

the density in the gas is uniform — a not too surprising result.

A useful quantity to know, as we shall see, is

$$G_{\mathbf{S}}(\mathbf{r} - \mathbf{r}') = \langle \Phi_0 | \psi_{\mathbf{S}}^\dagger(\mathbf{r}) \psi_{\mathbf{S}}(\mathbf{r}') | \Phi_0 \rangle, \quad (19-66)$$

the amplitude for removing a particle at \mathbf{r}' with spin \mathbf{s} from the ground

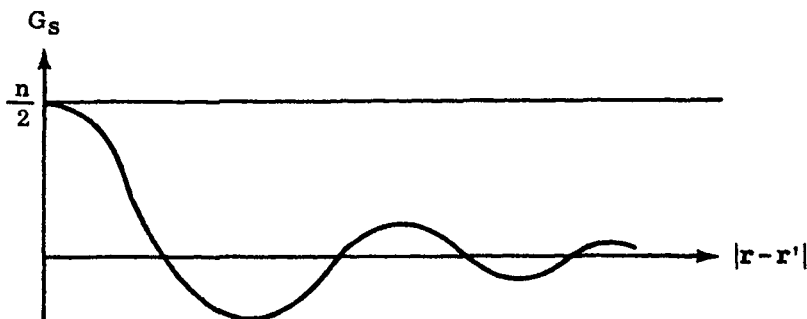


Fig. 19-1

The one-particle density matrix G_s for noninteracting spin $\frac{1}{2}$ fermions.

state and then returning to the ground state by replacing a particle with spin s at point \mathbf{r} . Writing the ψ 's in terms of the a 's, and using (19-64) we find

$$G_s(\mathbf{r} - \mathbf{r}') = \frac{1}{V} \sum_{\mathbf{p}} e^{-i\mathbf{p} \cdot (\mathbf{r} - \mathbf{r}')} n_{\mathbf{p}s}. \quad (19-67)$$

Converting the sum to an integral we have

$$\begin{aligned} G_s(\mathbf{r} - \mathbf{r}') &= \int_0^{p_f} \frac{d^3p}{(2\pi)^3} e^{-i\mathbf{p} \cdot (\mathbf{r} - \mathbf{r}')} \\ &= \frac{1}{4\pi^2} \int_0^{p_f} p^2 dp \int_{-1}^1 d\mu e^{-ip|\mathbf{r} - \mathbf{r}'|\mu} \\ &= \frac{3n}{2} \frac{\sin x - x \cos x}{x^3}, \end{aligned} \quad (19-68)$$

where $x = p_f |\mathbf{r} - \mathbf{r}'|$ and we have used (19-63). This amplitude is shown as a function of $|\mathbf{r} - \mathbf{r}'|$ in Fig. 19-1. Clearly, for $\mathbf{r} = \mathbf{r}'$, G_s equals the density $n/2$, of particles with spin orientation s . For small $|\mathbf{r} - \mathbf{r}'|$

$$G_s(\mathbf{r} - \mathbf{r}') = \frac{n}{2} \left[1 - \frac{(p_f |\mathbf{r} - \mathbf{r}'|)^2}{10} \right]. \quad (19-69)$$

G_s is called the *one-particle density matrix*.

PAIR CORRELATION FUNCTIONS

In a gas of fermions there is a certain tendency for particles of the same spin to avoid each other. This is a simple consequence of the exclusion principle: two particles of the same spin can't be at the same point in space, and therefore, the amplitude for their being close together must be relatively small. Let us calculate the relative probability of finding a particle at \mathbf{r}' if we know that there is one at \mathbf{r} . One way to formulate this problem is to remove (mathematically) a particle (with spin s) at \mathbf{r} from the system, leaving behind $N - 1$ particles in the state $|\Phi'(\mathbf{r}, s)\rangle = \psi_S(\mathbf{r})|\Phi_0\rangle$, and then ask for the density distribution of particles (with spin s') in this new state. This density is

$$\begin{aligned} \langle \Phi'(\mathbf{r}, s) | \psi_{S'}^\dagger(\mathbf{r}') \psi_{S'}(\mathbf{r}') | \Phi'(\mathbf{r}, s) \rangle &= \langle \Phi_0 | \psi_S^\dagger(\mathbf{r}) \psi_S(\mathbf{r}) \psi_{S'}^\dagger(\mathbf{r}') \psi_{S'}(\mathbf{r}') | \Phi_0 \rangle \\ &\equiv \left(\frac{n}{2}\right)^2 g_{SS'}(\mathbf{r} - \mathbf{r}'). \end{aligned} \quad (19-70)$$

