Polarons near the Čerenkov velocity

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(Received 20 April 1988)

We derive a set of nonlinear equations which describe the transport of optical polarons in strong electric fields. In the limit of weak electron-phonon coupling, the equations are used to calculate the external force required to maintain a constant polaron velocity and the velocity dependence of the polaron's effective mass for the velocities comparable to the Čerenkov velocity. The predictions of the transport equations are compared with mobility measurements in InSb and with the theory of Thornber and Feynman. The derivation of the transport equations is based upon a complex-time path-integral formulation of the transport of an electron interacting with a phonon field.

I. INTRODUCTION

An electron in the conduction band of an ionic crystal, through interaction with the phonon modes of the lattice, forms a quasiparticle known as a polaron. For low velocities and nonzero temperatures, a polaron in a constant electric field dissipates energy primarily through interaction with thermal phonons. However, at velocities near the Čerenkov velocity, radiation of phonons can become an important means of dissipation. These two transport regimes may be distinguished by quite different mobilities and effective masses.

Conventional approaches to transport have not been able to successfully describe the properties of the polaron near the Čerenkov velocity.[1] Kubo's formula applies only for low velocities, while the Boltzmann equation is limited to weak coupling and does not yield effective mass shifts. The method of Thornber and Feynman (TF),[2] based on path integrals, gives qualitatively reasonable results for all velocities and coupling strengths, but is quantitatively inaccurate. Finally, a mass renormalization approach developed by Karthauser[3] predicts a velocity-dependent effective mass containing an unphysical divergence at the Čerenkov velocity.

In this paper, we propose a set of approximate transport equations that overcome these problems. The equations contain the polaron's average position and its velocity-velocity correlation function as dynamical variables, and they apply for all coupling strengths and temperatures. The external electric field may be of arbitrary magnitude and time dependence, as long as it is spatially uniform.

The transport equations are derived by a technique similar to the one employed by TF, in that path integrals are used to eliminate the explicit appearance of the phonon coordinates. However, our method differs from that of TF in two important respects. The transport equations we derive are consistent with both momentum and energy conservation while those of TF, as its authors emphasize, obey only the conservation of momentum. Furthermore, the TF approach employs parameters taken from an equilibrium model of the polaron which is a dubious procedure near the Čerenkov velocity where the polaron is far from equilibrium. In contrast, the transport equations derived here are self-contained, requiring no reference to an equilibrium model. In addition, we use a complex-time path-integral technique rather than the double real-time technique used by TF, which significantly simplifies the derivation of our transport equations.

We solve the transport equations for a time-independent electric field in the limit of weak coupling and calculate the force needed to maintain a given velocity, as well as the dependence of the effective mass on the velocity. Results for the force are compared with experimental data from mobility measurements of InSb and with those of the TF method. We find that the effective mass changes rapidly near the Čerenkov velocity and becomes less than the band mass for large velocities. We also calculate the equilibrium effective mass as a function of temperature and discuss its relation to the effective mass at nonzero velocities.

II. THEORY

We start from the Fröhlich model for the polaron[4] which assumes the electron interacts only with the longitudinal-optical phonon modes that are approximated as having a flat dispersion relation characterized by a frequency ω_0. We also assume that the conduction band is isotropic and parabolic with a band mass m. Adopting units with $m=\omega_0=\hbar=1$, the Hamiltonian for the Fröhlich polaron at time t is

$$H(t)=\tfrac{1}{2}\mathbf{p}^2(t)+\mathbf{g}(t)\cdot\dot{\mathbf{x}}(t)+\sum_{\mathbf{k}} a_{\mathbf{k}}^{\dagger}(t)a_{\mathbf{k}}(t)+\left[\frac{\alpha 2\pi\sqrt{2}}{V}\right]^{1/2}\sum_{\mathbf{k}} k^{-1}[a_{\mathbf{k}}(t)e^{i\mathbf{k}\cdot\mathbf{x}(t)}+a_{\mathbf{k}}^{\dagger}(t)e^{-i\mathbf{k}\cdot\mathbf{x}(t)}] , \quad (1)$$

where $\mathbf{x}(t)$ and $\mathbf{p}(t)$ are the electron's position and momentum operators, $\dot{\mathbf{g}}(t)\equiv\mathbf{f}(t)$ is the external force caused by the electric field, α is the coupling constant, V is the volume of the system, and $a_{\mathbf{k}}(t)$ and $a_{\mathbf{k}}^{\dagger}(t)$ are the annihilation and creation operators for the phonon field. The system is assumed to be initially in equilibrium, with $\mathbf{g}(t)\rightarrow 0$ as $\mathrm{Re}\,t\rightarrow-\infty$. The Čerenkov velocity is the velocity at which the electron has enough energy to radiate phonons and is given by $u_c=u_0\sqrt{2}$, where $u_0=(\hbar\omega_0/m)^{1/2}$ (in our dimensionless units $u_0=1$).

We can express the phonon fields in terms of configuration-space variables. Defining

$$\Phi(\mathbf{y},t)=\frac{1}{\sqrt{2V}}\sum_{\mathbf{k}}[a_{\mathbf{k}}(t)e^{i\mathbf{k}\cdot\mathbf{y}}+a_{\mathbf{k}}^{\dagger}(t)e^{-i\mathbf{k}\cdot\mathbf{y}}]\ ,$$
$$\Pi(\mathbf{y},t)=\frac{-i}{\sqrt{2V}}\sum_{\mathbf{k}}[a_{\mathbf{k}}(t)e^{i\mathbf{k}\cdot\mathbf{y}}-a_{\mathbf{k}}^{\dagger}(t)e^{-i\mathbf{k}\cdot\mathbf{y}}]\ , \qquad (2)$$

