Alternative approach to the dynamics of polarons in one dimension

A. H. Castro Neto and A. O. Caldeira
Instituto de Física "Gleb Wataghin," Departamento de Física do Estado Sólido e Ciência dos Materiais, Universidade Estadual de Campinas, 13081 Campinas, São Paulo, Brazil
(Received 15 August 1991; revised manuscript received 19 November 1991)

We developed a method based on functional integration to treat the dynamics of polarons in one-dimensional systems. We treat the acoustical and the optical case in a unified manner, showing their differences and similarities. The mobility and the diffusion coefficients are calculated in the Markovian approximation in the strong-coupling limit.

I. INTRODUCTION

The main task of this paper is to develop a formalism to treat the dynamics of acoustical or optical polarons in the strong-coupling limit. Although we are applying the formalism to a specific problem we think that it can also be applied to a large class of phenomena, especially problems involving quantization of zero-frequency modes in theories which have solitons as solutions of their semiclassical equations of motion.

When we have a particle (electron) interacting with a given background (phonons in this case) and wish to study its effective dynamics, it is now well known that we must trace over the phonon coordinates and study the time evolution of the reduced density operator of the electronic system. However, in the specific case of electron-phonon coupling, the "effective propagator" for this operator is extremely cumbersome, preventing us from getting any simple result out of this standard analysis. Therefore, one should search for an extra step before blindly tracing the phonon coordinates out of the problem.

We start from a very intuitive point, treating the electron-phonon Hamiltonian as a "semi-classical" Hamiltonian.[1] This "semiclassical" picture provides us with solutions which are solitons, that is, solutions which do not change their shape with time. These solitons will be the basic entities for the future solution of the problem. We show that the best basis in which one can expand the field operators of the quantum Hamiltonian is obtained from the problem of an electron trapped in a self-consistent potential well. We will call it the "adiabatic basis" since the strong-coupling limit is the adiabatic limit (see Sec. II).

Once we have obtained the Hamiltonian in adiabatic form, we can eliminate the electronic part perturbatively, that is, we trace over the electron coordinates. This treatment gives rise to an effective Hamiltonian for the phonon system which has renormalized phonons and a zero-frequency mode, namely, the polaron. An important feature of this Hamiltonian is that it can be straightforwardly generalized for a noninteracting many-electron system.

Using the well-known "collective coordinate formalism," we transform the effective Hamiltonian into a Hamiltonian of a particle, the polaron, coupled to a new set of phonons. It can be shown that for a small polaron momentum the problem can be put in a very simple form.

Actually, this is a more systematic way to apply the ideas used by Schüttler and Holstein[2] to a quantum dissipation problem as the necessary step before the tracing procedure. Here, we shall repeat part of their arguments for the sake of completeness.

Finally, using the functional integral formalism, we can show that the polaron behaves as a Brownian particle due to the scattering of phonons. So, we have developed a method which allows us to calculate the physical quantities of interest, such as the damping parameter (mobility) and the diffusion coefficient without appealing to kinetic theory.

In Sec. II we will present the model and exhibit the adiabatic basis for the strong-coupling limit while in Sec. III we obtain the effective Hamiltonian for the polaron coupled to the renormalized phonons. In Sec. IV we use the functional integral formalism in order to show how this problem can be treated as a Brownian motion problem and in Sec. V we use the previous results to calculate the physical quantities of interest. Section VI contains our conclusions.

II. THE POLARON MODEL AND THE ADIABATIC EXPANSION

Since in this paper we will treat the problem of an electron coupled to acoustical or optical lattice vibrations (phonons) in a unified manner, we decided to develop these two problems in parallel, in order to show their differences and similarities.

A. Optical case

The optical polaron model is based on the Fröhlich Hamiltonian[3] for electrons coupled to longitudinal optical phonons. This Hamiltonian can be written in the second quantized form, in one dimension, as

$$H_0=\int dx\left\{\frac{\hat{\pi}^2}{2\nu}+\frac{\nu\omega_0^2}{2}\hat{\eta}^2+\frac{\hbar^2}{2m}\frac{\partial\hat{\psi}^\dagger}{\partial x}\frac{\partial\hat{\psi}}{\partial x}+\frac{D}{a}\hat{\eta}\hat{\psi}^\dagger\hat{\psi}\right\}, \tag{2.1}$$

here $\hat{\pi}$ and $\hat{\eta}$ are the momentum and position operator for the phonon field and $\hat{\psi}^\dagger$ and $\hat{\psi}$ the creation and destruction operators, respectively, for the electron field. They obey the following commutation rules:

$$[\hat{\eta}(x,t),\hat{\pi}(x',t)]=i\hbar\delta(x-x'),$$

$$\{\hat{\psi}(x,t),\hat{\psi}^\dagger(x',t)\}=\delta(x-x'),$$

where [,] denotes commutation and {,} anticommutation. All the other commutation (or anticommutation) relations are zero.

In (2.1), ω_0 is the frequency of the phonons, $\nu=M/a$ is the lattice density, M the ion mass, a the lattice parameter, m is the effective mass for the electrons in the conduction band, and D the coupling constant.

In order to analyze the physical content of (2.1) we will treat the operators as ordinary functions and interpret the electron field as the wave function for one electron in the lattice. In other words, we would say that we are treating the problem in the mean-field approximation where the operators are replaced by their mean values over configurations. It is emphasized that this is not an exact calculation but just an artifact to obtain the best basis in which we would expand the operators of the Hamiltonian (2.1) in order to get the strong-coupling regime. It can be easily shown that the following Lagrangian can generate the Hamiltonian (2.1):

$$L=\int dx\left\{\frac{\nu}{2}\left[\frac{\partial\eta}{\partial t}\right]^2-\frac{\nu\omega_0^2}{2}\eta^2+i\hbar\left[\psi^*\frac{\partial\psi}{\partial t}-\psi\frac{\partial\psi^*}{\partial t}\right]-\frac{\hbar^2}{2m}\frac{\partial\psi^*}{\partial x}\frac{\partial\psi}{\partial x}-\frac{D}{a}\eta\psi^*\psi\right\}, \tag{2.2}$$

where ψ is normalized:

$$\int dx\,|\psi(x,t)|^2=1\ . \tag{2.3}$$

The equations of motion for the Lagrangian (2.2) are

$$i\hbar\frac{\partial\psi}{\partial t}+\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}-\frac{D}{a}\eta\psi=0\ , \tag{2.4}$$

$$\frac{\partial^2\eta}{\partial t^2}+\omega_0^2\eta+\frac{D}{M}|\psi|^2=0\ . \tag{2.5}$$

Equation (2.4) is the Schrödinger equation for an electron in a potential given by

$$V(x,t)=\frac{D}{a}\eta(x,t)\ ,$$

while Eq. (2.5) is an equation for an oscillator with frequency ω_0 forced by the presence of an external field, $|\psi|^2$. The picture is that of an electron which distorts the lattice which, in its turn, produces a potential for the electron; a self-consistent interaction.

We are interested only in stationary solutions for the electrons, that is, solutions of the form

$$\psi(x,t)\equiv\phi_0(x)e^{-iE_0t/\hbar} \tag{2.6}$$

as well as in static solutions for the lattice (adiabatic solution)

$$\eta(x,t)\equiv\eta_0(x)\ . \tag{2.7}$$

From (2.4)–(2.7) we get

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{D}{a}\eta_0(x)\right]\phi_0(x)=E_0\phi_0(x)\ , \tag{2.8}$$

$$\eta_0(x)=-\frac{D}{M\omega_0^2}\phi_0^2(x)\ . \tag{2.9}$$

We can think of (2.8) and (2.9) as follows: we put the electron in the lattice and the latter adjusts itself to the presence of the former. As a consequence, the electron is trapped by the potential well formed around itself.

