2. Verify explicitly that the wave function (18-68) is totally antisymmetric.
3. Using Eqs. (9-71) and (9-72), calculate explicitly the low-energy cross section for elastic scattering of neutrons by (a) unpolarized protons; (b) unpolarized neutrons.
4. Construct the isotopic spin states of two pions. What is the symmetry of the spatial wave function in each case?

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 He^4. 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

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

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

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

$$[a_0, a_0^\dagger] = 1, \qquad (19\text{-}2)$$

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

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

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),

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

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

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

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

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

$$a_0^\dagger|0\rangle = |1\rangle, \qquad a_0^\dagger|1\rangle = 0. \qquad (19\text{-}6)$$

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

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

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:

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

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

$$a_0^2 = 0, \qquad (a_0^\dagger)^2 = 0 \qquad (19\text{-}9)$$

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

$$[a_0, a_0^\dagger] = 1, \qquad [a_0, a_0] = [a_0^\dagger, a_0^\dagger] = 0 \qquad (19\text{-}10)$$

while the fermion operators obey the anticommutation relations

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

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

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

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

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

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

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

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

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

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

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

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:

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

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

$$N = a_0^\dagger a_0 + a_1^\dagger a_1 \qquad (19\text{-}14)$$

is the *total number operator:*

$$N|n_1, n_2\rangle = (n_1+n_2)\,|n_1, n_2\rangle. \qquad (19\text{-}15)$$

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

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

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

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

$$a_1^\dagger|0,1\rangle = a_1^\dagger|1,1\rangle = 0 \qquad (19\text{-}16)$$

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

$$a_1|0,1\rangle = |0,0\rangle, \qquad a_1|1,1\rangle = |1,0\rangle. \qquad (19\text{-}17)$$

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

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

$$a_0|1,0\rangle = |0,0\rangle, \qquad a_0|0,0\rangle = 0. \qquad (19\text{-}18)$$

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†'s to interchange the two particles in the state $|1, 1\rangle$? First we remove one from the state φ_1, using a_1:

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

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

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

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

$$a_0^\dagger|0,1\rangle = -|1,1\rangle, \qquad (19\text{-}19)$$

in order that we get properly antisymmetrized states.

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

$$a_0^\dagger|1,1\rangle = 0 = a_0|0,1\rangle \qquad (19\text{-}20)$$

and

$$a_0|1,1\rangle = -|0,1\rangle. \qquad (19\text{-}21)$$

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

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

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

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

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

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

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

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

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 $a_1^\dagger$:

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

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 $|n_0, n_1, n_2, \ldots\rangle$. 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

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

$$[a_i, a_j] = 0 = [a_i^\dagger, a_j^\dagger]. \qquad (19\text{-}25)$$

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

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

where $|0\rangle$ is short for $|0, 0, 0, \ldots\rangle$, 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

$$|n_0, n_1, n_2, \ldots\rangle = \cdots (a_2^\dagger)^{n_2}(a_1^\dagger)^{n_1}(a_0^\dagger)^{n_0}|0\rangle \qquad (19\text{-}27)$$

and the operators obey anticommutation relations

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

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

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

$$N = \sum_i a_i^\dagger a_i \qquad (19\text{-}29)$$

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

$$[a_i^\dagger a_i, a_j^\dagger a_j] = 0. \qquad (19\text{-}30)$$

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

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

The **p**'s are restricted to values

$$p_x = \frac{2\pi n_x}{L_x}, \qquad n_x = 0, \pm 1, \pm 2, \ldots, \qquad (19\text{-}32)$$

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

The amplitude at the point **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

$$\psi_s^\dagger(\mathbf{r}) \equiv \sum_{\mathbf{p}} \frac{e^{-i\mathbf{p}\cdot\mathbf{r}}}{\sqrt{V}}\, a^\dagger_{\mathbf{p}s} \tag{19-33}$$

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

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

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

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

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

$$\psi_s(\mathbf{r}) \equiv \sum_{\mathbf{p}} \frac{e^{i\mathbf{p}\cdot\mathbf{r}}}{\sqrt{V}}\, a_{\mathbf{p}s}, \tag{19-35}$$