the Hamiltonian takes the form

$$H(t)=\tfrac{1}{2}\mathbf{p}^2(t)+\mathbf{g}(t)\cdot\dot{\mathbf{x}}(t)+\int d^3y\{\tfrac{1}{2}\Pi^2(\mathbf{y},t)+\tfrac{1}{2}\Phi^2(\mathbf{y},t)+U[\mathbf{x}(t)-\mathbf{y}]\Phi(\mathbf{y},t)\}\ , \qquad (3)$$

where

$$U(\mathbf{y})=\frac{(\alpha 4\pi\sqrt{2})^{1/2}}{V}\sum_{\mathbf{k}}\frac{1}{k}\cos(\mathbf{k}\cdot\mathbf{y})\ , \qquad (4)$$

and with Φ and Π obeying the canonical commutation relation

$$[\Phi(\mathbf{y},t),\Pi(\mathbf{y}',t)]=i\delta(\mathbf{y}-\mathbf{y}')\ . \qquad (5)$$

We define the generating functional

$$Z_c(\mathbf{g},t_0)=\mathrm{Tr}\left[T_c\exp\left[-i\int_c H(t)dt\right]\right]\ , \qquad (6)$$

where the time integration is performed along a complex contour c beginning at a real time t_0 and ending at $t_0-i\beta$ (see Fig. 1) with β^{-1} being the initial temperature times Boltzmann's constant. T_c time orders operators along the contour of integration so operators with "later" times are positioned to the left of operators with "earlier" times. The terms later and earlier are defined with respect to the specified direction of time along the contour. Assuming $\mathbf{g}(t)$ is analytic in t, the contour may be deformed without affecting Z_c as long as the end points are fixed.

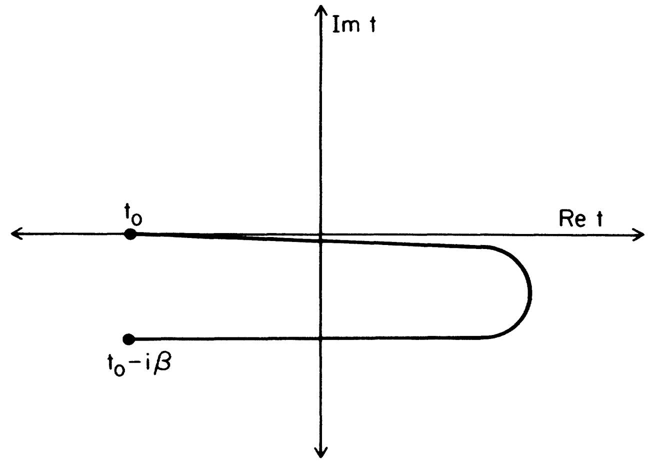

FIG. 1. The complex-time contour c.

The equilibrium partition function is given by

$$Z=\lim_{t_0\rightarrow-\infty}Z_c(\mathbf{g},t_0)\ . \qquad (7)$$

Expressions for real-time position correlation functions are found by choosing the contour to run through the real axis at times of physical interest, then taking functional derivatives with respect to $\mathbf{g}(t)$, and finally letting $t_0\rightarrow-\infty$. For example, the average value of the velocity is

$$\langle\dot{x}_j(t)\rangle=\frac{i}{Z}\lim_{t_0\rightarrow-\infty}\left[\frac{\delta}{\delta g_j(t)}Z_c(\mathbf{g},t_0)\right]\ , \qquad (8)$$

and the time-ordered, two-point correlation function is

$$\frac{d}{dt}\langle T_c x_i(t)\dot{x}_j(t')\rangle=-\frac{1}{Z}\lim_{t_0\rightarrow-\infty}\left[\frac{\delta}{\delta g_i(t)}\frac{\delta}{\delta g_j(t')}Z_c(\mathbf{g},t_0)\right]\ . \qquad (9)$$

Higher-order correlation functions are found by taking additional functional derivatives.

Since the generating functional is the trace of the evolution operator (albeit extended to complex times), it may be written in terms of path integrals as

$$Z_c(\mathbf{g},t_0)=\int D\mathbf{x}(t)D\mathbf{p}(t)D\Phi(\mathbf{y},t)D\Pi(\mathbf{y},t)\exp\left[i\int_c dt[\mathbf{p}(t)\cdot\dot{\mathbf{x}}(t)+\Pi(\mathbf{y},t)\dot{\Phi}(\mathbf{y},t)-H(t)]\right]\ , \qquad (10)$$

with the boundary conditions $\mathbf{x}(t_0)=\mathbf{x}(t_0-i\beta)$ and $\Phi(\mathbf{y},t_0)=\Phi(\mathbf{y},t_0-i\beta)$. The proof of Eq. (10) is a simple extension of the conventional arguments used for expressing real-time evolution operators as path integrals.[5,6]

As Φ, Π, and $\mathbf{p}$ enter the Hamiltonian quadratically, it is straightforward to do the path integrals over these coordinates explicitly[7] to find

$$Z_c(\mathbf{g},t_0)=Z_{\mathrm{ph}}\int D\mathbf{x}(t)\exp[iS_c(\mathbf{x})]\ , \qquad (11)$$

where Z_{ph} is the partition function for the free phonon field and $S_c(\mathbf{x})$ is an effective action for the electron, containing a phonon-induced retarded self-interaction, and is given by

$$S_c(\mathbf{x})=\int_c dt[\tfrac{1}{2}\dot{\mathbf{x}}^2(t)-\mathbf{g}(t)\cdot\dot{\mathbf{x}}(t)] - \int_c dt\int_c dt'\, W[\mathbf{x}(t)-\mathbf{x}(t'),t,t'] . \quad (12)$$

The function W is defined by

$$W(\mathbf{x},t,t')=-\frac{i}{2}\sum_{\mathbf{k}} A(k,|t-t'|_c)e^{i\mathbf{k}\cdot\mathbf{x}} \quad (13)$$

with

$$A(k,t)=\alpha\frac{2\pi\sqrt{2}(e^{-it}+e^{-\beta+it})}{Vk^2(1-e^{-\beta})} ,$$

and where $|t-t'|_c$ is equal to $(t-t')$ if t comes after t' on the contour and $(t'-t)$ if t comes before t'.

