Velocity Acquired by an Electron in a Finite Electric Field in a Polar Crystal

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The expectation value of the steady-state velocity acquired by an electron interacting with the longitudinal, optical phonons of a polar crystal in a finite electric field is analyzed quantum mechanically for arbitrary coupling strength, field strength, and temperature. The rate of loss of momentum by an electron drifting through the crystal in the applied field is expressed in a form in which the lattice coordinates (the phonons) have been eliminated exactly by path-integral methods. This expression is then evaluated by a path-integral approach similar to that used to calculate the impedance of electrons in polar crystals. We present numerical calculations of field (loss of energy per unit distance) versus velocity for three coupling strengths using the Fröhlich polaron model. In a single curve, all the expected phenomena appear, including a threshold field for producing hot electrons and a decreasing rate of energy loss with velocity for very fast electrons. Using only the experimentally measured values of the reststrahlen energy and the static and optical dielectric constants, we find an energy loss of 0.025 eV/Å for electrons near the threshold in Al_2O_3, which compares favorably with the experimental value of about 0.03 eV/Å. We conclude that optical-phonon scattering can indeed produce the high rate of energy loss that is present in tunnel-cathode structures.

I. INTRODUCTION

A NUMBER of years ago experimenters studying the operation of cold-cathode, tunnel-emission devices were surprised to find that electrons could lose as much as 0.01 eV/Å to 0.06 eV/Å to the insulator part of the device.[1,2] Theorists were hard-pressed to explain such results. Acoustic-phonon scattering can contribute at most 10^{-4} eV/Å; the band gap of the material ($\gtrsim$10 eV) is too large for pair production. As electrons are coupled moderately strongly to the longitudinal optical modes of the lattice, it was suggested that optical-phonon scattering might be important. Performing a meaningful calculation, however, was hindered because the standard perturbation approaches, involving mean-free-path or mean-free-time parameters and the Boltzmann equation assuming independent collisions, are not applicable. For example, the energy of an optical phonon is typically 0.05–0.1 eV for these materials. This fact would require a mean free path for phonon emission of only 3 and 4 Å and a mean free time of about 2×10^{-15} sec in terms of one-phonon processes. These parameters are even less at temperatures where absorption is also important. Either quantity emphasizes that quantum interferences between the emitted phonons are important. This immediately precludes the assumption of independent phonon emissions and, consequently, the use of Fermi's golden rule for the rate of emission. Electric fields of the size used in the experiments cannot be treated as perturbations, and the velocity of the electrons is not sufficiently large that the energy loss in any one collision is negligible. Thus, seeking to determine whether or not optical-phonon scattering can account for the very large rate of loss of electron energy observed, we at once face treating a transport problem in which an electron is simultaneously rapidly acquiring kinetic energy from a static electric field and rapidly losing that energy to a dissipative medium, a situation not assailable by existing perturbation or Boltzmann techniques.

Our approach is physical and direct. The simplest question we can ask is this: Given an applied field in the crystal, what is the expectation value of the velocity of the electron? We may start the electron from rest, in which case we ask for the expectation velocity after the steady state is reached. As we increase the field, we expect to reach a point where the electron's acceleration can no longer be controlled by the lattice. Above this threshold the electron is able to drift to ever increasing velocities unless other loss mechanisms with higher thresholds such as ionization are introduced. We carried out such a calculation[3] by extending to finite fields path-integral methods,[4,5] which have yielded such success in calculating the energy, effective mass, and impedance of the polaron for arbitrary coupling strength and temperature. The calculation was excessively lengthy and involved; however, it provided the key to the approach used here, which gives the same result by a much simpler and more physical method.

Under steady-state conditions the electron is, on the

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[1] For a review and assimilation of the experimental results see R. M. Handy, J. Appl. Phys. **37**, 4620 (1966). See also E. D. Savoye and D. E. Anderson, J. Appl. Phys. **38**, 3245 (1967).

[2] Specifically, when electric fields of about 0.01–0.06 eV/Å are applied to wide band-gap metal oxides (e.g., Al_2O_3), electrons, injected into the bottom of the conduction band by tunneling from near the Fermi level of the adjacent metal contact, are able to lose to the crystal a sizable fraction of the kinetic energy they acquire by falling through the impressed potential. This is measured by allowing the electrons to pass through a very thin metal contact on the opposite side and emerge into vacuum. Their energies are determined by using standard retarding field techniques. For Al_2O_3, 0.03 eV/Å is a commonly obtained value.

[3] K. K. Thornber, PhD thesis, Part II, 1966 (unpublished). The approach given here is also contained in this thesis.

[4] R. P. Feynman, Phys. Rev. **97**, 660 (1955), hereafter referred to as I.

[5] R. P. Feynman, R. W. Hellwarth, C. K. Iddings, and P. M. Platzman, Phys. Rev. **127**, 1004 (1962), hereafter referred to as FHIP.

average, acquiring kinetic energy by falling through the impressed potential, the energy per unit distance being just the applied field, and losing this energy by a net emission of optical phonons. Being a steady-state situation, the expectation value of the rate of change of electron momentum is zero. Therefore, we begin the calculation with the quantum-mechanical expression for the rate of change of electron momentum, and then determine the expectation value of each operator in the equation. The quantity $\langle\dot{\mathbf{p}}\rangle$ is zero, and we are left with an equation which balances the applied field, or rate of increase of electron momentum, against the rate of loss of momentum due to lattice scattering. This result is an explicit dependence for the field in terms of the steady-state velocity of the electron. The key feature then is not to ask what velocity is obtained for a given field. Rather, for a specific velocity, what field is necessary to maintain that velocity, or more generally, what energy is lost per unit distance by an electron whose expectation velocity is specified.

We assume that only the (polar) optical modes interact with the electron and that they do so in a very simple way. 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 with possibly an altered mass. No limit is placed on the strength of the coupling or the electric field, and the temperature is arbitrary. If the applied electric field is sufficiently strong to alter the phonon dispersion relation or the coupling, it is the altered values which must be used in our calculations.

Starting with the operator equation for the rate of change of momentum, we eliminate the lattice coordinates exactly using the path-integral method, and then evaluate this expression by an approximate approach similar to that used in I and FHIP. In FHIP the ac impedance of electrons in a polar crystal is determined for arbitrary coupling strength, temperature, and frequency of the small, oscillatory, applied electric field. Here we are interested in the zero-frequency but finite applied field situation.

The nonlinearities inherent in this transport problem emerge in a striking manner. Calculating energy loss per unit distance, which is the applied field for velocities below threshold and energy loss in the absence of an applied field for velocities above threshold, we obtain with increasing velocity first the strongly temperature-dependent, low-field mobility, as found by FHIP in the limit of zero frequency of the applied field. Then, for initial lattice temperatures below the reststrahlen energy, there is a rapid increase in the rate of energy loss as the electron's translational kinetic energy approaches this optical-phonon energy. This is followed by a temperature-*in*dependent threshold, or maximum loss of energy with distance, and finally a subsequent temperature-independent decrease as $\ln(v)/v^2$ for velocities well above threshold. For initial lattice temperatures above the optical-phonon energy, the low-field linear region passes smoothly through a broad temperature-dependent threshold which portrays the dominance of scattering from existing optical phonons. For very large velocities, the weak coupling limit of the solution gives the expected perturbation result. Thus, in a single family of field-velocity curves with temperature as the parameter, all the expected physical phenomena appear. Agreement with experiment is obtained for phenomena occurring the the vicinity of the threshold. We conclude that optical-phonon scattering can produce the large loss of electron energy observed in tunnel-emission devices.

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

If an electron is drawn through a crystal by an externally applied electric field, its momentum is changed by both the field and by the emission and absorption of phonons. Using operators, we may express this by a simple conservation equation

$$\dot{\mathbf{p}}=i[H,\mathbf{p}]/\hbar, \tag{1}$$

where H is the Hamiltonian for the system and $\mathbf{p}$ is the momentum operator of the electron.[6] The Hamiltonian is the sum of four terms—the kinetic energy of the electron and the Hamiltonian of the lattice, which commute with $\mathbf{p}$, and the interaction of the electron with the lattice $V_{(\mathbf{x},\mathbf{Q}_1,\ldots,\mathbf{Q}_n)}$ and with the applied field $-\mathbf{F}\cdot\mathbf{x}$, where $\mathbf{F}$ represents the applied force. Inserting into (1) gives

$$\dot{\mathbf{p}}=\mathbf{F}-i[\mathbf{p},V]/\hbar. \tag{2}$$

If we now evaluate the expectation value of both sides of (2), we obtain

$$\mathbf{F}=\langle i[\mathbf{p},V]\rangle/\hbar=\langle\nabla_{\mathbf{x}}V\rangle, \tag{3}$$

because in the steady state $\langle\dot{\mathbf{p}}\rangle=0$. This equation expresses the equality between the rate of increase and rate of decrease of electron momentum under steady-state conditions.

To calculate $\langle\nabla_{\mathbf{x}}V\rangle$, we must determine the density matrix ρ_t of the electron-lattice system in the steady state. To do so, we formulate the problem by specifying that at some time $t=t_1$ we inject the electron into the lattice, which itself is in thermal equilibrium in the presence of the applied electric field, and then wait until the steady state is reached, that is, until $\langle\dot{\mathbf{p}}\rangle=0$. Thus to within a normalizing constant $\rho_{t_1}=\exp(-\beta H_{\text{lattice}})$, $\beta=1/kT$. For $t>t_1$, we solve

$$i\frac{\partial\rho}{\partial t}=[H,\rho]/\hbar, \tag{4}$$

[6] Equation (1) is valid whether or not H is a function of time; however, to yield exact results it must be sandwiched between exact wave functions (or used with an exact density matrix) of H.

obtaining[7,8]

$$\rho_t=\exp\left(-i\int_{t_1}^{t}H_s ds/\hbar\right)\rho_{t_1}\exp\left(i\int_{t_1}^{t}H_{s'}ds'/\hbar\right). \quad (5)$$

This gives us the density matrix for $t>t_1$, a nonequilibrium situation. The $\langle\nabla_x V\rangle$ is now given by

$$\langle\nabla_x V\rangle_t=\mathrm{Tr}[(\nabla_x V)\rho_t], \quad (6)$$

and to obtain the steady state, we will let $t\to\infty$.

The model Hamiltonian preserving the essential physics of the problem of an electron interacting with the vibrational modes of the crystal in an electric field is

$$H=\mathbf{p}^2/2m-\mathbf{F}\cdot\mathbf{x}+\sum_{\mathbf{k}}\hbar\omega_{\mathbf{k}}a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}+V^{-1/2}\sum_{\mathbf{k}}(C_{\mathbf{k}}a_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{x}}+C_{\mathbf{k}}^{*}a_{\mathbf{k}}^{\dagger}e^{-i\mathbf{k}\cdot\mathbf{x}}). \quad (7)$$

Here $a_{\mathbf{k}}^{\dagger}$ and $a_{\mathbf{k}}$ are the creation and annihilation operators for phonons of momentum $\mathbf{k}$, frequency $\omega_{\mathbf{k}}$, coupled to the electron via the coupling coefficient $C_{\mathbf{k}}$; $\mathbf{p}$ is the momentum of the electron, $\mathbf{x}$ is its coordinate, m is its effective mass in a fixed lattice; V is the crystal volume; $\mathbf{F}=-e\mathbf{E}$, e is the magnitude of the electronic charge, $\mathbf{E}$ is the applied electric field in the crystal.

As a specific example, we shall later use Frohlich's model[9] of the polaron in which

$$C_{\mathbf{k}}=(-\hbar\omega_{\mathbf{k}}/k)(\hbar/2m\omega_{\mathbf{k}})^{1/4}(4\pi\alpha)^{1/2},$$

where

$$\alpha=(e^2/\hbar)(1/\epsilon_\infty-1/\epsilon_s)(m/2\hbar\omega_{\mathbf{k}})^{1/2},$$

$\omega_{\mathbf{k}}=1$ independent of $\mathbf{k}$, ϵ_s is the static dielectric constant of the material, and ϵ_∞ is the optical dielectric constant.

We now maintain the usual convention of setting $\hbar=1$, working with a unit volume, and incorporating e into $\mathbf{E}$ so that $-e\mathbf{E}\to\mathbf{E}$.