Substituting (2.9) in (2.8) we get

$$-\frac{\hbar^2}{2m}\frac{d^2\phi_0}{dx^2}-\frac{D^2}{Ma\omega_0^2}\phi_0^3=E_0\phi_0\ . \tag{2.10}$$

This is a nonlinear Schrödinger equation which can be solved exactly. There is a localized static solution which reads

$$\phi_0(x)=\frac{\sqrt{g}}{2}\operatorname{sech}\left[\frac{g(x-x_0)}{2}\right], \tag{2.11}$$

where

$$g=\frac{1}{a}\left[\frac{m}{M}\right]\left[\frac{D}{\hbar\omega_0}\right]^2 \tag{2.12}$$

and

$$E_0=-\frac{\hbar^2g^2}{8m} \tag{2.13}$$

is the binding energy of the electron in the potential well. x_0 is an arbitrary constant which gives the center of the packet described by (2.11).

The lattice displacements are given by (2.9)

$$\eta_0(x)=-2a\left[\frac{|E_0|}{D}\right]\operatorname{sech}^2\left[\frac{g(x-x_0)}{2}\right], \tag{2.14}$$

which is symmetric around the electron position.

The potential well where the electron is trapped is given by

$$V(x)=-2|E_0|\operatorname{sech}^2\left[\frac{g(x-x_0)}{2}\right]. \tag{2.15}$$

We can identify the parameter g as the strength of the interaction since the potential (2.15) becomes very weak for distances greater than g^{-1}. Therefore, g^{-1} defines the polaron length.

B. The acoustical case

For electrons interacting with acoustical phonons, the Hamiltonian can be written as[4]

$$H_A=\int dx\left\{\frac{\hat{\pi}^2}{2\nu}+\frac{\nu v_s^2}{2}\left[\frac{\partial\hat{\eta}}{\partial x}\right]^2+\frac{\hbar^2}{2m}\frac{\partial\hat{\psi}^\dagger}{\partial x}\frac{\partial\hat{\psi}}{\partial x}+D\frac{\partial\hat{\eta}}{\partial x}\hat{\psi}^\dagger\hat{\psi}\right\}, \quad (2.16)$$

where v_s is the sound velocity in the lattice and all other definitions are maintained.

The second term in (2.16) comes from the Debye dispersion relation for acoustical phonons

$$\omega=v_s|k| , \quad (2.17)$$

where k is the phonon wave vector.

For (2.16) the "semi-classical" Lagrangian is

$$L=\int dx\left\{\frac{\nu}{2}\left[\frac{\partial\eta}{\partial t}\right]^2-\frac{\nu v_s^2}{2}\left[\frac{\partial\eta}{\partial x}\right]^2+i\hbar\left[\psi^*\frac{\partial\psi}{\partial t}-\psi\frac{\partial\psi^*}{\partial t}\right]-\frac{\hbar^2}{2m}\frac{\partial\psi^*}{\partial x}\frac{\partial\psi}{\partial x}-D\frac{\partial\eta}{\partial x}\psi^*\psi\right\}, \quad (2.18)$$

which produces the following set of equations of motion:

$$i\hbar\frac{\partial\psi}{\partial t}+\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}-D\frac{\partial\eta}{\partial x}\psi=0 , \quad (2.19)$$

$$\frac{\partial^2\eta}{\partial t^2}-v_s^2\frac{\partial^2\eta}{\partial x^2}-\frac{D}{\nu}\frac{\partial|\psi|^2}{\partial x}=0 . \quad (2.20)$$

These equations are interpreted in the same way as for the optical case as a self-consistent interaction, where the potential that the electron feels is

$$V(x,t)=D\frac{\partial\eta}{\partial x} .$$

Unlike (2.4) and (2.5), this system of coupled equations admits a traveling solution. We can obtain a general solution for (2.19) and (2.20) defining a variable $\chi=x-x_0-vt$, where x_0 and v are arbitrary constants. We look for solutions of the form

$$\psi(x,t)=\phi_0(\chi)\exp\left\{\frac{i}{\hbar}(mvx-E_0't)\right\} \quad (2.21)$$

and

$$\eta(x,t)=\eta_0(\chi) . \quad (2.22)$$

From (2.19)–(2.22),

$$-\frac{\hbar^2}{2m}\frac{d^2\phi_0}{d\chi^2}+D\frac{d\eta}{d\chi}=\left[E_0'-\frac{mv^2}{2}\right]\phi_0(\chi) , \quad (2.23)$$

$$\frac{d\eta_0}{d\chi}=-\frac{D}{\nu(v_s^2-v^2)}\phi_0^2(\chi) . \quad (2.24)$$

Equation (2.23) is the Schrödinger equation in the variable ϕ and (2.24) has the form of a wave equation of the same variable. Substituting (2.24) in (2.23) we get

$$-\frac{\hbar^2}{2m}\frac{d^2\phi_0}{d\chi^2}-\frac{D^2}{\nu(v_s^2-v^2)}\phi_0^3=\left[E_0'-\frac{mv^2}{2}\right]\phi_0 . \quad (2.25)$$

Again we have obtained a nonlinear Schrödinger equation which is characteristic of a self-consistent interaction. The solution obtained if v is smaller than the velocity of the sound is

$$\phi_0(\chi)=\frac{\sqrt{g'}}{2}\text{sech}\left[\frac{g'\chi}{2}\right] , \quad (2.26)$$

where

$$g'=\frac{1}{a}\left[\frac{m}{M}\right]\left[\frac{D}{\hbar v_s/a}\right]^2\left[1-\frac{v^2}{v_s^2}\right]^{-1} \quad (2.27)$$

with the electron binding energy given by

$$E_0'=\frac{mv^2}{2}-\frac{\hbar^2 g'^2}{8m} . \quad (2.28)$$

The solution is unstable for $v>v_s$.

The interpretation is almost obvious: the electron and the lattice displacement move together with velocity v. Observe that the wave function (2.16) and the binding energy (2.28) have exactly the same shape as in the optical case for $v=0$ (the adiabatic case). We expect that the potential which the electron feels must be the same. From (2.24)

$$\eta_0(\chi)=-\frac{\hbar^2 g'}{2mD}\tanh\left[\frac{g'\chi}{2}\right] \quad (2.29)$$

and the potential is given by

$$V(\chi)=D\frac{d\eta_0}{d\chi}=-\frac{\hbar^2 g'^2}{4m}\text{sech}^2\left[\frac{g'\chi}{2}\right] . \quad (2.30)$$

Observe that, for $v=0$, (2.30) has the same shape of (2.15). This exhibits something fundamental in the physics of the two problems. Observe that the parameters g and g' have the same form for $v=0$:

$$\frac{1}{a}\left[\frac{m}{M}\right]\left[\frac{D}{E_c}\right]^2 ,$$

where E_c is the characteristic energy of the phonon system; $\hbar\omega_0$ in the optical case and $\hbar\omega_D$ in the acoustical case, where

$$\omega_D=v_s/a$$

is the Debye frequency. So, g and g' play the same role in both problems and, from now on, we will call them g. Actually, we will work only with the static case, $v=0$, observing that this means that we are not taking into account the kinetic energy of the lattice in (2.18) (Born-Oppenheimer approximation). This explains why we are using the term "adiabatic."

Here, it should be noticed that one must reconcile $g\gg 1$ (strong coupling) with the continuum model we have been using. It has been shown in Ref. 2 that there is a vast range of polaron sizes where both conditions are met.