Another equivalent way of asking the same question is first to remove a particle from \mathbf{r} using $\psi_S(\mathbf{r})$ and then one from \mathbf{r}' using $\psi_{S'}(\mathbf{r}')$; the relative amplitude for ending up in some $N - 2$ particle state $|\Phi_1^n\rangle$ is $\langle \Phi_1^n | \psi_{S'}(\mathbf{r}') \psi_S(\mathbf{r}) | \Phi_0 \rangle$. If we sum over a *complete* set of $N - 2$ particle states, we find that the total probability for removing the two particles is

$$\begin{aligned} \sum_i |\langle \Phi_1^n | \psi_{S'}(\mathbf{r}') \psi_S(\mathbf{r}) | \Phi_0 \rangle|^2 &= \langle \Phi_0 | \psi_S^\dagger(\mathbf{r}) \psi_S(\mathbf{r}) \sum_i |\Phi_1^n\rangle \langle \Phi_1^n | \psi_{S'}(\mathbf{r}') \psi_S(\mathbf{r}) | \Phi_0 \rangle \\ &= \langle \Phi_0 | \psi_S^\dagger(\mathbf{r}) \psi_S(\mathbf{r}) \psi_{S'}^\dagger(\mathbf{r}') \psi_{S'}(\mathbf{r}') | \Phi_0 \rangle. \end{aligned}$$

This is just the same result as (19-70).

To evaluate $g_{SS'}(\mathbf{r} - \mathbf{r}')$, we expand the ψ 's in (19-67) in terms of the a 's; this gives

$$\begin{aligned} \left(\frac{n}{2}\right)^2 g_{SS'}(\mathbf{r} - \mathbf{r}') &= \frac{1}{V^2} \sum_{\mathbf{p}\mathbf{p}'\mathbf{q}\mathbf{q}'} e^{-i(\mathbf{p}-\mathbf{p}')\cdot\mathbf{r}} e^{-i(\mathbf{q}-\mathbf{q}')\cdot\mathbf{r}'} \\ &\quad \times \langle \Phi_0 | a_{\mathbf{p}S}^\dagger a_{\mathbf{q}S'}^\dagger a_{\mathbf{q}'S'} a_{\mathbf{p}'S} | \Phi_0 \rangle. \end{aligned} \quad (19-71)$$

Now the expectation value vanishes unless the particles we put back have the same momentum and spin as the particles we remove. Thus if $s \neq s'$, \mathbf{p}' must equal \mathbf{p} , \mathbf{q}' must equal \mathbf{q} , and

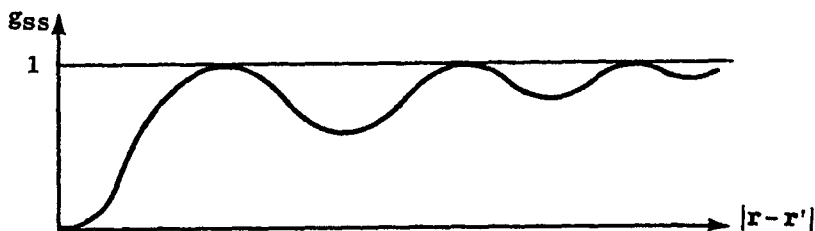


Fig. 19-2

The pair correlation function, for parallel spin, for noninteracting spin $\frac{1}{2}$ fermions.

$$\langle \Phi_0 | a_{ps}^\dagger a_{qs}^\dagger a_{qs} a_{ps} | \Phi_0 \rangle = \langle \Phi_0 | a_{ps}^\dagger a_{ps} a_{qs}^\dagger a_{qs} | \Phi_0 \rangle = n_{ps} n_{qs}. \quad (19-72)$$

Then (19-71) becomes

$$\left(\frac{n}{2}\right)^2 g_{ss'}(r - r') = \frac{1}{V^2} \sum_{pq} n_{ps} n_{qs'} = n_s n_{s'}$$

or

$$g_{ss'}(r - r') = 1, \quad \text{for } s \neq s'. \quad (19-73)$$

This says that the relative probability for finding particles at r and r' with different spin is independent of the distance $|r - r'|$; this is the same as the result for a classical noninteracting gas. The exclusion principle doesn't effect particles of opposite spin.

If the spins are the same, $s = s'$, then there are two possibilities: $p = p', q = q'$ or $p = q', q = p'$. [If $p' = q'$ then the expectation value vanishes since $a_{p's}^2 = 0$.] Thus

$$\begin{aligned} \langle \Phi_0 | a_{ps}^\dagger a_{qs}^\dagger a_{q's} a_{p's} | \Phi_0 \rangle &= \delta_{pp'} \delta_{qq'} \langle \Phi_0 | a_{ps}^\dagger a_{qs}^\dagger a_{qs} a_{ps} | \Phi_0 \rangle \\ &\quad + \delta_{pq'} \delta_{qp'} \langle \Phi_0 | a_{ps}^\dagger a_{qs}^\dagger a_{ps} a_{qs} | \Phi_0 \rangle \\ &= (\delta_{pp'} \delta_{qq'} - \delta_{pq'} \delta_{qp'}) \langle \Phi_0 | a_{ps}^\dagger a_{ps} a_{qs}^\dagger a_{qs} | \Phi_0 \rangle \\ &= (\delta_{pp'} \delta_{qq'} - \delta_{pq'} \delta_{qp'}) n_{ps} n_{qs}, \end{aligned} \quad (19-74)$$