If we insert the Hamiltonian (7) into (1) and carry out (2) and (3) we obtain

$$\mathbf{E}=\sum_{\mathbf{k}}\mathbf{k}\langle\hat{R}_{\mathbf{k}}\rangle, \quad (8a)$$

where

$$\hat{R}_{\mathbf{k}}=-i(C_{\mathbf{k}}^{*}a_{\mathbf{k}}^{\dagger}e^{-i\mathbf{k}\cdot\mathbf{x}}-C_{\mathbf{k}}a_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{x}}). \quad (8b)$$

The $\langle\hat{R}_{\mathbf{k}}\rangle$ may be interpreted as the net rate of emission (rate of emission less rate of absorption) of longitudinal optical phonons of wave vector $\mathbf{k}$, and $\mathbf{k}$ may be interpreted as the change of momentum of the electron. $\mathbf{E}$ is just the rate of increase of electron momentum. Equation (8a) expresses the fact that in steady state this gain and loss just balance. If we can evaluate $\langle\hat{R}_{\mathbf{k}}\rangle=\mathrm{Tr}(\rho_t\hat{R}_{\mathbf{k}})$ as a function of the expectation steady-state velocity of the electron, we shall obtain a relationship between the applied field and this velocity.

The problem of integrating $\mathrm{Tr}(\rho_t)$ over the crystal oscillator coordinates has been solved in I and FHIP. We use this result to determine $\mathrm{Tr}(\rho_t\hat{R}_{\mathbf{k}})$ in the following manner. If we write H_s and H_s' as

$$H_s=\mathbf{p}_s^2/2m-\mathbf{F}(s)\cdot\mathbf{x}_s+\sum_{\mathbf{q}}\omega_{\mathbf{q}}a_{\mathbf{q}}^{\dagger}a_{\mathbf{q}}+\sum_{\mathbf{q}}\{C_{\mathbf{q}}[1-\gamma\delta_{\mathbf{q},\mathbf{k}}\delta(s-t)]a_{\mathbf{q}}e^{i\mathbf{q}\cdot\mathbf{x}_s}+C_{\mathbf{q}}^{*}[1+\gamma\delta_{\mathbf{q},\mathbf{k}}\delta(s-t)]a_{\mathbf{q}}^{\dagger}e^{-i\mathbf{q}\cdot\mathbf{x}_s}\}$$

and

$$H_{s'}=\mathbf{p}_{s'}^2/2m-\mathbf{F}'(s')\cdot\mathbf{x}_{s'}+\sum_{\mathbf{q}}\omega_{\mathbf{q}}a_{\mathbf{q}}^{\dagger}a_{\mathbf{q}}+\sum_{\mathbf{q}}\{C_{\mathbf{q}}a_{\mathbf{q}}e^{i\mathbf{q}\cdot\mathbf{x}_{s'}}+C_{\mathbf{q}}^{*}a_{\mathbf{q}}^{\dagger}e^{-i\mathbf{q}\cdot\mathbf{x}_{s'}}\},$$

then

$$\mathrm{Tr}(\hat{R}_{\mathbf{k}}\rho_t)=\frac{\partial}{\partial\gamma}[\mathrm{Tr}(\rho_t)]|_{\gamma=0},$$

where ρ_t is given by (5) and $\rho_{t_1}=\exp(-\beta\sum_{\mathbf{k}}\omega_{\mathbf{k}}a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}})$. The result is

$$\langle\hat{R}_{\mathbf{k}}\rangle_{t_2}=\int\int R_{\mathbf{k}}e^{i\Phi_e}D(\mathbf{x})D(\mathbf{x}'), \quad (9a)$$

where $\int\int D(\mathbf{x})D(\mathbf{x}')$ is the path integral over $\mathbf{x}$ and $\mathbf{x}'$ between t_1 and t_2,

$$\Phi_e=\int_{t_1}^{t_2}(\tfrac{1}{2}m\dot{\mathbf{x}}_t^2+\mathbf{E}\cdot\mathbf{x}_t)dt-\int_{t_1}^{t_2}(\tfrac{1}{2}m\dot{\mathbf{x}}_t'^2+\mathbf{E}\cdot\mathbf{x}_t')dt+i\sum_{\mathbf{k}}|C_{\mathbf{k}}|^2\int_{t_1}^{t_2}dt\int_{t_1}^{t}dt'[T_{\omega_{\mathbf{k}}}(t-t')e^{-i\mathbf{k}\cdot(\mathbf{x}_{t'}-\mathbf{x}_{t''})}+T_{\omega_{\mathbf{k}}}^{*}(t-t')e^{i\mathbf{k}\cdot(\mathbf{x}_t-\mathbf{x}_{t'})}-T_{\omega_{\mathbf{k}}}(t-t')e^{i\mathbf{k}\cdot(\mathbf{x}_t-\mathbf{x}_{t''})}-T_{\omega_{\mathbf{k}}}^{*}(t-t')e^{-i\mathbf{k}\cdot(\mathbf{x}_{t'}-\mathbf{x}_{t'})}], \quad (9b)$$

$$T_{\omega_{\mathbf{k}}}(\tau)=e^{i\omega_{\mathbf{k}}\tau}/(1-e^{-\beta\omega_{\mathbf{k}}})+e^{-i\omega_{\mathbf{k}}\tau}/(e^{\beta\omega_{\mathbf{k}}}-1), \quad (9c)$$

and

$$R_{\mathbf{k}}=|C_{\mathbf{k}}|^2\int_{t_1}^{t_2}dt\left(\frac{e^{-i\omega_{\mathbf{k}}(t_2-t)}e^{i\mathbf{k}\cdot(\mathbf{x}_{t_2}-\mathbf{x}_t)}}{1-e^{-\beta\omega_{\mathbf{k}}}}-\frac{e^{i\omega_{\mathbf{k}}(t_2-t)}e^{-i\mathbf{k}\cdot(\mathbf{x}_{t_2}-\mathbf{x}_t)}}{e^{\beta\omega_{\mathbf{k}}}-1}+\frac{e^{i\omega_{\mathbf{k}}(t_2-t)}e^{-i\mathbf{k}\cdot(\mathbf{x}_{t_2}-\mathbf{x}_{t'})}}{1-e^{-\beta\omega_{\mathbf{k}}}}-\frac{e^{-i\omega_{\mathbf{k}}(t_2-t)}e^{i\mathbf{k}\cdot(\mathbf{x}_{t_2}-\mathbf{x}_{t'})}}{e^{\beta\omega_{\mathbf{k}}}-1}\right). \quad (9d)$$

Relation (9) includes all quantum interferences in the emission and absorption of phonons, real and virtual, and represents a substantial simplification of the problem in that the oscillator coordinates have been eliminated exactly. The expression (9), however, is still quite complicated, and we know of no exact way to perform the two-path integrals over the electronic coordinates. Thus we must use an approximate method.

[7] Here the time-ordered operator notation is used (see Ref. 8): Unprimed operators to the left and ordered right to left with increasing time, and primed operators to the right and ordered left to right with increasing time.

[8] R. P. Feynman, Phys. Rev. **84**, 108 (1951).

[9] H. Fröhlich, *Advances in Physics*, edited by N. F. Mott (Taylor & Francis, Ltd., London, 1954), Vol. 3, p. 325.

We point out, moreover, that the only term which gives us trouble and, therefore, which must be approximated, is the square bracketed term in the exact action, Φ_e (9b), and this involves only the electron-lattice interaction. Neither the electric field term in this action nor the R_k term, representing the Hamiltonian, need be altered. This is crucial, because the most sensitive dependence between the field and the velocity is governed by R_k. If, for example, the Hamiltonian is approximated in the usual way by the dipole approximation, the resulting R_k (and the new action) can give only the usual linear theory of field versus velocity. As we shall see in Sec. III, we may evaluate (9) by modifying Φ_e but not R_k. This ensures that the basic physical features of the problem will be maintained.

III. METHOD OF APPROXIMATION AND THE RESULT

The heart of the problem is how to represent the interaction of the small system, in which one is usually interested, with a dissipative system so that the problem may be treated directly, yet without losing its essential physical features. Approaching this problem from the quantum mechanics of Hamiltonians is difficult and cumbersome. One reason is that is is impossible to introduce loss into a one-particle Lagrangian or Hamiltonian. However, by using the path-integral approach, in particular the concept of the influence functional,[10] it is often possible to obtain enough physical insight into the nature of the dissipation to formulate a solvable approximation and to use this approximation in a well-defined manner. Additional accuracy can be obtained by introducing parameters or functions in the approximate influence functional which can be determined independently through a variational principle. Such a procedure was quite successful in treating the ground-state energy of the polaron.[4] However, neither in FHIP nor in the present paper has a variational principle emerged for the impedance, in the former study, or for the field-velocity dependence developed here.

A physically very reasonable approximation for the influence functional $\exp(i\Phi_e)$ of Eq. (9) was developed in I to treat the ground-state energy and in FHIP to treat the impedance of the polaron. These results indicate that this model yields the essential features of the physical phenomena expected. The approximation consists on modifying the eight terms in (9b) of the exact form

$$\sum_{\mathbf{k}} |C_k|^2 \exp(-i\mathbf{k}\cdot(\mathbf{x}_t'-\mathbf{x}_{t'}'))e^{i\omega_k(t-t')}.$$

These assume the approximate form

$$-Ce^{iw(t-t')}(\mathbf{x}_t'-\mathbf{x}_{t'}')^2,$$

where C is the relative strength and w is the frequency of the oscillator. The frequency in the thermal factors in (9b) is also changed from ω_k to w. In I, parameters C and w were determined so that this oscillator interaction approximates the effect of Φ_e as closely as possible in the sense of yielding a minimum ground-state energy. [In the Fröhlich model this term is $(\alpha/\sqrt{2})e^{i(t-t')}/\times|\mathbf{x}_t'-\mathbf{x}_{t'}'|$, a Coulombic interaction oscillating in time. However, if in the Fröhlich model one accounts for the discreteness of the ionic lattice by limiting the above summation over $\mathbf{k}$ to $|\mathbf{k}|\leq k_{\max}$ instead of summing over all $\mathbf{k}$, for small $|\mathbf{x}_t'-\mathbf{x}_{t'}'|$ the interaction is harmonic, being proportional to $(\mathbf{x}_t'-\mathbf{x}_{t'}')^2$.]

Our problem is somewhat different from that treated in I and FHIP, and hence we must modify this approximation somewhat. In calculating the ground-state energy[4] the mean velocity of the electron was zero, and hence there was no net translation. Here, however, the electron translates with some finite, expectation steady-state velocity $\mathbf{v}$ in addition to its fluctuations. Thus we should first transform the integrations in (9) to a reference frame moving with the electron. Formally this can be done simply with a change of variables. In this frame the electron fluctuates about its mean position as it does in the ground-state energy calculation.

This change of reference frames leads to another difference which should be included in the approximation. As will be seen shortly from Eq. (10c), the change of variables $\mathbf{x}_t=\mathbf{y}_t+\mathbf{v}t$, $\mathbf{x}_t'=\mathbf{y}_t'+\mathbf{v}t$ leads to a modification of the frequencies $\omega_k\rightarrow\omega_k\pm\mathbf{k}\cdot\mathbf{v}$. Hence, now one should couple the electron to a distribution of oscillators of various frequencies rather than to a single oscillator with a single frequency as was done in I and FHIP. This possibility was indicated in Sec. 7 of FHIP, and we shall make use of it here.

To carry out the above program we first change variables as indicated, absorbing constant factors into the normalization. The result of this is still an exact expression,[11] only now $\mathbf{y}$ is the coordinate of the electron with respect to its mean position in time:

$$E=\sum_{\mathbf{k}}\mathbf{k}\int\int R_k'e^{i\Phi_e'}D(\mathbf{y})D(\mathbf{y}'), \tag{10a}$$

where

$$\Phi_e'=\int_{t_1}^{t_2}(\tfrac{1}{2}m\dot{\mathbf{y}}_t^2+\mathbf{E}\cdot\mathbf{y}_t)dt-\int_{t_1}^{t_2}(\tfrac{1}{2}m\dot{\mathbf{y}}_t'^2+\mathbf{E}\cdot\mathbf{y}_t')dt$$
$$+i\sum_{\mathbf{k}}|C_k|^2\int_{t_1}^{t_2}dt\int_{t_1}^{t}dt'[S_{\omega_k}(t-t')e^{-i\mathbf{k}\cdot(\mathbf{y}_t'-\mathbf{y}_{t'}')}$$
$$+S_{\omega_k}^*(t-t')e^{i\mathbf{k}\cdot(\mathbf{y}_t-\mathbf{y}_{t'})}-S_{\omega_k}(t-t')e^{-i\mathbf{k}\cdot(\mathbf{y}_t-\mathbf{y}_{t'}')}$$
$$-S_{\omega_k}^*(t-t')e^{+i\mathbf{k}\cdot(\mathbf{y}_t'-\mathbf{y}_{t'})}], \tag{10b}$$

$$S_{\omega_k}(\tau)=\frac{e^{i\omega_k'\tau}}{1-e^{-\beta\omega_k}}+\frac{e^{-i\omega'-\mathbf{k}\tau}}{e^{\beta\omega_k}-1},\quad \omega_k'=\omega_k-\mathbf{k}\cdot\mathbf{v}, \tag{10c}$$

[10] R. P. Feynman and F. L. Vernon, Jr., Ann. Phys. (N. Y.) 24, 118 (1963).