Using the identities,[7]

$$0=\int D\mathbf{x}\frac{\delta}{\delta x_i(t)}\exp[iS_c(\mathbf{x})] ,$$
$$0=\frac{\delta}{\delta g_j(t')}\int D\mathbf{x}\frac{\delta}{\delta x_i(t)}\exp[iS_c(\mathbf{x})] , \quad (14)$$

one can show

$$\langle\ddot{\mathbf{x}}(t)\rangle=\mathbf{f}(t)-\sum_{\mathbf{k}}\mathbf{k}\int_c d\tau\, A(k,|t-\tau|_c) \times\langle T_c e^{i\mathbf{k}\cdot[\mathbf{x}(t)-\mathbf{x}(\tau)]}\rangle , \quad (15)$$

and

$$\langle T_c\ddot{x}_i(t)\dot{x}_j(t')\rangle=f_i(t)\langle\dot{x}_j(t')\rangle-\sum_{\mathbf{k}}\int_c d\tau\, A(k,|t-\tau|_c)\langle T_c k_i\dot{x}_j(t')e^{i\mathbf{k}\cdot[\mathbf{x}(t)-\mathbf{x}(\tau)]}\rangle . \quad (16)$$

Equation (15) is the expression for conservation of momentum of the polaron, with the second term on the right-hand side giving the force on the electron due to the phonon field. The physical meaning of Eq. (16) is less obvious, but the expression for energy conservation may be derived from it (see Appendix A).

To obtain a closed set of equations, we make the approximations

$$\langle T_c e^{i\mathbf{k}\cdot[\mathbf{x}(t)-\mathbf{x}(t')]}\rangle=B(\mathbf{k},t,t') ,$$
$$\langle T_c\dot{x}_j(t')e^{i\mathbf{k}\cdot[\mathbf{x}(t)-\mathbf{x}(\tau)]}\rangle=[\langle\dot{x}_j(t')\rangle+ik_iC_{ij}(t,\tau,t')]B(\mathbf{k},t,\tau) , \quad (17)$$

where

$$B(\mathbf{k},t,t')=\exp(i\mathbf{k}\cdot\langle\mathbf{x}(t)-\mathbf{x}(t')\rangle-\tfrac{1}{2}\langle T_c\{\mathbf{k}\cdot[\mathbf{y}(t)-\mathbf{y}(t')]\}^2\rangle) ,$$
$$C_{ij}(t,\tau,t')=\langle T_c\dot{y}_j(t')[y_i(t)-y_i(\tau)]\rangle , \quad (18)$$

and $\mathbf{y}(t)=\mathbf{x}(t)-\langle\mathbf{x}(t)\rangle$ is the fluctuation in the position of the electron about its mean value. As is shown in Appendix B, Eqs. (17) are exact for any theory based on an action $S_c(\mathbf{x})$ that is quadratic in $\mathbf{x}(t)$. Quadratic actions have been used successfully as approximate models for the equilibrium and linear-response properties of polarons for all coupling strengths;[8,9] it is, therefore, reasonable to use (17) to simplify Eqs. (15) and (16) for the nonlinear response, yielding

$$\langle\ddot{\mathbf{x}}(t)\rangle=\mathbf{f}(t)-\sum_{\mathbf{k}}\mathbf{k}\int_c d\tau\, A(k,|t-\tau|_c)B(\mathbf{k},t,\tau) , \quad (19)$$

and

$$\langle T_c\ddot{y}_i(t)\dot{y}_j(t')\rangle=-i\sum_{\mathbf{k}}\int_c d\tau\, A(k,|t-\tau|_c)k_ik_mC_{mj}(t,\tau,t')B(\mathbf{k},t,\tau) . \quad (20)$$

Note that the two-point function on the left-hand side of Eq. (20) contains the relative coordinate $\mathbf{y}(t)$. The assumption that $S_c(\mathbf{x})$ can be simulated by a quadratic action is also used in TF. However, unlike the TF method, here we do not specify a particular quadratic action.

To obtain equations containing only real times, we take $t'<t$ and choose c to run from $-\infty$ to t along the real axis, then back along the real axis from t to $-\infty$, and finally from $-\infty$ to $-i\beta-\infty$. The last part of c may be dropped from Eqs. (19) and (20), because $B(\mathbf{k},t,\tau)\to 0$ as $\mathrm{Re}\tau\to-\infty$ for $\mathbf{k}\neq 0$, as the correlation function $\langle T_c\{\mathbf{k}\cdot[\mathbf{y}(t)-\mathbf{y}(\tau)]\}^2\rangle$ increases without bound for $|t-\tau|\to\infty$.