C. The adiabatic expansion

As we have seen, for the acoustical as well as for the optical case, the potential well which traps the electron is the same. As a consequence the wave functions and binding energies are also the same. As we have treated the problem in a variational way, we expect that the wave function, (2.11) or (2.26), is the ground-state wave function for the electron in the adiabatic limit and zero temperature. Nevertheless, we expect that for finite temperatures the electron can be found in some excited state of this well due to its interaction with thermal phonons. As the interaction is self-consistent, the potential well must change its shape, changing the potential energy of the electron. If the temperature is not too high, so it does not remove the electron from the well, we might imagine that due to virtual transitions the electron absorbs energy from the lattice and immediately emits this energy, remaining in the ground state.

In order to find these excited states we have to solve the Schrödinger equation for the electron in the potential well, (2.15) or (2.30) (put $x_0=0$):

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\phi_n(x)-\frac{\hbar^2 g^2}{4m}\operatorname{sech}^2\left[\frac{gx}{2}\right]\phi_n(x)=E_n\phi_n(x)\ . \tag{2.31}$$

This equation can be solved exactly[5] and gives one bound state as expected [see (2.11) and (2.26)]:

$$\phi_0(x)=\frac{\sqrt{g}}{2}\operatorname{sech}\left[\frac{gx}{2}\right]$$

with energy

$$E_0=-\frac{\hbar^2 g^2}{8m}$$

and a set of doubly degenerate free states

$$\phi_n^F(x)=\frac{1}{\sqrt{L}}e^{ik_n x}\left\{\frac{k_n+ig\tanh(gx/2)/2}{k_n+ig/2}\right\} \tag{2.32}$$

with energy

$$E_n^F=\frac{\hbar^2 k_n^2}{2m}\ , \tag{2.33}$$

where k_n is the solution of

$$k_n=\frac{2n\pi}{L}-\frac{\delta(k_n)}{L},\quad n=0,\pm1,\pm2,\ldots \tag{2.34}$$

and $\delta(k)$ is the phase shift due to the scattering of the free states given by

$$\delta(k)=\arctan\left[\frac{kg}{k^2-g^2/4}\right]\ . \tag{2.35}$$

Here we have imposed periodic boundary condition in $x=\pm L/2$ with $L\rightarrow\infty$.

The "adiabatic expansion" is made by expanding the electron field operators in (2.1) or (2.16) in this basis, yielding

$$\hat\psi(x,t)=\phi_0(x)\hat a_0(t)+\sum_{n=1}^{\infty}\phi_n^F(x)\hat a_n(t)\ , \tag{2.36}$$

$$\hat\psi^\dagger(x,t)=\phi_0(x)\hat a_0^\dagger(t)+\sum_{n=1}^{\infty}\phi_n^{F*}(x)\hat a_n^\dagger(t)\ , \tag{2.37}$$

where a_n and $a_n^\dagger$ are, respectively, the destruction and creation operators for each state of (2.31). They obey the following anticommutation rules:

$$\{\hat a_n(t),\hat a_m^\dagger(t)\}=\delta_{nm}\ ,$$

$$\{\hat a_n(t),\hat a_m(t)\}=\{\hat a_n^\dagger(t),\hat a_m^\dagger(t)\}=0\ .$$

The field displacement as well as its conjugate momentum density can also be expanded in this basis as

$$\hat\eta(x,t)=\eta_0(x)+\sum_{k=-\infty}^{+\infty}\hat q_k(t)\frac{e^{ikx}}{\sqrt{N}}\ , \tag{2.38}$$

$$\hat\pi(x,t)=\sum_{k=-\infty}^{+\infty}\hat p_k(t)\frac{e^{ikx}}{\sqrt{N}}\ , \tag{2.39}$$

where $N=L/a$ is the number of ion sites and k is given by the periodic boundary conditions

$$k=\frac{2n\pi}{L},\quad n=0,\pm1,\pm2,\ldots\ .$$

As $\hat\eta$ and $\hat\pi$ are real, we must have

$$\hat q_k^\dagger=\hat q_{-k},\quad \hat p_k^\dagger=\hat p_{-k}\ ,$$

with the usual commutation rule

$$[\hat q_k(t),\hat p_{k'}(t)]=i\hbar\delta_{k,k'}\ .$$

If we substitute (2.36)–(2.39) in (2.1) and (2.16), and use the orthogonality of the adiabatic states

$$\int dx\,\phi_0(x)\phi_n^F(x)=0\ , \tag{2.40}$$

$$\int dx\,\phi_n^F(x)\phi_{n'}^F(x)=\delta_{nn'}\ , \tag{2.41}$$

and Eqs. (2.9), (2.14), and (2.31), we obtain

(i) for the optical case:

$$H_0=\epsilon_0+E_0a_0^\dagger a_0+\sum_{n=1}^{\infty}E_n^F a_n^\dagger a_n$$
$$+\sum_{k=-\infty}^{+\infty}\left\{\frac{\hat p_k\hat p_{-k}}{2M}+\frac{M\omega_0^2}{2}\hat q_k\hat q_{-k}\right.$$
$$\left.+\frac{D}{a}q_k\left[f^0(k)(a_0^\dagger a_0-1)+\sum_{n=0}^{\infty}\left[f_n(k)a_0^\dagger a_n+f_n^*(-k)a_n^\dagger a_0+\sum_{m=1}^{\infty}f_{nm}(k)a_n^\dagger a_m\right]\right]\right\}\ , \tag{2.42}$$

where

$$\epsilon_0=\frac{\nu\omega_0^2}{2}\int_{-\infty}^{+\infty}dx\ \eta_0^2(x)=\frac{\hbar^2 g^2}{12m}=\frac{2}{3}|E_0|\ , \tag{2.43}$$

$$f^0(k)=\frac{1}{\sqrt{N}}\int dx\ \phi_0^2(x)e^{ikx}\ , \tag{2.44}$$

$$f_n(k)=\frac{1}{\sqrt{N}}\int dx\ \phi_0(x)\phi_n^F(x)e^{ikx}\ , \tag{2.45}$$

$$f_{nm}(k)=\frac{1}{\sqrt{N}}\int dx\ \phi_n^{F*}(x)\phi_m^F(x)e^{ikx}\ , \tag{2.46}$$

(ii) for the acoustical case:

$$H_A=\epsilon_0+E_0a_0^\dagger a_0+\sum_{n=1}^{\infty}E_n^F a_n^\dagger a_n + \sum_{k=-\infty}^{+\infty}\left\{\frac{\hat{p}_k\hat{p}_{-k}}{2M}+\frac{Mv_s^2k^2}{2}\hat{q}_k\hat{q}_{-k} + ikDq_k\left[f_0(k)(a_0^\dagger a_0-1)+\sum_{n=0}^{\infty}\left[f_n(k)a_0^\dagger a_n+f_n^*(-k)a_n^\dagger a_0+\sum_{m=1}^{\infty}f_{nm}(k)a_n^\dagger a_m\right]\right]\right\}\ . \tag{2.47}$$

Notice that (2.42) and (2.47) are exact results, no approximations have been made so far.

Since we are interested in the strong-coupling limit, the phonons cannot excite the electron out of the well. Quantitatively this means that

$$\frac{|E_0|}{E_c}\gg 1\ ,$$

where E_c is the phonon characteristic energy and $|E_0|$ the modulus of the binding energy of the electron. The inequality above allows us to define an expansion parameter for the strong-coupling limit, α, as

$$\alpha=\frac{E_c}{|E_0|}\ll 1\ .$$

If now we scale the Hamiltonians (2.42) and (2.47) by the characteristic phonon energy, we can easily see that the pure electronic part is of the order of α^{-1} while the interaction term is of the order of $\alpha^{-1/2}$ and consequently much smaller than the former.[6,2] Using this result we will eliminate the electronic part of the Hamiltonian by a perturbative treatment and obtain a renormalized phonon Hamiltonian.

