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The Steady States of an Electron in a [illegible] Modulated Lattice, II.

by

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Abstract

This paper is a continuation of the previous report under the same title, dated May 18th 1953. In this paper a more general expression is obtained for the steady states, and a beginning is made towards developing a theory of electrical resistance at very low temperatures, based on the new point of view.

Introduction

The system under discussion consists of an electron and a lattice with its spectrum of normal modes, or phonons. The Hamiltonian involves three terms, the electron in the lattice field, the phonons, and the interaction between the electron and phonons that occurs because of the phonon modulations of the lattice potential. In Bardeen's recent work (1) this whole system is treated quantum-mechanically*, a suitable wave function being a product of two factors: (a) a Bloch function of the electron coordinates, and (b) a function of the generalized oscillator coordinates of the normal modes of the lattice. The significance of this procedure does not seem to have been generally

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* Bardeen's work was incorrectly assessed in the first report, p.10.

recognized. In our previous thinking on this problem, the interaction between electron and phonon has been taken as a time-dependent perturbation of the field in which the electron moves, the phonon being nothing more than the classical motion of the lattice points (2); and the resistance of the lattice was thought to be due to the scattering of the electron due to this time-dependent perturbation.

The new quantum-mechanical picture of the phonons has the effect of replacing the classical motion of the lattice points by harmonic oscillator probability functions, and the perturbation due to the interaction between phonons and electron no longer contains time explicitly, but is a function only of the generalized coordinates of the normal modes and the position variable of the electron wave function.

In such a system there can be no question of scattering from one state to another in the course of time because time is absent from the Hamiltonian completely. Standard perturbation theory, if applied correctly and consistently to this new problem, leads automatically to steady state solutions. Even though these steady state solutions may not in practice be found exactly, they do in principle exist. These solutions are steady in the sense that the system as a whole, electron plus lattice, does not change with time. One quantum of energy passes continually back and forth between the electron and lattice. From the classical point of view, when a quantum of energy passes from the electron to the lattice, it is there lost to heat, and electron scattering results. On the new point of view there is a resonance between lattice and electron, so the quantum is not lost but presently returned to the electron. Such a resonance was inconceivable classically but is an inevitable result of the true quantum picture.

Bearing these points in mind, one is led to more general wave functions than those used by Bardeen. In his work it was assumed that the phonons remain in their lowest zero-point energy states. On the present picture this can hardly be satisfactory, because energy necessarily passes back and forth between lattice and electron, so that the phonons get excited by the resonance process.

The resonance states

To describe the combined system, we use Bloch free-electron wave functions $u(k,r)$ where k is the wave-number vector. For the phonons we use the normal modes of the lattice: the displacement of a lattice point at equilibrium position Q, due to the p^{th} normal mode is classically

$$Y_p(Q) = A_p e^{iw_p t} \cos(\tfrac{1}{2}p.Q) \qquad (1)$$

where w_p is the angular frequency of the p^{th} mode, p is the vector $(2\pi/L)$ times the integral set of wave numbers, and the cosine is to be understood as the product of three cosines, one for each dimension of the crystal, side L. The coefficients

$$y_p(t) = A_p e^{iw_p t} \qquad (2)$$

are generalized coordinates for the phonon motion, and the classical Hamiltonian in terms of these coordinates is well-known (3):

$$H_{phon} = \tfrac{1}{2}\sum_p \dot{y}_p^2 + \tfrac{1}{2}\sum_p y_p^2 w_p^2 \qquad (3)$$

Following Bardeen, we now treat the phonon part of the problem by replacing the Hamiltonian (3) by the operator

$$H_{phon}\phi = -\tfrac{1}{2}\hbar^2\sum_p \partial^2\phi/\partial y_p^2 + \tfrac{1}{2}\sum_p w_p^2 y_p^2 \phi \qquad (4)$$

The eigenfunctions ϕ are products of Hermite polynomials of the simple harmonic oscillator, one for each normal mode coordinate, the eigenvalues being sums of the terms $(n_p + \tfrac{1}{2})\hbar w_p$:

$$\phi(\{n\},\{y\}) = \prod_p N_{np}\, e^{-\frac{1}{2}\alpha_p y_p^2}\, H_{np}(\sqrt{\alpha_p}\, y_p) \qquad (5)$$

where $\alpha_p = w_p/\hbar$, and N_{np} are normalization constants. This function depends on all the normal coordinates y_p, and the state is specified by the set of quantum numbers n_p, one for each mode, collectively represented by the symbol $\{n\}$.

