YAN SHI

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Abstract

Full Text

MATHEMATICAL PHYSICS

YAN SHI

THE METHOD OF CANONICAL TRANSFORMATION FOR STUDYING THE OVERHAUSER SPIN-DENSITY-WAVE STATE

(Presented by Academician N. N. Bogolyubov on 17 VI 1963)

The question of the ground and excited states of a system of interacting electrons has been studied by many authors ([1–3]). Recently Overhauser ([4,5]), in fact applying the idea of the microscopic theory of superconductivity ([6,7]), proposed, as the ground state in the Hartree–Fock approximation, to consider the so-called spin-density-wave state (s.d.w.).

As is known, in the theory of superconductivity the method of canonical transformation of N. N. Bogolyubov plays a major role (see ([7])). In the present work it will be shown that with the aid of this method it is easy to obtain all the basic results ([4,5]) and to generalize the theory of the s.d.w. to the case of the presence of a crystal lattice. In addition, the method of canonical transformation is very convenient for studying collective excitations.

Let us consider a system of N electrons situated in the periodic potential of the positive ions of a crystal lattice. We shall assume that the one-electron problem for the periodic potential has already been solved. For simplicity we consider the case where there is one valence electron for each ion, and we shall suppose that, as a result of the interaction among themselves, the electrons do not pass from one band to another. Then the Hamiltonian of the system can be written in the form

$$H = \sum_{k\sigma} E_k a^+_{k\sigma} a_{k\sigma} + \frac{1}{2N} \sum V_{k_1 k_2 k'_2 k'_1} a^+_{k_1\sigma_1} a^+_{k_2\sigma_2} a_{k'_2\sigma'_2} a_{k'_1\sigma'_1}, \qquad (1)$$

where $a^+_{k\sigma}, a_{k\sigma}$ are Fermi creation and annihilation operators of one-electron states (Bloch waves). In the second sum $k_1 + k_2 - k'_1 - k'_2 = 2\pi G$, where G is a reciprocal-lattice vector.

According to Overhauser ([4,5]), the most important interaction is that between electrons with wave vectors k and $k+Q$ and with opposite spins. We pass from the operators a to new Fermi operators b by the formulas

Fig. 1

Figure 1: Fig. 1

$$\begin{aligned} b_{k\uparrow} &= \cos\theta_k\, a_{k\uparrow} + \sin\theta_k\, a_{k+Q\downarrow}, \\ b_{k\downarrow} &= \sin\theta_k\, a_{k\uparrow} - \cos\theta_k\, a_{k+Q\downarrow}, \end{aligned} \tag{2}$$

where θ_k and Q are certain parameters, which are determined from the condition of minimum mean energy.

As the ground state we shall consider the state $|0\rangle$, for which the following conditions hold:

$$\begin{aligned} &b^+_{k\uparrow}|0\rangle = 0 \quad \text{for } k \in A; \\ &b_{k\uparrow}|0\rangle = 0 \quad \text{for } k \in \bar{A}; \\ &b_{k\downarrow}|0\rangle = 0 \quad \text{for all } k. \end{aligned} \tag{3}$$

Here the region A in k-space is the union of two regions—the region A_F, bounded by the Fermi surface, and the region A_F^Q, obtained from A_F by a shift through the vector $-Q$.

For symmetry reasons we shall assume that the vector Q is directed along one of the symmetry axes. Concerning the magnitude Q, we note that in the limiting case of the interaction being switched off, the ground state of the system must be the state of a degenerate Fermi gas. This corresponds to the solution: $\theta_k = 0$ in the region A_F, and $\pi/2$ in the region A_F^Q. In this case the magnitude Q must be such that the regions A_F and A_F^Q touch. (For example, if the Fermi surface is spherical, then Q is equal to twice its radius.) In the case of a nonvanishing interaction the values of Q are somewhat smaller, so that there is a small intersection of the two Fermi surfaces (Fig. 1).

The mean value of the energy in the state defined by the conditions (3) is equal to

$$\begin{aligned} \langle H\rangle = &\sum_{k\in A}\left(E_k\cos^2\theta_k + E_{k+Q}\sin^2\theta_k\right) - \\ &- \frac{1}{2N}\sum_{k_1k_2\in A}\Big(V_{k_1k_2,\,k_1k_2}\cos^2\theta_{k_1}\cos^2\theta_{k_2} + \\ &+ 2V_{k_1k_2+Q,\,k_1+Q\,k_2}\cos\theta_{k_1}\sin\theta_{k_1}\cos\theta_{k_2}\sin\theta_{k_2} + \\ &+ V_{k_1+Q\,k_2+Q,\,k_1+Q\,k_2+Q}\sin^2\theta_{k_1}\sin^2\theta_{k_2}\Big). \end{aligned} \tag{4}$$