Consider the pure electronic part as the nonperturbed Hamiltonian. Its eigenstates can be written in the Fock space as

$$|n_0,n_1,\ldots n_\infty\rangle\ , \tag{2.48}$$

where n_0 is the occupation number for the ground state. We simplify the calculation assuming that there is only one electron in the problem (see Appendix A for the case of many electrons); that is,

$$\sum_{j=0}^{\infty}n_j=1\ . \tag{2.49}$$

The ground state is given by

$$|\psi_0\rangle=|n_0=1;n_j=0\rangle,\quad j=1,2,3,\ldots \tag{2.50}$$

with energy E_0. This state is exactly the adiabatic state given by (2.11) or (2.26).

We can now apply the Rayleigh-Schrödinger perturbation theory to this problem. The first-order term is null because we have just one electron. The second-order correction is easily calculated and it gives

(i) for the optical case:

$$E_0^{(2)}=-\frac{D^2}{a^2}\sum_{kk'}V_0(k,k')\hat{q}_k\hat{q}_{-k'}\ , \tag{2.51}$$

where

$$V_0(k,k')=\sum_{n=0}^{\infty}\frac{f_n(k)f_n^*(k')}{E_n^F-E_0}\ , \tag{2.52}$$

(ii) for the acoustical case:

$$E_A^{(2)}=-D^2\sum_{kk'}kk'V_0(k,k')\hat{q}_k\hat{q}_{-k'}\ . \tag{2.53}$$

Therefore, we write the Hamiltonians for the renormalized phonons as

$$H_{O,A}=\epsilon+\sum_{k=-\infty}^{+\infty}\left\{\frac{\hat{p}_k\hat{p}_{-k}}{2M}+\frac{M}{2}\sum_{k'=-\infty}^{+\infty}[\Omega_{kk'}^{O,A}]^2\hat{q}_k\hat{q}_{-k'}\right\}\ , \tag{2.54}$$

where

$$\epsilon=\epsilon_0+E_0=-\frac{|E_0|}{3} \tag{2.55}$$

and

$$(\Omega_{kk'}^O)^2=\omega_0^2\delta_{kk'}-\frac{2D^2}{Ma^2}V_0(k,k')\ , \tag{2.56}$$

$$(\Omega_{kk'}^A)^2=v_s^2k^2\delta_{kk'}-\frac{2D^2}{M}kk'V_0(k,k')\ . \tag{2.57}$$

The Hamiltonian (2.54) was already obtained[6] some years ago for the acoustical case and it can be rewritten in a different form in terms of some new operators $\delta\hat{\eta}(x,t)$ and $\hat{\pi}(x,t)$ defined by [c.f., (2.38)]

$$\hat{q}_k(t)=\frac{1}{\sqrt{N}}\int\frac{dx}{a}e^{-ikx}\delta\hat{\eta}(x,t)\ , \tag{2.58}$$

$$\hat{p}_k(t)=\frac{1}{\sqrt{N}}\int dxe^{-ikx}\hat{\pi}(x,t)\ . \tag{2.59}$$

One can easily check that

$$[\delta\hat{\eta}(x,t),\hat{\pi}(x',t)]=i\hbar\delta(x-x')\ .$$

Now, using (2.58) and (2.59) in (2.54), we get

$$H_O=\epsilon+\int dx\left\{\frac{\hat{\pi}^2}{2\nu}+\frac{\nu\omega_0^2}{2}\delta\hat{\eta}^2-\frac{\nu\omega_0^2}{2}\delta\hat{\eta}\int dx'F(x,x')\delta\hat{\eta}(x')\right\} \tag{2.60}$$

and

$$H_A=\epsilon+\int dx\left\{\frac{\hat{\pi}^2}{2\nu}+\frac{\nu v_s^2}{2}\left[\frac{\partial\delta\hat{\eta}}{\partial x}\right]^2-\frac{\nu v_s^2}{2}\frac{\partial\delta\hat{\eta}}{\partial x}\int dx'F(x,x')\frac{\partial\delta\hat{\eta}}{\partial x'}\right\}, \tag{2.61}$$

where

$$F(x,x')=4g\phi_0(x)\phi_0(x')\sum_{n=1}^{\infty}\frac{\phi_n^{F*}(x)\phi_n^F(x')}{(k_n^2+g^2/4)}\ . \tag{2.62}$$

These results agree perfectly with those obtained by other methods.[2,7]

III. THE EFFECTIVE HAMILTONIAN

As we are interested in the excitation spectrum of the Hamiltonians (2.60) and (2.61), we have to diagonalize them. If we choose

$$\delta\hat{\eta}(x,t)=\sum_{n=0}^{\infty}\hat{q}_n(t)u_n(x)\ , \tag{3.1}$$

where u_n are the normalized eigenfunctions of (2.60) or (2.61),

$$\int\frac{dx}{a}u_n^*(x)u_m(x)=\delta_{nm}\ , \tag{3.2}$$

they must satisfy the following integrodifferential equations:

$$\text{(i)}\ \Omega_n^2u_n(x)=\omega_0^2u_n(x)-\omega_0^2\int dx'F(x,x')u_n(x') \tag{3.3}$$

for the optical case, while

$$\text{(ii)}\ \Omega_n^2u_n(x)=-v_s^2\frac{d^2u_n}{dx^2}+v_s^2\int dx'\frac{\partial}{\partial x}F(x,x')\frac{du_n(x')}{dx'} \tag{3.4}$$

for the acoustical case.

Observe that to solve (3.3) and (3.4) is equivalent in the momentum space to diagonalize (2.56) and (2.57). These equations often appear in works about polaron dynamics[2,8,9] and we do not intend to solve them in this work. For (3.3) there is a closed solution[9] which we will use later, while for (3.4) we will make some approximations which are suitable for our purposes.

An interesting and important solution of those equations can be found directly. These are the zero-mode solutions, that is, solutions with $\Omega_0=0$ (see Appendix B). For the optical case we have

$$u_0^{\text{OP}}(x)=\frac{\sqrt{15ag}}{2}\tanh\left[\frac{gx}{2}\right]\text{sech}^2\left[\frac{gx}{2}\right] \tag{3.5}$$

and for the acoustical case

$$u_0^{\text{AC}}(x)=\sqrt{3ag/8}\,\text{sech}^2\left[\frac{gx}{2}\right]\ . \tag{3.6}$$

Examining (3.5) and (3.6) and comparing with (2.14) and (2.29), we see that, in both cases,

$$u_0(x)=C\frac{d}{dx}\eta_0(x)\ , \tag{3.7}$$

where C is a constant which appears due to the normalization of u_0. The above relation clearly expresses the translational invariance of Hamiltonians (2.1) and (2.16). Notice that although we have put $x_0=0$ in (2.31), in order to obtain the adiabatic basis, the center of the soliton solutions (2.11), (2.14), (2.26), and (2.29) is arbitrary and therefore we must have u_n also expanded about this point; that is,

$$u_n\equiv u_n(x-x_0)\ . \tag{3.8}$$

Suppose that we move the center of the functions (2.14) or (2.29) by an infinitesimal quantity δx_0. Then,

$$\eta_0(x_0+\delta x_0)\simeq\eta_0(x_0)+\frac{u_0(x_0)\delta x_0}{C}\ , \tag{3.9}$$

where we have used (3.7). By (3.9) we conclude that the zero-mode frequency corresponds to the translation of the soliton, in other words, to the motion of the polaron.

Once we have the eigenfunctions of (3.3) and (3.4), we would expect to write the Hamiltonian in the form

$$H=\epsilon+\frac{\hat{P}_0^2}{2M}+\sum_{n=1}^{\infty}\left[\frac{\hat{P}_n^2}{2M}+\frac{M\Omega_n^2}{2}\hat{q}_n^2\right]\ , \tag{3.10}$$

where we have used that $\Omega_0=0$.