since for $\mathbf{q} \neq \mathbf{p}$ the $a_{\mathbf{p}S}$ anticommutes with $a_{\mathbf{q}S}^\dagger$ and $a_{\mathbf{q}S}$, while for $\mathbf{q} = \mathbf{p}$, the expectation value vanishes. Plugging (19-74) into (19-71) we find

$$\begin{aligned} \left(\frac{n}{2}\right)^2 g_{SS}(\mathbf{r}-\mathbf{r}') &= \frac{1}{V^2} \sum_{\mathbf{p}\mathbf{q}} [1 - e^{-i(\mathbf{p}-\mathbf{q}) \cdot (\mathbf{r}-\mathbf{r}')}] n_{\mathbf{p}S} n_{\mathbf{q}S} \\ &= \left(\frac{n}{2}\right)^2 - [G_S(\mathbf{r}-\mathbf{r}')]^2, \end{aligned} \tag{19-75}$$

where G_S is given by (19-67) and (19-68). Thus

$$g_{SS}(\mathbf{r}-\mathbf{r}') = 1 - \frac{9}{x^6} (\sin x - x \cos x)^2, \tag{19-76}$$

where $x = p_f |\mathbf{r}-\mathbf{r}'|$. The function $g_{SS}(\mathbf{r}-\mathbf{r}')$ is graphed in Fig. 19-2. We see that there is a substantial reduction in the probability for finding two fermions of the same spin at distances $\ll p_f^{-1}$. The exclusion principle causes large correlations in the motion of particles of the same spin. It is almost as if fermions of the same spin repelled each other at short distances. This effective "repulsion" arises just from the exchange symmetry of the wave function — not from any real forces between the particles. At large separation, g_{SS} approaches one, the same value as for opposite spins.

The function $g_{SS'}(\mathbf{r}-\mathbf{r}')$ is called the *pair correlation function*. If we use (19-75), (19-73), and (19-65), we can write our result for this function as

$$\begin{aligned} &\langle \Phi_0 | \psi_S^\dagger(\mathbf{r}) \psi_{S'}^\dagger(\mathbf{r}') \psi_{S'}(\mathbf{r}') \psi_S(\mathbf{r}) | \Phi_0 \rangle \\ &= \langle \Phi_0 | \psi_S^\dagger(\mathbf{r}) \psi_S(\mathbf{r}) | \Phi_0 \rangle \langle \Phi_0 | \psi_{S'}^\dagger(\mathbf{r}') \psi_{S'}(\mathbf{r}') | \Phi_0 \rangle \\ &\quad - \langle \Phi_0 | \psi_S^\dagger(\mathbf{r}) \psi_{S'}(\mathbf{r}') | \Phi_0 \rangle \langle \Phi_0 | \psi_{S'}^\dagger(\mathbf{r}') \psi_S(\mathbf{r}) | \Phi_0 \rangle. \end{aligned} \tag{19-77}$$

[This factorization of the pair correlation function depends *only* on the wave function of the N -particle system being a Slater determinant of single particle orbitals; for example, it is therefore valid for a system of noninteracting fermions in any potential well.]

Let us now evaluate the pair correlation function for a system of noninteracting spinless bosons in the state

$$|\Phi\rangle = |n_{\mathbf{p}_0}, n_{\mathbf{p}_1}, \dots\rangle. \tag{19-78}$$

The density in this state is

$$\langle \Phi | \psi^\dagger(\mathbf{r}) \psi(\mathbf{r}) | \Phi \rangle = \frac{1}{V} \sum_{\mathbf{p}} n_{\mathbf{p}} \equiv n. \quad (19-79)$$

The calculation of the pair correlation function begins with Eq. (19-71), whose form is equally valid for bosons. The expectation value $\langle \Phi | a_{\mathbf{p}}^\dagger a_{\mathbf{q}}^\dagger a_{\mathbf{q}} a_{\mathbf{p}} | \Phi \rangle$ is nonvanishing only if $\mathbf{p} = \mathbf{p}'$, $\mathbf{q} = \mathbf{q}'$ or $\mathbf{p} = \mathbf{q}'$, $\mathbf{q} = \mathbf{p}'$. These are not distinct cases though if $\mathbf{p} = \mathbf{q}$. Thus we have