It is convenient to define

$$\sigma_{ij}(t,t')=\langle y_i(t)\dot{y}_j(t')-\tfrac{1}{2}[y_i(t')\dot{y}_j(t') +\dot{y}_j(t')y_i(t')]\rangle , \quad (21)$$

allowing Eq. (19) to be rewritten as

$$\langle\ddot{\mathbf{x}}(t)\rangle=\mathbf{f}(t)-\int_{-\infty}^{t} d\tau\, 2\,\mathrm{Re}\sum_{\mathbf{k}}\mathbf{k}J(t,\tau,\mathbf{k}) , \quad (22)$$

where

$$J(t,\tau,\mathbf{k})=A(k,t-\tau)e^{i\mathbf{k}\cdot\langle\mathbf{x}(t)-\mathbf{x}(\tau)\rangle} \times\exp\left[-\int_\tau^t dt'k_ik_j\sigma_{ij}(t,t')\right] . \quad (23)$$

Setting

$$\dot{\sigma}_{ij}(t,t')=\frac{\partial\sigma_{ij}(t,t')}{\partial t} ,$$
$$\ddot{\sigma}_{ij}(t,t')=\frac{\partial\dot{\sigma}_{ij}(t,t')}{\partial t} ,$$

we can rewrite (20) as

$$\ddot{\sigma}_{ij}(t,t')=-\sigma_{mj}(t,t')\int_{-\infty}^{t}d\tau\,2\,\mathrm{Re}[G_{im}(t,\tau)]+\int_{t'}^{t}d\tau\,\sigma_{mj}(\tau,t')2\,\mathrm{Re}[G_{im}(t,\tau)]+\int_{-\infty}^{t'}d\tau\,2\,\mathrm{Re}[\sigma_{mj}(\tau,t')G_{im}^{*}(t,\tau)]\ , \quad (24)$$

where

$$G_{im}(t,\tau)=i\sum_{\mathbf{k}}k_i k_m J(t,\tau,\mathbf{k})\ . \quad (25)$$

It is important to remember that Eq. (24) applies only if $t>t'$. To obtain $\sigma_{ij}(t,t')$ for $t<t'$, one uses the condition

$$\dot{\sigma}_{ij}(t,t')=\dot{\sigma}_{ji}^{*}(t',t)\ , \quad (26)$$

which follows from the definition of σ_{ij}.

Equations (22) and (24) are the basis of our transport theory. To make the theory complete, one must also impose the boundary conditions

$$\sigma_{ij}(t,t)=\frac{i}{2}\delta_{ij}\ ,\quad \dot{\sigma}_{ij}(t,t)=\dot{\sigma}_{ji}(t,t)=\dot{\sigma}_{ij}^{*}(t,t)\ ,\quad \frac{d}{dt}\dot{\sigma}_{ij}(t,t)=\ddot{\sigma}_{ij}(t,t)+\ddot{\sigma}_{ji}^{*}(t,t)\ , \quad (27)$$

which follow from the definition of σ_{ij} and the commutation relation $[\mathbf{x}(t),\dot{\mathbf{x}}(t)]=i$.

If the electric field is independent of time, the transport equations have a steady-state solution of the form

$$\sigma_{ij}(t,t')=\begin{pmatrix}\sigma_1(t-t') & 0 & 0\\ 0 & \sigma_2(t-t') & 0\\ 0 & 0 & \sigma_3(t-t')\end{pmatrix}\ , \quad (28)$$

with the boundary conditions

$$\sigma_i(0)=\frac{i}{2}\ ,\quad \sigma_i(t)=-\sigma_i^{*}(-t)\ . \quad (29)$$

Taking the force to be in direction 3, symmetry implies

$$\sigma_1(t)=\sigma_2(t)\ , \quad (30)$$

leaving only two independent components.

Letting $\mathbf{u}$ be the polaron's constant average velocity, Eq. (22) becomes

$$\mathbf{f}=\int_0^{\infty}d\tau\,2\,\mathrm{Re}\sum_{\mathbf{k}}\mathbf{k}J(\tau,\mathbf{k})\ , \quad (31)$$

where

$$J(t,\mathbf{k})=A(k,t)e^{i\mathbf{k}\cdot\mathbf{u}t}\exp\left[-\int_0^{t}dt'\,k_i^2\sigma_i(t')\right]\ , \quad (32)$$

while from Eq. (24), we have

$$\ddot{\sigma}_i(t)=-\sigma_{(i)}(t)\int_0^{\infty}d\tau\,2\,\mathrm{Re}[G_{(i)}(\tau)]+\int_0^{t}d\tau\,\sigma_{(i)}(\tau)2\,\mathrm{Re}[G_{(i)}(t-\tau)]-\int_0^{\infty}d\tau\,2\,\mathrm{Re}[\sigma_{(i)}(\tau)G_{(i)}(t+\tau)]\ , \quad (33)$$

where

$$G_i(t)=i\sum_{\mathbf{k}}k_i^2 J(t,\mathbf{k})\ , \quad (34)$$

and with parentheses about a repeated index indicating it is not summed over. The TF method consists of using Eq. (31) together with an equilibrium approximation for $\sigma_i(t)$ based on Feynman's variational theorem.[8] Thus, the TF approach neglects the velocity dependence of $\sigma_i(t)$.

III. RESULTS FOR WEAK COUPLING

As an illustration of our transport theory, we now consider the limit of weak electron-phonon coupling for a time-independent electric field. If there were strictly no coupling between the electron and the phonon field (i.e., $\alpha=0$), the solution to Eq. (31) and (33) would be

$$\mathbf{f}=0\ ,\quad \sigma_i(t)=v_i^2 t+i/2\ , \quad (35)$$

where v_i^2, the mean square velocity fluctuation in the i direction, is undetermined. However, for any nonzero coupling, the boundary condition $\mathrm{Re}[\ddot{\sigma}_i(0)]=0$, which follows from (29), implies

$$\int_0^{\infty}d\tau\,2\,\mathrm{Re}[\sigma_{(i)}(\tau)G_{(i)}(\tau)]=0\ . \quad (36)$$

If the coupling is weak, one may evaluate this expression to lowest order in the coupling to find a condition that determines v_i^2. Physically, this means that any nonzero coupling, no matter how weak, forces the electron to adjust to the phonon heat bath.

