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Linear and Nonlinear Electronic Transport in Electron-Phonon Systems: Self-Consistent Approach within the Path-Integral Formalism

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The expectation value of the steady-state velocity acquired by an electron interacting with the phonons of a crystal in finite electric and magnetic fields is analyzed quantum mechanically for arbitrary coupling strength, field strengths, and temperature. The rate of loss of momentum by an electron drifting through the crystal in the applied fields is expressed in a form in which the lattice coordinates (the phonons) have been eliminated exactly by path-integral methods. The quadratic influence functional used to simulate the electron-lattice interaction is shown to be derivable from a self-consistent relation for the impedance tensor of the electron in its drifting frame of reference. This eliminates the ambiguity of which influence functional to use in path-integral treatments of electron transport. For zero applied electric and magnetic fields, it is shown that the self-consistency is equivalent to minimizing the free energy of the electron-phonon system at *finite* temperatures. The Feynman one-oscillator model is discussed in the light of the self-consistency relation. Several important changes are indicated by an approximate self-consistent solution for low temperature. The applied magnetic and electric field problem is briefly discussed. For optical-phonon scattering, it is shown that the cyclotron mass is the same as the dynamic effective mass in the absence of a magnetic field. For the Fröhlich polaron model, it is shown that, because of the influence of the magnetic field on the scattering rate, a longitudinal magnetoresistivity should exist equal to exactly one-half of the transverse value. Finally, two limitations of this general approach are noted and discussed briefly.

I. INTRODUCTION

The path-integral method offers a unique advantage in discussing electron-phonon systems.[1-5] If the electron-lattice interaction is linear in the lattice variables (the phonon approximation), then these lattice variables can be eliminated *exactly*, and the problem can then be written in terms of the electronic coordinates alone. The simplification thus achieved is remarkable as demonstrated in previous papers discussing the polaron problem.[1-5]

There is one difficulty, however. Written in terms of electron coordinates alone, the method cannot be completed without making some approximation. For weak coupling problems one may use one of several perturbation techniques. As the coupling increases, however, these expansion techniques quickly become unwieldy, and one searches for an alternative approach. The most successful alternative is due to Feynman[1] who attempted to simulate the exact influence functional by an approximate harmonic one which imitated the exact functional as well as possible while still permitting the calculation to be completed. After deriving a variational principle which gave an upper bound to the ground-state energy of an electron interacting with an arbitrary distribution of phonons, he used as influence functional the now well-known one-oscillator trial distribution whose strength and frequency are variational parameters used to minimize the ground-state energy at zero temperature. This method was soon generalized to finite temperature.[6]

Following this success for calculating self-energy, transport properties including mobility,[7] impendance,[2] and velocity-field characteristics[4,5] were investigated using harmonic in place of the exact influence functionals. However, there was no longer any guarantee that just because a particular choice of influence functional minimized the self-energy that this was necessarily the optimum choice for the particular transport problem under investigation. (Unfortunately, this problem of optimization still remains.) Nonetheless, Feynman *et al.*[2] (hereafter referred to as FHIP) were able to derive a self-consistent set of equations for the impedance from the minimization principle for the self-energy at *zero* temperature. The generalization to finite temperatures, though not explicitly stated, was implicitly evident from the nature of these equations and those derived in connection with the impedance.[8] These equations can be derived from the minimization principle for the free energy at *finite* temperature, as we show in Appendix A. They are also derived here using a method of rates.

More recently in the nonlinear problem of calculating the velocity-field dependence for arbitrary coupling, temperature, and field strength,[4,5] we were forced to fall back on the Feynman one-oscillator influence functional for lack of anything better. This was particularly unfortunate because in the region of maximum energy loss per unit distance the electron's relative motion is certainly appreciably

hotter than given by the one-oscillator model at the lattice temperature. Also, one can apply a strong magnetic field to calculate Hall mobility and cyclotron mass, and again one expects the harmonic influence functional to depend on the applied fields. Finally, while the one-oscillator model is physical for the polaron problem where an energy threshold exists for phonon emission, in order to deal with acoustic phonons where phonons of any energy can be emitted, it is clear one must have some procedure to determine a more physical model interaction. Moreover, little motivation for this can be sought from trying to minimize the free energy. For finite electric fields, energy loss is so important that the real and imaginary parts of the self-energy are comparable. For the drifting electron problem, one must pass to imaginary velocity variables. We do not pursue such approaches here.

This paper presents a simple physical self-consistent technique to calculate both linear and nonlinear transport properties of electron-phonon systems within the path-integral method. The expectation value of the rate of change of momentum operator equation is calculated for a general harmonic influence functional. The influence functional is then determined self-consistently by obtaining an expression for the impedance of the particle from both the rate equation and from an admittance equation. For example, consider the problem of finite applied magnetic and electric fields. The electron will acquire some steady-state expectation drift velocity. Transforming the problem to this drifting frame, one can now apply a small electric field to determine the impulse response of the electron under these conditions. This impulse response also can be related directly to the trial influence functional. Thus the impulse response is a functional of the influence functional, which is in turn a functional of the impulse response. This then yields a self-consistent relation for these functionals. Once the influence functional is determined, the drift velocity can be related to the strengths of the electric and magnetic fields, the desired solution.

We permit any number of phonon modes of any character to interact with the electron, since modes of different character but of comparable strength cannot be treated separately. Since we are primarily interested in the effect of the phonon scattering, it is assumed that in the undeformed lattice the electron would move as a free particle, possibly with an altered mass tensor. While it is possible to treat the effects of the undeformed lattice on the electron in this formalism, we make no claim that such band-structure effects beyond an effective mass tensor can be represented nearly as well as the phonon-scattering effects. We are not interested in the problem of the electron weakly coupled to the phonons. Our primary interest lies in those problems where the amount of scattering by phonons may exceed that due to the fixed lattice. That such is quite possible has been more fully discussed before.[5]

We begin by stating the problem and deriving the self-consistent set of equations. The integration over electron paths is slightly more general than before. We include the possibility of a finite uniform magnetic field and permit the crystal to be oriented arbitrarily with respect to this field. The influence functional and impedance are then tensors rather than scalars as before. This, however, requires little additional effort over the previous treatment. We then consider the self-consistent influence functional for the impedance problem of FHIP and find that the Feynman one-oscillator model approximates a distribution of oscillators in the same way that a simple pole approximates a cut from threshold to infinity in scattering theory. We also comment on Hall mobility, cyclotron mass, and magnetoresistance for the Fröhlich polaron in perpendicular electric and magnetic fields. Finally, two limitations of this general approach are noted and discussed briefly.

II. FORMULATION OF TRANSPORT PROBLEM IN TERMS OF ELECTRON COORDINATES ALONE

The relevant Hamiltonian for transport problems, which describes the interaction of the electron with the applied time-invariant electric and magnetic fields $\vec{E}$ and $\vec{H}=\vec{\nabla}\times\vec{A}$, a small oscillatory electric field $\vec{e}_t$, and all varieties of phonons n, may be written

$$\begin{aligned} H=&\tfrac{1}{2}(\vec{p}-q\vec{A}/c)\cdot(1/\overleftrightarrow{m})\cdot(\vec{p}-q\vec{A}/c)\\ &-q\vec{E}\cdot\vec{x}-q\vec{e}_t\cdot\vec{x}+\textstyle\sum_n\sum_{\vec{k}}\hbar\omega_{\vec{k},n}a^\dagger_{\vec{k},n}a_{\vec{k},n}\\ &+V^{-1/2}\textstyle\sum_n\sum_{\vec{k}}(C_{\vec{k},n}a_{\vec{k},n}\exp(i\vec{k}\cdot\vec{x})\\ &+C^*_{\vec{k},n}a^\dagger_{\vec{k},n}\exp(-i\vec{k}\cdot\vec{x}))\,, \end{aligned} \tag{1}$$

where $1/\overleftrightarrow{m}$ is the (symmetric) reciprocal effective-mass tensor, V is the volume of the system, and $C_{\vec{k},n}$ is the amplitude for an electron to absorb a phonon of type n and wave vector $\vec{k}$. With this H we can calculate expectation values of any operator $\hat{O}$ at time t as follows:

$$\langle\hat{O}\rangle_t\equiv \mathrm{Tr}(\hat{O}\rho_t)/\mathrm{Tr}\rho_t\,, \tag{2}$$

where ρ_t is the density matrix given by

$$\rho_t=\exp(-i\textstyle\int_{t_1}^t H_s ds/\hbar)\,\rho_{t_1}\exp(+i\int_{t_1}^t H'_{s'}ds'/\hbar). \tag{3}$$