$$\begin{aligned} \langle \Phi | a_{\mathbf{p}}^\dagger a_{\mathbf{q}}^\dagger a_{\mathbf{q}} a_{\mathbf{p}} | \Phi \rangle &= (1 - \delta_{\mathbf{p}\mathbf{q}}) (\delta_{\mathbf{p}\mathbf{p}'} \delta_{\mathbf{q}\mathbf{q}'} \langle \Phi | a_{\mathbf{p}}^\dagger a_{\mathbf{q}}^\dagger a_{\mathbf{q}} a_{\mathbf{p}} | \Phi \rangle \\ &\quad + \delta_{\mathbf{p}\mathbf{q}'} \delta_{\mathbf{q}\mathbf{p}'} \langle \Phi | a_{\mathbf{p}}^\dagger a_{\mathbf{q}}^\dagger a_{\mathbf{p}} a_{\mathbf{q}} | \Phi \rangle) + \delta_{\mathbf{p}\mathbf{q}} \delta_{\mathbf{p}\mathbf{p}'} \delta_{\mathbf{q}\mathbf{q}'} \langle \Phi | a_{\mathbf{p}}^\dagger a_{\mathbf{p}}^\dagger a_{\mathbf{p}} a_{\mathbf{p}} | \Phi \rangle \\ &= (1 - \delta_{\mathbf{p}\mathbf{q}}) (\delta_{\mathbf{p}\mathbf{p}'} \delta_{\mathbf{q}\mathbf{q}'} + \delta_{\mathbf{p}\mathbf{q}'} \delta_{\mathbf{q}\mathbf{p}'} n_{\mathbf{p}} n_{\mathbf{q}} + \delta_{\mathbf{p}\mathbf{q}} \delta_{\mathbf{p}\mathbf{p}'} \delta_{\mathbf{q}\mathbf{q}'} n_{\mathbf{p}} (n_{\mathbf{p}} - 1)). \end{aligned} \quad (19-80)$$

Putting this into (19-71) we find

$$\begin{aligned} \langle \Phi | \psi^\dagger(\mathbf{r}) \psi^\dagger(\mathbf{r}') \psi(\mathbf{r}') \psi(\mathbf{r}) | \Phi \rangle \\ = n^2 + \left| \frac{1}{V} \sum_{\mathbf{p}} n_{\mathbf{p}} e^{-i\mathbf{p} \cdot (\mathbf{r} - \mathbf{r}')} \right|^2 - \frac{1}{V^2} \sum_{\mathbf{p}} n_{\mathbf{p}} (n_{\mathbf{p}} + 1). \end{aligned} \quad (19-81)$$

This result differs from the fermion result in two respects: the sign of the second term is positive (a consequence of the exchange symmetry of boson wave functions), and the presence of the last term, which arises because one can have many bosons in the same state.

For example, if *all* the particles are in only one state \mathbf{p}_0 , then (19-81) becomes

$$n^2 + n^2 - \left[\frac{1}{V^2} N(N+1) \right] = \frac{N(N-1)}{V^2}. \quad (19-82)$$

This says simply that the relative amplitude for removing the first particle is N/V , while the amplitude for removing the second is $(N-1)/V$, since there are only $N-1$ particles left after removing the first.

Consider next the case that $n_{\mathbf{p}}$ is a smoothly varying distribution. To be definite let us take

$$n_{\mathbf{p}} = c e^{-\alpha(\mathbf{p} - \mathbf{p}_0)^2/2}, \quad (19-83)$$

which essentially represents a beam of particles of momentum centered, with a Gaussian spread, about \mathbf{p}_0 . If we take the limit of

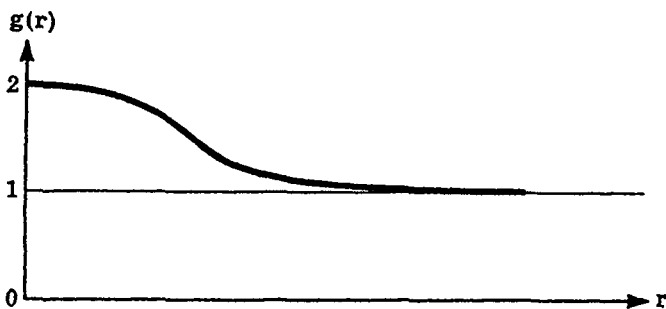


Fig. 19-3

The pair correlation function for noninteracting spin zero bosons.

large volume, keeping n fixed, then the last term in (19-81) is of the order $1/V$ smaller than the first two terms, and we can drop it. Converting the sums to integrals, (19-81) becomes

$$\begin{aligned} \langle \Phi | \psi^\dagger(\mathbf{r})\psi^\dagger(\mathbf{r}')\psi(\mathbf{r}')\psi(\mathbf{r}) | \Phi \rangle &\equiv n^2 g(\mathbf{r} - \mathbf{r}') \\ &= n^2 + \left| \int \frac{d^3p}{(2\pi)^3} n_{\mathbf{p}} e^{-i\mathbf{p} \cdot (\mathbf{r} - \mathbf{r}')} \right|^2 = n^2 \left(1 + e^{-(\mathbf{r} - \mathbf{r}')^2/\alpha} \right). \end{aligned} \quad (19-84)$$

The $e^{-(\mathbf{r} - \mathbf{r}')^2/\alpha}$ term is the effect of exchange. We see that it *increases* the probability for two bosons to be found at small separations. In fact, the probability for finding two bosons right on top of each other, $\mathbf{r} = \mathbf{r}'$, is *twice* the value for finding two at a large $|\mathbf{r} - \mathbf{r}'|$, as in Fig. 19-3.