Assuming the coupling is weak enough so that Eq. (35) provides a good approximation to $\sigma_i(t)$, we use Eq. (36) to find v_i^2. With this assumption, (36) becomes

$$v_{(i)}^2\int_0^{\infty}d\tau\,\mathrm{Re}[G_{(i)}(\tau)]\tau=\tfrac{1}{2}\int_0^{\infty}d\tau\,\mathrm{Im}[G_i(\tau)]\ , \quad (37)$$

where

$$G_i(t)=i\sum_{\mathbf{k}}k_i^2 A(k,t)e^{i\mathbf{k}\cdot\mathbf{u}t}\times\exp[-\tfrac{1}{2}(k_j^2 v_j^2 t^2+ik^2 t)]\ . \quad (38)$$

In equilibrium, $u=0$ and Eq. (37) has the solution $v_i^2=\beta^{-1}$, as expected from the equipartition theorem. For $u\neq 0$, Eq. (37) must be solved numerically. Results of such a calculation for temperatures T of 0, 0.271, and 1.0 in units of $T_0\equiv\hbar\omega_0/k_B$ (which typically corresponds to a few-hundred kelvins) are depicted in Fig. 2. The velocity fluctuations remain nearly constant until $u\approx 0.7$ at which point they begin to increase rapidly, up to many times their equilibrium values for $u=u_c$. Furthermore, the fluctuations parallel to the applied field (direction 3) are larger than those transverse to the field (direction 1), with the difference being more dramatic at low temperatures. At $T=0$ and $u<u_c/2$, the velocity fluctuations appear, based on our numerical results, to be precisely zero.

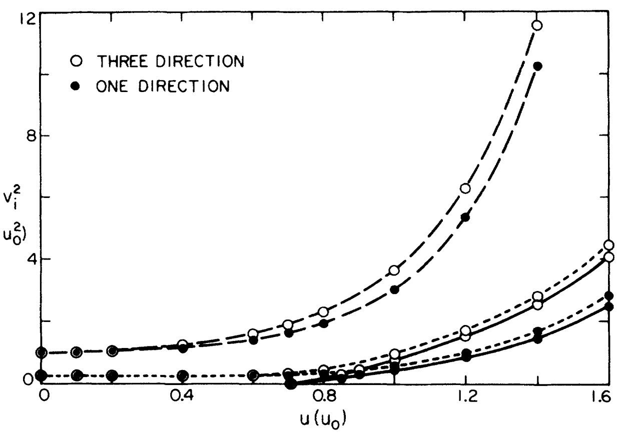

FIG. 2. The velocity fluctuations v_i^2 vs u for $T=0$ (solid line), $T=0.271$ (small-dashed line), and $T=1.0$ (large-dashed line). $u_0=(\hbar\omega_0/m)^{1/2}$.

Using the v_i^2's and Eq. (31), the force required to maintain the steady-state velocity u is calculated. The results, together with those predicted by the TF method, are shown in Fig. 3 for temperatures of 0, 0.271, and 1.0. For small values of u, the relationship between f and u is linear. Nonlinearities begin around $u=0.7$ and the force reaches a maximum at $u\approx 1.0-1.4$. If the external force exceeds this critical maximum value, then there is no steady-state solution to the transport equations, since a negative slope implies the solution is unstable.

That the force is zero until $u=u_c/2$ for $T=0$ may be explained by a physical argument due to Shockley.[10] Consider an electron at a temperature $T=0$ in a weak electric field. If initially at rest, the electron accelerates uniformly, since there are no thermal phonons to scatter the electron, and since its kinetic energy is too small to create a phonon. When its velocity reaches u_c the electron will, with high probability, emit an optical phonon before its velocity increases much more (as the field is weak), causing the electron to lose most of its kinetic energy. This process, known as streaming motion, repeats *ad infinitum*, and so the electron's velocity, averaged over many cycles, is $u_c/2$. Experimentally, electric field versus velocity measurements at low temperatures ($T\approx 0.02$) in AgBr and AgCl do indeed show a sharp rise at $u=u_c/2$.[11]

For weak coupling, the TF theory corresponds to using Eq. (31) with all the v_i^2's set to their equilibrium value of β^{-1}. Although the TF method gives results qualitatively similar to ours, there is a substantial numerical difference. For $T=0$, the TF theory predicts that f is zero until $u>u_c$, while we find the experimentally observed result that f is zero only until $u>u_c/2$. In general, the TF calculation suggests that nonlinearities appear at higher velocities than we find, and that the critical velocities, beyond which there is no steady-state solution, are larger than ours. The differences between these two methods are not surprising considering the rapid variation of the v_i's with u, for $u>0.7$. The shortcoming of the TF approach is that it uses an equilibrium expression for $\sigma_i(t)$ even when the polaron is far from equilibrium.

A comparison with experimental data in InSb at $T=0.271$ is given in Fig. 4. The parameters for InSb are $\alpha=0.0197$, $m=0.0138m_e$, and $\omega_0=3.69\times 10^{13}$ sec^{-1}, where m_e is the bare mass of the electron.[12] The experiment was performed in a weak magnetic field with the particle velocity being determined from the Hall coefficient.[13] The experimental result for f/u is larger than the theoretical one, but this may be attributed to scattering mechanisms such as impurities and acoustic phonons which have not been included in the theory. However, the general dependence on velocity of the calculated result seems consistent with the experiment, while the TF result does not.

Warmenbol *et al.* have done a Monte Carlo simulation of the Boltzmann equation and are able to fit similar experimental results.[12] Although our theory does no better than the Boltzmann equation in predicting f/u for weak coupling, our theory has the advantages that it yields effective mass shifts and that it applies also when the coupling is strong.