In (3) the standard Feynman ordered-operator convention applies.[9]

We are interested in two expectation quantities here. We shall determine the linear impulse response, the quantity calculated in FHIP, and the rate of change of momentum, the quantity calculated in Thornber and Feynman (TF), [5] with two important differences. First, the full impulse-response tensor is calculated in the drifting frame to zero order, the influence functional being sufficiently accurate that the first-order calculation of FHIP is not necessary. Second, the rate of change of momentum will contain both a dc and an ac part. The dc part is similar to the calculation of TF, while the ac part is taken together with the impulse response to form the self-consistent set of equations which determine the approximate influence functional. For zero applied $\vec{E}$ and $\vec{H}$, the self-consistent set reduces to that derivable from the self-consistent set of equations which minimize the free energy at finite temperature (Appendix A). At zero temperature the self-consistency requirement reduces to that derived in FHIP from the minimization condition of the self-energy.

The expression for the rate of change of *kinetic* momentum $\vec{m}\dot{\vec{x}}$,

$$\dot{\vec{x}} = (i/\hbar)[H, \vec{x}] = (1/\vec{m})(\vec{p} - q\vec{A}/c),$$

is given by

$$\vec{m}\ddot{\vec{x}} = i/\hbar[H, \vec{m}\dot{\vec{x}}] = q\vec{E} + q\vec{e}_t + (q/c)\dot{\vec{x}}\times\vec{H} - \sum_{n,\vec{k}} \vec{k}\hat{R}_{\vec{k},n}, \tag{4}$$

where

$$\hat{R}_{\vec{k},n} = -i(C^*_{\vec{k},n}a^\dagger_{\vec{k},n}e^{-i\vec{k}\cdot\vec{x}} - C_{\vec{k},n}a_{\vec{k},n}e^{i\vec{k}\cdot\vec{x}}). \tag{5}$$

As in TF, $\hat{R}_{\vec{k},n}$ is the operator for the net rate of phonon emission (emission less absorption). [10]

As the first steps in evaluating the expectation value of (4), we eliminate the phonon coordinates exactly, cast the problem into the path-integral method, transform to a frame of reference drifting with the expectation value of the electron's velocity $\vec{v}$ in the absence of $\vec{e}_t$, and set q, c, $\hbar$, and V equal to unity. The result is

$$\vec{E} + \vec{v}\times\vec{H} + \vec{e}_t + \langle\dot{\vec{y}}\rangle_t \times \vec{H} - \vec{m}\cdot\langle\ddot{\vec{y}}\rangle_t = \sum_{n,\vec{k}} \vec{k}\langle\hat{R}_{\vec{k},n}\rangle_t\ , \tag{6a}$$

where $\langle\dot{\vec{y}}\rangle_t$ and $\langle\ddot{\vec{y}}\rangle_t$ are the expectation values of the velocity and acceleration of the linear response to $\vec{e}_t$, and where

$$\langle\hat{R}_{\vec{k},n}\rangle_{t_2} = \frac{\int\int R'_{\vec{k},n}e^{i\Phi'_e}D(y_t)D(y'_t)}{\int\int e^{i\Phi'_e}D(y_t)D(y'_t)}\ , \tag{6b}$$

$$\begin{aligned}\Phi'_e = &\int_{t_1}^{t_2} dt[\tfrac{1}{2}\dot{\vec{y}}_t\cdot\vec{m}\cdot\dot{\vec{y}}_t + (\vec{E}+\vec{v}\times\vec{H})\cdot\dot{\vec{y}}_t + \vec{e}_t\cdot\vec{y}_t + \tfrac{1}{2}\dot{\vec{y}}_t\cdot\vec{H}\times\vec{y}_t]\\
&+ \int_{t_1}^{t_2} dt[\tfrac{1}{2}\dot{\vec{y}}'_t\vec{m}\cdot\dot{\vec{y}}'_t + (\vec{E}+\vec{v}\times\vec{H})\dot{\vec{y}}'_t + \vec{e}_t\cdot\vec{y}'_t + \tfrac{1}{2}\dot{\vec{y}}'_t\cdot\vec{H}\times\vec{y}'_t]\\
&+ i\sum_{n,\vec{k}}|C_{\vec{k},n}|^2\int_{t_1}^{t_2} dt\int_{t_1}^{t} dt'[S_{\omega_{\vec{k},n}}(t-t')e^{-i\vec{k}\cdot(\vec{y}_t-\vec{y}'_{t'})}\\
&+ S^*_{\omega_{\vec{k},n}}(t-t')e^{i\vec{k}\cdot(\vec{y}_t-\vec{y}_{t'})} - S_{\omega_{\vec{k},n}}(t-t')e^{i\vec{k}\cdot(\vec{y}_t-\vec{y}_{t'})} - S^*_{\omega_{\vec{k},n}}(t-t')e^{i\vec{k}\cdot(\vec{y}_t-\vec{y}_{t'})}],\end{aligned} \tag{6c}$$

$$S_{\omega_{\vec{k},n}}(\tau) = T_{\omega_{\vec{k},n}}(\tau)e^{-i\vec{k}\cdot\vec{v}\tau}\ , \tag{6d}$$

$$T_{\omega_{\vec{k},n}}(\tau) = \frac{e^{i\omega_{\vec{k},n}\tau}}{1-e^{-\beta\omega_{\vec{k},n}}} + \frac{e^{-i\omega_{\vec{k},n}\tau}}{e^{\beta\omega_{\vec{k},n}}-1}\ , \tag{6e}$$

and

$$\begin{aligned}R'_{\vec{k},n} = |C_{\vec{k},n}|^2\int_{t_1}^{t_2} dt\ &\frac{\exp[-i(\omega_{\vec{k},n}-\vec{k}\cdot\vec{v})(t_2-t)]\exp[i\vec{k}\cdot(\vec{y}_{t_2}-\vec{y}_t)]}{1-e^{-\beta\omega_{\vec{k},n}}} - \frac{\exp[i(\omega_{\vec{k},n}-\vec{k}\cdot\vec{v})(t_2-t)]\exp[-i\vec{k}\cdot(\vec{y}_{t_2}-\vec{y}_t)]}{e^{\beta\omega_{\vec{k},n}}-1}\\
&+ \frac{\exp[i(\omega_{\vec{k},n}-\vec{k}\cdot\vec{v})(t_2-t)]\exp[-i\vec{k}\cdot(\vec{y}_{t_2}-\vec{y}'_t)]}{1-e^{-\beta\omega_{\vec{k},n}}} - \frac{\exp[-i(\omega_{\vec{k},n}-\vec{k}\cdot\vec{v})(t_2-t)]\exp[i\vec{k}\cdot(\vec{y}_{t_2}-\vec{y}'_t)]}{e^{\beta\omega_{\vec{k},n}}-1}\ .\end{aligned} \tag{6f}$$

In (6) some simplification has been achieved by noting that $\vec{A} = -\frac{1}{2}\vec{x}\times\vec{H}$. It should also be stressed that terms of order H^2 have *not* been neglected. They do not exist in the Lagrangian formalism. For the Hamiltonian as given, this (nonrelativistic) expression is exact and applicable for arbitrary applied $\vec{E}$ and $\vec{H}$.