Coupling between the electron and phonons is secured through the phonon modulation of the lattice potential. If the phonon amplitudes are not too great, we may neglect anharmonic effects, and the potential modulation is proportional to the relative displacements of the lattice points, so that we may write for this modulation:

$$V = \sum_p K_p\, y_p \sin(\tfrac{1}{2}p\cdot r) \qquad (6)$$

where again a product of three sines is understood, y_p is the normal mode coordinate of eq.(2), and K_p a proportionality constant depending on the form of the lattice potential. Note that V is not a function of time explicitly.

The combined Hamiltonian is now

$$H = -(\hbar^2/2m)\nabla^2 + H_{phon} + V_{latt} + V \qquad (7)$$

where V_{latt} is the potential of an electron in the ideal lattice. If V were zero, the eigenfunctions of H would be

$$\Psi_0[(\{n\},k)(\{y\},r)] = u(k,r)\phi(\{n\},\{y\}) \qquad (8)$$

We now regard V as a perturbation, not time-dependent, and therefore seek linear combinations of eigenfunctions like (8) for the perturbed Hamiltonian. Bardeen does this by forming linear combinations of the Bloch functions, retaining the oscillator factor ϕ unchanged. This procedure is not consistent with our present picture, which must allow for excitation of the phonons also. Instead we therefore form the more general linear combination as follows:

$$\Psi[(\{n\},k)(\{y\},r)] = u(k,r)\phi(\{n\},\{y\}) + \sum_{(\{m\},j) \neq (\{n\},k)} C(\{m\},j)\, u(j,r)\phi(\{m\},\{y\}) \qquad (9)$$

[illegible] that the [illegible] $c(\{m\},j)$ are [illegible]

[illegible] of electrons is to be represented by a determinant formed from (5) with respect to some specified spectrum of k vectors. For the present we shall not be concerned with the effects of the exclusion principle, and will omit the complications of formalism needed to handle the determinant forms.

Standard perturbation procedure applied to (9) leads at once to

$$c(\{m\},j)\left[E^{o}(\{n\},k) - E^{o}(\{m\},j)\right] =$$

$$\delta(\{m\},\{n\})(j|V_{latt}|k) + \sum_{p}(j|\sin \mathbf{p}\cdot\mathbf{r}|k)(\{m\}|y_p|\{n\})K_p \qquad (10)$$

where $$E^{o}(\{n\},k) = \sum_{p} n_p \hbar w_p + \hbar^2 k^2/2m^* \qquad (11)$$

Here the matrix elements $(j|\ |k)$ are with respect to the Bloch functions, and the elements $(\{m\}|\ |\{n\})$ are with respect to the oscillator functions. The mass m^* is the effective mass of the electron for the Bloch functions.

Now the elements $(\{m\}|y_p|\{n\})$ of the matrix of y_p are all zero except those for which one and only one member, m_p of the set $\{m\}$ differs from the corresponding member n_p of the set $\{n\}$ by unity:

$$m_p = n_p \pm 1 \qquad (12)$$

in which case

$$(\{m\}|y_p|\{n\}) \text{ is either } (n_p + 1)^{\frac{1}{2}}\hbar/2w_p \text{ or } n_p^{\frac{1}{2}}\hbar/2w_p \qquad (13)$$