THE HANBURY-BROWN AND TWISS EXPERIMENT

The *Hanbury-Brown and Twiss experiment*¹ provides a simple way of observing this tendency of bosons to clump together. Basically, the experiment measures the probability of observing two photons simultaneously at different points in a beam of incoherent light (which as we've seen, can be described in terms of the occupation numbers of the photon states). The actual measuring apparatus uses a half silvered mirror, Fig. 19-4, to split the beam into two identical beams; this avoids the problem of one detector

¹Nature 177, 27 (1956); 178, 1447 (1956).

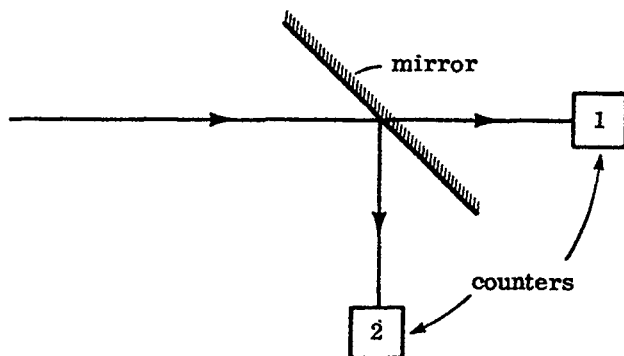


Fig. 19-4

The half-silvered mirror and counters in the Hanbury-Brown and Twiss experiment.

casting a shadow on the other. The amplitude for a photon to be transmitted, or reflected by the mirror, is $1/\sqrt{2}$. Hanbury-Brown and Twiss measured the light intensities $I_1(t)$ observed in detector 1 at time t , and $I_2(t + \tau)$ observed in detector 2 at a later time $t + \tau$, and averaged the product of the intensities over t , keeping τ fixed. This is equivalent to determining the relative probability of observing two photons at two points separated by a distance $c\tau$ in the beam, where c is the speed of light. The observed average correlated intensities $I_1(t)I_2(t + \tau)$, as a function of τ , turned out to have just the form we derived for $g(r)$, in Fig. 19-3, with $r = c\tau$.

This experiment looks like a fine verification of the laws of quantum mechanics for identical bosons. On the contrary, it can be understood completely in terms of classical electromagnetism. What the experiment teaches us is that the boson nature of the photon is already contained in the superposition principle obeyed by classical electromagnetic fields. To see this, let us suppose, as in Fig. 19-5, that in the source of the beam there are just two emitters, A and B. Assume that A emits coherent light with amplitude α and wave num-

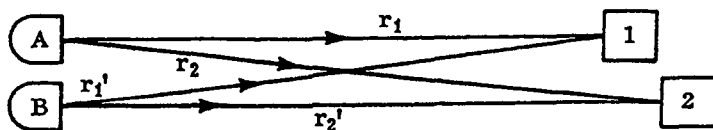


Fig. 19-5

ber k , B emits coherent light with amplitude β and wave number k' , that the relative phase of these two sources is random, and that the light from each has the same polarization. The light from A falling on detector 1 has amplitude αe^{ikr_1} where r_1 is the distance to detector 1 from A ; the light from B on 1 has amplitude $\beta e^{ik'r_1'}$ where r_1' is the distance from B to 1. Thus the total amplitude falling on 1, according to the superposition principle, is

$$a_1 = \alpha e^{ikr_1} + \beta e^{ik'r_1'} \quad (19-85)$$

(times some polarization vector) while the intensity is

$$I_1 = |\alpha|^2 + |\beta|^2 + 2 \operatorname{Re} \alpha^* \beta e^{i(k'r_1' - kr_1)}. \quad (19-86)$$

If we average over the relative phase of α and β (equivalent to averaging over t in the Hanbury-Brown and Twiss experiment) we find

$$\bar{I}_1 = |\alpha|^2 + |\beta|^2. \quad (19-87)$$

Similarly the amplitude falling on the second counter is

$$a_2 = \alpha e^{ikr_2} + \beta e^{ik'r_2'} \quad (19-88)$$

(times a polarization vector) where r_2 is the distance from A to 2 and r_2' is the distance from B to 2. Thus

$$I_2 = |\alpha|^2 + |\beta|^2 + 2 \operatorname{Re} \alpha^* \beta e^{i(k'r_2' - kr_2)} \quad (19-89)$$

and averaged,

$$\bar{I}_2 = |\alpha|^2 + |\beta|^2. \quad (19-90)$$

The product of the averaged intensities, $\bar{I}_1 \bar{I}_2$ is independent of the distance between detectors 1 and 2. However, the product of the intensities is

$$\begin{aligned} I_1 I_2 = |a_1 a_2|^2 = & |\alpha^2 e^{ik(r_1+r_2)} + \beta^2 e^{ik'(r_1'+r_2')} \\ & + \alpha\beta(e^{ikr_1} e^{ik'r_2'} + e^{ik'r_1'} e^{ikr_2})|^2, \end{aligned} \quad (19-91)$$

multiplying this out and averaging over the relative phase of α and β (which eliminates the terms proportional to $\alpha\beta|\alpha|^2$, $\alpha\beta|\beta|^2$, etc.) we find

$$\begin{aligned} \overline{I_1 I_2} &= |\alpha|^4 + |\beta|^4 + |\alpha|^2 |\beta|^2 |e^{ikr_1} e^{ik'r_2'} + e^{ik'r_1'} e^{ikr_2}|^2 \\ &= \bar{I}_1 \bar{I}_2 + 2|\alpha|^2 |\beta|^2 \cos [k'(r_1' - r_2') - k(r_1 - r_2)]. \end{aligned} \quad (19-92)$$