Next, we do two things: If we set $\vec{e}_t = 0$, then $\langle \dot{\vec{y}} \rangle_t$ and $\langle \ddot{\vec{y}} \rangle_t$ are zero and (6) gives a nonlinear relation between $\vec{v}$ and $\vec{E}$ and $\vec{H}$ from which, for example, exact formal expressions for Hall and drift mobility can be easily obtained, etc. If we next permit $\vec{e}_t$ to serve as a small probe signal, we can determine the "differential" impedance as a function of frequency of the particle in its drifting state. Before carrying this out and also calculating the impulse response directly using (2), it is necessary to approximate the influence functional (6c), so that the two path integrals over the electronic coordinates in (6b) can be performed. This we perform in Sec. III.

III. METHOD OF APPROXIMATION AND SELF-CONSISTENCY

As written the influence functional (6c) expresses the dependence of the motion of the electron at time t on its position at all times t' where $t' < t$. In order to simulate this interaction and yet use a harmonic influence functional so that the path integral may be performed, we approximate Φ'_e by Φ'_0:

$$\Phi'_0 = \int_{t_1}^{t_2} dt \left(\tfrac{1}{2}\dot{\vec{y}}_t \cdot \overleftrightarrow{m} \cdot \dot{\vec{y}}_t + \vec{e}_t \cdot \vec{y}_t + \tfrac{1}{2}\dot{\vec{y}}_t \cdot \vec{H} \times \vec{y}_t\right) - \int_{t_1}^{t_2} dt \left(\tfrac{1}{2}\dot{\vec{y}}'_t \cdot \overleftrightarrow{m} \cdot \dot{\vec{y}}'_t + \vec{e}_t \cdot \vec{y}'_t + \tfrac{1}{2}\dot{\vec{y}}'_t \cdot \vec{H} \times \vec{y}'_t\right)$$

$$- i \int_{t_1}^{t_2} dt \int_{t_1}^{t} dt' [(\vec{y}'_t - \vec{y}'_{t'}) \cdot \overleftrightarrow{G}^*(t-t') \cdot (\vec{y}'_t - \vec{y}'_{t'}) + (\vec{y}_t - \vec{y}_{t'}) \cdot \overleftrightarrow{G}(t-t') \cdot (\vec{y}_t - \vec{y}_{t'})$$

$$- (\vec{y}_t - \vec{y}'_{t'}) \cdot \overleftrightarrow{G}^*(t-t') \cdot (\vec{y}_t - \vec{y}'_{t'}) - (\vec{y}'_t - \vec{y}_{t'}) \cdot \overleftrightarrow{G}(t-t') \cdot (\vec{y}'_t - \vec{y}_{t'})] . \tag{7}$$

If we express $\overleftrightarrow{G}(t-t')$ as

$$\overleftrightarrow{G}(t-t') = \int_{-\infty}^{\infty} d\Omega \, \overleftrightarrow{G}(\Omega) \, e^{-i\Omega(t-t')} , \tag{8}$$

then, apart from the tensor nature of $\overleftrightarrow{G}(\Omega)$ and $\overleftrightarrow{m}$ and the presence of the magnetic field $\vec{H}$, (7) is essentially identical to the Φ discussed in Appendix B of TF. As shown in TF this is the most general harmonic form one can expect to have to represent Φ'_e. The tensor nature of (7) partially simulates the anisotropy induced by crystal structure and applied fields. Since $\overleftrightarrow{G}(\Omega)$ represents a distribution of oscillators, it is a real function of Ω. Since the argument of the double integral in (7) is a quadratic form, $\overleftrightarrow{G}$ can without loss of generality be taken to be symmetric. As discussed in TF, there can be no linear driving forces in the moving frame (apart from the auxiliary $\vec{e}_t \cdot \vec{y}_t$ terms). In fact, if one were to expand each term of the form $\exp[-i\vec{k} \cdot (\vec{y}'_t - \vec{y}'_{t'})]$ in (6c) as

$$\{[1 - i\vec{k} \cdot (\vec{y}'_t - \vec{y}'_{t'}) - \tfrac{1}{2}[\vec{k} \cdot (\vec{y}'_t - \vec{y}'_{t'})]^2\}$$

$$\times \exp[-\vec{k} \cdot \overleftrightarrow{L}(t-t') \cdot \vec{k}] ,$$

where the additional factor exp [ ] is analogous to the Debye-Waller factor, and where $\overleftrightarrow{L}$ is yet to be defined, one would find that terms of order 1 cancel trivially, terms of order $\vec{y}_t$ and $\vec{y}'_t$ separately cancel the $(\vec{E} + \vec{v} \times \vec{H})$ terms using (6a) with $\vec{e}_t = 0$, a further internal consistency, and the terms of order $\vec{y}_t^2$, etc., give (7) complete with the same $\overleftrightarrow{G}(\Omega)$ we shall find self-consistently below.

The path integral with (7) as the influence functional is easily evaluated as outlined in Appendix B. Using this result it is straightforward to calculate the admittance, the Fourier transform of the linear impulse response function:

$$Y_{ij}(\omega) = \int_{-\infty}^{\infty} d(t_2 - t_1) \, e^{i\omega(t_2 - t_1)}$$

$$\times \iint y_{it_2}(y_{jt_1} - y'_{jt_1}) \, ie^{i\Phi'_0} D(\vec{y}_t) D(\vec{y}'_t) \tag{9a}$$

$$= \int_0^{\infty} dt \, e^{i\omega t} i[L_{ij}(t) - L^*_{ij}(t)] \tag{9b}$$

$$= \int_0^{\infty} dt \, e^{i\omega t_i} \int_{-\infty}^{\infty} \frac{d\nu}{2\pi i} \left(\frac{1}{\overleftrightarrow{Z}_\nu} - \frac{1}{\overleftrightarrow{Z}^\dagger_\nu}\right)_{ij} e^{-i\nu t} \tag{9c}$$

$$= + \left(\frac{1}{\overleftrightarrow{Z}_\omega}\right)_{ij} . \tag{9d}$$

Thus the $\overleftrightarrow{Z}_\omega$ which we defined in Appendix B and which is a functional of $\overleftrightarrow{G}(\Omega)$ is simply the differential impedance, the inverse of the differential admittance. Notice that impedance and admittance here refer to position response rather than velocity response as in FHIP, $\vec{y}_\omega = \overleftrightarrow{Y}_\omega \cdot \vec{e}_\omega$, $\vec{e}_\omega = \overleftrightarrow{Z}_\omega \cdot \vec{y}_\omega$.

We now derive our second expression for $\overleftrightarrow{Z}_\omega$ from the linear (in $\vec{e}_t$) terms of (6a), using of course (7) in place of (6c) for the influence functional and (9d) for the admittance. The result is

$$\overleftrightarrow{Z}_\omega = -\overleftrightarrow{m}\omega^2 - i\omega\underline{\epsilon}\vec{H} + \int_0^\infty d\xi(1-e^{i\omega\xi})\,\mathrm{Im}[\overleftrightarrow{S}(\xi)], \tag{10}$$

$$\overleftrightarrow{S}(\xi)_{ij} = \sum_{n,\vec{k}} |\, C_{\vec{k},n}|^2 k_i k_j\, 2T_{\omega_{\vec{k},n}}(\xi)\, e^{-i\vec{k}\cdot\vec{v}\xi}\, e^{-\vec{k}\cdot\underline{L}(\xi)\cdot\vec{k}}. \tag{10'}$$

$\underline{\epsilon}$ is defined by $\vec{A}\cdot\underline{\epsilon}\cdot\vec{B}\cdot\vec{C} = A_i\epsilon_{ijk}B_jC_k = \vec{A}\cdot\vec{B}\times\vec{C}$ and

$$\underline{\overleftrightarrow{L}}(\xi) \equiv \overleftrightarrow{L}(\xi) - \overleftrightarrow{L}(0) = \int_{-\infty}^{\infty} \frac{d\nu}{2\pi i}\left[\frac{1}{\overleftrightarrow{Z}_\nu}\left(4\pi i\overleftrightarrow{G}(-\nu)\right)\frac{1}{\overleftrightarrow{Z}_\nu^\dagger}\right](1-e^{-i\nu\xi}). \tag{10''}$$

The $\overleftrightarrow{L}(\xi)$ is defined in (B9). To obtain (10'') we have used (B9), (B12), (B14), and (B15).