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

The commutation relations of the ψ's and $\psi^\dagger$'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

$$\psi_s(\mathbf{r})\psi_{s'}(\mathbf{r}') \mp \psi_{s'}(\mathbf{r}')\psi_s(\mathbf{r}) = 0, \tag{19-36}$$

and similarly

$$\psi_s^\dagger(\mathbf{r})\psi_{s'}^\dagger(\mathbf{r}') \mp \psi_{s'}^\dagger(\mathbf{r}')\psi_s^\dagger(\mathbf{r}) = 0. \tag{19-37}$$

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

$$\psi_s(\mathbf{r})\psi_{s'}^\dagger(\mathbf{r}') \mp \psi_{s'}^\dagger(\mathbf{r}')\psi_s(\mathbf{r}) = \sum_{\mathbf{p}\mathbf{p}'} \frac{e^{i\mathbf{p}\cdot\mathbf{r}}e^{-i\mathbf{p}'\cdot\mathbf{r}'}}{V}(a_{\mathbf{p}s}a^\dagger_{\mathbf{p}'s'} \mp a^\dagger_{\mathbf{p}'s'}a_{\mathbf{p}s})$$

$$= \sum_{\mathbf{p}\mathbf{p}'} \frac{e^{i\mathbf{p}\cdot\mathbf{r}}e^{-i\mathbf{p}'\cdot\mathbf{r}'}}{V}\delta_{\mathbf{p}\mathbf{p}'}\delta_{ss'} = \delta(\mathbf{r}-\mathbf{r}')\delta_{ss'},$$

so that

$$\psi_s(\mathbf{r})\psi_{s'}^\dagger(\mathbf{r}') \mp \psi_{s'}^\dagger(\mathbf{r}')\psi_s(\mathbf{r}) = \delta(\mathbf{r}-\mathbf{r}')\delta_{ss'}. \tag{19-38}$$

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

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

(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 $\psi^\dagger$'s, (19-39) has the proper symmetry under interchanges of the $\mathbf{r}_i$. For example, for fermions

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

since

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

Furthermore

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

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 $|\mathbf{r}_1, \ldots, \mathbf{r}_n\rangle$ with $\psi(\mathbf{r})$ we get

$$\psi(\mathbf{r})|\mathbf{r}_1, \ldots, \mathbf{r}_n\rangle = \frac{1}{\sqrt{n!}}\psi(\mathbf{r})\psi^\dagger(\mathbf{r}_n)\cdots\psi^\dagger(\mathbf{r}_1)|0\rangle$$

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

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

$$\psi(\mathbf{r})|\mathbf{r}_1, \ldots, \mathbf{r}_n\rangle = \frac{1}{\sqrt{n!}}[\delta(\mathbf{r}-\mathbf{r}_n)|\mathbf{r}_1, \ldots, \mathbf{r}_{n-1}\rangle \pm \delta(\mathbf{r}-\mathbf{r}_{n-1})|\mathbf{r}_1, \ldots, \mathbf{r}_{n-2}, \mathbf{r}_n\rangle + \cdots + (\pm 1)^{n-1}\delta(\mathbf{r}-\mathbf{r}_1)|\mathbf{r}_2, \ldots, \mathbf{r}_n\rangle]. \qquad (19\text{-}41)$$

Thus removing a particle at $\mathbf{r}$ can work only if $\mathbf{r} = \mathbf{r}_n$, or $\mathbf{r}_n = \mathbf{r}_{n-1}, \ldots,$ 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 $\psi^\dagger$ 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 $\langle \mathbf{r}_1, \ldots, \mathbf{r}_n|$, which is the row vector conjugate to the state $|\mathbf{r}_1 \ldots \mathbf{r}_n\rangle$, is

$$\langle \mathbf{r}_1 \ldots \mathbf{r}_n| = [\psi^\dagger(\mathbf{r}_n) \cdots \psi^\dagger(\mathbf{r}_1)|0\rangle]^\dagger = \langle 0|\psi(\mathbf{r}_1) \cdots \psi(\mathbf{r}_n),$$

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

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

$$\langle \mathbf{r}_1', \ldots, \mathbf{r}_{n'}'|\mathbf{r}_1, \ldots, \mathbf{r}_n\rangle = \frac{\delta_{nn'}}{n!}\sum_P (\pm 1)^P P\delta(\mathbf{r}_1-\mathbf{r}_1')\delta(\mathbf{r}_2-\mathbf{r}_2')\cdots\delta(\mathbf{r}_n-\mathbf{r}_n') \qquad (19\text{-}42)$$

where the sum is over all permutations of the coordinates $\mathbf{r}_1', \ldots, \mathbf{r}_n'$, 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 $\varphi(\mathbf{r}_1, \ldots, \mathbf{r}_n)$. This state is simply the coherent sum of localized states $|\mathbf{r}_1, \ldots, \mathbf{r}_n\rangle$ with relative phases $\varphi(\mathbf{r}_1, \ldots, \mathbf{r}_n)$. Thus