The effective mass of a polaron in equilibrium has been investigated by many authors, using various definitions.[1] At zero temperature, Karthauser calculates a velocity-dependent effective mass (defined as the ratio of the

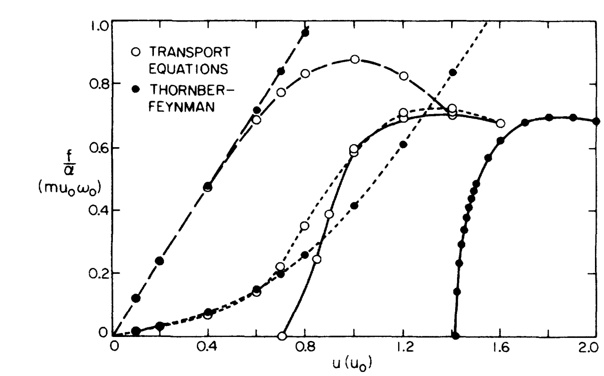

FIG. 3. f/α vs u for $T=0$ (solid line), $T=0.271$ (small-dashed line), and $T=1.0$ (large-dashed line).

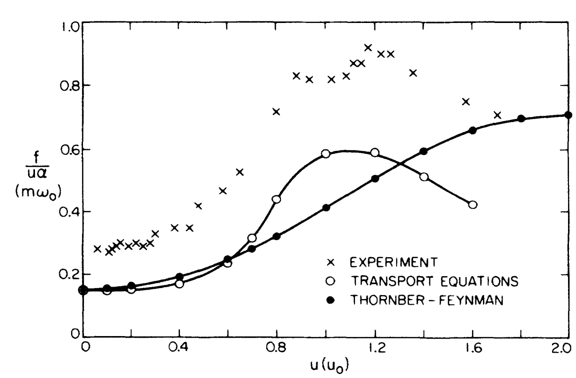

FIG. 4. $f/(u\alpha)$ vs u compared with experiment for $T=0.271$.

polaron's momentum to its velocity) but which has a divergence at the Čerenkov velocity.[3] We define the effective mass by perturbing a steady-state polaron of velocity $\mathbf{u}$ with a small time-dependent external force $\delta\mathbf{f}$. The average deviation of the electron's velocity is

$$\langle \delta\dot{x}_i(t)\rangle = \int_{-\infty}^{t} dt'\, \delta f_j(t') R_{ij}(t-t') , \tag{39}$$

with

$$R_{ij}(t) \equiv \delta_{(i)j} \frac{(-i)}{2\pi} \int_{-\infty}^{\infty} d\omega \frac{\omega}{\zeta_{(i)}(\omega)-\omega^2} e^{-i\omega t} . \tag{40}$$

We then take for the effective mass

$$m_i^*(\omega) = 1 - \mathrm{Re}\left[\frac{\zeta_i(\omega)}{\omega^2}\right] . \tag{41}$$

In words, we fit the response of the electron to a Drude model; the imaginary part of $\zeta_i(\omega)$ is related to the relaxation time. By defining the effective mass in terms of the response to an external perturbation, we assure that it is, in principle, experimentally observable. Note that the effective mass is not generally isotropic.

We define the zero-frequency, weak-coupling mass shift as

$$\delta m_i^* = \alpha \lim_{\omega\to 0} \lim_{\alpha\to 0} \left[\frac{1}{\alpha}[m_i^*(\omega,\alpha)-1]\right] . \tag{42}$$

The order of these limits is important, because the effective mass depends on whether $\omega\tau_r$, where τ_r is the relaxation time, is large or small compared to 1 (in equilibrium, however, the limits do commute). We choose the order of the limits to correspond to large $\omega\tau_r$; the case with small $\omega\tau_r$ is less interesting, since the damping is so strong that inertial effects would be difficult to observe. Experimentally, the effective-mass shift given by Eq. (42) could be observed in the response of the electron to an electric-field perturbation of frequency ω with $\omega_0 \gg \omega \gg \tau_r^{-1}$.

Using Eq. (22), we find

$$\delta m_i^* = -\int_0^{\infty} dt\, \mathrm{Re}[G_i(t)] t^2 , \tag{43}$$

where $G_i(t)$ is evaluated with the zeroth-order result for $\sigma_i(t)$ given in (35).

If $T=0$ and $u<u_c/2$ so that $v_i^2=0$, we find

$$\delta m_3^* = \frac{\alpha}{\nu^3}\left[\arcsin\nu + \frac{\nu^3}{2(1-\nu^2)^{3/2}} - \frac{\nu}{(1-\nu^2)^{1/2}}\right] ,$$
$$\delta m_1^* = \frac{\alpha}{2\nu^3}\left[\frac{\nu}{(1-\nu^2)^{1/2}} - \arcsin\nu\right] , \tag{44}$$

where $\nu = u/\sqrt{2}$. An identical result for δm_1^* is derived by Karthauser. The singularity at $\nu=1$ is not physical, since the result is valid only when $\nu<\frac{1}{2}$. For small ν, (44) becomes

$$\delta m_3^* = \alpha(\tfrac{1}{6}+\tfrac{9}{20}\nu^2+\dots) ,$$
$$\delta m_1^* = \alpha(\tfrac{1}{6}+\tfrac{3}{20}\nu^2+\dots) , \tag{45}$$

showing that the mass of the polaron increases with velocity. The equilibrium mass shift of $\alpha/6$ is the well-known result of Lee, Low, and Pines.[14] At $\nu=\frac{1}{2}$, we find

$$\delta m_3^* = \tfrac{4}{3}\alpha\left[\pi - \frac{5}{\sqrt{3}}\right] \approx 0.340\alpha ,$$
$$\delta m_1^* = 2\alpha\left[\frac{2}{\sqrt{3}} - \frac{\pi}{3}\right] \approx 0.215\alpha . \tag{46}$$

