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Text Book: Philip Phillips - Advanced Solid State Physics, Cambridge university Press, 2nd ed., Cambridge (2012)

Fermion Operator

Consider two single-particle states ϕ_1 and ϕ_2. The normalized wave function that is antisymmetric with respect to particle interchange is

$$\langle r_1, r_2 | \, n_1, n_2 \rangle = \frac{1}{\sqrt{2}} \left[\phi_1(1)\phi_2(2) - \phi_1(2)\phi_2(1) \right] \tag{1}$$

This state can be constructed from the determinant of ϕ_1 and ϕ_2:

$$D_2 = \frac{1}{\sqrt{2!}} \left| \begin{pmatrix} \phi_1(1) & \phi_2(1) \\ \phi_1(2) & \phi_2(2) \end{pmatrix} \right| \tag{2}$$

The general rule for constructing an antisymmetric wave function out of n single-particle states is

$$D_n = \left\langle r_1, r_2, \cdots \middle| \, n_\alpha, n_\beta, \cdots \right\rangle = \frac{1}{\sqrt{n!}} \left\| \phi_1 \cdots \phi_n \right\| \tag{3}$$

where $\| \quad \|$ represents the determinant. D_n contains all antisymmetrized permutations of the orbital set $\phi_1 \cdots \phi_n$ and hence may be written as

$$D_n = \left\langle r_1, r_2, \cdots \middle| \, n_\alpha, n_\beta, \cdots \right\rangle = \frac{1}{\sqrt{n!}} \sum_P (-1)^P P \left[\phi_1 \cdots \phi_n \right] \tag{4}$$

with P as the permutation operator. A general many-particle fermionic state can be written as

$$|n_1, n_2, \cdots\rangle = a_1^\dagger a_2^\dagger \cdots |0\rangle \tag{5}$$

Complete antisymmetry under particle interchange is built into this many-body state as a result of the anticommuting property of the fermion operators. Note that there is no $\sqrt{n!}$ normalization factor. In first quantization, however, an explicit $\sqrt{n!}$ factor appears, because particle are placed in particular single-particle state and all possible permutations are summed over. In second quantization, no labels are attached to the particles.

Consider the one body operator $\hat{H}_1$. In second quantized form, a general one-body operator is restricted to have a single creation-annihilation operator pairs. In general, we can write a one-body operator as

$$\hat{H}_1 = \sum_{\nu,\lambda} c_{\lambda\nu} a_\lambda^\dagger a_\nu \tag{6}$$

To determine the coefficient $c_{\lambda\nu}$, we simply evaluate the matrix element $\left\langle \mu \middle| \hat{H}_1 \middle| \gamma \right\rangle$.

Orthogonality of the single-particle state implies that$\left\langle \mu \middle| \hat{H}_1 \middle| \gamma \right\rangle = c_{\mu\gamma}$

Therefore the most general way of writing a one-body operator in second quantization is,

$$\hat{H}_1 = \sum_{\nu,\lambda} \langle \lambda | \hat{H}_1 | \nu \rangle \, a_\lambda^\dagger a_\nu \tag{7}$$

In the event that the single-particle state are eigenfunctions of $\hat{H}_1$, then $\hat{H}_1 |\nu\rangle = \epsilon_\nu |\nu\rangle$. Then equation (7) becomes

$$\hat{H}_1 = \sum_\lambda \epsilon_\lambda a_\lambda^\dagger a_\lambda = \sum_\lambda n_\lambda \epsilon_\lambda \tag{8}$$

In the case that the $\hat{H}_1$ is a one-body energy operator, the average of $H\hat{(}1)$ determines the average energy of the system.