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

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

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

and from (19-42) we then find

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

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

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

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

$$\langle \Phi|\Phi\rangle = \int d^3r_1 \cdots d^3r_n\, \varphi^*(\mathbf{r}_1, \ldots, \mathbf{r}_n) \times \langle \mathbf{r}_1, \ldots, \mathbf{r}_n|\int d^3r_1' \cdots d^3r_n'|\mathbf{r}_1', \ldots, \mathbf{r}_n'\rangle\varphi(\mathbf{r}_1', \ldots, \mathbf{r}_n')$$

$$= \int d^3r_1 \cdots d^3r_n d^3r_1' \cdots d^3r_n'\, \varphi^*(\mathbf{r}_1, \ldots, \mathbf{r}_n) \times \varphi(\mathbf{r}_1', \ldots, \mathbf{r}_n')\frac{1}{n!}\sum_P (\pm 1)^P P\delta(\mathbf{r}_1-\mathbf{r}_1')\cdots\delta(\mathbf{r}_n-\mathbf{r}_n')$$

$$= \int d^3r_1 \cdots d^3r_n |\varphi(\mathbf{r}_1, \ldots, \mathbf{r}_n)|^2 = 1. \qquad (19\text{-}45)$$

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

$$|\Phi\rangle = \int d^3r_1 \cdots d^3r_n |\mathbf{r}_1, \ldots, \mathbf{r}_n\rangle\langle \mathbf{r}_1, \ldots, \mathbf{r}_n|\Phi\rangle. \qquad (19\text{-}46)$$

In other words, the operator

$$1_n = \int d^3r_1 \cdots d^3r_n |\mathbf{r}_1, \ldots, \mathbf{r}_n\rangle\langle \mathbf{r}_1, \ldots, \mathbf{r}_n| \qquad (19\text{-}47)$$

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

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

Thus

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

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

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

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:

$$\langle\Phi'|\rho(\mathbf{r})|\Phi\rangle = \langle\Phi'|\psi^\dagger(\mathbf{r})\psi(\mathbf{r})|\Phi\rangle = \langle\Phi'|\psi^\dagger(\mathbf{r})1\psi(\mathbf{r})|\Phi\rangle$$

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

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

$$\langle\Phi'|\rho(\mathbf{r})|\Phi\rangle = \int d^3r_1\cdots d^3r_{n-1}\langle\Phi'|\psi^\dagger(\mathbf{r})|\mathbf{r}_1\ldots\mathbf{r}_{n-1}\rangle\langle\mathbf{r}_1\ldots\mathbf{r}_{n-1}|\psi(\mathbf{r})|\Phi\rangle$$

$$= n\int d^3r_1\cdots d^3r_{n-1}\langle\Phi'|\mathbf{r}_1,\ldots,\mathbf{r}_{n-1},\mathbf{r}\rangle\langle\mathbf{r}_1,\ldots,\mathbf{r}_{n-1},\mathbf{r}|\Phi\rangle.$$

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

$$\langle\Phi'|\rho(\mathbf{r})|\Phi\rangle = \int d^3r_1\cdots d^3r_n\langle\Phi'|\mathbf{r}_1\cdots\mathbf{r}_n\rangle\sum_i\delta(\mathbf{r}-\mathbf{r}_i)\langle\mathbf{r}_1\cdots\mathbf{r}_n|\Phi\rangle, \tag{19-51}$$

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 $\langle\mathbf{r}_1\ldots\mathbf{r}_n|\Phi'\rangle$ and $\langle\mathbf{r}_1\ldots\mathbf{r}_n|\Phi\rangle$. 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

$$\rho(\mathbf{r}) = \sum_s\psi_s^\dagger(\mathbf{r})\psi_s(\mathbf{r}), \tag{19-52}$$