For nonzero v_i^2, we obtain the expressions

$$\delta m_3^* = \alpha\frac{4\sqrt{2\pi}}{(1-e^{-\beta})}\int_0^1 ds\, \Gamma(s,u,v_i^2)s^2 ,$$
$$\delta m_1^* = \alpha\frac{2\sqrt{2\pi}}{(1-e^{-\beta})}\int_0^1 ds\, \Gamma(s,u,v_i^2)(1-s^2) , \tag{47}$$

where

$$\Gamma(s,u,v_i^2) = \sum_{n=0}^{\infty} \frac{(2su)^{2n}}{(2n)!} g_n\{2[v_3^2 s^2 + v_1^2(1-s^2)]\} , \tag{48}$$

and

$$g_n(y) = \left[\frac{\partial}{\partial y}\right]^{n+1} [y^{-1/2} I_0(y^{-1})\exp(-y^{-1})] , \tag{49}$$

with I_0 being the modified Bessel function of zeroth order. The series for Γ generally converges rapidly and typically only a few terms are needed.

In equilibrium, Eqs. (47)–(49) yield

$$\delta m_1^* = \delta m_3^* = \alpha\frac{2\sqrt{2\pi}\vartheta^{3/2}}{3\sinh\vartheta}[(\vartheta-\tfrac{1}{2})I_0(\vartheta) - \vartheta I_1(\vartheta)] , \tag{50}$$

where $\vartheta=\beta/2$. This temperature-dependent mass shift is shown in Fig. 5. Previous calculations of the temperature dependence of the effective-mass shift are discussed in Ref. 1. Different definitions of the effective mass lead to widely differing results. We prefer our definition, since it is based directly on the polaron's physical inertia.

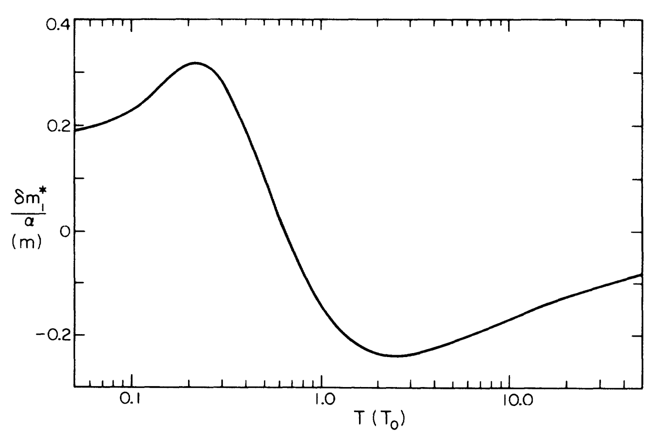

FIG. 5. $\delta m_i^*/\alpha$ vs T in equilibrium. $T_0=\hbar\omega_0/k_B$.

The velocity dependence of the effective-mass shift is shown in Fig. 6 for temperatures of 0, 0.271, and 1.0. For $u \approx u_c/2$, the δm_i^* change rapidly and approach zero from below as $u \to \infty$. Comparing with Fig. 5, we see that the variation of the mass shift with temperature is qualitatively similar to the variation of the zero-temperature mass shift with velocity. This similarity is reasonable since an increase in the temperature causes an increase in the typical velocity (i.e., the root-mean-square velocity) of the polaron.

To understand why the effective-mass shifts become negative for large u, we consider the classical polaron. In the classical limit, one can use Eq. (A4) and the fact that classically $\sigma_i(t)$ is zero (for $T=0$) to show

$$\delta m_3^* = \frac{1}{2}\frac{\partial^2}{\partial u^2}V(u) , \tag{51}$$

where $V(u)$ is the potential energy of the polaron. Evaluating $V(u)$ gives

$$V(u) = -\frac{\alpha\pi}{\sqrt{2}u} . \tag{52}$$

$V(u)$ is negative, since the interaction between the electron and the phonon field lowers the system's energy, and it approaches zero for large u because the electron and the phonon field decouple in this limit. The second derivative of any function with this behavior must be negative for some value of u [for $V(u)$ it is negative for all positive u]. Thus, a negative mass shift is a classical effect, arising from the decoupling at large velocities of the electron from the phonon field.

We are not aware of any experimental measurements of the velocity dependence of the effective-mass shift. As we expect the variation to be significant for $u \approx u_c/2$, if α is not too small ($\alpha \approx 0.1$ gives a variation of a few percent at $T=0$), such a measurement would be an important test of the transport equations.

IV. SUMMARY

We have derived a set of approximate transport equations suitable for studying the behavior of polarons near

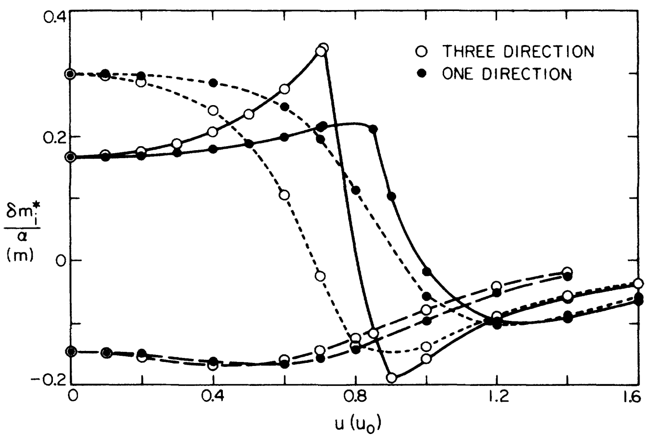

FIG. 6. $\delta m_i^*/\alpha$ vs u for $T=0$ (solid line), $T=0.271$ (small-dashed line), and $T=1.0$ (large-dashed line).

the Čerenkov velocity. We have solved these equations for weak coupling and have shown that the solutions are consistent with experimental observations. We have also shown our approach to be more accurate than that of Thornber and Feynman. Finally, we have calculated the effective-mass shift for weak coupling and find that it changes rapidly near the Čerenkov velocity. We encourage experimental measurement of this quantity as a test of our theory.