Now if $\overleftrightarrow{L}(\xi)$ were simply a functional of $\overleftrightarrow{Z}_\omega$, then we would have a self-consistent relation at this point for $\overleftrightarrow{Z}_\omega$. However, $\overleftrightarrow{L}(\xi)$ contains $\overleftrightarrow{G}(\Omega)$ as well. We proceed as follows. It is straightforward to verify that

$$\int_0^\infty d\xi(1-e^{i\omega\xi})\,\mathrm{Im}[\overleftrightarrow{S}(\xi)] = -4\omega^2\int_{-\infty}^{\infty} d\Omega\frac{P}{\Omega}\overleftrightarrow{G}(\Omega) \times \frac{1}{\Omega^2-(\omega+i\epsilon)^2}, \tag{11}$$

where

$$G(\Omega)_{ij} = \tfrac{1}{2}\sum_{n,k} |C_{k,n}|^2 k_i k_j \int_{-\infty}^{\infty}\frac{d\xi}{2\pi}\, e^{-i\Omega\xi} \times T_{\omega_{k,n}}(\xi)\, e^{-i\vec{k}\cdot\vec{v}\xi}\, e^{-\vec{k}\cdot\underline{L}(\xi)\cdot\vec{k}}. \tag{11'}$$

By (9d) and (B12) this $\overleftrightarrow{G}(\Omega)$ must be the same function as our trial oscillator distribution (8), and hence the same symbol is used. Thus (10) and (11) give $\overleftrightarrow{Z}_\nu$ in terms of $\overleftrightarrow{G}(\Omega)$, (11') gives $\overleftrightarrow{G}(\Omega)$ in terms of $\underline{\overleftrightarrow{L}}(\xi)$, and (10'') gives $\underline{\overleftrightarrow{L}}(\xi)$ in terms of $\overleftrightarrow{G}(\Omega)$ and $\overleftrightarrow{Z}_\nu$. The set of equations [(10), (11), (11'), and (10'')] thus forms a self-consistent relationship from which $\overleftrightarrow{G}$, $\underline{\overleftrightarrow{L}}$, and $\overleftrightarrow{Z}$ may be determined for arbitrary magnetic field $\vec{H}$, translational velocity $\vec{v}$, reciprocal-lattice temperature β, and electron-phonon interaction $|C_{\vec{k},n}|^2$. Furthermore, returning to (6a) and now setting $\vec{e}_t = 0$ (and of course, replacing Φ_e' by Φ_0'), we find for the generalization of the basic result of TF:

$$\vec{E}+\vec{v}\times\vec{H} = \sum_{n,\vec{k}}\vec{k}\,|C_{\vec{k},n}|^2\int_{-\infty}^{\infty}d\xi\; T_{\omega_{\vec{k},n}}(\xi) \times e^{-i\vec{k}\cdot\vec{v}\xi}\, e^{-\vec{k}\cdot\underline{\overleftrightarrow{L}}(\xi)\cdot\vec{k}}, \tag{12}$$

where now $\underline{\overleftrightarrow{L}}(\xi)$ can be determined self-consistently. Equation (12) relates the expectation value of the steady-state velocity of the electron to the applied static electric and magnetic fields $\vec{E}$ and $\vec{H}$.

Equation (10'') may be cast into a somewhat different form from which comparison with the FHIP result for zero temperature $\vec{E}$ and $\vec{H}$ may be readily made. By changing the contour of the ξ integration in (11') from the real axis ξ to $\xi+\frac{1}{2}i\beta$, it is then apparent that

$$\overleftrightarrow{G}(\Omega) = e^{\Omega\beta/2}\overleftrightarrow{\Theta}_{\vec{v}}(\Omega), \tag{13a}$$

where

$$\overleftrightarrow{\Theta}_{\vec{v}}(\Omega) = \tfrac{1}{2}\sum_{n,\vec{k}}|C_{\vec{k},n}|^2\vec{k}\vec{k}\int_{-\infty}^{\infty}\frac{d\xi}{2\pi}\, e^{-(\beta/2)\vec{k}\cdot\vec{v}} \times\frac{\cos(\Omega-\vec{k}\cdot\vec{v})\xi\,\cos\omega_{\vec{k},n}\xi}{\sinh\frac{1}{2}\beta\omega_{k,n}}\, e^{-\vec{k}\cdot\underline{L}'(\xi)\cdot\vec{k}}. \tag{13b}$$

It follows at once from (B14)–(B16) that

$$i4\pi\overleftrightarrow{G}(-\nu) = \overleftrightarrow{Z}_-^*(\nu) - \overleftrightarrow{Z}_-(\nu) = [e^{\beta\nu}\overleftrightarrow{\Theta}_{\vec{v}}(\nu)\overleftrightarrow{\Theta}_{\vec{v}}^{-1}(-\nu)-1]^{-1}\cdot(\overleftrightarrow{Z}_\nu^\dagger - \overleftrightarrow{Z}_\nu), \tag{13c}$$

and similarly that

$$i4\pi\overleftrightarrow{G}(\nu) = \overleftrightarrow{Z}_+^*(\nu) - \overleftrightarrow{Z}_+(\nu) = [1-e^{-\beta\nu}\overleftrightarrow{\Theta}_{\vec{v}}(-\nu)\overleftrightarrow{\Theta}_{\vec{v}}^{-1}(\nu)]^{-1}\cdot(\overleftrightarrow{Z}_\nu^* - \overleftrightarrow{\tilde{Z}}_\nu). \tag{13d}$$

If we assume $\vec{v}=0$ (no applied static electric field $\vec{E}$), then $\overleftrightarrow{\Theta}_{\vec{v}}(\nu) = \overleftrightarrow{\Theta}_{\vec{v}}(-\nu)$ and (10'') becomes

$$\underline{\overleftrightarrow{L}}(\xi) = \int_{-\infty}^{\infty}\frac{d\nu}{2\pi i}\left(\frac{1}{\overleftrightarrow{Z}_\nu}-\frac{1}{\overleftrightarrow{\tilde{Z}}_\nu}\right)\frac{1-e^{-i\nu\xi}}{e^{\beta\nu}-1} = \int_{-\infty}^{\infty}\frac{d\nu}{2\pi i}\left(\frac{1}{\overleftrightarrow{\tilde{Z}}_\nu}\,\frac{1-e^{i\nu\xi}}{1-e^{-\beta\nu}}+\frac{1}{\overleftrightarrow{Z}_\nu}\,\frac{1-e^{-i\nu\xi}}{e^{\beta\nu}-1}\right). \tag{10'''}$$

If the magnetic field is zero, then $\overleftrightarrow{\tilde{Z}}_\nu = \overleftrightarrow{Z}_\nu$ and we have

$$\underline{\overleftrightarrow{L}}(\xi) = \int_{-\infty}^{\infty}\frac{d\nu}{2\pi i}\,\frac{1}{\overleftrightarrow{Z}_\nu}\left(\frac{1-e^{i\nu\xi}}{1-e^{-\beta\nu}}+\frac{1-e^{-i\nu\xi}}{e^{\beta\nu}-1}\right). \tag{10''''}$$

Equations (10), (10'), and (10'''') with $\vec{v}=0=\vec{H}=\vec{E}$ are the finite-temperature generalization of the self-consistent set of equations for Z_ν derived in FHIP by minimizing the polaron self-energy at zero temperature. They are derived here at finite temperature in Appendix A.