Again the matrix elements $(j|c\{n\}_p^{\pm}.r|k)$ vanish unless

$$j - k = p \tag{14}$$

in which case the element equals unity. Thus we may express the eigenfunctions (9) in the form

$$\Psi(\{n\},k)(\{y\},r) = u(k,r)\phi(\{n\},\{y\}) +$$

$$\sum_{j\neq k} \frac{(j|V_{latt}|k)u(j,r)\phi(\{n\},\{y\})}{E^0(\{n\},k) - E^0(\{n\},j)} +$$

$$\sum_p \frac{(K_p\hbar/2w_p)(n_p+1)^{\frac{1}{2}}\, u(k+p,r)\phi(\{n^+\},\{y\})}{E^0(\{n\},k) - E^0(\{n^+\},k+p)} +$$

$$\sum_p \frac{(K_p\hbar/2w_p)\, n_p^{\frac{1}{2}}\, u(k+p,r)\phi(\{n^-\},\{y\})}{E^0(\{n\},k) - E^0(\{n^-\},k+p)} \tag{15}$$

where $\{n^+\}$ is identical with $\{n\}$ except that $n_p^+ = n_p + 1$ and $\{n^-\}$ is identical with $\{n\}$ except that $n_p^- = n_p - 1$.

The energy of this state to second order terms is

$$E(\{n\},k) = E^0(\{n\},k) + L^{-3}\int V_{latt}\, dr +$$

$$\sum_j{}' (j|V_{latt}|k)^2 \Big/ \left[E^0(\{n\},k) - E^0(\{n\},j)\right] +$$

$$\sum_p (K_p\hbar/2w_p)^2(n_p+1) \Big/ \left[E^0(\{n\},k) - E^0(\{n^+\},k+p)\right] +$$

$$\sum_p (K_p\hbar/2w_p)^2\, n_p \Big/ \left[E^0(\{n\},k) - E^0(\{n^-\},k+p)\right] \tag{16}$$

The last two expressions represent the resonance energy of the electron, in second order, in response to entire acoustical spectrum present in the lattice.

The above approximation fails only when degeneracy occurs between states for which the numerators do not vanish identically. This occurs with the expression in the second line of (16) at the Bloch zone boundaries, and is removed in the familiar fashion leading to energy discontinuities at the zone boundaries. The resonance terms give similar trouble when the wave number vector k has any of the special values at which

$$(\hbar^2/2m^*)(k + p)^2 - \hbar^2k^2/2m^* = \pm \hbar w_p \qquad (17)$$

when the kinetic energy change in the electron exactly equals the accompanying change in acoustical energy. If θ is the angle between the vectors k and p, and if c is the velocity of propagation of the phonon in the lattice, this condition can be written

$$2k \cos\theta = - p \pm m^*c/\hbar \qquad (18)$$

The trouble is removed in the same way as with the zone boundaries. For any state k for which (18) is true, the state $k+p$ must be included in the wave function in zeroth order. The linear combination in zeroth order that diagonalizes the singular matrix ($\underline{A}$) is easily found to be: Case i, positive sign in eq.(18).

$$\Psi_0 = 2^{-\frac{1}{2}}\left[u(k,r)\phi(\{n^*\},y) \pm u(k+p,r)\phi(\{n\}_i,y)\right] \qquad (19)$$

The two signs here give the two alternative perturbed zeroth-order wave functions corresponding to the two unperturbed wave functions at $(\{n\}, k)$ and $(\{n^{+}\}, k+p)$. Case ii, negative sign in eq.(19):

$$\Psi_o = 2^{-\frac{1}{2}}\left[u(k,r)\phi(\{n^{-}\},y) \pm u(k+p,r)\phi(\{n\},y)\right] \qquad (20)$$

The first order perturbation energy accompanying these zeroth order resonances is:

$$\begin{aligned} &\text{Case i:} && \pm \tfrac{1}{2}\hbar K_p(n_p+1)^{\frac{1}{2}}/w_p \\ &\text{Case ii:} && \pm \tfrac{1}{2}\hbar K_p\, n_p^{\frac{1}{2}}/w_p \end{aligned} \qquad (21)$$

The lowest energies are in general those in resonance with the lowest frequency phonons.

Evidently the currents carried by these resonance states are oscillatory in time, but their mean values are simple means between the free-particle currents corresponding to the wave number vectors k and k+p. The resistance of the lattice due to these pure phonon interactions is therefore absolutely zero. A state of zero current is always available by combining two resonance states corresponding to opposite currents, and will in general be lower in energy than a state of finite net current.