ACKNOWLEDGMENTS

This work was supported in part by the National Science Foundation under Grants No. DMR-80-2063 and No. DMR-87-03434, and through the Northwestern University Materials Research Center under Grant No. DMR-85-20280. J.H.J. wishes to thank F. M. Peeters for useful discussions and the National Science Foundation for partial support. This work was based in part on a doctoral thesis of J.H.J., Princeton University.

APPENDIX A

In this appendix, we derive the expression for energy conservation from Eq. (16). By letting $t' \to t$ with t' coming before t on the contour in Eq. (16), and then again with t' coming after t, we find

$$\langle \ddot{x}_i(t)\dot{x}_j(t)\rangle = f_i(t)\langle \dot{x}_j(t)\rangle - \sum_{\mathbf{k}} \int_c d\tau\, A(k,|t-\tau|_c)\langle T_c e^{i\mathbf{k}\cdot\mathbf{x}(t)} k_i \dot{x}_j(t) e^{-i\mathbf{k}\cdot\mathbf{x}(\tau)}\rangle \tag{A1}$$

and

$$\langle \dot{x}_j(t)\ddot{x}_i(t)\rangle = f_i(t)\langle \dot{x}_j(t)\rangle - \sum_{\mathbf{k}} \int_c d\tau\, A(k,|t-\tau|_c)\langle T_c k_i \dot{x}_j(t) e^{i\mathbf{k}\cdot\mathbf{x}(t)} e^{-i\mathbf{k}\cdot\mathbf{x}(\tau)}\rangle . \tag{A2}$$

Adding these, contracting on the indices, and dividing by 2 yields

$$\frac{1}{2}\frac{d}{dt}\langle \dot{\mathbf{x}}^2(t)\rangle = \mathbf{f}(t)\cdot\langle \dot{\mathbf{x}}(t)\rangle + i\sum_{\mathbf{k}} \int_c d\tau\, A(k,|t-\tau|_c)\frac{d}{dt}\langle T_c e^{i\mathbf{k}\cdot[\mathbf{x}(t)-\mathbf{x}(\tau)]}\rangle . \tag{A3}$$

We then use the product rule for derivatives to get

$$\frac{d}{dt}\left[\tfrac{1}{2}\langle \dot{\mathbf{x}}^2(t)\rangle - i\sum_{\mathbf{k}}\int_c d\tau\, A(k,|t-\tau|_c)\langle T_c e^{i\mathbf{k}\cdot[\mathbf{x}(t)-\mathbf{x}(\tau)]}\rangle\right]$$
$$= \mathbf{f}(t)\cdot\langle \dot{\mathbf{x}}(t)\rangle - i\sum_{\mathbf{k}}\int_c d\tau \langle T_c e^{i\mathbf{k}\cdot[\mathbf{x}(t)-\mathbf{x}(\tau)]}\rangle \frac{d}{dt}A(k,|t-\tau|_c)\ . \qquad (A4)$$

The left-hand side of Eq. (A4) is the rate of change of the energy of the polaron, while the right-hand side is the rate of energy transfer to the polaron from the external force minus the rate of energy transfer from the polaron to the phonons.

APPENDIX B

Here we prove that Eqs. (17) are exact for actions $S_c(\mathbf{x})$ that are quadratic in $\mathbf{x}(t)$. We begin with the exact expressions

$$\langle T_c e^{i\mathbf{k}\cdot[\mathbf{x}(t_2)-\mathbf{x}(t_1)]}\rangle = \frac{1}{Z}\lim_{t_0\to-\infty} Z_c\{\mathbf{g}(t)+\mathbf{k}[\Theta_c(t-t_2)-\Theta_c(t-t_1)],\, t_0\}\ ,$$

$$\langle T_c \dot{x}_j(t') e^{i\mathbf{k}\cdot[\mathbf{x}(t_2)-\mathbf{x}(t_1)]}\rangle = \frac{i}{Z}\lim_{t_0\to-\infty}\left[\frac{\delta}{\delta g_j(t')}Z_c\{\mathbf{g}(t)+\mathbf{k}[\Theta_c(t-t_2)-\Theta_c(t-t_1)],\, t_0\}\right]\ , \qquad (B1)$$

where $\Theta_c(t-t')$ is 1 if t comes after t' on the contour and 0 if t comes before t'.

For quadratic actions, the path integral in Eq. (11) can be done exactly and leads to a generating functional of the form

$$Z_c(\mathbf{g},t_0) = Z\exp\left[\tfrac{1}{2}\int_c d\tau \int_c d\tau'\, g_i(\tau) M_{ij}(\tau,\tau') g_j(\tau')\right]\ , \qquad (B2)$$

where $M_{ij}(\tau,\tau')$ is a function symmetric in τ and τ' and in i and j. Using Eq. (8), the average particle velocity is

$$\langle \dot{x}_i(t)\rangle = i\lim_{t_0\to-\infty}\left[\int_c d\tau\, M_{ij}(t,\tau) g_j(\tau)\right]\ . \qquad (B3)$$

The exponential disappears, since after taking the functional derivative, we can deform the contour in the exponent to a straight line from t_0 to $t_0-i\beta$, and then taking the limit $t_0\to-\infty$ and using $\mathbf{g}(t)\to 0$ as $\mathrm{Re}\,t\to-\infty$, one finds that the argument of the exponent tends to zero. Similarly, we obtain

$$\frac{d}{dt}\langle T_c y_i(t)\dot{y}_j(t')\rangle = -M_{ij}(t,t')\ . \qquad (B4)$$

Applying Eqs. (B2)–(B4) to (B1) leads directly to (17).

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