At first sight (3.10) shows a free particle with momentum P_0 and a set of decoupled harmonic oscillators. Nevertheless, it is not possible to take it seriously because, initially, we have implicitly assumed that the lattice displacement cannot be indefinitely large. From (2.51) and (2.53) we see that the energy correction depends on the lattice displacement which must be finite in order for the perturbation theory to be valid.

Let us observe that, due to (3.9), the polaron displacement is proportional to the displacement of its center, that is,

$$q_0=\delta x_0/C \ . \tag{3.11}$$

From (3.1), we have

$$\delta\eta(x,t)=q_0u_0+\sum_{n=1}^{\infty}q_nu_n$$

or, using (3.7) and (3.11),

$$\delta\eta(x,t)=\delta x_0\frac{\partial\eta_0}{\partial x_0}+\sum_{n=1}^{\infty}q_nu_n \ . \tag{3.12}$$

Therefore, we can assume that x_0 is a true dynamic variable, that is, $x_0=x_0(t)$. So, based on (3.12), we will rewrite expansion (3.1) as

$$\delta\hat{\eta}(x,t)=\eta_0[x-\hat{x}_0(t)]+\sum_{n=1}^{\infty}\hat{q}_n(t)u_n[x-\hat{x}_0(t)] \ . \tag{3.13}$$

This procedure is known as "collective coordinate formalism."[10] Observe that (3.13) changes the kinetic part of (2.60) or (2.61) because $\hat{x}_0$ is also a function of time. It is shown[2] that the new Hamiltonian in the presence of the polaron position operator, $\hat{x}_0$, is given by

$$\begin{aligned}H=\epsilon+\sum_{n=1}^{\infty}\left[\frac{\hat{p}_n^2}{2M}+\frac{M\Omega_n^2}{2}\hat{q}_n^2\right]\\+\frac{1}{8M_0}\left\{\left[\hat{P}-\sum_{n,m=1}^{\infty}G_{nm}\hat{q}_n\hat{p}_n\right],\left[1+\sum_{n=1}^{\infty}S_n\hat{q}_n\right]^{-1}\right\}\\-\frac{\hbar^2M}{8M_0^2}\sum_{n=1}^{\infty}S_n^2\left[1+\sum_{m=1}^{\infty}S_m\hat{q}_m\right]^{-1} \ .\end{aligned} \tag{3.14}$$

Here $\{,\}$ denotes anticommutation and $\hat{P}$ is the momentum operator associate to $\hat{x}_0$:

$$[\hat{x}_0(t),\hat{P}(t)]=i\hbar$$

and

$$[\hat{q}_n(t),\hat{p}_m(t)]=i\hbar\delta_{nm}$$

with all the other commutators being zero.

In (3.14) we have

$$M_0=\nu\int_{-\infty}^{+\infty}dx\left[\frac{d\eta_0}{dx}\right]^2 \tag{3.15}$$

as being the classical soliton mass which becomes

$$M_0=\frac{m}{8}\left[\frac{E_0}{\hbar\omega_0}\right]^2$$

for the optical case, and

$$M_0=\frac{32}{3}m\left[\frac{E_0}{\hbar v_s g}\right]^2$$

for the acoustical case.

The new quantities

$$S_n=\frac{M}{M_0}\int\frac{dx}{a}\frac{d\eta_0}{dx}\frac{du_n}{dx} \tag{3.16}$$

and

$$G_{nm}=\int\frac{dx}{a}u_m(x)\frac{du_n(x)}{dx} \tag{3.17}$$

couple the polaron to the renormalized phonons.

In the strong-coupling limit (3.14) can be simplified.[8] Due to (3.5), (3.6), (2.14), (2.29), and (3.7), we can rewrite S_n as

$$S_n\sim\frac{M}{M_0}\frac{1}{\sqrt{ag}}\left[\frac{E_0}{D}\right]\int\frac{dx}{a}u_0(x)\frac{du_n(x)}{dx} \ .$$

As the integral only gives a numerical factor, this yields

$$S_n\sim\frac{M}{M_0}\frac{1}{\sqrt{ag}}\left[\frac{E_0}{D}\right]\frac{1}{a} \ .$$

Now, from (3.15),

$$\frac{M}{M_0}\sim\frac{M}{m}\left[\frac{E_c}{E_0}\right]^2$$

and

$$q_n\sim\frac{\hbar}{(ME_c)^{1/2}}$$

so

$$\sum_n S_nq_n\sim\left[\frac{E_c}{|E_0|}\right]^{1/2}\ll 1$$

and, therefore, this sum is very small in the strong-coupling limit. Within this approximation we get

$$H\simeq\epsilon+\sum_{n=1}^{\infty}\left[\frac{\hat{p}_n^2}{2M}+\frac{M\Omega_n^2}{2}\hat{q}_n^2\right]+\frac{1}{2M_0}\left[\hat{P}-\sum_{n,m=1}^{\infty}G_{nm}\hat{q}_m\hat{p}_n\right]^2 \ . \tag{3.18}$$

The second term in (3.18) is the energy of noninteracting phonons and the third term can be interpreted as the kinetic energy of the polaron. Observe that

$$\dot{\hat{x}}_0=\frac{1}{i\hbar}[\hat{x}_0,\hat{H}]=\frac{1}{M_0}\left[\hat{P}-\sum_{n,m=1}^{\infty}G_{nm}\hat{q}_m\hat{p}_n\right] \tag{3.19}$$

and so $\hat{P}$ cannot be the polaron momentum because, since

$$\dot{\hat{P}}=\frac{1}{i\hbar}[\hat{P},\hat{H}]=0 \ ,$$

it is a constant of motion. From (3.19) we interpret $M_0\dot{\hat{x}}_0$ as the polaron momentum and $\sum_{nm}G_{nm}\hat{q}_m\hat{p}_n$ as the momentum of the phonon field. Observe that Hamiltonian (3.18) is very close to the electromagnetic Hamiltonian, where the coupling between the particle and the field are obtained via the potential vector (see Sec. IV).

If we define the destruction and creation operators

$$\hat{b}_n=\left[\frac{M\Omega_n}{2\hbar}\right]^{1/2}\left[\hat{q}_n+i\frac{\hat{p}_n}{M\Omega_n}\right] , \tag{3.20}$$

$$\hat{b}_n^\dagger = \left[\frac{M\Omega_n}{2\hbar} \right]^{1/2} \left[\hat{q}_n - i\frac{\hat{p}_n}{M\Omega_n} \right] , \qquad (3.21)$$

which obviously obey

$$[\hat{b}_n, \hat{b}_m^\dagger] = \delta_{nm} ,$$

one can rewrite H as

$$H = \epsilon + \sum_{n=1}^{\infty} \hbar\Omega_n (b_n^\dagger b_n + \tfrac{1}{2}) + \frac{1}{2M_0}(\hat{P} - \hat{P}_{\text{ph}})^2 , \qquad (3.22)$$

where

$$\hat{P}_{\text{ph}} = \sum_{n,m=1}^{\infty} \frac{\hbar}{2i} \left[\left[\frac{\Omega_n}{\Omega_m} \right]^{1/2} + \left[\frac{\Omega_m}{\Omega_n} \right]^{1/2} \right] G_{nm} b_m^\dagger b_n + \sum_{n,m=1}^{\infty} \frac{\hbar}{4i} \left[\left[\frac{\Omega_n}{\Omega_m} \right]^{1/2} - \left[\frac{\Omega_m}{\Omega_n} \right]^{1/2} \right] \times G_{nm} (b_m b_n - b_m^\dagger b_n^\dagger) . \qquad (3.23)$$

Here we have used the fact that, from (3.15), G_{nm} is antisymmetric in the interchange of m and n,

$$G_{nm} = -G_{mn} . \qquad (3.24)$$

Observe that the momentum of the phonon field consists of two parts; a diagonal part [the first term on the right-hand side of (3.23)] which commutes with the phonon-number operator,

$$\hat{N} = \sum_{n=1}^{\infty} \hat{b}_n^\dagger \hat{b}_n ,$$

and, therefore, conserves the number of phonons in the system. This term is responsible for scattering. The other term does not commute with the number operator and is related with absorption or emission of phonons by the polaron (Cerenkov process). We will restrict our problem to typical polaron kinetic energies much smaller than the phonon energies, in other words, small velocities. In this limit the occurrence of emission or absorption of phonons is not possible due to the simultaneous conservation of momentum and energy. In terms of our parameters this means that

$$|\dot{x}_0| \ll \sqrt{E_c/M_0} . \qquad (3.25)$$

Only scattering, and therefore virtual transitions, will be relevant for our problem.