A possible resistance mechanism

As emphasized in the previous report, the resistance of the phonon-modulated lattice ceases to be zero only through random transitions among the phonon states induced by thermal fluctuations. To find a mechanism for such random transitions it is not necessary to include anharmonic terms in the Hamiltonian. In an ideal crystal model, set up for the discussion of the Debye theory of specific heat, the phonons are standing waves produced by reflection at the perfect boundaries. We now consider a single domain having all the ideal characteristics required, except that it is surrounded by a thermal bath. Here its surface is subjected to random pressure fluctuations, which, translated, means it is bombarded by random acoustic impulses. The standing waves within the crystal are then subject to random changes in phase through the motion of the reflecting boundaries. Such phase shifts show up in eq.(2) in the form

$$y_p' = y_p \, e^{i\delta_p} \tag{22}$$

where y_p' is the modified generalized coordinate and the phase shift is δ_p corresponding to the p^{th} mode. The Hermitian form of Hamiltonian perturbation corresponding to such a phase shift in eq.(3) is easily shown to have the form

$$H_p' = \tfrac{1}{2}w_p^2 \sin(2\delta_p) \, y_p^2 \tag{23}$$

and when the phase shift is sufficiently small we may write

$$H_p' = w_p^2 \, y_p^2 \, \delta_p \tag{24}$$

The matrix of this perturbation with respect to the unperturbed harmonic oscillator wave functions of H_{phon} contains only three sets of components as follows:

$$
\begin{aligned}
(n_p|H'_p|n_p+2) &= \tfrac{1}{4}\hbar w_p\delta_p\sqrt{(n_p+1)(n_p+2)} \\
(n_p|H'_p|n_p) &= \tfrac{1}{2}\hbar w_p\delta_p\,(n_p+1) \qquad (25) \\
(n_p|H'_p|n_p-2) &= \tfrac{1}{4}\hbar w_p\delta_p\sqrt{(n_p)(n_p-1)}
\end{aligned}
$$

The perturbed oscillator wave function, to first order in δ_p, is

$$\phi_p = \phi_{op} + \tfrac{1}{8}\delta_p\phi_{+p}\sqrt{(n_p+1)(n_p+2)} - \tfrac{1}{8}\delta_p\phi_{-p}\sqrt{n_p(n_p-1)} \qquad (26)$$

where ϕ_{op} is the unperturbed oscillator function, ϕ_{+p} is the unperturbed oscillator function with n_p+2 replacing n_p, and ϕ_{-p} the same with n_p-2 replacing n_p. The probability that the system be removed from its original state ϕ_{op} by the single phase jump is therefore $\tfrac{1}{8}\delta_p^2(1+n_p+n_p^2)$ If G_p such phase jumps occur per unit time, we can define a relaxation time τ_p for the scattering out of the original state:

$$1/\tau_p = \tfrac{1}{8}G_p\delta_p^2\,(1+n_p+n_p^2) \qquad (27)$$

At ordinary temperatures those transitions in phase and resulting transitions in phonon states, would be so rapid, presumably, that it is useless to picture the electrons as forming resonance states with the individual phonon states: τ_p, the life-time of the phonon state being too short. The standard picture of resistance in which the electrons are scattered out of their ordinary momentum states, is then the more realistic. But at sufficiently low temperatures, we may reasonably suppose that the life-time of the phonon states becomes long enough and the picture here developed becomes useful: namely that the electrons form resonance states with the phonon states, and get shaken out of these resonance states only through the phonon-transitions with a frequency given by (27).

It is clear now that on the present model, electrical resistance can vanish at a finite temperature only if the phase jumps due to fluctuations disappear. Let us consider what happens when a phase shift is produced at a fluctuating boundary. The phase shift cannot immediately affect the standing wave as a whole, but is propagated throughout the crystal with the speed of sound. Meanwhile an energy of misfit exists in the lattice at the area of contact between the old and the new phase regions. It therefore takes a positive energy to produce the phase shifts, and it is quite conceivable that at low enough temperatures the fluctuation mechanism may be unable to supply the required energy. It is possible to prove, in terms of a plausible model, that a transition temperature exists below which phase coherence begins to build up.(5). Such a phase coherence would increase the life-time of phonon states and open the way for superconductivity.

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