One would have obtained (10''') for $\vec{v}\neq 0$ if in the approximate influence functional (7), one had assumed that the electron-lattice interaction could be simulated by terms of the form

$$\vec{\vec{G}}(\Omega)\left(\frac{e^{i\Omega(t-t')}}{1-e^{-\beta\Omega}}+\frac{e^{-i\Omega(t-t')}}{e^{\beta\Omega}-1}\right), \quad 0\le\Omega<\infty$$

rather than by the more general form

$$\vec{\vec{G}}(\Omega)\,e^{i\Omega(t-t')}, \quad -\infty<\Omega<\infty.$$

The deviation of the thermal factor in (13c) and (13d) from the Planck factor simulates the relative heating of the lattice in the vicinity of the electron owing to the loss of energy from the electron to the lattice at finite steady-state drift velocity $\vec{v}$. Thus the temperature characterizing the relative motion of the electron now acquires a dependence on the drift velocity $\vec{v}$, and this dependence arises both from the velocity dependence of $\vec{\vec{Z}}_\nu$ and from the internally consistent deviation from a Planck distribution of the occupation of the trial oscillators.

Using Eqs. (10) and (11) for $\vec{H}=0$, it follows that

$$\mathrm{Im}\vec{\vec{Z}}_\omega=-2\pi[\,\vec{\vec{G}}(\omega)-\vec{\vec{G}}(-\omega)]\,. \qquad (11'')$$

This establishes a very simple, almost intuitive relation between the absorptive part of the impedance and the trial distribution of oscillators which absorb the energy. For $\vec{v}=0$ it follows from (13a) and (13b) that

$$\mathrm{Im}\vec{\vec{Z}}_\omega=-2\pi\vec{\vec{G}}(\omega)\,(1-e^{-\beta\omega}), \qquad (11''')$$

an expression which we shall use extensively in Sec. IV.

IV. APPROXIMATE SELF-CONSISTENT SOLUTION

In this section we examine an approximate self-consistent solution to the Fröhlich[11] model of the polaron in the absence of the applied electric and magnetic fields $\vec{E}$ and $\vec{H}$. In the Fröhlich model the electron is assumed to interact only with the longitudinal optic modes of the lattice in a very simple isotropic way. The energy of these modes $\omega_{\vec{k}}$ is a constant ω_0 and

$$|C_k|^2=\frac{\omega_0^2}{k^2}\frac{1}{(2m\omega_0)^{1/2}}\,4\pi\alpha\,, \qquad (14a)$$

where

$$\alpha=(1/\epsilon_0-1/\epsilon_s)\,(m/2\omega_0)^{1/2}. \qquad (14b)$$

The ϵ_s is the static dielectric constant of the material and ϵ_0 the optical dielectric constant. Using this model it is possible to greatly simplify the self-consistent equations derived in Sec. III.

For an isotropic interaction Eq. (11'''') assumes the simple form[12]

$$G(\omega)=-\frac{1}{2\pi}\,\frac{\mathrm{Im}Z_\omega}{1-e^{-\beta\omega}}\,, \qquad (15)$$

relating the trial oscillator distribution $G(\omega)$ to the absorption. Let us compare this relation with the examples given in FHIP, Figs. 1–3. FHIP assumed a very simple physical oscillator distribution

$$G_F(\omega)=C\,\delta(\omega-w)=\tfrac{1}{4}\,w(v^2-w^2)\,\delta(\omega-w), \qquad (16)$$

where C, the electron-oscillator interaction, and w, the oscillator frequency, were calculated by minimizing the self-energy of the electron at zero temperature. Using this oscillator distribution in Eqs. (10)–(10'') with $\vec{H}$ and $\vec{v}$ set equal to zero and with $\beta=100$, they calculated $-\mathrm{Im}Z_\omega$, which in their paper is referred to as $\mathrm{Im}\chi_\omega$. For low temperature, a self-consistent solution would require $G_F(\omega)=C\,\delta(\omega-w)=\mathrm{Im}\chi_\omega/2\pi$. By contrast the $\alpha=3$ and $\alpha=5$ results show that $\mathrm{Im}\chi_\omega$ is relatively smooth in ω, whereas for $\alpha=7$, relatively sharp peaks occur at $\omega\gtrsim n\nu+1$, $n=0,1,2,\ldots$.[13] If we were to use this $\mathrm{Im}\chi_\omega$ as a new trial distribution, then, as discussed below, a series of peaks at $\omega\approx n\nu+m\cdot 1$ would arise in $\mathrm{Im}\chi_\omega$. For $n=0$ these correspond to the absorption of quanta by the polaron and the subsequent emission of m optical phonons, the polaron remaining in the ground state. For $n=1$, the series might represent the polaron excited in addition to the emission of m phonons, etc. Of course, the coupling would have to exceed $\alpha=7$ for this structure to be resolved. For $\alpha=3$ structure in $\mathrm{Im}\chi_\omega$ is probably too broadened to be greatly affected by fine tuning $G(\omega)$.

Let us now return to our self-consistent set of Eqs. (10), (11), (11'), and (10'') and write them in scalar form for the Fröhlich polaron $\vec{E}=\vec{H}=0$:

$$-\mathrm{Im}Z_\nu=\frac{\alpha\omega_0^{3/2}}{(2\pi m)^{1/2}}\,\frac{1}{3}\,\frac{\sinh\frac{1}{2}\beta\nu}{\sinh\frac{1}{2}\beta\omega_0}\times\int_0^\infty\frac{\cos\nu\xi\,\cos\omega_0\xi}{[\bar{K}'_\beta(\xi)]^{3/2}}\,d\xi, \qquad (17a)$$

$$Z_\nu=-m(\nu+i\epsilon)^2-(\nu+i\epsilon)\int_{-\infty}^{\infty}\frac{d\Omega}{\pi}\,\frac{-\mathrm{Im}Z_\Omega/\Omega}{\Omega-(\nu+i\epsilon)}\,, \qquad (17b)$$

$$\bar{K}'_\beta(\xi)=\int_0^\infty\frac{d\nu}{\pi}\,\frac{-\mathrm{Im}Z_\nu}{|Z_\nu|^2}\,\frac{\cosh\frac{1}{2}\beta\nu-\cos\nu\xi}{\sinh\frac{1}{2}\beta\nu}\,. \qquad (17c)$$

If, as a starting point, one were to assume

$$K'_\beta(\xi)=(\xi^2+\tfrac{1}{4}\beta^2C')/2m^*\beta$$

essentially an effective-mass approximation, then for low temperature (large β), $-\mathrm{Im}Z_\nu$ would acquire a piece of structure of the form

$$e^{\beta(\nu-\omega_0)/2}\,|\nu-\omega_0|K_1(\beta\sqrt{C'}\,|\nu-\omega_0|/2).$$