For a well collimated beam, $r_1 - r_2 \approx r_1' - r_2'$ so that (19-93) becomes

$$\overline{I_1 I_2} = \bar{I}_1 \bar{I}_2 + 2|\alpha|^2 |\beta|^2 \cos [(k' - k)(r_1 - r_2)]. \quad (19-93)$$

Thus we find a term in the correlated intensities that depends on the relative separation of the two detectors; this term is maximum when the two detectors are at the same point. Now finally we should average the result (19-93) over all the different k and k' present in the beam. Then we find, for a Gaussian distribution, exactly the form (19-84). The photon bunching effect is thus a consequence of the superposition principle for light applied to noisy sources.²

From a quantum mechanical point of view we can interpret the three terms on the right side (19-91) as follows. The α^2 term is the amplitude for the two observed photons both to have come from A; this leads to the $|\alpha|^4$ term in (19-92). The β^2 term is the amplitude for them both to have come from B; this produces the $|\beta|^4$ term in (19-92). The $\alpha\beta$ term is the amplitude for one of the photons to have come from A and the other from B. There are two ways for this to occur — the photon from A can strike 1 while the photon from B strikes 2, or vice versa. These two ways are indistinguishable, and it is just the interference between them that leads to the \cos term in (19-92).

Try to imagine the results of the Hanbury-Brown and Twiss experiment if it were performed with a beam of electrons.

THE HAMILTONIAN

There is still one very important operator we have not yet learned how to write in second quantized language — the Hamiltonian. If the particles interact by means of a two-body potential $v(\mathbf{r} - \mathbf{r}')$ then the interaction energy operator is

$$\mathcal{V} = \frac{1}{2} \sum_{SS'} \int d^3r d^3r' v(\mathbf{r} - \mathbf{r}') \psi_S^\dagger(\mathbf{r}) \psi_{S'}^\dagger(\mathbf{r}') \psi_{S'}(\mathbf{r}') \psi_S(\mathbf{r}). \quad (19-94)$$

²This is discussed further by E. Purcell in *Nature* 178, 1449 (1956).

Note carefully the order of the operators. The order is the same as that used in (19-70) to determine the pair distribution function. It is left as an exercise to verify (19-94) by writing out a matrix element $\langle \Phi' | \mathcal{V} | \Phi \rangle$ of (19-94) in terms of the wave functions of the states. We can interpret the potential energy operator (19-94) as first trying to remove particles from \mathbf{r} and \mathbf{r}' ; if it is successful it counts a $v(\mathbf{r} - \mathbf{r}')$ and then replaces the particles, replacing the last removed particle first. It then sums over all pairs of points \mathbf{r} and \mathbf{r}' , whence the factor $1/2$.

The second quantized Hamiltonian for particles of mass m acting pairwise is, using (19-58), thus

$$H = \sum_{\mathbf{S}} \int d^3\mathbf{r} \frac{1}{2m} \nabla \psi_{\mathbf{S}}^\dagger(\mathbf{r}) \cdot \nabla \psi_{\mathbf{S}}(\mathbf{r}) \tag{19-95}$$

$$+ \frac{1}{2} \sum_{\mathbf{S}\mathbf{S}'} \int d^3\mathbf{r} d^3\mathbf{r}' v(\mathbf{r} - \mathbf{r}') \psi_{\mathbf{S}}^\dagger(\mathbf{r}) \psi_{\mathbf{S}'}^\dagger(\mathbf{r}') \psi_{\mathbf{S}'}(\mathbf{r}') \psi_{\mathbf{S}}(\mathbf{r}).$$

Let us evaluate the ground state energy of a gas of spin $1/2$ fermions, treating the interaction v as a perturbation. To lowest order the energy is simply the kinetic energy,

$$E^{(0)} = \sum_{\mathbf{p}\mathbf{s}} \frac{p^2}{2m} = 2 \int_0^{P_f} V \frac{d^3p}{(2\pi)^3} \frac{p^2}{2m} = \frac{3}{5} \frac{P_f^2}{2m} N. \tag{19-96}$$