Consider now a general 2-body operator

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$$\hat{H}_2 = \frac{1}{2}\sum_{i,j}\hat{V}(i,j) \tag{9}$$

In the electron gas, $\hat{V}(i,j) = e^2/|\hat{r}_i - \hat{r}_j|$, the Coulomb energy. A two-body operator can at most create two particle-hole excitations in a general many-body state. The general form of the operator that creates such excitations is $a_k^\dagger a_l^\dagger a_j a_i$. As a consequence, a general 2-body operator in second-quantized form can be written as

$$\hat{H}_2 = \frac{1}{2}\sum_{i,j,k,l} V_{i,j,k,l}\, a_k^\dagger a_l^\dagger a_j a_i \tag{10}$$

The interacting electron Hamiltonian containing both one- and two- body terms can be recast as

$$\hat{H}_e = \sum_{\nu,\lambda}\langle\nu|\hat{H}_1|\lambda\rangle a_\nu^\dagger a_\lambda + \frac{1}{2}\sum_{i,j,k,l}\langle k\, l|\frac{e^2}{r_1 - r_2}|i\, j\rangle\; a_k^\dagger a_l^\dagger a_j a_i \tag{11}$$

To make contact with the electron gas, it is customary to transform to momentum space, in which the single-particle plane-wave states,

$$\phi_p(r) = \frac{e^{i\,p\cdot r/\hbar}}{\sqrt{V}} \tag{12}$$

diagonalize exactly the electron kinetic energy. These states are defined in a box of volume V with periodic boundary conditions imposed. Particles with spin σ are added or removed from these states by the operators $a_{p\sigma}^\dagger$ or $a_{p\sigma}$, respectively. We introduce the *field operator*

$$\Psi_\sigma^\dagger(r) = \sum_p \frac{e^{-i\,p\cdot r/\hbar}}{\sqrt{V}} a_{p_\sigma}^\dagger \tag{13}$$

which creates an electron at r with spin σ. The Hermitian conjugate field, $\Psi_\sigma(r)$, annihilates a particle with spin σ at r. Field operators create and annihilate particles at particular positions. In so doing, they do not add or remove particles from a particular momentum states with amplitude $e^{\pm p\cdot r/\hbar}/\sqrt{V}$. The product of the creation and annihilation field operators

$$\Psi_\sigma^\dagger(r)\Psi_\sigma(r) = \frac{1}{V}\sum_{p,p'} e^{-ir\cdot(p-p')/\hbar}\; a_{p_\sigma}^\dagger a_{p'_\sigma} \tag{14}$$

defines the particle density operator. Consequently if we integrate equation (14) over r,

$$\begin{aligned}\hat{n}_\sigma &= \int \Psi^\dagger_\sigma(r)\Psi_\sigma(r)dr \\ &= \frac{1}{V}\int \sum_{p,p'} e^{-ir\cdot(p-p')/\hbar}\, a^\dagger_{p_\sigma} a_{p'_\sigma} dr \\ &= \sum_p a^\dagger_{p_\sigma} a_{p_\sigma} \\ &= \sum_p \hat{n}_{p\sigma}\end{aligned}$$

we obtain the total particle density for the electron with spin σ.

We can construct a general many-body state $\left|r_{1\sigma_1}\cdots r_{n\sigma_n}\right\rangle$,

$$\left|r_{1\sigma_1}\cdots r_{n\sigma_n}\right\rangle = \frac{1}{\sqrt{n!}}\Psi^\dagger_{\sigma_1}(r_1)\cdots\Psi^\dagger_{\sigma_n}(r_n)\left|0\right\rangle \tag{15}$$

from vacuum state, using the field operator $\Psi^\dagger_{\sigma_l}(r_i)$. The rules applying $\Psi^\dagger_{\sigma_l}$ and Ψ_{σ_l} to $\left|r_{1\sigma_1}\cdots r_{n\sigma_n}\right\rangle$ are

$$\Psi^\dagger_{\sigma_{n+1}}(r_{n+1})\left|r_{1\sigma_1}\cdots r_{n\sigma_n}\right\rangle = \sqrt{n+1}\,(-1)^{\eta_{n+1}}\left|r_{1\sigma_1}\cdots r_{n+1\sigma_{n+1}}\right\rangle \tag{16}$$

and

$$\Psi_\sigma(r)\left|r_{1\sigma_1}\cdots r_{n\sigma_n}\right\rangle = \frac{1}{\sqrt{n}}\sum_\alpha \delta(r-r_\alpha)(-1)^{\eta_\alpha}\left|r_1\cdots r_{\alpha-1}, r_{\alpha+1}\cdots r_n\right\rangle \tag{17}$$

Here, η_α is the number of occupied states to the left of r_α.

Homework-03

1. All problems in Philip Philips Book, corresponding chapter.