[11] In (10b) we have used $|C_{-k}|^2=|C_k|^2$ and $\omega_k=\omega_{-k}$ to change the sign of $\mathbf{k}$ in the last two exponentials. These follow quite generally from the time-reversal symmetry of the physical phenomena characterizing the interaction and the oscillators.

and

$$R_{\mathbf{k}}' = |C_{\mathbf{k}}|^2 \int_{t_1}^{t_2} dt \Bigg(\frac{e^{-i\omega_{\mathbf{k}}'(t_2-t)} e^{i\mathbf{k}\cdot(\mathbf{y}_{t_2}-\mathbf{y}_t)}}{1-e^{-\beta\omega_{\mathbf{k}}}} - \frac{e^{i\omega_{\mathbf{k}}'(t_2-t)} e^{-i\mathbf{k}\cdot(\mathbf{y}_{t_2}-\mathbf{y}_t)}}{e^{\beta\omega_{\mathbf{k}}}-1} + \frac{e^{i\omega_{\mathbf{k}}'(t_2-t)} e^{-i\mathbf{k}\cdot(\mathbf{y}_{t_2}-\mathbf{y}_{t'})}}{1-e^{-\beta\omega_{\mathbf{k}}}} - \frac{e^{-i\omega_{\mathbf{k}}'(t_2-t)} e^{i\mathbf{k}\cdot(\mathbf{y}_{t_2}-\mathbf{y}_{t'})}}{e^{\beta\omega_{\mathbf{k}}}-1} \Bigg). \quad (10d)$$

To see how we take advantage of this transformation and introduce the approximate influence functional, expand the square-bracketed expression in Eq. (10b) in powers of $\mathbf{k}\cdot\mathbf{y}$. The zeroth-order term vanishes; a first-order term and all higher odd-order terms enter which would be absent in the untransformed (or $\mathbf{v}=0$) integrals; all even-order terms above the zeroth enter as before,[4,5] except for the altered frequencies ($\omega_{\mathbf{k}} \rightarrow \omega_{\mathbf{k}}'$) in the time-dependent phases of the integrand. As mentioned above, in I and FHIP (where $\mathbf{v}=0$) the spirit was to simulate the harmonic and all higher-order terms by a single-harmonic term with frequency and coupling strength derivable from minimizing the free energy. Here, besides introducing a distribution of oscillators to represent the new spectrum of frequencies, we see that in the $\mathbf{v}\neq 0$ frame the potential is clearly not symmetric in the $\pm\mathbf{v}$ direction. This suggests using a linear term of the form

$$\int_{t_1}^{t_2} \mathbf{F}_0(t)\cdot(\mathbf{y}_t-\mathbf{y}_{t'})dt \quad (11)$$

to simulate all of the odd terms of the expansion. $\mathbf{F}_0(t)$ would then also have to be determined from some other principle. Unfortunately such a term can have no effect on the result.[12]

The arguments given above suggest that the dynamical behavior of the electron might be described approximately if we replace the exact influence functional by $\exp(i\Phi_0)$, where now

$$\Phi_0 = \int_{t_1}^{t_2} (\tfrac{1}{2}m\dot{y}_t^2 - \tfrac{1}{2}m\dot{y}_{t'}^2)dt - i\int_0^\infty d\Omega\, G(\Omega) \int_{t_1}^{t_2} dt \int_{t_1}^{t} dt' \times [T_\Omega(t-t')(\mathbf{y}_t'-\mathbf{y}_{t'}')^2 + T_\Omega^*(t-t')(\mathbf{y}_t-\mathbf{y}_{t'})^2 - T_\Omega(t-t')(\mathbf{y}_t-\mathbf{y}_{t'}')^2 - T_\Omega^*(t-t')(\mathbf{y}_t'-\mathbf{y}_{t'})^2] \quad (12)$$

and where T_Ω is as given in (9c).[13] As discussed above, we have introduced the oscillator distribution $G(\Omega)$ for $|C_k|^2$ to partially compenstate for the error introduced by using a parabolic potential in place of the true potential. Making this substitution and using the general path integral evaluated in Appendix A, we obtain the explicit relation shown between the applied electric field $\mathbf{E}$ in the lattice and the expectation, steady-state velocity $\mathbf{v}$ of the electron.

$$\mathbf{E} = \int_{-\infty}^{\infty} d\xi \sum_{\mathbf{k}} |C_{\mathbf{k}}|^2 \mathbf{k} \Bigg(\frac{e^{i(\omega_{\mathbf{k}}-\mathbf{k}\cdot\mathbf{v})\xi}}{1-e^{-\beta\omega_{\mathbf{k}}}} - \frac{e^{-i(\omega_{\mathbf{k}}-\mathbf{k}\cdot\mathbf{v})\xi}}{e^{\beta\omega_{\mathbf{k}}}-1} \Bigg) e^{-k^2\bar{K}_\beta(\xi)} \quad (13a)$$

$$= \int_{-\infty}^{\infty} d\xi \sum_{\mathbf{k}} |C_k|^2 \mathbf{k} T_{\omega_{\mathbf{k}}}(\xi) e^{-i\mathbf{k}\cdot\mathbf{v}\xi} e^{-k^2\bar{K}_\beta(\xi)}. \quad (13b)$$

Recalling our basic equation (8a), we may interpret this result as an expression for the electric field $\mathbf{E}$ needed to balance the net loss of energy per unit distance (or momentum per unit time) to the polar crystal to maintain the steady-state translational velocity $\mathbf{v}$ of the electron, whose interaction with the lattice is characterized by the $C_{\mathbf{k}}$ of (7). In (13) we have set

$$\bar{K}_\beta(\xi) = K_\beta(\xi) - K_\beta(0) = \int_0^\infty d\omega [-\Gamma(\omega)] \Bigg(\frac{1-e^{i\omega\xi}}{1-e^{-\beta\omega}} + \frac{1-e^{-i\omega\xi}}{e^{\beta\omega}-1} \Bigg). \quad (13c)$$

$K_\beta(\xi)$ and $\Gamma(\omega)$ are introduced and discussed in Appendix A.

In Sec. IV we develop a physical feel for (13) by examining several limiting cases and comparing these with results obtainable by other means. Then in Sec. V we shall use the Fröhlich polaron model for $|C_{\mathbf{k}}|^2$ and $\omega_{\mathbf{k}}$ and the one-oscillator approximation[4] for $G(\Omega)$ to obtain numerical results. The physics we have maintained in our method will then be strikingly apparent.

For the present section let us make several observations regarding our result (13). There are really two ways in which $\mathbf{E}$ depends on $\mathbf{v}$: The explicit dependence, which in the phase of the integrand is a very sensitive dependence, and which we have preserved in its correct form, and (possibly) an implicit dependence in $\bar{K}_\beta(\xi)$ which would arise indirectly through the choice for our result of a best possible distribution of oscillators $G(\Omega)$

[12] The coefficient of the first-order term in the expansion of (10b) is independent of time. This suggests $\mathbf{F}_0$ should be independent of time. If this is the case, then the final result (13) is in fact found to be *in*dependent of this constant. Hence nothing is gained by inserting such a term. One can easily let $\mathbf{F}_0(t)$ be a function of t and carry out the path integrals as in Appendix A without additional complication. But then one is faced with what such a time dependent $\mathbf{F}_0(t)$ would represent physically in the context of our problem. Surely such a coefficient must be translationally invariant in absolute time as are coefficients of all higher processes, and only $\mathbf{F}_0(t)=$const satisfies this requirement. (The reason that the $\mathbf{F}_0=$const case does not lead to additional terms in the final result is easy to see. A uniform applied field superimposed on a harmonic potential is just a shifted harmonic potential of the same strength. This clearly can have no effect on the fluctuations of the electron in its well.)

[13] At this point the reader should note that we have in using $G(\Omega)T_\Omega(t-t')$ in (12) not used the most general approximation suggested by our expansion of (10b). Such an expression would be $G_1(\Omega)\exp[i\Omega(t-t')]+G_2(\Omega)\exp[-i\Omega(t-t')]$ for $0\leq\Omega<\infty$, or simply $G'(\Omega)\exp[i\Omega(t-t')]$ for $-\infty<\Omega<\infty$. Our form assumes that the effective oscillators are not only in thermal equilibrium but in equilibrium at the initial lattice temperature. We work out the problem for this more general approximation in Appendix B. The result may be used to evaluate $\mathbf{E}$ versus $\mathbf{v}$ if one wished to use for the distribution of oscillators just that one given by the quadratic terms of (10b). This would introduce a velocity dependence into the trial influence functional which is absent in (12).

with steady-state velocity.[14–16] For lack of a better criterion we will not consider this latter possibility. We should note, however, that if we change the integration of ξ from $\mathrm{Im}(\xi)=0$ to $\mathrm{Im}(\xi)=\frac{1}{2}\beta$, we obtain a form convenient for numerical work,

$$\mathbf{E}=\int_{-\infty}^{\infty}d\xi\sum_{\mathbf{k}}|C_{\mathbf{k}}|^2\mathbf{k}\frac{\cos(\omega_{\mathbf{k}}\xi)}{\sinh(\frac{1}{2}\beta\omega_{\mathbf{k}})}\times e^{-i\mathbf{k}\cdot\mathbf{v}(\xi+i\beta/2)}e^{-k^2\bar{K}_\beta'(\xi)}, \quad (14a)$$

where now

$$\bar{K}_\beta'(\xi)=\int_0^{\infty}d\omega[-\Gamma(\omega)]\times\left(\tanh(\tfrac{1}{4}\beta\omega)+\frac{1-\cos(\omega\xi)}{\sinh(\frac{1}{2}\beta\omega)}\right) \quad (14b)$$

and where, in reality, only the real part of $e^{-ik_xv(\xi+i\beta/2)}$ enters. In this form the coefficients of k^2 in the exponent is purely real, so that to the extent whereby the phase of the integrand is the sensitive function of the velocity $\mathbf{v}$, the dependence of $\overline{\mathbf{K}}_\beta'$ on velocity will be less important.

Up to this point we have been using applied field, rate of change of electron momentum, and loss of energy per unit distance interchangeably. Naturally, we would expect that as we apply stronger and stronger electric fields a point is reached, where no steady-state drift velocity will exist for the electron. Indeed, our result (13) contains this as we point out in our discussion of the numerical result for the Fröhlich model. How can we interpret our result for velocity above this threshold, especially when throughout our discussion we have imposed the steady-state condition that the expectation values do not change in time.

Rewriting (2) with the help of (8) but not imposing the steady-state restriction we have

$$\mathbf{E}-\dot{\mathbf{p}}=\sum_{\mathbf{k}}\mathbf{k}\hat{R}_{\mathbf{k}}, \quad (15)$$

which, as described in Sec. II, expresses, in the spirit of the correspondence principles, the balance between the rate of increase of electron momentum in the applied field $\mathbf{E}$ and the rate of decrease due to scattering by the crystal and due to inertial acceleration. The steady-state criterion entered twice in our solution: first in setting $\langle\dot{\mathbf{p}}\rangle=0$, second in the evaluation of $\langle\hat{R}_{\mathbf{k}}\rangle$. We shall see that under certain restricted conditions, if $\mathbf{E}$ is interpreted as the rate of momentum lost to the lattice in scattering, (13) may be physically meaningful even when the steady state is not possible.

