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ON THE ELECTRON-LATTICE INTERACTION BY THE METHOD OF BARDEEN AND PINES

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Abstract: A generalization of the method developed by Bardeen and Pines is performed by taking into account all three modes of acoustic vibrations in a monatomic lattice and including lowest-order non-RPA contributions into calculation.

1. *Introduction*

The basic feature of an electron-lattice system is that electrons tend to screen the field produced by ions and electrons themselves. Bardeen$^{1)}$ was the first to calculate the electron-phonon matrix element for normal metals in the Hartree approximation. This method was generalized by Toya$^{2)}$ to determine the phonon spectrum. Further progress was achieved when Fröhlich$^{3)}$ and Nakajima$^{4)}$ applied the canonical transformation method to the problem under consideration. By carrying out an appropriate transformation they derived a new Hamiltonian in which electrons are decoupled from phonons. This gives the longitudinal phonon dispersion relation, the corresponding effective electron-phonon matrix element, and the electron-electron interaction which appears as a consequence of the electron-phonon coupling. The approach by Bardeen and Pines$^{5)}$ was especially fruitful. They gave an extension of the collective-description method developed by Bohm and Pines$^{6)}$ to include excitations of the crystal lattice.

Toya$^{7)}$ and Bailyn$^{8)}$ included exchange and correlation effects into Bardeen's original procedure. Hone$^{9)}$ gave an alternative way of deriving physically equivalent results. Bross[10)] and Bross and Holz[11)] extended previous calculations to include transversal lattice vibrations. Since the integral equation derived by generalizing Nakajima's procedure to exchange terms has singular behaviour for zero momentum transfers, the screened potential is used instead of the bare Coulomb electron-electron potential in all practical calculations. This step can be easily understood in the framework of the Bohm-Pines collective theory. The long-range part of the electron-electron interaction describes plasma oscillations in metal, so that electrons interact effectively via short-range forces.

In the last few years a number of papers have contributed to a more detailed knowledge of phonon frequencies in solids. Batiyev and Prokovsky[12)] obtained expressions for phonon and electron energies by a diagrammatic technique. Sham[13)] developed a pseudopotential formalism for calculating the phonon spectrum and applied it to Na. Vosko, Taylor and Keech[14)] examined the influence of the electron-phonon interaction on lattice dynamics and determined phonon frequencies in Na, Al and Pb. Sham[15)] gave a microscopic formulation of the dynamical matrix in insulating crystals. Pick, Cohen and Martin [16)] derived expressions for force constants in terms of the electronic dielectric function. Brovman and Kagan[17)] found general expressions for the dynamical matrix in non-transition metals.

The purpose of the present paper is to examine the role of the electron-phonon interaction in metals by confining ourselves to the canonical transformation method. By generalizing the procedure of Bardeen and Pines the whole treatment will be performed along the same lines as in Refs.[10), 11)], with the difference that in our work an auxiliary plasmon field is explicitly introduced. This removes the singularity in the integral equation and modifies the phonon-induced electron-electron interaction.

2. *Canonical transformation*

We start from the Hamiltonian of a monatomic metal in which conduction electrons interact with the phonon field[18)]

$$H_{e\,ph} = \sum_{sp} E_p N_{sp} + \frac{1}{2} \sum_{k} V_k \varrho_k^{\star} \varrho_k + \frac{1}{2} \sum_{\sigma k} (\pi_{\sigma k}^{\star} \pi_{\sigma k} + \Omega_{\sigma k}^2 q_{\sigma k}^{\star} q_{\sigma k}) + \sum_{\sigma k} v_{\sigma k}' q_{\sigma k} \varrho_k^{\star}. \quad (1)$$

E_p is the Bloch energy of an electron, N_{sp} is the electron occupation operator in the state with momentum $\vec{p}$ and spin s, which is given in terms of electron creation and annihilation operators as

$$N_{sp} = c_{sp}^{\star}\, c_{sp},$$

ϱ_k is the electron density fluctuation operator

$$\varrho_k = \sum_{sp} c^*_{sp} c_{sp+k},$$

$\pi_{\sigma k}$ and $q_{\sigma k}$ are the conjugate pair describing the lattice vibration of the wave vector $\vec{k}$ and polarization $\sigma = 1, 2, 3$, Ω_k is the bare phonon frequency, $v'_{\sigma k}$ is the bare electron-phonon matrix element, and V_k describes the electron-electron interaction. If N denotes the ionic concentration, M the ionic mass, $\vec{e}_{\sigma k}$ the unit polarization vector, $\vec{R}_j$ the equilibrium position of the j-th atom, and $v(\vec{r} - \vec{R}_j)$ the electron-ion potential energy, we have

$$v'_{\sigma k} = -\frac{1}{\sqrt{NM}} \sum_j \vec{e}_{\sigma k} < \vec{p} + \vec{k} \,|\, \nabla v(\vec{r} - \vec{R}_j) \,|\, \vec{p} >, \tag{2}$$

$$V_k = \frac{4\pi e^2}{k^2} \,|\, < \vec{p} + \vec{k} \,|\, e^{i\vec{k}\vec{r}} \,|\, \vec{p} > |^2. \tag{3}$$

In the above expressions we have assumed that the matrix elements formed by Bloch waves depend only on the initial and final electron wave vectors. The nature of this approximation is discuseed by Brovman and Kagan$^{17)}$. This step is not essential for the present treatment, and it serves only to make the whole calculation as simple as possible.

