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A HAMILTONIAN FOR SUPERCONDUCTORS

by

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ABSTRACT

From consideration of the physical situation in the normal state of superconductors, namely that there are electron-electron, electron-ion, and ion-ion interactions, we show that the Hamiltonian for superconductors is similar to those obtained by the BCS group, as well as the Hubbard Hamiltonian. In our approximations, the electron-electron interaction is separated into two parts, namely the screened Coulombic, and collective interactions. Finally, only those terms in which electrons are paired, such as ($\underline{k}$, $-\underline{k}$), are chosen.

DERIVATION OF THE HAMILTONIAN

Various schemes have been put forward to explain the phenomenon of superconductivity, which remains an active area of research. Here, we assume that the Hamiltonian has the form

$$H = \sum_j \underline{p}^2/2m + \tfrac{1}{2}\sum_{i\neq j} e^2/|\underline{r}_i - \underline{r}_j| + \text{higher corrections} \qquad (1)$$

where $\underline{p}^2/2m$ is the kinetic energy of the free electron. The second term is the electron-electron interaction. The higher corrections include such effects as ion-ion and ion-electron interactions which have been neglected because the isotopic effect is now believed to be less important. Using the expansion

$$1/(|\underline{r}_i - \underline{r}_j|) \equiv V^{-1}\sum_k (4\pi/k^2)\exp(i\underline{k}\cdot(\underline{r}_i - \underline{r}_j))$$

and defining the frequency of oscillation of electrons as

$$\omega_e = (4\pi e^2 N_e/mV)^{\frac{1}{2}},$$

eq (1) becomes

$$H = \sum_j \underline{p}^2/2m + \tfrac{1}{2}\sum_{i\neq j}(\omega_e^2 m/N_e k^2)\exp(i\underline{k}\cdot(\underline{r}_i - \underline{r}_j)) \qquad (2)$$

where N_e is the number of electrons, V is the volume of the system, and m the mass of the electron. Using the following transformations:

$$Q_k = (m/N_e k^2)^{\frac{1}{2}}\sum_j \exp(i\underline{k}\cdot\underline{r}_j)$$

$$Q_{-k} = (m/N_e k^2)^{\frac{1}{2}} \sum_i \exp(-i\underline{k} \cdot \underline{r}_i),$$

we find

$$H = \sum_j \underline{p}^2/2m + \tfrac{1}{2} \sum_{k<k_c} \omega_e^2 Q_{-k} Q_k$$

$$+ \tfrac{1}{2} \sum_{i \neq j} \sum_{k>k_c} (\omega_e^2 m/N_e k^2) \exp(i\underline{k} \cdot (\underline{r}_i - \underline{r}_j))$$

where the electron-electron term has been separated into a collective part (the second term), and a screened Coulombic interaction part H_{sc} (the last term). Defining the canonical conjugates to Q_k and Q_{-k} as

$$p_k = (mN_e)^{-\frac{1}{2}} \sum_j (\underline{k} \cdot \underline{p}_j) \exp(i\underline{k} \cdot \underline{r}_j)/|\underline{k}|$$

$$p_{-k} = (mN_e)^{-\frac{1}{2}} \sum_j (\underline{k} \cdot \underline{p}_j^*) \exp(-i\underline{k} \cdot \underline{r}_j)/|\underline{k}|,$$

eq (2) becomes

$$H = \tfrac{1}{2} \sum_k p_k p_{-k} + \tfrac{1}{2} \sum_{k<k_c} \omega_e^2 Q_{-k} Q_k + H_{sc} \tag{3}$$

We now define the creation and annihilation operators for electrons, b_k^+ and b_k respectively, from the following equations:

$$Q_k = (\hbar/2\omega_e)^{\frac{1}{2}} (b_k + b_{-k}^+)$$

$$p_k = i(\tfrac{1}{2}\hbar\omega_e)^{\frac{1}{2}} (b_k^+ - b_{-k})$$

Finally, we define the density matrix as

$$\rho(k) = (2\pi)^{\frac{1}{2}} \sum_i \exp(i\underline{k} \cdot \underline{r}_i) \equiv \sum_{K,\sigma} b_{K\sigma}^+ b_{K'\sigma}$$

$$\rho(-k) = (2\pi)^{\frac{1}{2}} \sum_j \exp(-i\underline{k} \cdot \underline{r}_j) \equiv \sum_{K,\sigma'} b_{-K\sigma'}^+ b_{-K'\sigma'}$$

where $K = k + q$ and $K' = k' + q$. Then, eq (3) becomes

$$H = \tfrac{1}{2} \sum_k \hbar\omega_e b_k^+ b_k + \tfrac{1}{2} \sum_{k<k_c} \hbar\omega_e b_k b_k^+$$

$$+ \sum_{k>k_c} (2e^2/Vk^2) b_{k+q,\sigma}^+ b_{k'+q,\sigma} b_{-k,\sigma'}^+ b_{-k',\sigma'} \tag{4}$$

In eq (4), use was made of the fact that summation over allowed values of $-k$ merely duplicates the sum over k. Following the commutation rules for fermions:

$$[b_k, b_{k'}^+] = \hbar f_{kk'}$$

q (4) becomes

$$H = \sum_k \varepsilon_k b_{k\uparrow}^+ b_{k\uparrow} + \sum_{k<k_c} \varepsilon_k b_{k\downarrow} b_{k\downarrow}^+$$

$$-\tfrac{1}{2} \sum V b_{k+q,\uparrow}^+ b_{-k,\downarrow}^+ b_{-k',\downarrow} b_{k'+q,\uparrow} \tag{5}$$

Following the prescription of Bardeen, that is, taking only the

$q = 0$ part of the interaction, eq (5) becomes

$$H = \sum_{k} {}_{k} b^{+}_{k\uparrow} b_{k\uparrow} + \sum_{k<k_c} \varepsilon_k b_{k\downarrow} b^{+}_{k\downarrow} - \tfrac{1}{2} \sum_{k} V b^{+}_{k\uparrow} b^{+}_{-k\downarrow} b_{-k'\downarrow} b_{k'\uparrow} \tag{6}$$

This final expression for the Hamiltonian is similar to the various results in current use.

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