The K_1 is the modified Bessel function of the second kind, $n=1$. [$C'=1+4R/\beta$, $R=(v^2-w^2)/w^2v$, in the FHIP one-oscillator model.] Explicitly, one would find

$$-\mathrm{Im}\,Z_\nu = M_1 \frac{\sinh\frac{1}{2}\beta\nu}{\sinh\frac{1}{2}\beta\omega_0}\frac{\beta^{1/2}}{\Gamma(\frac{3}{2})} \times[|\nu-\omega_0|K_1(\beta(\sqrt{C'})|\nu-\omega_0|/2) + |\nu+\omega_0|K_1(\beta(\sqrt{C'})|\nu+\omega_0|/2)] ,$$

where

$$M_1 = (\tfrac{1}{3}\alpha\omega_0^{3/2})(m^*/m)^{1/2}(m^*/\sqrt{C'}) .$$

This is illustrated in Fig. 1, curve AA, for $\omega_0=1$, $\beta=100$, and $R=4$. Taking this expression for $-\mathrm{Im}\,Z_\nu$ and inserting it into (17c) we obtain, in addition to the term corresponding to the effective-mass approximation, a term of the form $\exp(-\frac{1}{2}\beta\omega_0)\times\cos(\nu\xi)/[(\frac{1}{2}\beta\sqrt{C'})^2+\xi^2]^{3/2}$ for $K'_\beta(\xi)$. When this second $K'_\beta(\xi)$ is substituted into (17a), a series of structures represented by $K_{(5n-3)/2}$ Bessel functions of higher order centered about $n\omega_0$ arises.[8,14] This is shown in curve BBB of Fig. 1, where we have taken

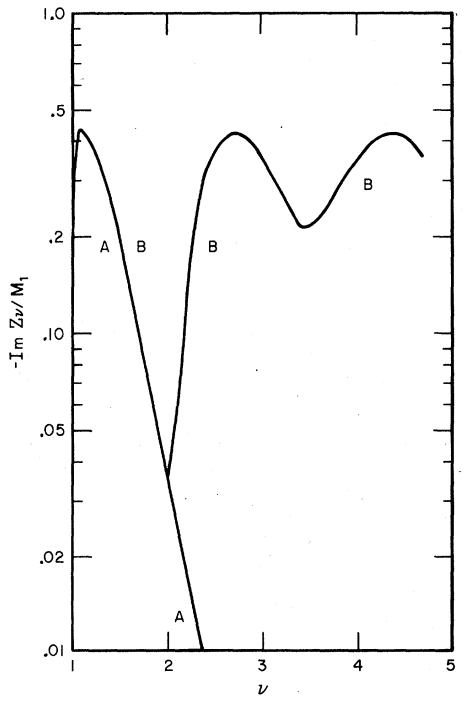

FIG. 1. $-\mathrm{Im}Z_\nu/M_1$ is plotted vs frequency $1\le\nu<5$ for $\beta=100$. Curve AA is the absorption in the effective-mass approximation. Curve BBB is the absorption when curve AA is used for the trial oscillator distribution $G(\nu)=-\mathrm{Im}Z_\nu/2\pi(1-e^{-\beta\omega})$. Further iteration modifies the relative magnitude of the structure.

$M_1m^*/\pi^{1/2}C'^{3/4}|Z\omega_0|^2$ to be 20. Although starting with an effective-mass approximation is quite unrealistic if one is interested in Z_ν for ν much in excess of $\omega_0=1$, a one-oscillator model already introduces structure of physical interest.

The above considerations suggest the following *ansatz* for the imaginary part of the impedance at low temperature (large β):

$$-\mathrm{Im}\,Z_\nu = M_1\sinh\tfrac{1}{2}\beta\nu\sum_{n=1}\{C_n\beta^{1/2}[\Gamma(\tfrac{1}{2}(5n-3)+\tfrac{1}{2})]^{-1} \times(\sinh\tfrac{1}{2}\beta\omega_0)^{-n}X(\nu,\ n,\ \beta\tfrac{1}{2}\sqrt{C'})\}, \qquad (18a)$$

where

$$X(\nu,\ n,\ \beta\tfrac{1}{2}\sqrt{C'}) = |\nu-n\omega_0|^{(5n-3)/2} \times K_{(5n-3)/2}(\tfrac{1}{2}\beta\sqrt{C'}|\nu-n\omega_0|) + |\nu+n\omega_0|^{(5n-3)/2}K_{(5n-3)/2}(\tfrac{1}{2}\beta\sqrt{C'}|\nu+n\omega_0|) \qquad (18b)$$

and where C' is defined below somewhat more generally than as used in FHIP or in TF. By inserting (18a) into (17c) and then calculating (17a), one can by matching like powers of $X(\nu,\ n,\ \beta\frac{1}{2}\sqrt{C'})$ obtain a recursion relation for the coefficients C_n. The other factors multiplying X normalize the magnitude of $(\sinh\beta\nu)X(\nu,\ n,\ \beta\frac{1}{2}\sqrt{C'})$ at its local maximum. Thus C_n/C_m gives the ratio of $-\mathrm{Im}\,Z_{\nu_n}/-\mathrm{Im}\,Z_{\nu_m}$, where ν_m is the local maximum of $(\sinh\beta\nu)\times X(\nu,\ m,\ \beta\frac{1}{2}\sqrt{C'})$ in the vicinity of $m\omega_0$.[15] If we choose $C_1=1$, then

$$M_1 = (\tfrac{1}{3}\alpha\omega_0^{3/2})(m^*/m)^{1/2}(m^*/\sqrt{C'}) ,$$

as given above.

The form of (18a) is not exact. There are approximations which must be made in deriving the recursion series for the C_n, and these must be made perfectly clear. If we start with Eq. (17a), then we know that for very small ν we have

$$\mathrm{Re}\,Z_\nu \approx m^*\nu^2, \quad m^* \equiv L_{\nu\to 0}\mathrm{Re}\,Z_\nu/\nu^2 , \qquad (19a)$$

and

$$\mathrm{Im}\,Z_\nu \approx -b\nu ,$$

where

$$b = O(e^{-\beta\omega_0}) . \qquad (19b)$$

In (19a) m^* is the low-frequency effective mass of the polaron (zero net drift velocity), and in (19b) b represents the very small probability that the electron can be scattered by phonon absorption in a cold lattice. Thus in the region $0<\nu<\exp(-\beta\omega_0)$, the integrand is of the order of $e^{\beta\omega_0}$: Hence $-\mathrm{Im}Z_\nu/|Z_\nu|^2$ may be treated as a δ function. The result of this

is that

$$\overline{K}'_\beta(\xi) = \frac{1}{2m^*\beta}\left(\tfrac{1}{4}\beta^2 C' + \xi^2\right) - \int_{0+}^{\infty} \frac{d\nu}{\pi} \frac{-\operatorname{Im} Z_\nu}{|Z_\nu|^2} \frac{\cos\nu\xi}{\sinh\frac{1}{2}\beta\nu}, \tag{20a}$$

where

$$C' \equiv 1 + (4/\beta)R,$$
$$R \equiv 2m^* \int_{0+}^{\infty} \frac{d\nu}{\pi} \frac{-\operatorname{Im} Z_\nu}{|Z_\nu|^2} \frac{\cosh\nu\xi}{\sinh\frac{1}{2}\beta\nu}. \tag{20b}$$

It is apparent from (19a), (17b), and (20b) that m^* and R are obtained from gross averages of $-\operatorname{Im} Z_\nu$.