It should be noted that $\vec{k}$ labelling the phonon variable in the electron-phonon coupling term may run out of the first Brillouin zone. In this case one chooses the value for $q_{\sigma k}$ which corresponds to the reduced wave vector.

In the collective-description method we consider the extended Hamiltonian

$$H = H_{e\,ph} + \frac{1}{2} \sum_k P^*_k P_k \tag{4}$$

together with a set of corresponding subsidiary conditions

$$P_k \Psi = 0, \qquad k < k_c, \tag{5}$$

where P_k is the momentum of the plasmon field and k_c is the largest wave number describing the collective behaviour of electrons. Relations (4) and (5) represented the starting point in the approach by Bardeen and Pines with difference that they took into account only longitudinal lattice waves.

Now we make a canonical transformation with the generating function

$$S' = \sum_{k<k_c} Q_k \left(-i \sqrt{V_k}\, \varrho^*_k + \sum_\sigma u_{\sigma k}\, q_{\sigma k}\right), \tag{6}$$

Q_k being the coordinate conjugate to P_k. In the transformed Hamiltonian

$$H' = e^{-\frac{i}{\hbar}S'} H_{e\,ph} e^{\frac{i}{h}S'}$$

we shall omit the nondiagonal contributions to the pure electron part and the phonon-plasmon coupling. Then after applying the sum rule[13)]

$$\sum_{sp} | < \vec{p} | e^{-i\vec{k}\vec{r}} | \vec{p} + \vec{k} > |^2 (E_{p+k} - E_p) N_{sp} = \frac{\hbar^2 k^2 N}{2m}, \tag{7}$$

where N and m denote the concentration and the mass of electrons, respectively, and introducing the follwing abbreviations

$$H_0 = \sum_{sp} E_p N_{sp} - \frac{1}{2} \sum_{spp'} V_{p-p'} N_{sp} N_{sp'} \Theta(|\vec{p}' - \vec{p}| - k_c) + \\ + \frac{1}{2} \sum_{\sigma k < \sigma_c} (\pi^\star_{\sigma k} \pi_{\sigma k} + \omega_k^2 q^\star_{\sigma k} q_{\sigma k}), \tag{8}$$

$$H_1 = \frac{1}{2} \sum_{spp'} V_{p-p'} N_{sp} N_{sp'} \Theta(|\vec{p}' - \vec{p}| - k_c) + \frac{1}{2} \sum_{k > k_c} V_k \varrho^\star_k \varrho_k, \tag{9}$$

$$H_2 = \sum_{sp\sigma k < k_c} v_{\sigma k p} c^\star_{sp} c_{sp-k} q_{\sigma k}, \tag{10}$$

$$H_3 = \sum_{sp\sigma k < k_c} (J_{\sigma k} - v_{\sigma k p}) c^\star_{sp} c_{sp-k} q_{\sigma k}, \tag{11}$$

$$H_4 = \frac{1}{2} \sum_{\sigma k < k_c} q^\star_{\sigma k} [q_{\sigma k} (\Omega^2_{\sigma k} - \omega_k^2) - \sum_{\sigma'} q_{\sigma' k} u_{\sigma k} u^\star_{\sigma' k}]. \tag{12}$$

$$H_5 = \frac{1}{2} \sum_{k < k_c} \Big[P^\star_k P_k + \Big(\frac{4\pi N e^2}{m} + \sum_{\sigma\sigma'} u_{\sigma k} u^\star_{\sigma' k} \Big) Q^\star_k Q_k + \\ + \frac{2}{\hbar} \sqrt{V_k}\, Q_k \sum_{sp} (E_p - E_{p-k}) c^\star_{sp} c_{sp-k} \Big] + \\ + \frac{1}{2} \sum_{\sigma k > k_c} (\pi^\star_{\sigma k} \pi_{\sigma k} + \Omega^2_{\sigma k} q^\star_{\sigma k} q_{\sigma k} + 2 v^l_{\sigma k} q_{\sigma k} q^\star_k), \tag{13}$$

the transformed Hamiltonian may be written as

$$H' = H_0 + H_1 + H_2 + H_3 + H_4 + H_5. \tag{14}$$

In the above expressions Θ is the usual step function

$$\Theta(x) = \begin{cases} 0 & x < 0 \\ 1 & x > 0, \end{cases} \tag{15}$$

ω_k is the renormalized phonon frequency, $v_{\sigma kp}$ is the effective electron-phonon matrix element, $J_{\sigma k}$ is given by

$$J_{\sigma k} = v'_{\sigma k} + i\sqrt{V_k}\, u^{*}_{\sigma k}, \tag{16}$$

while $u_{\sigma k}$ will be determined after the second transformation.