The average kinetic energy per particle is $3/5$ of the Fermi energy. The first-order change $E^{(1)}$ in the energy is simply the expectation value of \mathcal{V} in the unperturbed ground state. Thus

$$E^{(1)} = \frac{1}{2} \int d^3\mathbf{r} d^3\mathbf{r}' v(\mathbf{r} - \mathbf{r}') \sum_{\mathbf{S}\mathbf{S}'} \langle \Phi_0 | \psi_{\mathbf{S}}^\dagger(\mathbf{r}) \psi_{\mathbf{S}'}^\dagger(\mathbf{r}') \psi_{\mathbf{S}'}(\mathbf{r}') \psi_{\mathbf{S}}(\mathbf{r}) | \Phi_0 \rangle \tag{19-97}$$

$$= \frac{1}{2} \int d^3\mathbf{r} d^3\mathbf{r}' v(\mathbf{r} - \mathbf{r}') \sum_{\mathbf{S}\mathbf{S}'} \left(\frac{n}{2}\right)^2 g_{\mathbf{S}\mathbf{S}'}(\mathbf{r} - \mathbf{r}'),$$

where $g_{\mathbf{S}\mathbf{S}'}(\mathbf{r} - \mathbf{r}')$ is the pair correlation function. Using (19-73), and (19-75), we find

$$E^{(1)} = \frac{1}{2} \int d^3\mathbf{r} d^3\mathbf{r}' v(\mathbf{r} - \mathbf{r}') [n^2 - \sum_{\mathbf{S}} G_{\mathbf{S}}(\mathbf{r} - \mathbf{r}')^2]. \tag{19-98}$$

The n^2 term gives $Nnv_0/2$, where $v_0 = \int d^3\mathbf{r} v(\mathbf{r})$; it represents the average interaction of a uniform density of particles with itself, leaving out all correlation effects. This energy is called the direct, or Hartree, energy. The second term, called the *exchange energy*,

$$E_{\text{ex}} = -\frac{1}{2} \int d^3r d^3r' v(\mathbf{r} - \mathbf{r}') \sum_{\mathbf{s}} G_{\mathbf{s}}(\mathbf{r} - \mathbf{r}')^2, \quad (19-99)$$

is the correction to the direct energy due to exchange. It accounts for the fact that particles of the same spin tend to stay apart; for this reason the effects of the short-ranged part of $v(\mathbf{r} - \mathbf{r}')$ are overcounted in the direct energy and the exchange energy subtracts out this overcounting, as well as the self-interactions included in the direct term. From (19-68) we find that the exchange energy is given by

$$\frac{E_{\text{ex}}}{N} = -\frac{9n}{4} \int d^3r \frac{(\sin p_f r - p_f r \cos p_f r)^2}{(p_f r)^6} v(r). \quad (19-100)$$

Thus to first order, the ground state energy per particle is

$$E_0 = \frac{3}{5} \frac{p_f^2}{2m} + \frac{nv_0}{2} + \frac{E_{\text{ex}}}{N}. \quad (19-101)$$

As an example, we consider a gas of electrons of average density n interacting through a Coulomb interaction

$$v(\mathbf{r} - \mathbf{r}') = \frac{e^2}{|\mathbf{r} - \mathbf{r}'|}. \quad (19-102)$$

The conduction electrons in a metal form such a gas. In any physical situation, one never has an isolated gas, but rather, there are always enough positive charges present to make the overall system electrically neutral. To a first approximation, in a metal or plasma, one can replace the positive ions by a uniform background of positive charge of density $+ne$. The electrostatic self-energy of this background, $(1/2) \int d^3r d^3r' (e^2 n^2 / |\mathbf{r} - \mathbf{r}'|)$, plus the average electrostatic interaction between the positive background and the electrons, $-\int d^3r d^3r' (e^2 n^2 / |\mathbf{r} - \mathbf{r}'|)$, exactly cancels the Hartree energy of the electrons. [This cancellation is not accidental, the electrostatic energy of an overall neutral system can only be proportional to the volume, in the limit of a large system - not to a higher power of the volume.] Thus the net interaction energy of the electron gas, to first order, is just the exchange energy:

$$\frac{E_{\text{ex}}}{N} = -\frac{9\pi n e^2}{p_f^2} \int_0^\infty \frac{dx}{x^5} (\sin x - x \cos x)^2 = -\frac{3}{4\pi} p_f e^2. \quad (19-103)$$

How valid is the perturbation expansion we have begun? What is small? The only dimensionless parameter (called r_s) that one can construct for the electron gas in its ground state is the ratio of the

average interparticle spacing, d , to the Bohr radius, $a_0 = \hbar^2/me^2$. Defining d by $(4\pi d^3/3)n = 1$, so that

$$d = \frac{(9\pi/4)^{1/3}}{P_f} \quad (19-104)$$

we have

$$r_s = \frac{d}{a_0} = \left(\frac{9\pi}{4}\right)^{1/3} \left(\frac{me^2}{P_f}\right). \quad (19-105)$$

Expressed in terms of r_s , the energy per particle, (19-96) plus (19-103), is

$$E = \left(\frac{2.21}{r_s^2} - \frac{0.916}{r_s}\right) \left(\frac{e^2}{2a_0}\right). \quad (19-106)$$

The first term is the kinetic energy and the second the exchange energy; $e^2/2a_0$ is the Rydberg. (19-106) must be an upper bound to the energy by the Rayleigh-Ritz variation principle, since it is the expectation value of H in the unperturbed ground state. This estimate is valid for small r_s , or dense gases.