We now insert $-\operatorname{Im} Z_\nu$ (18a) into the integral in (20a). In principle, we would also have to calculate $\operatorname{Re} Z_\nu$ from (17b) and insert this into (20b) as well. For low temperature, however, this is not necessary. In the vicinity of $n\omega_0$, $-\operatorname{Im} Z_\nu/\sinh\frac{1}{2}\beta\nu$ behaves like $X(\nu, n, \beta\frac{1}{2}\sqrt{C'})$, which is a very sharply peaked $\exp(-\frac{1}{2}\beta|\nu - n\omega_0|)$ at $n\omega_0$. By contrast $|Z_\nu|^2$ is relatively smooth[16] in intervals of the order of $\Delta\nu \approx 1/\beta$. Using this approximation, $\overline{K}'_\beta(\xi)$ may be readily evaluated from (20a):

$$\overline{K}'_\beta(\xi) = \frac{1}{2m^*\beta}\left(\tfrac{1}{4}\beta^2 C' + \xi^2\right) - M_1 \sum_{n=1}^{\infty} \left(C_n (\beta/\pi)^{1/2} \frac{1}{(\sinh\frac{1}{2}\beta\omega_0)^n} \frac{1}{|Z_{n\omega_0}|^2} (\beta\sqrt{C'})^{(5n-3)/2} \frac{\cos n\omega_0\xi}{[\xi^2 + (\frac{1}{2}\beta\sqrt{C'})^2]^{(5n-3)/2+1/2}} \right). \tag{20c}$$

This expression for $\overline{K}'_\beta(\xi)$ may be inserted into (17a) to obtain $-\operatorname{Im} Z_\nu$. To perform this most expediently we use a trick from FHIP, page 1011. For large β the nth term in the summation in (20c) is of the order of $\exp(-\frac{1}{2}\beta n\omega_0)$. If we treat this sum as being small, then we may expand $[\overline{K}'_\beta(\xi)]^{-3/2}$ in terms of this summation. A typical term in the integrand of (17a) will then be $\cos\nu\xi\ \cos\omega_0\xi(\cos n\omega_0\xi)^m$. A phase match will occur for numerous integral multiples of ω_0, but only for $\nu = \pm(1+nm)\omega_0$ will the $\sinh\frac{1}{2}\beta\nu$ factor in $-\operatorname{Im} Z_\nu$ offset $(\sinh\frac{1}{2}\beta\omega_0)^{-(nm+1)}$ to yield a contribution to $-\operatorname{Im} Z_\nu$ which is not exponentially small in the limit of low temperature. One then obtains an expansion for $-\operatorname{Im} Z_\nu$ of the same form as the ansatz (18):

$$-\operatorname{Im} Z_\nu = M_1 \sinh\tfrac{1}{2}\beta\nu \left[\beta^{1/2} \left[\Gamma\left(\tfrac{1}{2}(5\cdot 1 - 3) + \tfrac{1}{2}\right) \right]^{-1} (\sinh\tfrac{1}{2}\beta\omega_0)^{-1} X(\nu, 1, \beta\tfrac{1}{2}\sqrt{C'}) + \sum_{m=1}^{\infty} (M_1 m^*/\pi^{1/2} C^{3/4})^m \right.$$
$$\times \frac{3\times 5\cdots(2m+1)}{2\times 4\cdots(2m)} \left(\sum_{n_1=1}^{\infty} \cdots \sum_{n_m=1}^{\infty} C_{n_1}\cdots C_{n_m} \frac{1}{|Z_{n_1\omega_0}|^2} \cdots \frac{1}{|Z_{n_m\omega_0}|^2} \beta^{1/2} \left\{ \Gamma\left[\tfrac{1}{2}(5(n_1+\cdots+n_m+1) - 3) + \tfrac{1}{2}\right] \right\}^{-1} \right.$$
$$\left. \left. \times (\sinh\tfrac{1}{2}\beta\omega_0)^{-(n_1+\cdots+n_m+1)} X(\nu, n_1+\cdots+n_m+1, \beta\tfrac{1}{2}\sqrt{C'}) \right) \right]. \tag{21}$$

Equating coefficients of like powers of $X(\nu, n, \beta\frac{1}{2}\sqrt{C'})$ in (18) and (21), we find

$$C_1 = 1,$$
$$C_2 = \tfrac{3}{2} C_1 \frac{m^*}{(\sqrt{\pi})C^{3/4}} \frac{1}{|Z_{\omega_0}|^2} M_1,$$
$$C_3 = \tfrac{3}{2} C_2 \frac{m^*}{(\sqrt{\pi})C^{3/4}} \frac{1}{|Z_{2\omega_0}|^2} M_1 + \tfrac{15}{8} C_1^2 \left(\frac{m^*}{(\sqrt{\pi})C^{3/4}} \right)^2 \frac{1}{|Z_{\omega_0}|^4} M_1^2, \text{ etc.} \tag{22}$$

Of course, m^*, C', and $Z_{n\omega_0}$ must still be determined from $-\operatorname{Im} Z_\nu$.

Thus self-consistently we obtain the physically appealing result that $\operatorname{Im} Z_\nu$ contains definite structure at the threshold for the emission of successively one, two, three, etc., phonons, however buried this structure may be due to the enveloping $\sinh\frac{1}{2}\beta\nu$ factor. For low temperatures at least this structure should be included in the trial oscillator distribution $G(\Omega)$. Whether the C_n are enhanced in the neighborhood of $\nu \approx n\nu + 1$, the location of the structure in $\operatorname{Im}\chi_\omega$ in the Feynman one-oscillator model, has not been checked. For low temperatures $\operatorname{Im} Z_\nu$ is small for $-\omega_0 < \nu < \omega_0$ and finite for $|\nu| > \omega_0$. Thus the self-consistent oscillator distribution $G(\nu)$ approximates cuts along the real axis for $|\nu| > \omega_0$, and the Feynman one-oscillator model is a single-pole approximation of this cut.

V. FRÖHLICH POLARON IN ELECTRIC AND MAGNETIC FIELDS

In this section we briefly examine the motion of the Fröhlich polaron in applied electric and magnetic fields. We shall calculate the cyclotron mass, the Hall mobility, and the magnetoresistivity. Not surprisingly the cyclotron mass is found to have

essentially the same value as the polaron effective mass. In this theory the Hall mobility (small magnetic field) is found to be the same as the drift mobility. However, the longitudinal magnetoresistivity is found to be exactly one-half the transverse result. At first glance, such a result may seem unphysical since the electron is drifting parallel to the magnetic field and ordinarily would not be affected by it. It must be remembered, however, that the electron is scattered in all directions, and hence it can be acted upon by the magnetic field to an extent comparable to an electron drifting transverse to the field.

To determine the above transport properties we return to Eq. (12). If we assume we have a cubic crystal with the magnetic field H parallel to the z axis and expand the right-hand side of (12) to lowest order in $\vec{v}$, the steady-state expectation velocity, then we obtain

$$\vec{E}+\vec{v}\times\vec{H}=\tfrac{1}{2}\beta\sum_{\vec{k},n}\vec{k}\cdot\vec{v}\,|C_{\vec{k},n}|^2\int_{-\infty}^{\infty}d\xi\,\frac{\cos\omega_{\vec{k},n}\xi}{\sinh\frac{1}{2}\beta\omega_{\vec{k},n}}$$

$$\times\exp\{-\tfrac{1}{2}(k_x^2+k_y^2)[\overline{K}'_{-}(\xi)+\overline{K}'_{-}(\xi)]\}e^{-k_z^2\overline{K}'_0(\xi)}\,, \tag{23a}$$

where now[17]

$$\overline{K}'_{+,-,0}(\xi)=\int_{-\infty}^{\infty}\frac{d\nu}{2\pi i}\left(\frac{1}{Z_{+,-,0}(\nu)}\right)\left(\frac{\cosh\frac{1}{2}\beta\nu-\cos\nu\xi}{\sinh\frac{1}{2}\beta\nu}\right), \tag{23b}$$

$$Z_{\pm}(\xi)=-m(\nu+i\epsilon)^2\pm(\nu+i\epsilon)H-4(\nu+i\epsilon)^2$$

$$\times\int_{-\infty}^{\infty}d\Omega\,\frac{G_{\pm}(\Omega)}{\Omega^2-(\nu+i\epsilon)^2}\,, \tag{23c}$$

$$Z_0(\nu)=-m(\nu+i\epsilon)^2-4(\nu+i\epsilon)^2\int_{-\infty}^{\infty}d\Omega\,\frac{P}{\Omega}\,\frac{G_0(\Omega)}{\Omega^2-(\nu+i\epsilon)^2}\,. \tag{23d}$$

In going from (13) to (23a) the variable ξ has been changed to $\xi+\frac{1}{2}i\beta$. Because of the high symmetry in the x-y plane, $\vec{G}(\Omega)$ is quite generally diagonal and $G_+(\Omega)=G_-(\Omega)$ [see Eq. (11″)]. The effect of the magnetic field is contained in the quadratic argument of the exponent and will clearly play a similar role whether $\vec{v}$ is perpendicular or parallel to $\vec{H}$.