With this approximation the polaron dynamics will be described by the following effective Hamiltonian:

$$H = \frac{1}{2M_0} \left[\hat{P} - \sum_{n,m=1}^{\infty} \hbar g_{nm} \hat{b}_m^\dagger \hat{b}_n \right]^2 + \sum_{n=1}^{\infty} \hbar\Omega_n \hat{b}_n^\dagger \hat{b}_n , \qquad (3.26)$$

where

$$g_{nm} = \frac{1}{2i} \frac{(\Omega_n + \Omega_m)}{\sqrt{\Omega_n \Omega_m}} G_{nm} . \qquad (3.27)$$

As we will show in the next section the Hamiltonian (3.26) describes the dynamics of a Brownian particle, that is, a heavy particle in a bath of light particles which collide with it.

IV. FUNCTIONAL INTEGRAL METHOD

The starting point for the calculations of the transport properties of the polaron is the well-known Feynman-Vernon formalism[11] that the authors have recently applied[12] to the Hamiltonian (3.26).

We are interested only in the quantum statistical properties of the polaron and the phonons act only as a source of relaxation and diffusion processes. Consider the density operator for the system polaron plus phonons, $\hat{\rho}(t)$. This operator evolves in time according to

$$\hat{\rho}(t) = e^{-i\hat{H}t/\hbar} \hat{\rho}(0) e^{i\hat{H}t/\hbar} , \qquad (4.1)$$

where $\hat{H}$ is given by (3.26) and $\hat{\rho}(0)$ is the density operator at $t=0$ which we will assume to be decoupled as a product of the polaron density operator, $\hat{\rho}_S(0)$, and the phonon density operator, $\hat{\rho}_R(0)$:

$$\hat{\rho}(0) = \hat{\rho}_S(0) \hat{\rho}_R(0) , \qquad (4.2)$$

where the symbol $\underline{S}$ refers to the polaron (system of interest) and $\underline{R}$ to the phonons (the reservoir of excitations).

Condition (4.2) means that we put the electron in the lattice which is in thermal equilibrium at temperature T. So, we consider the phonons as described by their equilibrium distribution,

$$\hat{\rho}_R(0) = \frac{e^{-\beta\hat{H}_R}}{Z} , \qquad (4.3)$$

where

$$Z = \text{tr}_R(e^{-\beta\hat{H}_R}) \qquad (4.4)$$

with

$$\beta = \frac{1}{K_B T} . \qquad (4.5)$$

Here tr_R denotes the trace over the phonon variables and K_B is the Boltzmann constant. $\hat{H}_B$ is the free-phonon Hamiltonian which is given by the last term on the right-hand side of (3.26).

As we said, we are interested only in the quantum dynamics of the system S, so, we define a reduced density operator

$$\hat{\rho}_s(t) = \text{tr}_R[\hat{\rho}(t)] , \qquad (4.6)$$

which contains all the information about S when it is in contact with R.

Projecting now (4.6) in the coordinate representation of the polaron system

$$\hat{x}_0 |q\rangle = q|q'\rangle \qquad (4.7)$$

and in the coherent state representation for bosons (the phonons)

$$\hat{b}_n |\alpha_n\rangle = \alpha_n |\alpha_n\rangle , \qquad (4.8)$$

we have[13] (see also Appendix C)

$$\rho_s(x,y,t)=\int dx'\int dy' J(x,y,t;x',y',0)\rho_s(x',y',0) . \tag{4.9}$$

Here we have used (4.1), (4.2), (4.6), and the completeness relation for the representations above, namely,

$$\int dq|q\rangle\langle q|=1 , \tag{4.10}$$

$$\int \frac{d^2\alpha}{\pi}|\alpha\rangle\langle\alpha|=1 , \tag{4.11}$$

where $d^2\alpha=d(\mathrm{Re}\alpha)d(\mathrm{Im}\alpha)$ as usual.

In (4.9), J is the superpropagator of the polaron, which can be written as

$$J=\int_{x'}^{x}Dx\int_{y'}^{y}Dy e^{(i/\hbar)(S_0[x]-S_0[y])}F[x,y] , \tag{4.12}$$

where

$$S_0[x]=\int_0^t dt'\left\{\frac{M_0\dot{x}^2(t')}{2}\right\} \tag{4.13}$$

is the classical action for the free particle. F is the so-called influence functional

$$F[x,y]=\int\frac{d^2\boldsymbol{\alpha}}{\pi^N}\int\frac{d^2\boldsymbol{\beta}}{\pi^N}\int\frac{d^2\boldsymbol{\beta}'}{\pi^N}\rho_R(\boldsymbol{\beta}^*,\boldsymbol{\beta}')e^{-|\alpha|^2-|\beta|^2/2-|\beta'|^2/2}\int_{\boldsymbol{\beta}}^{\boldsymbol{\alpha}^*}D^2\boldsymbol{\alpha}\int_{\boldsymbol{\beta}^*}^{\boldsymbol{\alpha}}D^2\boldsymbol{\gamma}\, e^{S_I[x,\alpha]+S_I^*[y,\gamma]} , \tag{4.14}$$

where $\boldsymbol{\beta}$ denotes the vector $(\beta_1,\beta_2,\beta_3,\ldots,\beta_N)$ and S_I is a complex action related to the reservoir plus interaction

$$S_I[x,\boldsymbol{\alpha}]=\int_0^t dt'\left\{\frac{1}{2}\left[\boldsymbol{\alpha}\cdot\frac{d\boldsymbol{\alpha}^*}{dt'}-\boldsymbol{\alpha}^*\cdot\frac{d\boldsymbol{\alpha}}{dt'}\right]-\frac{1}{\hbar}(H_R-\dot{x}h_I)\right\} \tag{4.15}$$

with

$$H_R=\sum_{n=1}^{\infty}\hbar\Omega_n\alpha_n^*\alpha_n , \tag{4.16}$$

$$h_I=\sum_{n,m=1}^{\infty}\hbar g_{nm}\alpha_m^*\alpha_n . \tag{4.17}$$

Here we have obtained a result which is very close to the electromagnetic coupling where the Hamiltonian depends on the vector potential, $\mathbf{A}$, through

$$\left[\mathbf{p}-\frac{e\,\mathbf{A}}{c}\right]^2$$

but the Lagrangian depends on

$$\mathbf{v}\cdot\mathbf{A} .$$

In our case the Lagrangian formulation simplifies the problem transforming a nonlinear problem into a linear one. The action (4.15) is quadratic in $\boldsymbol{\alpha}$, so it can be solved exactly. Observe that the Euler-Lagrange equations for (4.15) are