In actual metals, $1.8 \leq r_s \leq 5.5$. For $r_s \leq 2.3$, (19-106) is negative indicating, since it is an upper bound, that the system binds together. The exclusion principle plays an important role in this binding, keeping apart parallel spin particles, and thereby lowering their electrostatic energy. Actually the energy should be still lower than (19-106) due to the fact that even electrons of opposite spin tend to stay apart, because of the repulsive Coulomb interactions. The exact expansion of the energy in r_s begins as³

$$E = \left(\frac{2.21}{r_s^2} - \frac{0.916}{r_s} + 0.0622 \ln r_s - 0.094 + \dots\right) \frac{e^2}{2a_0}. \quad (19-107)$$

The difference between (19-107) and (19-106) is called the *correlation energy*. The $\ln r_s$ means that the energy is not a simple analytic function of r_s . One can see, from the relative size of the terms in (19-107), that this expansion of E in terms of r_s is not valid for metallic densities.

It is often useful to write the interaction energy operator in terms of the a_p operators. Writing the ψ 's in terms of the a_p we find

³M. Gell-Mann and K. Brueckner. *Phys. Rev.* 106, 364 (1957).

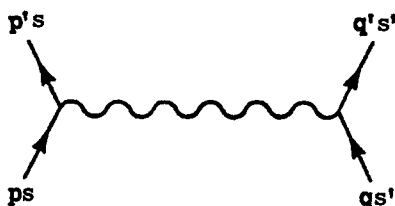


Fig. 19-6

$$v = \frac{1}{2V} \sum_{pp'qq'} \sum_{ss'} v_{p'-p} \delta_{p+q, p'+q'} a_{p's}^\dagger a_{q's'}^\dagger a_{qs'} a_{ps} \quad (19-108)$$

where $v_{\mathbf{k}} = \int d^3r e^{-i\mathbf{k}\cdot\mathbf{r}} v(\mathbf{r})$. One can think of the interaction operator written this way as a sum over scattering processes of the form shown in Fig. 19-6. The momentum $\mathbf{p} + \mathbf{q}$ of the scattering particles is conserved and the amplitude for the scattering is $v_{\mathbf{p}'-\mathbf{p}}$.

Finally, let us consider briefly the second quantized operators in the Heisenberg representation. Recall that in this representation the equation of motion of any operator $X(t)$ not dependent explicitly on time is

$$i \frac{\partial X(t)}{\partial t} = [X(t), H(t)]. \quad (19-109)$$

When H doesn't depend explicitly on time, (19-109) is equivalent to

$$X(t) = e^{iHt} X e^{-iHt}. \quad (19-110)$$

The commutation relations (19-36), (19-37), and (19-38) remain valid as long as all the operators are at the *same* time. Then by simple evaluation of commutators, one can verify that $\psi_{\mathbf{S}}(\mathbf{r}t)$ obeys the equation of motion, for H given by (19-95):

$$i \frac{\partial \psi_{\mathbf{S}}(\mathbf{r}t)}{\partial t} = -\frac{\nabla^2}{2m} \psi_{\mathbf{S}}(\mathbf{r}t) + \left[\sum_{\mathbf{S}'} \int d^3r' v(\mathbf{r}-\mathbf{r}') \psi_{\mathbf{S}'}^\dagger(\mathbf{r}') \psi_{\mathbf{S}'}(\mathbf{r}') \right] \psi_{\mathbf{S}}(\mathbf{r}t).$$

(19-111)

This equation has the same structure as the Schrödinger equation, only the ψ 's are operators. The term in square brackets is roughly the operator for the potential energy felt by a particle at \mathbf{r} due to the other particles. This term is an operator, and not a simple numerical function because a particle in a many particle system constantly affects the potential it feels from the other particles. As a consequence, Eq. (19-111) is far more difficult to solve than a single particle Schrödinger equation, and one can usually only solve it approximately.

PROBLEMS

- Construct explicit 4×4 matrices to represent the fermion creation and annihilation operators a_0 , a_0^\dagger , a_1 , and a_1^\dagger for two levels. Check the anticommutation relations.
- (a) Calculate, to first order in the interparticle interaction, the energy of an $N + 1$ particle system of spin $1/2$ fermions with one particle of momentum \mathbf{p} outside an N -particle Fermi sea (quasi-particle state). Repeat for the state of $N - 1$ particles with a particle of momentum \mathbf{p} removed from an N -particle Fermi sea (hole state). Measure the energies from the N -particle ground state energy.
(b) Evaluate the quasi-particle and hole energies for a Coulomb interaction (remember the uniform positive background).
- Suppose that the wave function of an N -fermion system is a Slater determinant of orthonormal functions φ_i . Using the second quantized formalism show that the pair correlation function of the state factors as for plane waves, Eq. (19-77). [The operators $a_i = \int d^3r \varphi_i^*(\mathbf{r})\psi(\mathbf{r})$ play a useful role.]
- Two electrons are in plane wave states in a box. Calculate to first order in the Coulomb interaction the energy difference of parallel and antiparallel spin alignments [exchange interaction].