Qualitatively our result (13) can be divided into two regions in the velocity $\mathbf{v}$. The function $\mathbf{E}(\mathbf{v})$ rises montonically from zero at $\mathbf{v}=0$ to a threshold E_{Th} at some v_{Th}, and then falls montonically to zero for infinite $\mathbf{v}$. Physically these two situations correspond to what we shall call the stable and the unstable regions, respectively. For $v<v_{\mathrm{Th}}$, should the velocity of the electron increase, the corresponding loss increases above that which the electron gains from the applied field. Consequently, its velocity must decrease. Similarly, if the velocity decreases, it will gain from the field more than it loses to the lattice, and hence its velocity will increase. In this sense the motion is stable: the electron drifts with an expectation velocity $\mathbf{v}$, and its average loss of momentum per unit time, its average loss of energy per unit distance, to the lattice is just balanced by the applied field.

For $v>v_{\mathrm{Th}}$ this situation is quite different. First, we stress that we do not mean $E>E_{\mathrm{Th}}$ for this situation. To be sure, if the field exceeds the threshold for a given temperature, that is, the maximum rate of loss to the crystal at that temperature, the steady-state velocity is no longer meaningful, at least in the manner which we have used it. For $E>E_{\mathrm{Th}}$ the problem is no longer a steady-state one: the electron accelerates indefinitely (unless, of course, another mode of energy loss is introduced, such as pair production). Thus, in this paper our treatment applies only to applied fields below threshold.

If now the field is below threshold and the velocity exceeds v_{Th}, the loss to the crystal is still given by (13), assuming a steady-state situation, and this loss can be compensated by an applied field. This situation, of course, is unstable. If the velocity decreases, the loss increases, which further decreases the velocity, etc., until a stable steady state is reached at the applied field, but for the corresponding $v<v_{\mathrm{Th}}$. Thus, while our results give us the loss for steady-state velocity above threshold, this situation as a steady-state phenomenon is probably not physically realizable.

An alternative interpretation for $v>v_{\mathrm{Th}}$ is apparent from Eq. (15). If there is no applied field, then determining the expectation value of (15) would give us a time-dependent relation for the loss of momentum in time. If in addition $\dot{v}\tau\ll v$, where v is the electron velocity and τ is a valid "collision time," then (13) could be used to obtain the rate of loss of electron momentum to the crystal. And if there is appreciable persistence of the initial momentum, a rather unlikely situation except in the limit of very fast particles, (13) can provide the rate of loss of energy with distance. For example, while it can be hard to calculate loss in a transient situation, here we visualize applying a field which just compensates the loss, and we perform the somewhat easier steady-state solution to determine this loss.

[14] If we could find a variational principle for the field-velocity dependence, we would obtain the best $G(\Omega)$ possible for our result as a function coupling strength, temperature, and velocity. Using the one-oscillator distribution[4] and the variational principle for the free energy, the parameters are found to be relatively sensitive to coupling strength but insensitive to temperature (Refs. 15 and 16). We must assume here that the dependence with velocity is also insensitive.

[15] Y. Osaka, Progr. Theoret. Phys. (Kyoto) **22**, 437 (1959).

[16] M. A. Krivogloz and S. I. Pekar, Bull. Acad. Sci. USSR **21**, (1957); **21**, 13 (1957); **21**, 29 (1957).

This leads to an interesting situation. Suppose we apply an electric field $E_0<E_{\rm Th}$ to the crystal and then somehow inject electrons with velocity $v_i>v_{\rm Th}$. Given $E_0<E_{\rm Th}$, (13) is satisfied for *two* values of velocities v_0 and v_1 and $v_0<v_{\rm Th}<v_1$. If now $v_i>v_1$, the electron will lose less energy per unit distance to the crystal than it can gain from the applied field. In this case the electron is accelerated until pair production dominates. If $v_i<v_1$, then the electron will lose more energy per unit distance to the lattice than it gains from the applied field. In this latter case the electron will decelerate until steady state is reached for $v=v_0$. This essentially serves the function of a particle detector for velocity.

IV. COMPARISON WITH OTHER RESULTS

To obtain additional insight into our relation (13) we turn to three special limiting cases: the weak coupling limit, the small-field, small-velocity limit, and the low-frequency limit (of the impedance).

A. Weak Coupling Limit

Let us briefly consider the special case of the electron in the crystal lattice under the hypothesis that the interaction is so weak that we may consider the collisions with optical phonons to occur essentially independently; that is, sufficiently separated in time so that the quantum interferences between these collisions are negligible. Under these conditions $\bar{K}_\beta(\xi)$ in (13) assumes its free-particle value[17] of $(-i\xi+\xi^2/\beta)/2m$.

This result may be obtained more simply as follows. The above weak coupling criterion permits us to use Fermi's Golden rule to calculate the transition rate between free-electron states $|p\rangle$ and $|p'\rangle$ due to scattering with optical phonons. If we average over a thermal distribution of phonons, then the rate to pass from $|p\rangle$ to $|p'\rangle$ by phonon absorption is simply

$$2\pi|C_{\rm k}|^2\delta(-k^2/2m-\mathbf{p}\cdot\mathbf{k}/m+\omega_{\rm k})/(e^{\beta\omega_{\rm k}}-1), \quad (16a)$$

where $\mathbf{k}=\mathbf{p}'-\mathbf{p}$, and that by phonon emission is

$$2\pi|C_{\rm k}|^2\delta(-k^2/2m+\mathbf{p}\cdot\mathbf{k}/m-\omega_{\rm k})/(1-e^{-\beta\omega_{\rm k}}). \quad (16b)$$

Writing

$$\delta(x)=\left(\int_{-\infty}^{\infty}e^{-ix\xi}d\xi\right)\Big/2\pi,$$

and equating the electric field, or gain of momentum per unit time, to the loss of momentum per unit time to the lattice as given by these rates, we obtain the relation

$$\mathbf{E}=\int_{-\infty}^{\infty}d\xi\sum_{\rm k}|C_{\rm k}|^2\mathbf{k}\left(\frac{e^{i(\omega_{\rm k}-\mathbf{k}\cdot\mathbf{v})\xi}}{1-e^{-\beta\omega_{\rm k}}}-\frac{e^{-i(\omega_{\rm k}-\mathbf{k}\cdot\mathbf{v})\xi}}{e^{\beta\omega_{\rm k}}-1}\right)\times\exp-\frac{k^2}{2m}\left(-i\xi+\frac{\xi^2}{\beta}\right), \quad (17)$$

where the zero-order distribution for the electrons is taken as a drifted Maxwellian whose mean velocity is equal to the steady-state velocity $\mathbf{v}$. This is just our result (13) with $\bar{K}_\beta(\xi)$ replaced by its free-particle value.[17] As the coupling is increased, the importance of higher-order scattering is represented in our result by $\bar{K}_\beta(\xi)$, departing significantly from this free-particle value. One effect of this is to enhance the apparent mass of the electron.[4]

It should be emphasized that this weak coupling limit of our result does *not* agree with the mobility obtained from standard Boltzmann treatments applicable for sufficiently low temperature.[18] It differs slightly in its temperature dependence as discussed in FHIP (p. 1014 and Sec. VI). Based on the method used here to obtain our relation (13), the explanation for this difference given in FHIP no longer applies. At present we do not understand this disagreement.

B. Small Static Field (Low-Velocity) Limit

The drift of electrons in a polar crystal in a very small, static, electric field can be treated in a manner closely paralleling the treatment in FHIP for arbitrary coupling and temperature.[3] The result of such a calculation is

$$\mathbf{E}=\int_{-\infty}^{\infty}d\xi\sum_{\rm k}|C_{\rm k}|\mathbf{k}(-i\xi\mathbf{k}\cdot\mathbf{v})T_{\omega_{\rm k}}(\xi)e^{-k^2\bar{K}_\beta(\xi)}. \quad (18)$$

If we take the low-velocity limit of our result (13), we obtain just this result. This is important because there is no *a priori* reason why the approximate method of summing the expansion used in FHIP should be equivalent to the method of rates used here. This equivalence is also brought out by using this method of rates to derive the general result for the (ac) impedance of FHIP. This calculation is outlined in Sec. IV C below.

C. Low-Frequency Limit of Impedance

Another check on our result is to find the zero-frequency limit of the real part of the impedance calculated in FHIP [Eq. (41)]. This limit gives the electronic mobility for arbitrary coupling and temperature, and agrees with the low-velocity limit of our result (13). As was stressed in FHIP, careful attention had to be given

[17] Reference 4, p. 664; Ref. 5, p. 1012. In the weak coupling limit and for a single-oscillator model, the free energy is a minimum for $w_0=1$, $v_0=1$. The choice gives what we call the free-particle $\bar{K}_\beta(\xi)$. The trial oscillator has the frequency of the lattice and is not coupled to the electron. $\Gamma(\omega)=\delta'(\omega)/m$ in our notation here.

[18] A novel Boltzmann treatment for arbitrary coupling has been carried out by L. P. Kadanoff, Phys. Rev. **130**, 1364 (1963). Again his result and our result (24) differ by the same factor $\frac{2}{3}\beta$.

to this limit because the approach used to sum the expansion of the admittance was subject to question for zero frequency. Their result, however, is not subject to question at zero frequency: it can be derived using our approach which avoids the zero-frequency problem. We outline this briefly.

To determine the impedance of the electron in the polar crystal, we may write the expectation value of (15) after steady state is reached (in this case after the transients have decayed) as

$$(-i\omega)Z_\omega\bar{x}e^{-i\omega t}+\omega^2\bar{x}e^{-i\omega t}=\sum_{\mathbf{k}}\mathbf{k}\langle\hat{R}_{\mathbf{k}}\rangle_t, \tag{19}$$

where Z_ω is the impedance defined by $Z\dot{x}=E$, $\bar{x}$ is the (complex) amplitude of the vibration, and $e^{-i\omega t}$ is the time dependence of the oscillation of frequency ω [FHIP use $\exp(ivt)$]. Perform the $\langle\hat{R}_{\mathbf{k}}\rangle_t$, as in Sec. II, making the change of variables $x_t=y_t+\bar{x}e^{-i\omega t}$ in the path integral and expand this result for $\bar{x}$ small.[19] The result is

$$i\omega Z_\omega=\omega^2-\int_0^\infty d\xi(1-e^{i\omega\xi})\,\mathrm{Im}[S(\xi)], \tag{20a}$$

where

$$S(\xi)=\sum_{\mathbf{k}}|C_{\mathbf{k}}|^2\tfrac{2}{3}k^2T_{\omega\mathbf{k}}(\xi)e^{-k^2\bar{R}_\beta(\xi)} \tag{20b}$$

is identical to the final result of FHIP for all frequencies.

The physical features of this result were discussed in great detail in FHIP. In particular, it was possible to show how the expression for the dissipation at low temperature could be written to show explicitly how the absorption and emission of both phonons and photons from the fields were represented complete with cross sections for these processes. It is difficult, however, to represent the essentially continuous change of state of an electron in a static electric field by the emission and absorption of photons. Thus in describing our result it was convenient to go back to the classical idea of balancing rates of momentum gain with loss.