$$\dot{\alpha}_n+i\Omega_n\alpha_n-i\dot{x}\sum_{m=1}^{\infty}g_{mn}\alpha_m=0 , \tag{4.18}$$

$$\dot{\alpha}_n^*-i\Omega_n\alpha_n^*+i\dot{x}\sum_{m=1}^{\infty}g_{nm}\alpha_m^*=0 , \tag{4.19}$$

which must be solved subject to the boundary conditions

$$\alpha_n(0)=\beta_n , \tag{4.20}$$

$$\alpha_n^*(t)=\alpha_n^* . \tag{4.21}$$

Due to (3.24) we have $g_{nn}=0$, so, the modes are not coupled among themselves. This makes (4.18) and (4.19) easy to solve. That set of equations represents a set of harmonic oscillators forced by the presence of the polaron. The result can be written as

$$\alpha_n(\tau)=e^{-i\Omega_n\tau}\left[\beta_n+\sum_{m=1}^{\infty}W_{nm}(\tau)\beta_m\right] , \tag{4.22}$$

$$\alpha_n^*(\tau)=e^{i\Omega_n\tau}\left[\alpha_n^*e^{-i\Omega_n t}+\sum_{m=1}^{\infty}\tilde{W}_{nm}(\tau)e^{-i\Omega_m t}\alpha_m^*\right] , \tag{4.23}$$

where W_{nm} and $\tilde{W}_{nm}$ are functionals of $x(t)$ which obey the following equations:

$$W_{nm}(\tau)=\int_0^{\tau}W_{nm}^{(0)}(t')dt'+\sum_{k=1}^{\infty}\int_0^{\tau}W_{nk}^{(0)}(t')W_{nk}(t')dt' , \tag{4.24}$$

$$\tilde{W}_{nm}(\tau)=\int_{\tau}^{t}\tilde{W}_{nm}^{(0)}(t')dt'+\sum_{k=1}^{\infty}\int_{\tau}^{t}\tilde{W}_{nk}^{(0)}(t')\tilde{W}_{km}(t')dt' , \tag{4.25}$$

where

$$W_{nm}^{(0)}(\dot{x}(t'),t')=ig_{nm}\dot{x}(t')e^{i(\Omega_n-\Omega_m)t'} , \tag{4.26}$$

$$\tilde{W}_{nm}^{(0)}(\dot{x}(t'),t')=W_{nm}^{(0)}(\dot{x}(t'),t') \tag{4.27}$$

[observe that $W_{nm}(t)=\tilde{W}_{mn}(0)$].

Now we expand the action (4.15) around the classical solution (4.22) and (4.23) and obtain, after some integrations in (4.14),

$$F[x,y]=\prod_{n=1}^{\infty}(1-\Gamma_{nn}[x,y]\bar{n}_n)^{-1} , \tag{4.28}$$

where

$$\Gamma_{nm}=W_{nm}^*[y]+W_{mn}[x]+\sum_{l=1}^{\infty}W_{lm}^*[y]W_{ln}[x] \tag{4.29}$$

with

$$\bar{n}_n=(e^{\beta\hbar\Omega_n}-1)^{-1} . \tag{4.30}$$

Notice that (4.28) and (4.29) are exact, no approximations have been made so far.

We see from (4.24) and (4.25) that W_{nm} can be expressed as a power series of the Fourier transform of the polaron velocity, $\dot{x}$, so, due to the small polaron velocity condition (3.25), we expect that only few terms in (4.24) will be sufficient for a good description of the polaron dynamics.

Another way to see this is to notice that (4.24) and (4.25) are the scattering amplitudes from mode k to mode j. The terms that appear in the sum represent the virtual transitions between these two modes. With these two arguments in mind we will make use of the Born approximation. In matrix notation,

$$W(\tau)\approx\int_0^\tau W^{(0)}(t')dt' + \int_0^\tau W^{(0)}(t')\int_0^{t'} W^{(0)}(t'')dt''dt' \ . \qquad (4.31)$$

Therefore, in the approximation of small polaron velocity the terms in (4.29) are small and we can rewrite, as a good approximation,

$$F[x,y]\simeq\exp\left\{\sum_{n=1}^{\infty}\Gamma_{nn}[x,y]\bar{n}_n\right\} . \qquad (4.32)$$

Observe that if the interaction is turned off ($\Gamma\rightarrow 0$) or the temperature is zero ($T=0$) the functional (4.29) is one, and, as we would expect the polaron moves as a free particle.

Substituting the Born approximation (4.31) in (4.32) and the latter in (4.12) we find

$$J=\int_{x'}^{x}Dx\int_{y'}^{y}Dy\exp\left\{\frac{i}{\hbar}\tilde{S}[x,y]+\frac{1}{\hbar}\tilde{\phi}[x,y]\right\} , \qquad (4.33)$$

where

$$\tilde{S}=\int_0^t dt'\left\{\frac{M_0}{2}[\dot{x}^2(t')-\dot{y}^2(t')]+[\dot{x}(t')-\dot{y}(t')]\int_0^t dt''\Gamma_I(t'-t'')[\dot{x}(t'')+\dot{y}(t'')]\right\} \qquad (4.34)$$

and

$$\tilde{\phi}=\int_0^t dt'\int_0^t dt''\{\Gamma_R(t'-t'')[\dot{x}(t')-\dot{y}(t')] \times[\dot{x}(t'')-\dot{y}(t'')]\} \qquad (4.35)$$

with

$$\Gamma_R(t)=\hbar\theta(t)\sum_{n,m=1}^{\infty}g_{nm}^2\bar{n}_n\cos(\Omega_n-\Omega_m)t , \qquad (4.36)$$

$$\Gamma_I(t)=\hbar\theta(t)\sum_{n,m=1}^{\infty}g_{nm}^2\bar{n}_n\sin(\Omega_n-\Omega_m)t . \qquad (4.37)$$

Now, if we define the new variables R and r as

$$R=\frac{x+y}{2} , \qquad (4.38)$$

$$r=x-y , \qquad (4.39)$$

the equations of motion for the action in (4.34) read

$$\ddot{R}(\tau)+2\int_0^t dt'\gamma(\tau-t')\dot{R}(t')=0 , \qquad (4.40)$$

$$\ddot{r}(\tau)-2\int_0^t dt'\gamma(t'-\tau)\dot{r}(t')=0 , \qquad (4.41)$$

where

$$\gamma(t)=\frac{1}{M_0}\frac{d\Gamma_I}{dt} \qquad (4.42)$$

or, using (4.37),

$$\gamma(t)=\frac{\hbar\theta(t)}{M_0}\sum_{n,m=1}^{\infty}g_{nm}^2\bar{n}_n(\Omega_n-\Omega_m)\cos(\Omega_n-\Omega_m)t \qquad (4.43)$$

is the damping function.

In terms of these newly defined variables, we can easily see that (4.40) and (4.41) have the same form of the equations previously obtained in the case of quantum Brownian motion,[14] except for the fact that they now present memory effects. It should be emphasized that although (4.40) and (4.41) have only indirect physical meaning, through the study of the motion of the center of a wave packet and the spreading of its width, $\gamma(t)$ really plays the role of the damping parameter in the equation of motion of the former (see Ref. 14 for details).

Furthermore, we shall prove that (4.43) can be written in the form

$$\gamma(t)=\bar{\gamma}(T)\delta(t) , \qquad (4.44)$$

where $\bar{\gamma}(T)$ is a damping parameter which is temperature dependent and $\delta(t)$ is the Dirac δ function. The form (4.44) is known as the Markovian approximation because in this case the memory is purely local and does not depend on the previous motion of the particle.