The accompanying set of subsidiary conditions now reads

$$\Big(P_k - i\sqrt{V_k}\,\varrho^{*}_{k} + \sum_{\sigma} u_{\sigma k}\, q^{*}_{\sigma k}\Big)\Psi' = 0, \qquad k < k_c, \tag{17}$$

Ψ' being the transformed wave function.

For the next generating function we choose

$$S = i \sum_{sp\sigma k < k_c} c^{*}_{sp}\, c_{sp-k} \left(f_{\sigma kp}\, q_{\sigma k} - i g_{\sigma kp}\, \pi^{*}_{\sigma k}\right). \tag{18}$$

Up to the second-order terms in the electron-phonon coupling, a new Hamiltonian can be expanded as

$$H_{\text{new}} = H' + \frac{i}{\hbar}[H_0 + H_1 + H_2 + H_3, S] + \frac{1}{2}\left(\frac{i}{\hbar}\right)^2 [[H_0 + H_1, S], S] + \dots. \tag{19}$$

In the following calculation we shall keep the RPA and diagonal exchange terms. The latter are caused by the second term in H_1, which describes short-range forces between electrons.

Conditions to be imposed on the unspecified quantities $u_{\sigma k}$, $f_{\sigma kp}$, $g_{\sigma kp}$, $v_{\sigma kp}$ and ω_k are as follows:

— the parameter $u_{\sigma k}$ is defined by the requirement that phonon variables should not enter the subsidiary conditions in the lowest order of the coupling constant. This leads to

$$u_{\sigma k} = \frac{i\sqrt{V_k}}{\hbar} \sum_{sp} (N_{sp} - N_{sp-k}) f^{*}_{\sigma kp}; \tag{20}$$

— we demand that

$$\frac{i}{\hbar}[H_0, S] + H_2 = 0, \tag{21}$$

which is easily solved to give

$$g_{\sigma kp} = -\frac{\hbar f_{\sigma kp}}{\varepsilon_p - \varepsilon_{p-k}}, \tag{22}$$

$$f_{\sigma kp} = \hbar v_{\sigma kp} \frac{\varepsilon_p - \varepsilon_{p-k}}{(\varepsilon_p - \varepsilon_{p-k})^2 - \hbar^2 \omega_k^2}. \tag{23}$$

Here ε_p is the one-electron energy including the Hartree-Fock screened contribution

$$\varepsilon_p = E_p - \sum_{p'} V_{p-p'} N_{sp'} \Theta(|\vec{p}' - \vec{p}| - k_c). \tag{24}$$

Inserting (20) and (23) into (16), we arrive at

$$J_{k\sigma} = v_{\sigma k}^l + V_k \sum_{sp} v_{\sigma kp} (\varepsilon_p - \varepsilon_{p-k}) \frac{N_{sp} - N_{sp-k}}{(\varepsilon_p - \varepsilon_{p-k})^2 - \hbar^2 \omega_k^2}; \tag{25}$$

— the term $i\,[H_1, S]/\hbar$ describes the effect of the electron interaction calculated in the Hartree-Fock approximation on the electron-phonon coupling. We require that this commutator is compensated by the term from expression (11):

$$\frac{i}{\hbar}[H_1, S] + H_3 = 0. \tag{26}$$

This implies that $v_{\sigma kp}$ satisfies the integral equation

$$v_{\sigma kp} = v_{\sigma k}^l + \sum_{p'} v_{\sigma kp'} (\varepsilon_{p'} - \varepsilon_{p'-k}) \frac{N_{sp'} - N_{sp'-k}}{(\varepsilon_{p'} - \varepsilon_{p'-k})^2 - \hbar^2 \omega_k^2} \cdot$$

$$\cdot [2V_k - V_{p-p'} \Theta(|\vec{p}' - \vec{p}| - k_c]. \tag{27}$$

In the adiabatic approximation $\omega_k \to 0$, (27) reduces to the equation derived by Bailyn$^{8)}$ and Hone$^{9)}$ for the effective matrix element describing electron scattering on longitudinal phonons;