V. NUMERICAL RESULTS FOR FRÖHLICH POLARON MODEL

Physically we would expect that as the steady-state velocity of the electron increases so that its kinetic energy approaches the energy of the optical phonons, the emission of optical phonons will become dominant and the velocity will tend to saturate with increasing field. As the velocity exceeds this threshold, the loss to the lattice should diminish with increasing velocity, as we would expect from a perturbation treatment for a very fast electron. For $\beta>1$, the loss should be essentially independent of temperature above threshold: It goes as $\coth\beta$. As the temperature is increased above the optical-phonon energy, scattering from thermal phonons will tend to suppress these features and increase the threshold field and threshold velocity. Our numerical results (Figs. 1–3) show these effects nicely. Numerical results for the weak coupling limit have been given by Stratton.[20]

We now evaluate our result (13) numerically using the Fröhlich[9] model of the polaron for $|C_k|^2$ and ω_k and the single-oscillator influence functional[4,5] for coupling strengths of $\alpha=3$, 5, 7, and for reciprocal temperatures β between 20 and 0.001. In our units β is the ratio of the energy of the longitudinal optical mode to the average thermal energy of the lattice kT. Typical longitudinal reststrahlen energies range between about one-third room temperature and six times room temperature.[21]

For numerical work it is convenient to use the form of our result given in (14) with $m=1$. For the Feynman model, $\bar{K}_\beta'(\xi)$ becomes

$$\bar{K}_\beta'(\xi)=\frac{1}{2}\frac{w_0^2}{v_0^2}\left[\left(\frac{v_0^2-w_0^2}{w_0^2v_0}\right)\times\frac{\cosh(\frac{1}{2}\beta v_0)-\cos v_0\xi}{\sinh(\frac{1}{2}\beta v_0)}+\frac{\xi^2}{\beta}+\tfrac{1}{4}\beta\right], \tag{21}$$

where w_0, v_0 are determined by minimizing the free energy at zero temperature.[4] The values used here are $v_0=3.4$, $w_0=2.5$ for $\alpha=3$; $v_0=4.0$, $w_0=2.1$ for $\alpha=5$; $v_0=5.8$, $w_0=1.6$ for $\alpha=7$ (FHIP, p. 1012).[22] Performing those integrals which can be evaluated analytically we obtain

$$E=\frac{4\alpha}{v^2\beta\pi^{1/2}\sinh(\frac{1}{2}\beta)}\int_0^{v(\sqrt{\beta})\,v_0/w_0}x^2dx\times\int_0^\infty ds\frac{\cos(\frac{1}{2}\beta s)}{[A(s)]^{3/2}}\exp\left(-x^2\frac{s^2-1}{2A(s)}\right)\times[\cos(x^2s/A(s))-s\sin(x^2s/A(s))], \tag{22a}$$

where

$$A(s)=s^2+1+\frac{4}{\beta}\frac{v_0^2-w_0^2}{w_0^2v_0}\frac{\cosh(\frac{1}{2}\beta v_0)-\cos(\frac{1}{2}s_0v\beta)}{\sinh(\frac{1}{2}\beta v_0)}. \tag{22b}$$

The magnitude of β limits the velocities for which these expressions can be integrated using Simpson's rule on an IBM 7094 computer. For small β it is possible to integrate beyond the velocity threshold, for $\beta>10$ the threshold can only be approached due to the violent sinusoidal oscillation. To complete the curves it was

[19] If we use $\bar{x}/(-i\omega)$ in place of $\bar{x}$, then the limit $\omega\to 0$ is easily seen to cause no difficulty.

[20] R. Stratton, Proc. Roy. Soc. (London) **A246**, 406 (1958).

[21] The longitudinal reststrahlen $\hbar\omega_L$ can be determined from the experimentally measured transverse reststrahlen ($\hbar\omega_T$) frequency using $\omega_L/\omega_T=(\epsilon_s/\epsilon_\infty)^{\frac{1}{2}}$, where ϵ_s is the static dielectric constant and ϵ_∞ is the electronic contribution to the dielectric constant. It can alternately be found as in Ref. 23.

[22] While one would expect these values to be valid only for large β (low temperature), we use them for all temperatures. In fact, for high temperatures the $E-v$ relation no longer depends significantly on w_0, v_0. This may be seen by expanding $A(\xi)$ (22b) for small β: $A(s)\approx(v_0^2/w_0^2)(s^2+1)$, and setting $z=(w_0/v_0)x$ in (22a). Therefore we expect the numerical results to be about as good as would be obtained if different v_0, w_0 were inserted at each temperature.

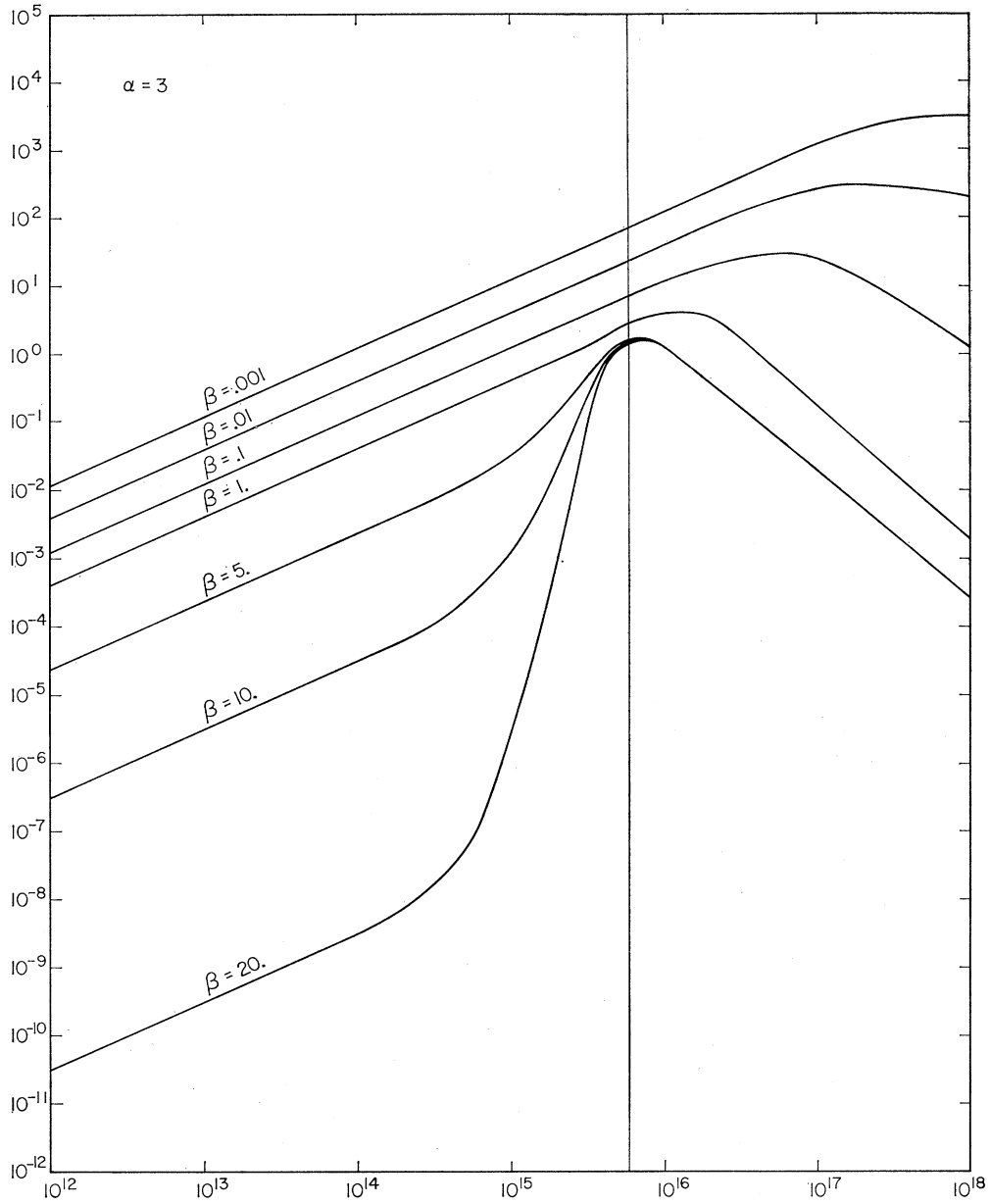

FIG. 1. The energy loss per unit distance E' (vertical axis suffered by an electron whose steady-state velocity is v' (horizontal axis) for a coupling constant of $\alpha=3$ and oscillator parameters $w=2.5$, $v=3.4$.

necessary to return to (21) and expand $\bar{K}_\beta'(\xi)$ to second order in ξ. This is justified for large β, where the $\cos v_0\xi$ dependence is unimportant, and for small β, where most of the contribution to the $\int d\xi$ of (14) comes for $\xi \lesssim \beta$. Thus writing $\bar{K}_\beta'(\xi)=(1/2\beta)(A\xi^2+B)$ and performing the $\int d\xi$, first we obtain

$$E=\frac{\alpha}{2v^2}\left(\frac{\beta}{\pi}\right)^{1/2}\frac{1}{\sinh(\frac{1}{2}\beta)}\int_0^{v/\sqrt{A}} x\,dx \times\int_{-\infty}^{\infty} dk\frac{k}{|k|}\exp\left[-\frac{\beta k^2}{8A}\left(\frac{4B}{\beta^2}-A\right)\right] \times\left(e^{\beta/2}e^{-(\beta/2)(x-k/2-1/k)^2}+e^{-\beta/2}e^{-\beta/2(x-k/2+1/k)^2}\right), \quad (23a)$$

where

$$A=1+(1-w_0^2/v_0^2)\{v_0\beta/[2\sinh(\tfrac{1}{2}v_0\beta)]-1\} \quad (23b)$$

and

$$B=\beta\frac{w_0^2}{v_0^2}\left(\frac{v_0^2/w_0^2-1}{v_0}\tanh(\tfrac{1}{4}\beta v_0)+\tfrac{1}{4}\beta\right). \quad (23c)$$

These integrals are sufficiently well-behaved that they can be easily handled numerically. For the low-field mobility we obtain

$$\frac{1}{\mu}=\tfrac{2}{3}\alpha\left(\frac{1}{A^{3/2}}\right)\frac{\beta}{\sinh(\frac{1}{2}\beta)}\frac{1}{\sqrt{C}}\left(\frac{\beta}{\pi}\right)^{1/2}K_1(\tfrac{1}{2}\beta\sqrt{C}), \quad (24)$$

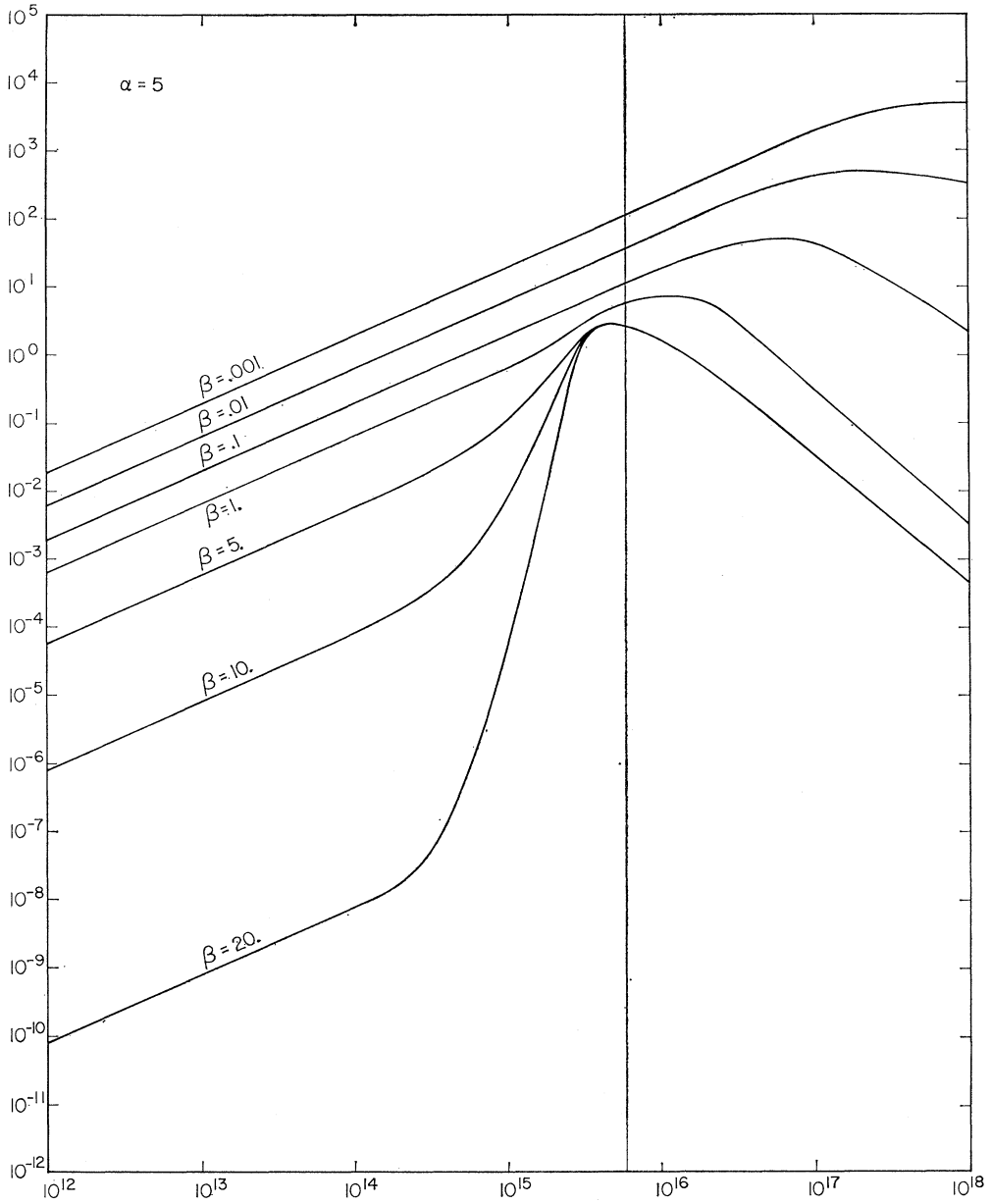

FIG. 2. The energy loss per unit distance E' (vertical axis) suffered by an electron whose steady-state velocity is v' (horizontal axis) for a coupling constant of $\alpha=5$ and oscillator parameters $w=2.1$, $v=4.0$.

where $C=4B/AB^2$ and K_1 is the modified Bessel function of order 1. For sufficiently large velocity the rate of momentum loss becomes $2(\sqrt{2}\alpha/v^2)\ln v$, the rate of energy loss $2(\sqrt{2}\alpha/v)\ln v$, the result of perturbation theory.

