Lattice Waves and Electron States

One electron approximation:

Let us suppose we have a set of orthonormal solutions of some one-particle wave equation. We write a solution of a one-particle wave equation as $\phi_j(x)$, where

$$H\phi_j(x) = \epsilon_j \phi_j(x) \quad \text{——— (1)}$$

Note that we do not label the electron with a number index, such as r in x_r. The eigenfunction label j will include the specification of the spin state, for example, $\uparrow$ or $\downarrow$, or α or β.

Next from the field operator

$$\psi(x) = \sum_j c_j \phi_j(x) ; \quad \psi^+(x) = \sum_j c_j^+ \phi_j^*(x) \quad \text{——— (2)}$$

where c_j is an operator with properties to be specified below; $\phi_j(x)$ remains an eigenfunction and not an operator, so that it is essentially a c-number function of the coordinate x. The field operator $\psi(x)$ and the fermion operators c_j operate on a state vector which we write as Φ. This state vector is in the space of the occupation numbers of the one electron states. Thus

$$\Phi_{vac} = |000\cdots0\cdots\rangle = |vac\rangle \quad \text{——— (3)}$$

is the vacuum state in which all the occupation numbers n_j of the one-electron states are zero - no particles are present in the system. The unperturbed ground state of a system of N fermions in the independent particle approximation will be written as Φ_0, where

$$\Phi_0 = |1_1 1_2 1_3 \cdots 1_N 0_{N+1} 0_{N+2} \cdots 0\cdots\rangle \quad \text{——— (4)}$$

where the states are numbered in order of increasing energy. We note that $\psi^+(x)$ is an operator which adds a particle to the system at x.

The requirements of the pauli principle are satisfied if the fermion operators c, c^+ satisfy the anticommutation relations.

$$c_l c_m^+ + c_m^+ c_l = \delta_{lm} ; \quad c_l c_m + c_m c_l = 0 ; \quad c_l^+ c_m^+ + c_m^+ c_l^+ = 0 \quad \text{— (5)}$$

We write these as

$$\{c_l, c_m^\dagger\} = \delta_{lm} ; \quad \{c_l, c_m\} = 0 ; \quad \{c_l^\dagger, c_m^\dagger\} = 0 \qquad \text{—— (6)}$$

For a system with only a single state we represent $c^\dagger$ and c in the following way:

$$c^\dagger = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \frac{1}{2}(\sigma_x + i\sigma_y) ; \quad c = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \frac{1}{2}(\sigma_x - i\sigma_y) . \qquad \text{—— (7)}$$

where the σ's are the pauli matrices. Thus

$$c^\dagger c + c c^\dagger = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \text{—— (8)}$$

Further,

$$\left.\begin{aligned} cc + cc &= 2 \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} ; \\ c^\dagger c^\dagger + c^\dagger c^\dagger &= 2 \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} . \end{aligned}\right\} \qquad \text{—— (9)}$$

The 2×2 matrices are to be understood as operating on a two component state vector in the occupation number of the particle;

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} ; \quad |0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \qquad \text{—— (10)}$$

Corresponding to the possible fermion state occupancy numbers, 1 and 0.

We have the property

$$c^\dagger c |1\rangle = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = 1\begin{pmatrix} 1 \\ 0 \end{pmatrix} = 1|1\rangle ; \qquad \text{—— (11)}$$

and

$$c^\dagger c |0\rangle = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0\begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0|0\rangle \qquad \text{—— (12)}$$

Thus

$$\hat{n} = c^\dagger c \qquad \text{—— (13)}$$

is the number operator and has the eigenvalues 1 and 0 for the eigen states $|1\rangle$ and $|0\rangle$, respectively.