— the phonon spectrum is determined by the condition that H_4 should cancel the corresponding part of $i\,[H_2 + H_3, S]/2\hbar$. This yields the linear homogeneous algebraic system

$$q_{\sigma k}(\omega_k^2 - \Omega_{\sigma k}^2) + i \sum_{\sigma'} q_{\sigma' k} v_{\sigma' k}^l \frac{u_{\sigma k}}{\sqrt{V_k}} = 0, \tag{28}$$

from which it follows

$$\det \left| i\, v'_{\sigma' k} \frac{u_{\sigma k}}{\sqrt{V_k}} + (\omega_k^2 - \Omega_{\sigma k}^2)\, \delta_{\sigma' \sigma} \right| = 0. \tag{29}$$

Inserting the roots ω_{1k}, ω_{2k} and ω_{3k} of the dispersion relation (29) into (19) after applying relations (20), (21) and (26), the new Hamiltonian becomes

$$H_{\text{new}} = \sum_{sp} E_p N_{sp} + \frac{1}{2} \sum_{\sigma k < k_c} (\pi_{\sigma k}^{\star} \pi_{\sigma k} + \omega_{\sigma k}^2 q_{\sigma k}^{\star} q_{\sigma k}) +$$

$$+ \frac{1}{2} \sum_{k > k_c} V_k \varrho_k^{\star} \varrho_k + H_5 + \frac{\hbar^2}{2} \sum_{sp\sigma k < k_c} J_{\sigma k}^{\star} v_{\sigma k p} \varrho_k \cdot \frac{c_{sp}^{\star} c_{sp-k}}{(\varepsilon_p - \varepsilon_{p-k})^2 - \hbar^2 \omega_\sigma^2}. \tag{30}$$

The shift in electron energy caused by lattice vibrations is equal to the diagonal part of the last term in (30)

$$\Delta E_e = \frac{\hbar^2}{2} \sum_{sp\sigma k < k_c} J_{\sigma k}^{\star} v_{\sigma k p} N_{sp-k} \frac{1 - N_{sp}}{(\varepsilon_p - \varepsilon_{p-k})^2 - \hbar^2 \omega_{\sigma k}^2}.$$

Disregarding the non-RPA contributions and assuming that $v'_{\sigma k}$ is different from zero only for the longitudinal mode, one arrives at the results derived in the original work by Bardeen and Pines. On the other hand, the last term in (30) goes over into the corresponding result derived by Bross10) if $J_{\sigma k}$ is replaced by the bare matrix element $v'_{\sigma k}$. It must be emphasized, however, that this resemblance is only formal, because in the derivation of the dispersion relation (29) we did not neglect the coupling of the different phonon modes.

References

1) J. Bardeen, Phys. Rev. **52** (1973) 688;
2) T. Toya, Busseiron Kenkyu **59** (1952) 179;
3. H. Fröhlich, Proc. Roy. Soc. **A215** (1952) 291;
4) S. Nakajima, Proceedings of the International Conference on Theoretical Physics, Kyoto and Tokyo, September 1952, Science Council of Japan, Tokyo 1954;
5) J. Bardeen and D. Pines, Phys. Rev. **99** (1955) 1140;
6) D. Bohm and D. Pines, Phys. Rev. **92** (1953) 609;
7) T. Toya, J. Res. Inst. Catal. **6** (1958) 161;
8) M. Bailyn, Phys. Rev. **117** (1960) 974;
9) D. Hone, Phys. Rev. **120** (1960) 1600;
10) H. Bross, Phys. Letters **13** (1964) 15;
11) H. Bross and A. Holz, Z. Naturforschung **20a** (1965) 504;
12) E. G. Batiyev and V. L. Pokrovsky, ŽETF **46** (1964) 262;
13) L. J. Sham, Proc. Roy. Soc. **A283** (1965) 33;
14) S. H. Vosko, R. Taylor and G. H. Keech, Canad. J. Phys. 43 (1965) 1187;
15) L. J. Sham, Phys. Rev. **118** (1969) 1431;
16) R. M. Pick, M. H. Cohen and R. M. Martin, Phys. Rev. **B1** (1971) 910;
17) E. G. Brovman and J. Kagan in Dynamic Properties of Solids I, p. 191, edited by G. K. Horton and A. A. Maradudin, North-Holland Publishing Company, Amsterdam (1974);
18) D. Pines, Elementary Excitations in Solids, W. A. Benjanim, New York-Amsterdam (1963);
19) P. Nozieres and D. Pines, Phys. Rev. **109** (1958) 741.

O MEĐUDJELOVANJU ELEKTRONA S REŠETKOM U METODI BARDEENA I PINESA

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Sadržaj

Metoda Bardeena i Pinesa u teoriji elektron-fonon interakcije poopćena je uzimajući u obzir sva tri akustička titranja monoatomne kristalne rešetke i uključujući u račun popravke najnižeg reda aproksimaciji slučajnih faza.