If we compare the curves for $\alpha=3$, 5, and 7, we note that apart from an over-all increase in loss due to increased coupling, the threshold region shifts to lower electron velocity. (The vertical line corresponds to the velocity where $\frac{1}{2}mv^2=\hbar\omega_L$ or in our units $v=\sqrt{2}$.) This shift is a manifestation of the increase in the effective mass of the electron resulting from the electron-lattice coupling as discussed in I. This shift is most clearly evident in (23a) for low temperatures: $\sqrt{A}\rightarrow w_0/v_0$ and $\frac{1}{8}\beta(4B/A\beta^2-1)\rightarrow(v_0^2/w_0^2-1)/v_0$. While the latter term narrows the threshold region for increasing coupling, the former contracts the velocity scale $v\rightarrow vv_0/w_0$. Thus near threshold $\frac{1}{2}m(vv_0/w_0)^2=\hbar\omega_L$ or $\frac{1}{2}(mv_0^2/w_0^2)v^2=\hbar\omega_L$, and mv_0^2/w_0^2 is very nearly the effective electron mass (FHIP, p. 1008).

For convenience, the scales of the graphs have been changed from the E, v that we have used in our equations to E', v', where $E'=E(m_e)^{1/2}/\hbar=E/2.75$ and $v'=v/(m_e)^{1/2}=v\times0.418\times10^{16}$. To obtain F the force on

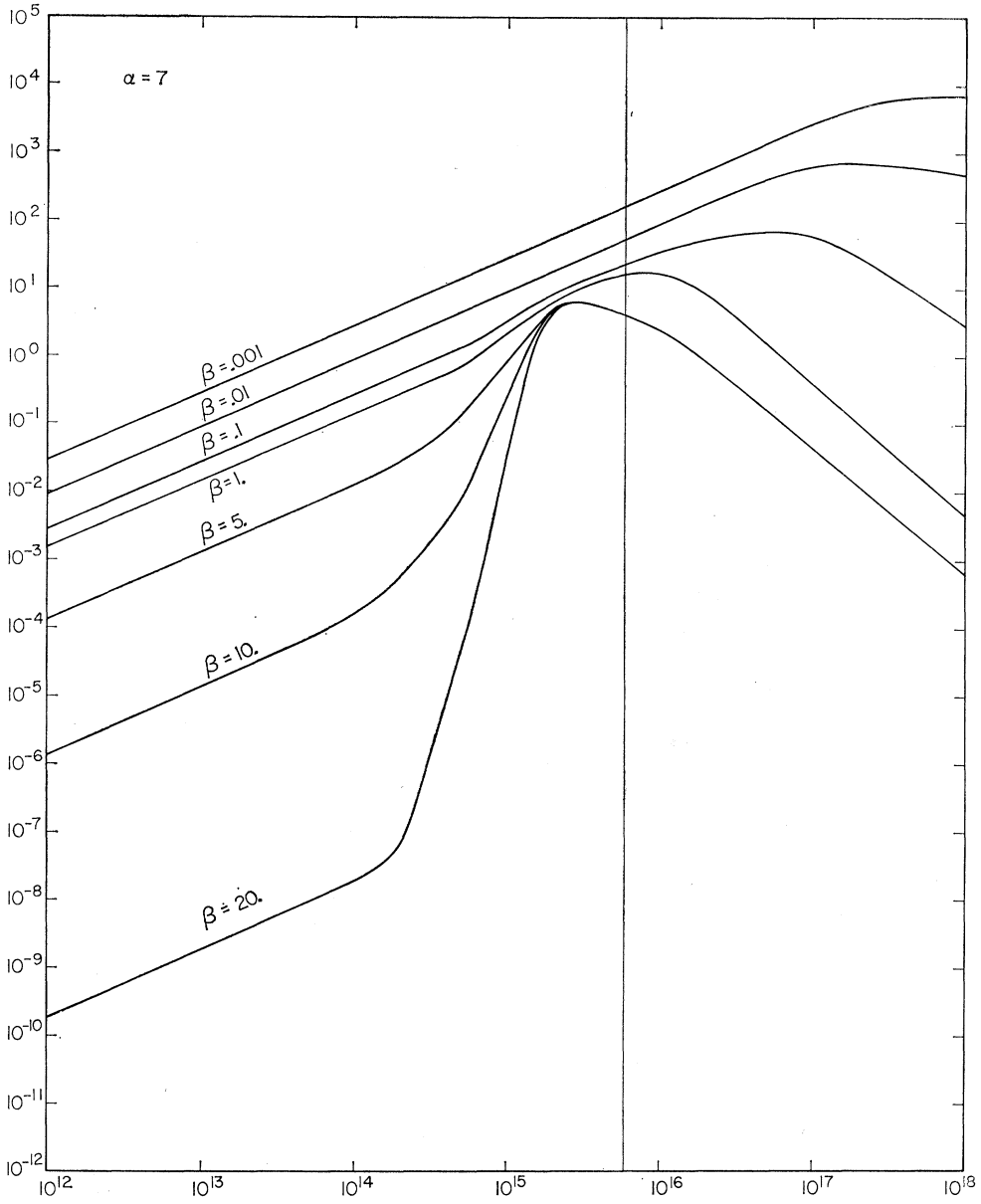

FIG. 3. The energy loss per unit distance E' (vertical axis) suffered by an electron whose steady-state velocity is v' (horizontal axis) for a coupling constant of $\alpha=7$ and for oscillator parameters $w=1.6$, $v=5.8$.

the electron in eV/Å and v_r the velocity in Å/sec one uses

$$F=(m/m_e)^{1/2}(\hbar\omega_L)^{3/2}E' \quad (\text{eV/Å}), \qquad (25a)$$

$$v_r=(m_e/m)^{1/2}(\hbar\omega_L)^{1/2}v' \quad (\text{Å/sec}), \qquad (25b)$$

where m_e is the rest mass of the electron, m is its fixed-lattice effective mass, and $\hbar\omega_L$ is the energy of the longitudinal optical phonons in eV. We see that to calculate the coupling constant α in the Fröhlich model all we need apart from m are three experimentally determined quantities—the static and optical dielectric constants and the reststrahlen frequency.

To obtain a feel for the magnitude of the energy loss to a lattice which we would predict based on the above, let us consider the specific example of Al_2O_3. The optical-phonon structure[23] of Al_2O_3 is a good deal more complicated than can be described with the Fröhlich model: The strongest contributions to the dielectric dispersion correspond to modes whose longitudinal frequencies (energies) are 0.060, 0.064, and 0.078 eV. Let us take 0.07 eV as an average $\hbar\omega_L$, $\epsilon_\infty=3.1$, and $\epsilon_s=9.0$ and unit effective mass. These values give $\alpha=2.7$, and the low-temperature (temperature-independent) threshold

[23] A. S. Barker, Jr., Phys. Rev. **132**, 1474 (1963).

($E'=1.5$ for $\alpha=3$, 2.8 for $\alpha=5$, and 5.8 for $\alpha=7$) is $F=0.025$ eV/Å. (We have reduced the $\alpha=3$ value by the factor 2.7/3.0: the v_0 and w_0 change by a much smaller percentage for these α.) If the reststrahlen of 0.12 eV which Handy[1] uses is more appropriate, this would give $F=0.043$ eV/Å. The extent to which these results are directly applicable to the Al_2O_3 films on which losses of about 0.03 eV/Å have been measured may not be too clear: The films may be polycrystalline or amorphous, the band structure may not permit the unit mass assumption we have assumed here, the electron's velocity in the crystal is uncertain, etc. The point is that optical-phonon scattering can indeed produce the high rate of energy loss that seems to be present in these layers.

VI. FURTHER REMARKS

In the spirit of our method of rates, Sec. II, one can also evaluate the operator equation for the rate of change of electron kinetic energy:

$$\frac{d}{dt}(\mathbf{p}^2/2m)=i[H,\mathbf{p}^2/2m]$$

$$=(\mathbf{F}\cdot\mathbf{p}+\mathbf{p}\cdot\mathbf{F})/2m-\sum_{\mathbf{k}}R_{\mathbf{k}}', \qquad (26)$$

where

$$R_{\mathbf{k}}''=-i\{C_{\mathbf{k}}^*a_{\mathbf{k}}^\dagger\mathbf{k}\cdot[e^{i\mathbf{k}\cdot\mathbf{x}},\mathbf{p}]_+ -C_{\mathbf{k}}a_{\mathbf{k}}\mathbf{k}\cdot[e^{-i\mathbf{k}\cdot\mathbf{x}},\mathbf{p}]_+\}. \qquad (27)$$

Taking the expectation value of this expression, invoking the steady-state limit, recalling that $\mathbf{F}$ is independent of distance, and using the notational change indicated following Eq. (7), one finds

$$\mathbf{E}\cdot\mathbf{v}=\sum_{\mathbf{k}}\langle R_{\mathbf{k}}''\rangle. \qquad (28)$$

In the steady state, (28) expressed simply the balance of the rate at which energy is acquired from the applied field and the rate at which energy is lost to the lattice.

A more transparent and useful expression for this relation of energy transfer can be obtained from

$$\dot{H}=i[H,H]=0, \qquad (29)$$

which, when expectation values are calculated and the steady-state limit is taken, yields

$$\mathbf{E}\cdot\mathbf{v}=\frac{d}{dt}\langle\sum_{\mathbf{k}}\omega_{\mathbf{k}}a_{\mathbf{k}}^\dagger a_{\mathbf{k}}\rangle \qquad (30a)$$

$$=\sum_{\mathbf{k}}\omega_{\mathbf{k}}\langle R_{\mathbf{k}}\rangle, \qquad (30b)$$

where $R_{\mathbf{k}}$ is given by (8b). (In the steady state neither the electron kinetic energy nor the electron-lattice interaction energy changes with time.) Since $R_{\mathbf{k}}$ is the operator for the net rate of emission of optical phonons (emission less absorption), (30b) is seen at once to express the balance between the rate of gain and the rate of loss of electron energy from the field and to the lattice, respectively. Eliminating the lattice variables as in Sec. II and approximating the expression as in Sec. III gives the field-velocity relation

$$\mathbf{E}\cdot\mathbf{v}=\int_{-\infty}^{\infty}d\xi\sum_{\mathbf{k}}|C_{\mathbf{k}}|^2\omega_{\mathbf{k}}\left(\frac{e^{i(\omega_{\mathbf{k}}-\mathbf{k}\cdot\mathbf{v})\xi}}{1-e^{-\beta\omega_{\mathbf{k}}}} -\frac{e^{-i(\omega_{\mathbf{k}}-\mathbf{k}\cdot\mathbf{v})\xi}}{e^{\beta\omega_{\mathbf{k}}}-1}\right)e^{-k^2\bar{K}_\beta(\xi)}. \qquad (31)$$

This result agrees with (13) *only* when $\bar{K}_\beta(\xi)$ is independent of ξ.

As a test of the consistency of our approach, this disagreement is unfortunate. For $\beta<2$, $E<E_{\mathrm{Th}}$, $v<v_{\mathrm{Th}}$ (Th represents threshold), the discrepancy is not serious. For higher temperatures, (31) goes sour: For example, the low-field mobility tends to increase again with increasing temperature whereas it sould continue to decrease. The fact that (13) was obtained in two *independent* ways, and that it is qualitatively correct physically for all temperatures, velocities, and field strengths leads us to discount but not forget the trouble with (31).

[One could, of course, permit the electron (or effective oscillator) "temperature" in (12) to differ from the lattice temperature in (10d) and solve both (13) and (31) for E and this electron temperature self-consistently. This is analogous to the drifted-Maxwellian approximation.[20] We did not pursue this possibility.]