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

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

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

$$N = \sum_s\int d^3r\sum_{\mathbf{p}}\frac{e^{-i\mathbf{p}\cdot\mathbf{r}}}{\sqrt{V}}a^\dagger_{\mathbf{p}s}\sum_{\mathbf{p}'}\frac{e^{i\mathbf{p}'\cdot\mathbf{r}}}{\sqrt{V}}a_{\mathbf{p}'s} \tag{19-54}$$

$$= \sum_s\sum_{\mathbf{p}\mathbf{p}'}a^\dagger_{\mathbf{p}s}a_{\mathbf{p}'s}\int d^3r\,\frac{e^{i(\mathbf{p}'-\mathbf{p})\cdot\mathbf{r}}}{V}.$$

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

$$N = \sum_{\mathbf{p}s}a^\dagger_{\mathbf{p}s}a_{\mathbf{p}s}, \tag{19-55}$$

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

$$T = \sum_{\mathbf{p}s}\frac{p^2}{2m}a^\dagger_{\mathbf{p}s}a_{\mathbf{p}s}. \tag{19-56}$$

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

$$a^\dagger_{\mathbf{p}s} = \int d^3r\,\frac{e^{i\mathbf{p}\cdot\mathbf{r}}}{\sqrt{V}}\psi_s^\dagger(\mathbf{r})$$

$$a_{\mathbf{p}s} = \int d^3r\,\frac{e^{-i\mathbf{p}\cdot\mathbf{r}}}{\sqrt{V}}\psi_s(\mathbf{r}). \tag{19-57}$$

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

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

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

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

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

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

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

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

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

$$n_{\mathbf{p}\uparrow} = \langle\Phi_0|a_{\mathbf{p}\uparrow}^\dagger a_{\mathbf{p}\uparrow}|\Phi_0\rangle = \begin{cases} 1, & |p| \le p_f \\ 0, & |p| \ge p_f \end{cases}, \tag{19-61}$$

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

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

Converting the sum to an integral gives

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

Thus

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

where n is the average particle density.

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

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

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

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

whereupon

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

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

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

$$G_s(\mathbf{r}-\mathbf{r}') = \langle\Phi_0|\psi_s^\dagger(\mathbf{r})\psi_s(\mathbf{r}')|\Phi_0\rangle, \tag{19-66}$$

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

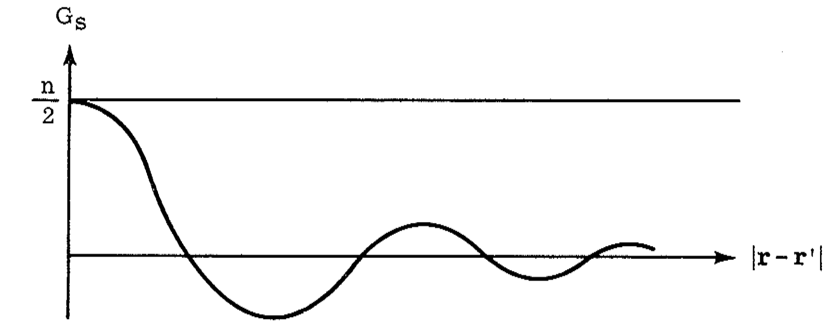

Fig. 19-1
The one-particle density matrix G_s for noninteracting spin ½ fermions.

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

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

Converting the sum to an integral we have

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

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 $|\mathbf{r}-\mathbf{r}'|$

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

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

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

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 $|\Phi_i''\rangle$ is $\langle \Phi_i''|\psi_{s'}(\mathbf{r}')\psi_s(\mathbf{r})|\Phi_0\rangle$. If we sum over a *complete* set of N − 2 particle states, we find that the total probability for removing the two particles is

$$\begin{aligned} \sum_i |\langle \Phi_i''|\psi_{s'}(\mathbf{r}')\psi_s(\mathbf{r})|\Phi_0\rangle|^2 &= \langle \Phi_0|\psi_s^\dagger(\mathbf{r})\psi_{s'}^\dagger(\mathbf{r}') \sum_i |\Phi_i''\rangle\langle \Phi_i''|\psi_{s'}(\mathbf{r}')\psi_s(\mathbf{r})|\Phi_0\rangle \\ &= \langle \Phi_0|\psi_s^\dagger(\mathbf{r})\psi_{s'}^\dagger(\mathbf{r}')\psi_{s'}(\mathbf{r}')\psi_s(\mathbf{r})|\Phi_0\rangle. \end{aligned}$$

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

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

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