The cyclotron mass follows easily from (23c). The cyclotron frequency will, in general, be much less than the threshold for the emission of optical phonons. Hence, in the low-frequency limit we have

$$Z_+(\nu)=-m^*\nu^2+\nu H\,. \tag{24}$$

This is zero for $\nu=H/m^*$, the effective mass m^* being given by (19a), except for the magnetic field dependence of $G_+(\Omega)$, which goes as H^2 for small H. Apart from this dependence, the cyclotron mass corresponds to the same physical quantity as the polaron effective mass in this theory.

Except for terms in H^2, the same equality holds between drift and Hall mobilities in this theory. Suppose $\vec{v}$ is taken to be in the $\vec{x}$ direction. Then from (23a) it follows that $|E_y|=v_xH=E_xH\mu_D$, where μ_D is the drift mobility; hence $\mu_H=\mu_D$. That one is not evaluating the expectation value of the scattering operator in these two cases with different weighting functions is a difficulty with this approach in its present form. This is discussed in Sec. VI.

To determine the magnetoresistivity, the effect of the magnetic field on the mobility of electrons parallel and perpendicular to the field, we must assume some phonon model. As indicated at the beginning of this section, we shall use the Fröhlich model (14a) and (14b). Inserting this $|C_{\vec{k}}|^2$ into (23a), we find for the parallel and perpendicular mobilities

$$\begin{pmatrix}1/\mu_{\parallel}\\1/\mu_{\perp}\end{pmatrix}=\frac{\beta}{4}\,\frac{\alpha\omega_0^{3/2}}{(\sqrt{2\pi m})}\int_{-\infty}^{\infty}d\xi\,\frac{\cos\omega_0\xi}{\sinh\frac{1}{2}\omega_0\beta}$$

$$\times\int_0^1 d\mu\begin{pmatrix}\mu^2\\\frac{1}{2}(1-\mu^2)\end{pmatrix}[K(\xi,\mu)]^{-3/2}\,, \tag{25a}$$

where $\mu=\cos\theta$ and where

$$K(\xi,\mu)=\overline{K}'_0(\xi)\{1+(1-\mu^2)$$

$$\times[\tfrac{1}{2}(\overline{K}'_{+}(\xi)+\overline{K}'_{-}(\xi))-\overline{K}'_0(\xi)]/\overline{K}'_0(\xi)\}\,. \tag{25b}$$

Since the factor of $(1-\mu^2)$ in (25b) will be of the order of H^2, we may expand $K(\xi,\mu)^{-3/2}$ to first order, obtaining the standard path-integral result for the mobility from the H^0 term and the magnetoresistivity from the H^2 term. Call $r_{\parallel}$ the magnetoresistivity parallel to the magnetic field and $r_{\perp}$ that perpendicular to the field ($1/\mu_{\parallel}\equiv 1/\mu_0+r_{\parallel}H^2$; $1/\mu_{\perp}\equiv 1/\mu_0+r_{\perp}H^2$). Performing the angular integral in (25a), we obtain

$$r_{\parallel}/r_{\perp}=\tfrac{1}{2}\,. \tag{26}$$

For the Fröhlich polaron this result is quite general: it is independent of having a self-consistent or even a best possible oscillator distribution $\vec{G}(\Omega)$ for the given field. However, (26) is only true for very small applied magnetic fields. For fields sufficiently large that the current vs magnetic field deviates from a quadratic, one must, of course, perform (25a) as it stands. If the electric field is also strong, the general result (12) must be used.

A word of clarification is in order regarding (26). This is a result concerning (the curvature in H of) resistivities, whereas in actual practice it is mag-

exponentially rapidly, this being the emission threshold. Even here, however, the real part is relatively smooth. For weak coupling, the $m\nu^2$ term in $\mathrm{Re}Z_\nu$ dominates; for stronger coupling, $\mathrm{Re}Z_{\omega_0}/\mathrm{Im}Z_{\omega_0} \approx \beta^{1/2}$, $\nu = \omega_0$. Thus $|Z_\nu|^2$ can be taken to be relatively smooth compared to $X(\nu, n, \beta^{\frac{1}{2}}\sqrt{C'})$.

[17] $Z_\pm(\nu)$ here is to be distinguished from $\overrightarrow{Z}_\pm(\nu)$ in Appendix B. No confusion should arise from this.

[18] J. W. Hodby, J. A. Borders, and F. C. Brown, J. Phys. C 3, 335 (1970).

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Magnetoresistance of Very Pure Polycrystalline Aluminum†

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The behavior of the resistance of polycrystalline aluminum wires as a function of magnetic field and purity at temperatures of 4, 15, and 19.6 K is reported. Both longitudinal and transverse configurations were measured. The residual resistance ratios of the specimens varied from 1600 to 31 000. The measured magnetoresistance ($\Delta R/R_0$) is separated into a saturating and a linear part. The value of the saturating component is high at 19.6 K but is shown to be less than 6, even in the limit of infinite specimen purity. The linear component varies with both temperature and purity. Possible sources for the large saturating magnetoresistance values and for the variations observed in the linear portion are discussed. An analysis scheme is presented which allows prediction of the saturating component from zero-field resistance values. A deviation from Matthiessen's rule observed here, and by several other experimenters, is presented and discussed.

I. INTRODUCTION

The magnetoresistance of aluminum has been studied extensively.[1–5] Both single- and polycrystalline specimens have been measured. Most of the measurements were made only at 4 K on specimens of relatively low purity. Frequently, the specimens used were very small in at least one dimension, leading to the possibility of size effects. Several experiments, however, have been performed on large high-purity specimens and at temperatures up to 20 K.[6,7] These measurements indicate that the magnetoresistance ($\Delta R/R_0$) rises dramatically with temperature, reaching as much as four times the value measured at 4 K.

The experiment reported here was designed to cover a range both of temperature (4–20 K), and of specimen purity [residual resistance ratio (RRR) = 1000 – 30 000]. Magnetoresistance measurements were made both in the transverse and longitudinal configurations. We hoped, by this technique, to arrive at a phenomenology which would characterize the magnetoresistance of aluminum, at least in the form of polycrystalline wires, over this range.

It has become almost axiomatic that the more simple metals, in the free-electron sense, exhibit magnetoresistance effects which are at odds with theory.[8] Aluminum,[1–7] indium,[9] potassium,[10] and sodium[10] all show a linear magnetoresistance at high fields. A typical curve for aluminum is shown in Fig. 1. Furthermore, no simple metal which has been investigated over a wide range of purity and temperature has been observed to obey Kohler's rule. This indicates that the relative effects of different scattering mechanisms are more complex than the rule anticipates. More recent theoretical treatments such as those by Young,[11,12] and Pippard,[13] although promising some success in particular cases, have not yet shown wide applicability.

The Fermi surface of aluminum is well known and theoretical calculations of the major features have been adequately confirmed by de Haas-van Alphen and other experiments.[14] In one instance, transverse-magnetoresistance rotation diagrams for several crystal orientations were calculated, based on early models of the surface; however, agreement with available experimental data was not good.[15]

Recently, a good deal of discussion has taken place as to the presence or absence of magnetic breakdown effects which could lead to extended orbits on the Fermi surface.[7,13,14,16] The situation is still not totally clear, but it seems that magnetic breakdown may well occur in aluminum with the field along the ⟨100⟩ direction.

An extended orbit configuration, whatever its cause, would be expected to lead to a significant anisotropy of single-crystal transverse-magnetoresistance rotation diagrams. Early experiments showed no such large anisotropy,[2] whereas more recent work on higher-purity aluminum[7] does show a considerable effect.

Finally, the creation of a significant linear mag-