There are several important qualitative features of the behavior of the electron apparent from Figs. 1–3 which should be mentioned. First, even for very low temperatures (large β) there is a range of velocities near v_{Th} over which the electron-lattice scattering is so severe that, as discussed in Sec. I, a quasiparticle picture of the electron is not possible. The lifetime is so short and catastrophic that the electronic state cannot be viewed as decaying exponentially in time. (In fact, the broadening is roughly two orders of magnitude larger than the energy.) Mott pointed out to us that under such conditions electrons and holes in this energy region in highly ionic materials would behave quite differently than a rigid-lattice band-theory calculation would predict, and, as we have just noted, a quasiparticle approximation will not remedy this difficulty. Fortunately Al_2O_3 is an extreme case, and even for most alkali halides the troublesome region is confined to a few tenths of an eV.

However, the scattering is not sufficiently strong that the electron never breaks out of the polaron state. As pointed out to us by P. M. Platzman, the electron has a *finite* apparent "mass" for all velocities. (Near v_{Th} the large apparent mass is dominated by resistive losses

rather than lossless reactive coupling typical of quasiparticles.)

At very low velocities and at very high velocities, where a quasiparticle picture is valid, we expect that the mass appropriate for Eq. (7) is a fixed lattice mass characteristic of the band electrons at the appropriate energy. More complicated band structures may be simulated by more complicated kinetic-energy expressions. However, near the threshold region where the electron–optical-phonon interaction clearly dominates all other interactions and the electron is well-localized due to the magnitude of the scattering, it seems best to use the free-electron mass in (7) as we have done in Sec. V. Of course, if the electron–optical-phonon coupling is sufficiently small, the quasiparticle picture and a band mass may be used for all velocities.

In connection with the quasiparticle picture, one other clarification is necessary. An electron whose energy is less than the threshold for phonon emission cannot emit a phonon. Hence, at *zero* temperature and in the *absence* of an applied electric field, such an electron with its cloud of phonons forms an eigenstate of the system—a quasiparticle with infinite lifetime and an $E(k)$ self-energy relation.[24] Such a description may be useful in the presence of a very small applied field. However, for the strong fields of interest here, where the magnitude of the gain and loss of energy is important, the mixing of such particle states in the field makes these an inconvenient basis to work with. This is most clearly seen by noting that the motion of a particle whose expectation velocity is below threshold but above the linear mobility region is clearly dominated by phonon *emission*. [In fact, for $\beta>2$ and with increasing velocity, the electron quickly passes from the temperature-dependent, phonon-absorption dominated, linear field-velocity (mobility) regime to the temperature-independent, phonon-emission dominated, nonlinear field-velocity regime.] In this transition region from absorption to emission dominated transport, the electron is simultaneously (a) rapidly acquiring translational kinetic energy from the applied field, (b) having this energy transformed into the thermal, kinetic energy of the electron's relative motion and into the electron-lattice interaction energy, and (c) finally dissipating this energy to the lattice via phonon emission. Hence in a quasiparticle picture, the state of interest in this regime is some complicated combination of continuum states (with finite lifetime) which has an expectation velocity *below* threshold, and not a single quasiparticle state with a momentum corresponding to this velocity. This precludes a simple treatment or interpretation in terms of diagrams and illustrates the convenience indicated in the introduction of treating the problem as a single unit without separately treating the zero-field electron state, phonon emission and absorption, and the influence of the field.

[24] G. Whitfield and R. Puff, Phys. Rev. **139**, A338 (1965).

VII. CONCLUSIONS

In this paper we have treated the motion of an electron in a polarizable crystal under the influence of a static electric field. Starting with the crystal in thermodynamic equilibrium, the electron was injected and an approximate expression for its subsequent steady-state drift velocity was determined for arbitrary coupling strength, temperature, and applied field using path integral methods. The approximation is based on finding the distribution of oscillators which would give the best agreement between the exact field-velocity dependence and our result (13). We have not found a principle to give this distribution but have reason to believe such a principle exists. In lieu of this, we have used the one-oscillator distribution of I which minimizes the free energy at zero temperature. As we have seen, this is sufficient to represent all the expected physical behavior between the velocity and rate of loss of momentum, and, where appropriate, the energy loss per unit distance. The numerical results obtained are physically reasonable in view of existing experimental results. They predict the large applied fields necessary to pull the electron out of the polaron state.

In I and FHIP a correction term was also evaluated when the influence function $e^{i\Phi_e}$ was approximated by $e^{i\Phi_0}$. That is,

$$\int\int e^{i\Phi_e}=\int\int e^{i\Phi_0}e^{i(\Phi_e-\Phi_0)}\approx\int\int e^{i\Phi_0}+\int\int i(\Phi_e-\Phi_0)e^{i\Phi_0}.$$

Evaluating the second term was not necessary here because the rate Eq. (8) already contained the electron-lattice interaction in a convenient from. One might be able to improve the accuracy of our result by including the term $\vec{R}_k i(\Phi_e-\Phi_0)e^{i\Phi_0}$ in the calculation of $\langle\vec{R}_k\rangle$.

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APPENDIX A: CALCULATION OF PATH INTEGRAL

In this Appendix we outline the calculation of

$$\int\int e^{i\bar{\Phi}_0} D[\mathbf{y}(t)]D[\mathbf{y}'(t)], \tag{A1}$$

where

$$\bar{\Phi}_0=\Phi_0+\int_{t_1}^{t_2}[\mathbf{F}(t)\cdot\mathbf{y}_t-\mathbf{F}'(t)\cdot\mathbf{y}_t']dt$$

and where Φ_0 is given by Eq. (12). In order to avoid the usual problems which arise in performing path integrals over finite intervals with complex exponents (especially the presence of undamped transitents), we change the limits of the time integrals from $\int_{t_1}^{t_2}$ to $\int_{-\infty}^{\infty}$, while at the same time changing $\mathbf{F}(t)$ and $\mathbf{F}'(t)$ appropriately to ensure that physically we are still working with the same problem. To facilitate this transition, we recall that the path integral may be interpreted as a kernel or propagator.[25] Thus if in $\mathbf{F}(t)$ and $\mathbf{F}'(t)$ we represent the $\mathbf{E}$ field to be turned on at $t=t_1$ from a zero value for $t<t_1$, the propagation from $t\approx-\infty$ to $t=t_1$ will result in zero displacement of the electron. Similarly, the fields may be turned off at $t=t_2$. Clearly, this applies also to the $\mathbf{k}$ "field" in $R_{\mathbf{k}}'$ (10d). Because we will use a number of different $\mathbf{F}(t)$ and $\mathbf{F}'(t)$, we consider general $\mathbf{F}$ and $\mathbf{F}'$ here.

Thus we must evaluate

$$\int\int e^{i\bar{\Phi}_0'} D[\mathbf{y}(t)]D[\mathbf{y}'(t)], \tag{A2}$$

where

$$\bar{\Phi}_0'=\int_{-\infty}^{\infty}dt(\tfrac{1}{2}m\dot{\mathbf{y}}_t^2+\mathbf{F}(t)\cdot\mathbf{y}_t)-\int_{-\infty}^{\infty}dt(\tfrac{1}{2}m\dot{\mathbf{y}}_t'^2+\mathbf{F}'(t)\cdot\mathbf{y}_t)$$
$$-i\int_0^{\infty}d\Omega G(\Omega)\int_{-\infty}^{\infty}dt\int_{-\infty}^{t}dt'\{T_\Omega(t-t')(\mathbf{y}_t'-\mathbf{y}_{t'}')^2$$
$$+T_\Omega^*(t-t')(\mathbf{y}_t-\mathbf{y}_{t'})^2-T_\Omega(t-t')(\mathbf{y}_t-\mathbf{y}_{t'})^2$$
$$-T_\Omega^*(t-t')(\mathbf{y}_t'-\mathbf{y}_{t'})^2\}. \tag{A3}$$

First express $\mathbf{x}$, $\mathbf{x}'$, $\mathbf{F}$, and $\mathbf{F}'$ by their Fourier transforms:

$$\begin{aligned}
\xi_\nu&=\int_{-\infty}^{\infty}\mathbf{y}_te^{+i\nu t}dt, & \mathbf{y}_t&=\int_{-\infty}^{\infty}\frac{d\nu}{2\pi}\xi_\nu e^{-i\nu t},\\
\xi_\nu'&=\int_{-\infty}^{\infty}\mathbf{y}_t'e^{+i\nu t}dt, & \mathbf{y}_t'&=\int_{-\infty}^{\infty}\frac{d\nu}{2\pi}\xi_\nu' e^{-i\nu t},\\
\mathbf{f}_\nu&=\int_{-\infty}^{\infty}\mathbf{F}(t)e^{+i\nu t}dt, & \mathbf{F}(t)&=\int_{-\infty}^{\infty}\frac{d\nu}{2\pi}\mathbf{f}_\nu e^{-i\nu t},\\
\mathbf{f}_\nu'&=\int_{-\infty}^{\infty}\mathbf{F}'(t)e^{+i\nu t}dt, & \mathbf{F}'(t)&=\int_{-\infty}^{\infty}\frac{d\nu}{2\pi}\mathbf{f}_\nu' e^{-i\nu t}.
\end{aligned} \tag{A4}$$

Inserting these in (A3) gives for (A2)

$$\int\int e^{iX}D(\xi_\nu)D(\xi_\nu'), \tag{A5}$$

where

$$X=\int_{-\infty}^{\infty}\frac{d\nu}{2\pi}(\tfrac{1}{2}m\nu^2\xi_\nu\cdot\xi_{-\nu}+\mathbf{f}_\nu\cdot\xi_{-\nu})-\int_{-\infty}^{\infty}\frac{d\nu}{2\pi}(\tfrac{1}{2}m\nu^2\xi_\nu'\cdot\xi_{-\nu}'+\mathbf{f}_\nu'\cdot\xi_{-\nu}')$$
$$+2\int_0^{\infty}G(\Omega)d\Omega\int_{-\infty}^{\infty}\frac{d\nu}{2\pi}\Big[\xi_\nu'\cdot\xi_{-\nu}'\Big(\frac{1}{1-e^{-\beta\Omega}}\frac{\nu}{\Omega(\Omega+\nu+i\epsilon)}-\frac{1}{e^{\beta\Omega}-1}\frac{\nu}{\Omega(\Omega+\nu-i\epsilon)}\Big)$$
$$-\xi_\nu\cdot\xi_{-\nu}\Big(\frac{1}{1-e^{-\beta\Omega}}\frac{\nu}{\Omega(\Omega+\nu-i\epsilon)}-\frac{1}{e^{\beta}-1}\frac{\nu}{\Omega(\Omega+\nu+i\epsilon)}\Big)-2\pi i\xi_\nu'\cdot\xi_{-\nu}\Big(\frac{\delta(\Omega+\nu)}{1-e^{-\beta\Omega}}+\frac{\delta(\Omega-\nu)}{e^{\beta\Omega}-1}\Big)\Big]. \tag{A6}$$

We note that since $\mathbf{x}_t$, $\mathbf{x}_t'$, $\mathbf{F}(t)$, $\mathbf{F}'(t)$ are real, $\xi_\nu=\xi_{-\nu}^*$, $\xi_\nu'=\xi_{-\nu}'^*$, $\mathbf{f}_\nu=\mathbf{f}_{-\nu}^*$, $\mathbf{f}_{-\nu}'^*=\mathbf{f}_\nu'$. Thus by changing $\int_{-\infty}^{\infty}d\nu$ to $\int_0^{\infty}d\nu$, we obtain for (A2)

$$\int\int e^{iX'}D(\xi_\nu)D(\xi_\nu^*)D(\xi_\nu')D(\xi_\nu'^*),\quad \nu\geq 0 \tag{A7}$$

where

$$X'=\int_0^{\infty}\frac{d\nu}{2\pi}\{[Z_1(\nu)+Z_2(\nu)]\xi_\nu\cdot\xi_\nu^*-[Z_1^*(\nu)+Z_2^*(\nu)]\xi_\nu'\cdot\xi_\nu'^*+[Z_2^*(\nu)-Z_2(\nu)]\xi_\nu'\cdot\xi_\nu^*$$
$$+[Z_1^*(\nu)-Z_1(\nu)]\xi_\nu'^*\cdot\xi_\nu+\mathbf{f}_\nu\cdot\xi_\nu^*+\mathbf{f}_\nu^*\cdot\xi_\nu-\mathbf{f}_\nu'\cdot\xi_\nu'^*-\mathbf{f}_\nu'^*\cdot\xi_\nu'\} \tag{A8}$$

and

$$Z_1(\nu)=\tfrac{1}{2}m\nu^2+2\int_0^{\infty}d\Omega\frac{G(\Omega)}{1-e^{-\beta\Omega}}\frac{2\nu^2}{\Omega(\Omega^2-\nu^2-i\epsilon)}, \tag{A9a}$$

[25] R. P. Feynman, Rev. Mod. Phys. 20, 367 (1948).

$$Z_2(\nu)=\tfrac{1}{2}m\nu^2-2\int_0^\infty d\Omega\frac{G(\Omega)}{e^{\beta\Omega-1}}\frac{2\nu^2}{\Omega(\Omega^2-\nu^2+i\epsilon)}. \tag{A9b}$$

These are defined *only* for $\nu\geq 0$. In $1/\Omega$, the principal value is to be understood.