Fig. 1

The variation of the mean energy with respect to θ_k must vanish for a stationary solution; this leads to the equation

$$(-E_k + E_{k+Q}) \sin 2\theta_k + \frac{1}{N} \sum_{k' \in A} \big(V_{kk',\,kk'} \sin 2\theta_k \cos^2 \theta_{k'} \tag{5}$$

$$- \operatorname{Re} V_{k\,k'+Q,\,k+Q\,k'} \cos 2\theta_k \sin 2\theta_{k'} - V_{k+Q\,k'+Q,\,k+Q\,k'+Q} \sin 2\theta_k \sin^2 \theta_{k'} \big) = 0.$$

Equation (5) may be written in the form

$$(-\varepsilon_k + \varepsilon_{k+Q}) \sin 2\theta_k - 2g_k \cos 2\theta_k = 0; \tag{6}$$

where

$$\varepsilon_k = E_k - \frac{1}{N} \sum_{k' \in A} V_{kk',\,kk'} \cos^2 \theta_{k'}; \tag{7}$$

$$\varepsilon_{k+Q} = E_{k+Q} - \frac{1}{N} \sum_{k' \in A} V_{k+Q\,k'+Q,\,k+Q\,k'+Q} \sin^2 \theta_{k'}; \tag{8}$$

$$g_k = \frac{1}{N} \sum_{k' \in A} \operatorname{Re} V_{k\,k'+Q,\,k+Q\,k'} \sin \theta_{k'} \cos \theta_{k'}. \tag{9}$$

The spectrum of one-particle excitations in the b-operators is calculated as the mean value of the energy over the corresponding one-particle states of the type $\langle b^+_{k\uparrow} H b_{k\uparrow} \rangle_{\text{av}}$, $\langle b_{k\downarrow} H b^+_{k\downarrow} \rangle_{\text{av}}$. As a result we obtain

$$\widetilde{E}_{k\uparrow} = \varepsilon_k \cos^2 \theta_k + \varepsilon_{k+Q} \sin^2 \theta_k - g_k \sin 2\theta_k, \tag{10}$$

$$\widetilde{E}_{k\downarrow} = \varepsilon_k \sin^2 \theta_k + \varepsilon_{k+Q} \cos^2 \theta_k + g_k \sin 2\theta_k.$$

Consequently, the minimization equation can also be written in the form

$$g_k = \frac{1}{N} \sum_{k' \in A} \operatorname{Re} V_{k\,k'+Q,\,k+Q\,k'} \frac{g_{k'}}{\widetilde{E}_{k'\downarrow} - \widetilde{E}_{k'\uparrow}} \tag{11}$$

or

$$g_k = \frac{1}{N} \sum_{k' \in A} \operatorname{Re} V_{k\,k'+Q,\,k+Q\,k'} \frac{g_{k'}}{2 \left[(\varepsilon_{k'} - \varepsilon_{k'+Q})^2/4 + g^2_{k'} \right]^{1/2}}. \tag{12}$$

Let us note that, when the interaction is switched off, we obtain only one trivial solution, $g_k = 0$. In the case of a nonvanishing interaction, however, there exists also a nontrivial solution. It differs from zero in the neighborhood of the point of intersection (k_0) of the regions A_F and A_F^Q, and goes to zero far from it. To obtain the explicit form of the nontrivial solution, we replace the potential V by a constant γ, and approximate the parameter g_k by a constant g near k_0 over a distance L, and by zero far away. Generally speaking, the regions A_F and A_F^Q may intersect at several points, and these points may prove to be inequivalent. In this case, for each type of inequivalent point we must introduce a parameter g_i. For g_i we obtain, from equation (12), a system of transcendental equations. In the simplest case, when the regions A_F and A_F^Q intersect at a single point, or all intersection points are equivalent, we obtain an explicit expression for g:

$$g = \mu L/2 \operatorname{sh}(8\pi^3\mu/\gamma S), \tag{13}$$

where

$$\mu = -\frac{Q}{Q} \operatorname{grad} \varepsilon_k \big|_{k=k_0} \qquad (k_0 Q = Q^2/2).$$

S —the transverse area between the solution (13) and the trivial one —is

$$\frac{\Delta\langle H\rangle}{N} = -\frac{\mu L^2 S}{32\pi^3}\left(\operatorname{cth}\frac{8\pi^3\mu}{\gamma S} - 1\right)$$

and is negative definite.

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Central Scientific-Research
Physico-Technical Laboratory
of the Academy of Sciences of the ArmSSR

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Note: Figure translations are in progress. See original paper for figures.