We are now permitted to regard ξ_ν and ξ_ν^* independently for the following reason. The Fourier transform of $\mathbf{x}_t$ has a real part $\mathbf{a}_\nu$ (even in ν) and an imaginary part $\mathbf{b}_\nu$ (odd in ν). To integrate $\mathbf{x}(t)$ over all possible paths is equivalent to integrating $\mathbf{a}_\nu$ and $\mathbf{b}_\nu$ independently over all possible values, but only for those $\nu\geq 0$. And as ξ_ν and ξ_ν^* are simply linear combinations of $\mathbf{a}_\nu$ and $\mathbf{b}_\nu$, they are to be integrated independently. Hence, performing the integrals in (A7), we obtain for (A2)

$$\exp\left[i\int_0^\infty\frac{d\nu}{2\pi}\left(\frac{\mathbf{f}_\nu^*\cdot(\mathbf{f}_\nu'-\mathbf{f}_\nu)}{Z_2(\nu)+Z_1^*(\nu)}+\frac{\mathbf{f}_\nu'\cdot(\mathbf{f}_\nu'^*-\mathbf{f}_\nu^*)}{Z_2^*(\nu)+Z_1(\nu)}+\frac{(\mathbf{f}_\nu'-\mathbf{f}_\nu)\cdot(\mathbf{f}_\nu'^*-\mathbf{f}_\nu^*)[Z_1(\nu)-Z_1^*(\nu)]}{[Z_2(\nu)+Z_1^*(\nu)][Z_2^*(\nu)+Z_1(\nu)]}\right)\right]. \tag{A10}$$

Letting $Z(\nu)=Z_1(\nu)+Z_2^*(\nu)$, we find

$$Z(\nu)=m\nu^2+4\int_0^\infty d\Omega\frac{G(\Omega)}{\Omega}\frac{\nu^2}{\Omega^2-\nu^2-i\epsilon},\quad \nu\geq 0 \tag{A11}$$

and (A2) becomes

$$\exp\left[i\int_0^\infty\frac{d\nu}{2\pi}\left(\frac{\mathbf{f}_\nu^*\cdot(\mathbf{f}_\nu'-\mathbf{f}_\nu)}{Z^*(\nu)}+\frac{\mathbf{f}_\nu'\cdot(\mathbf{f}_\nu'^*-\mathbf{f}_\nu^*)}{Z(\nu)}-\frac{(\mathbf{f}_\nu'-\mathbf{f}_\nu)\cdot(\mathbf{f}_\nu'^*-\mathbf{f}_\nu^*)[Z^*(\nu)-Z(\nu)]}{Z(\nu)Z^*(\nu)(1-e^{-\beta\nu})}\right)\right]. \tag{A12}$$

Returning to (A4) we replace f_ν and f_ν' by their integral representations to obtain finally for (A2)

$$\exp\left[\int_{-\infty}^\infty dt\int_{-\infty}^t dt'[\mathbf{F}(t)-\mathbf{F}'(t)]\times[\mathbf{F}(t')K_\beta^*(t-t')-\mathbf{F}'(t')K_\beta(t-t')]\right], \tag{A13}$$

where

$$K_\beta(\tau)=\int_0^\infty d\nu\,\Gamma(\nu)\left(\frac{e^{i\nu\tau}}{1-e^{-\beta\nu}}+\frac{e^{-i\nu\tau}}{e^{\beta\nu}-1}\right) \tag{A14}$$

and

$$\Gamma(\nu)=\frac{1}{2\pi i}\left(\frac{1}{Z(\nu)}-\frac{1}{Z^*(\nu)}\right). \tag{A15}$$

To use (A13) to evaluate say the first term in (10a), one lets $\mathbf{F}(\eta)=\mathbf{k}[\delta(t_2-\eta)-\delta(t-\eta)]$ and $\mathbf{F}'(\eta)=0$, which reproduces this term in (A2), and then evaluates (A13). Many other examples of this useful trick may be found in FHIP.

The careful reader will note that several terms have been omitted from (A13). These terms are

$$\int_{-\infty}^\infty dt\int_{-\infty}^t dt'[F(t)F(t')-F'(t)F'(t')]\times\int_0^\infty\frac{d\nu}{2\pi i}\left[\frac{1}{Z(\nu)}e^{i\nu(t-t')}+\frac{1}{Z^*(\nu)}e^{-i\nu(t-t')}\right],$$

which would otherwise appear in the argument of the exponential of (A13), except for the fact that

$$A(t-t')=\int_0^\infty\frac{d\nu}{2\pi i}\left[\frac{1}{Z(\nu)}e^{i\nu(t-t')}+\frac{1}{Z^*(\nu)}e^{-i\nu(t-t')}\right]$$

must equal zero. This may be seen in several ways:

(1) One may calculate $\langle\mathbf{x}^2\rangle$ by calculating $\langle\mathbf{x}_{t_2}^2\rangle$ or $\langle\mathbf{x}_{t_2}\cdot\mathbf{x}_{t_2}'\rangle$ or $\langle\mathbf{x}_{t_2}'^2\rangle$ using the above-mentioned trick. The result, of course, must be the same in either case, but the contribution of this extra term A is $+2A$ if $\langle x_{t_2}^2\rangle$ is used, zero if $\langle\mathbf{x}_{t_2}\cdot\mathbf{x}_{t_2}'\rangle$ is used, and $-2A$ if $\langle x_{t_2}'^2\rangle$ is used.

(2) This contribution to purely real quantities is also purely imaginary.

(3) Since $\nu\geq 0$, $Z(\nu)$ of (A11) may be written equivalently as

$$Z(\nu)=m(\nu+i\epsilon)^2+4\int_0^\infty d\Omega\frac{G(\Omega)}{\Omega}\frac{(\nu+i\epsilon)^2}{\Omega^2-(\nu+i\epsilon)^2}.$$

This tells us that in the $\int_0^\infty d\nu/Z(\nu)$ we are to integrate just above the cut in $Z(\nu)$ along the positive real axis and in $\int_0^\infty d\nu/Z^*(\nu)$, just below this cut. Furthermore, $Z(\nu)$ behaves as an impedence, and therefore by causality it can have no zeroes (or other troublesome singularities) in the upper half-plane, likewise $Z^*(\nu)$ in the lower half-plane. Recalling $t-t'>0$, one shifts the contour to the positive imaginary axis for the $1/Z(\nu)$ part of the integral and to the negative imaginary axis for the $1/Z^*(\nu)$ part. These then cancel identically.

APPENDIX B: FURTHER CALCULATIONS

In this Appendix we evaluate

$$\int\int e^{i\Phi}D(y_t)D(y_t'), \tag{B1}$$

where

$$\Phi=\int_{-\infty}^{\infty}dt[\tfrac{1}{2}m\dot{y}_t{}^2+F(t)y_t]-\int_{-\infty}^{\infty}dt[\tfrac{1}{2}m\dot{y}_t{}'^2+F'(t)y_t']$$
$$-i\int_{-\infty}^{\infty}d\Omega G_y'(\Omega)\int_{-\infty}^{\infty}dt\int_{-\infty}^{t}dt'[e^{i\Omega(t-t')}(y_t'-y_{t'}')^2$$
$$+e^{-i\Omega(t-t')}(y_t-y_{t'})^2-e^{i\Omega(t-t')}(y_t-y_{t'}')^2$$
$$-e^{-i\Omega(t-t')}(y_t'-y_{t'})^2]. \quad \text{(B2)}$$

We now proceed as in Appendix A. In fact, there is little point to repeat those steps here. The important difference in evaluating (B1) is to split the range of integration of Ω into two regions, $-\infty<\Omega<0$ and $0<\Omega<\infty$, when defining quantities analogous to Z_1 and Z_2 in (A9a) and (A9b). One then obtains for (B1) the expression

$$\exp\left(\int_{-\infty}^{\infty}dt\int_{-\infty}^{t}dt'[F(t)-F'(t)]\right.$$
$$\left.\times[F(t')L^*(t-t')-F'(t')L(t-t')]\right), \quad \text{(B3)}$$

where

$$L(\tau)=\int_0^{\infty}\frac{d\nu}{2\pi i}\left(\frac{Z_+{}^*(\nu)-Z_+(\nu)}{Z(\nu)Z^*(\nu)}e^{i\nu\tau}\right.$$
$$\left.+\frac{Z_-{}^*(\nu)-Z_-(\nu)}{Z(\nu)Z^*(\nu)}e^{-i\nu\tau}\right) \quad \text{(B4)}$$

and where

$$Z_+(\nu)=\tfrac{1}{2}m\nu^2+4\nu^2\int_0^{\infty}\frac{d\Omega}{\Omega}\frac{G_y'(\Omega)}{(\Omega-i\epsilon)^2-\nu^2},$$

$$Z_-(\nu)=\tfrac{1}{2}m\nu^2+4\nu^2\int_{-\infty}^{0}\frac{d\Omega}{\Omega}\frac{G_y'(\Omega)}{(\Omega-i\epsilon)^2-\nu^2},$$

$$Z(\nu)=Z_+(\nu)+Z_-{}^*(\nu)$$
$$=m(\nu+i\epsilon)^2+4(\nu+i\epsilon)^2\int_{-\infty}^{\infty}\frac{d\Omega}{\Omega}G_y'(\Omega)\frac{1}{\Omega^2-(\nu+i\epsilon)^2},$$

for $\nu\geq 0$.

Having this result we can, for example, calculate $L(\tau)$, and hence any path integral for the quadratic approximation obtained directly from the quadratic terms of (9b). One must be very careful here, however, to note that the Z's will be different in the direction parallel and perpendicular to the drift velocity. This is easily incorporated here. Equation (B1) was calculated above for one dimension. Products of the solution for the other two directions give the three-dimensional result. Thus, for the $\hat{x}$ direction

$$G_x'(\Omega)=\tfrac{1}{2}\sum_{\mathbf{k}}|C_{\mathbf{k}}|^2k_x{}^2\left(\frac{\delta[\Omega-(\omega_{\mathbf{k}}-\mathbf{k}\cdot\mathbf{v})]}{1-e^{-\beta\omega_{\mathbf{k}}}}\right.$$
$$\left.+\frac{\delta[\Omega+(\omega_{\mathbf{k}}-\mathbf{k}\cdot\mathbf{v})]}{e^{\beta\omega_{\mathbf{k}}}-1}\right).$$

$G_y'(\Omega)$ and $G_z'(\Omega)$ are found similarly, the only difference being that $k_x{}^2$ is replaced by $k_y{}^2$ and $k_z{}^2$, respectively. Finally, it should be noted that

$$[Z_+{}^*(\nu)-Z_+(\nu)]_x=-4i\pi G_x'(\nu), \qquad \nu\geq 0$$
$$[Z_-{}^*(\nu)-Z_-(\nu)]_x=-4\pi i G_x'(-\nu), \qquad \nu\geq 0$$
$$[Z^*(\nu)-Z(\nu)]_x=-4\pi i[G_x'(\nu)-G_x'(\nu)], \qquad \nu\geq 0$$

and

$$\frac{1}{ZZ^*}=\left(\frac{1}{Z}-\frac{1}{Z^*}\right)\frac{1}{Z^*-Z}$$

and

$$\frac{P}{\Omega}\frac{1}{\Omega^2-(\nu+i\epsilon)^2}$$
$$=\frac{1}{(\nu+i\epsilon)^2}\left(-\frac{P}{\Omega}+\frac{1/2}{\Omega-(\nu+i\epsilon)}+\frac{1/2}{\Omega+(\nu+i\epsilon)}\right),$$

which in actual practice simplify matters greatly.