If we use (4.40) and (4.41) with (4.44) and expand the phase of (4.33) around this classical solution we get the well-known result for the quantum Brownian motion[14] where the damping parameter γ (temperature independent) is replaced by $\bar{\gamma}(T)$ and the diffusive part is replaced by (4.35). As a consequence, the diffusion parameter in momentum space will be given by

$$D(t)=\hbar\frac{d^2\Gamma_R}{dt^2} = -\hbar^2\theta(t)\sum_{n,m=1}^{\infty}g_{nm}^2\bar{n}_n(\Omega_n-\Omega_m)^2 \times\cos(\Omega_n-\Omega_m)t . \qquad (4.45)$$

We will also prove that $D(t)$ has the Markovian form

$$D(t)=\bar{D}(T)\delta(t) , \qquad (4.46)$$

where $\bar{D}(T)$ and $\bar{\gamma}(T)$ obey the classical fluctuation-dissipation theorem at low temperatures.[15]

In what follows we shall define a function $S(\omega,\omega')$ which will, in analogy to the spectral function $J(\omega)$ of the standard model,[14] allow one to replace all the summations over k by integrals over frequencies:

$$S(\omega,\omega')=\sum_{n,m=1}^{\infty} g_{nm}^2\delta(\omega-\Omega_n)\delta(\omega'-\Omega_n) \, . \tag{4.47}$$

Notice, however, that unlike $J(\omega)$ in Ref. 14, this new function $S(\omega,\omega')$ is related to the scattering of the environmental excitations between states of frequencies ω and ω' (as seen from the laboratory frame). Moreover, due to (3.24) it is easy to see that

$$S(\omega,\omega')=S(\omega',\omega) \, . \tag{4.48}$$

From now on we shall call $S(\omega,\omega')$ the "scattering function."

Notice that we can rewrite (4.43) and (4.45) as

$$\gamma(t)=\frac{\hbar\theta(t)}{2M_0}\int_0^\infty d\omega\int_0^\infty d\omega' S(\omega,\omega')(\omega-\omega')[n(\omega)-n(\omega')]\cos(\omega-\omega')t \tag{4.49}$$

and

$$D(t)=-\frac{\hbar^2\theta(t)}{2}\int_0^\infty d\omega\int_0^\infty d\omega' S(\omega-\omega')(\omega-\omega')^2[n(\omega)+n(\omega')]\cos(\omega-\omega')t \, . \tag{4.50}$$

Concluding, we have established that the Hamiltonian (3.26) leads to a Brownian dynamics, that is, the polaron moves as a particle in a viscous environment where its relaxation and diffusion are due to the scattering of phonons.

V. MOBILITY AND DIFFUSION

Equations (4.43) and (4.45) show that the polaron transport properties depend essentially on the coupling parameter g_{nm}. From (3.17) we see that this parameter can be obtained if we know the eigenfunctions of (3.3) and (3.4).

First of all we can show that (3.3) and (3.4) have solutions with definite parities. This is easily seen by changing x by $-x$ in (3.3) and (3.4) and x' by $-x'$ in the integral term. From (2.62) we observe that $F(-x,-x')=F(x,x')$ and therefore $u_n(x)$ and $u_n(-x)$ obey the same eigenvalue equation. In other words, the Hamiltonians commute with the parity operator and therefore it is possible to classify their eigenfunctions as odd or even. Now we must study the optical and the acoustical cases separately.

A. Optical case

Turkevich and Holstein[9] obtained the exact solutions for (3.3). For the odd modes the eigenfunctions are

$$u_n(x)=\sqrt{ag/2}\left[\frac{2n+5}{(n+2)(n+3)}\right]^{1/2} \times[1-Y^2(x)]\frac{dP_{n+2}}{dY}, \quad n=0,2,4,6\ldots, \tag{5.1}$$

where

$$Y(x)=\tanh\left[\frac{gx}{2}\right] \tag{5.2}$$

and P_n are the Legendre polynomials.

The eigenvalues of the problem are

$$\Omega_n=\omega_0\left[1-\frac{4}{n^2+5n+4}\right]^{1/2} \, . \tag{5.3}$$

In particular, the zero mode, $n=0$ and $\Omega_0=0$, is given by (3.5).

The even modes can be written as

$$u_\alpha(x)=\sqrt{ag/2}\left[\frac{2\alpha+5}{(\alpha+2)(\alpha+3)}\right]^{1/2} \times\frac{[1-Y^2(x)]}{2}\frac{d}{dY}[P_{\alpha+2}(Y)-P_{\alpha+2}(-Y)] \, , \tag{5.4}$$

where the allowed values of $\underline{\alpha}$ are solutions of

$$\psi(\alpha+3)-\psi(1)=\frac{\pi}{2}\tan\left[\frac{\alpha\pi}{2}\right]$$

and ψ is the digamma function. Its eigenvalues are given by

$$\Omega_\alpha=\omega_0\left[1-\frac{4}{\alpha^2+5\alpha+4}\right]^{1/2} .$$

We will use the convention given in Table I.

As the labels for the even solutions are not integers we define $\epsilon_n=n-\alpha$ as the difference between our classification and the label. Table I shows us that the eigenfrequencies go quickly to ω_0 while ϵ_n goes to zero.

From (3.17) we note that G_{nm} only couples functions with opposite parity. Substituting (5.1) and (5.4) in (3.17), we get

$$G_{nm}=-\frac{2g}{\pi}\frac{\sin[\pi(n-m+\epsilon_m)]}{\pi[(n-m+\epsilon_m)^2-1]}K_{nm} \, , \tag{5.5}$$

where

TABLE I. Conventions for classification of the eigenfunctions.

n	α	Ω_n/ω_0	$\epsilon_n=n-\alpha$
0	0	0	0
1	0.523	0.648	0.477
2	2	0.882	0
3	2.601	0.912	0.394
4	4	0.949	0
5	4.648	0.958	0.352
6	6	0.971	0
7	6.674	0.975	0.326
8	8	0.981	0
9	8.692	0.983	0.308
10	10	0.987	0

$$K_{nm}=\frac{[(n+2)(n+3)(2n+5)(m-\epsilon_m+2)(m-\epsilon_m+3)(2m-2\epsilon_m+5)]^{1/2}}{[(n+m+\epsilon_m)^2+10(n+m-\epsilon_m)+24]} \tag{5.6}$$

for $n=0,2,4,6\ldots, m=1,3,5,7\ldots$.

Observe that (5.5)) is strongly peaked around $n=m\pm 1$. Therefore, the most important contributions to summations involving G_{nm} will come from these forms (observe that ϵ_m goes to zero as m goes to infinity):

$$G_{nm}\simeq gK_{nm}[\delta(n-m-1)-\delta(n-m+1)] \tag{5.7}$$

for n even and m odd.

From (4.47) and (3.27) we get

$$S(\omega,\omega')=-\frac{g^2}{4}\sum_n\{C_{nn-1}^2[\delta(\omega-\Omega_n)\delta(\omega'-\Omega_{n-1})+\delta(\omega-\Omega_{n-1})\delta(\omega'-\Omega_n)] + C_{nn+1}^2[\delta(\omega-\Omega_n)\delta(\omega'-\Omega_{n+1})+\delta(\omega-\Omega_{n+1})\delta(\omega'-\Omega_n)]\}\ , \tag{5.8}$$

where n is even and

$$C_{nm}=\frac{(\Omega_n+\Omega_m)}{\sqrt{\Omega_n\Omega_m}}K_{nm}\ . \tag{5.9}$$

Substituting (5.8) in (4.48) we find

$$\gamma(t)=-\frac{\hbar g^2}{8M_0}\theta(t)\sum_n\{C_{nn-1}^2(\Omega_n-\Omega_{n-1})[n(\Omega_n)-n(\Omega_{n-1})]\cos(\Omega_n-\Omega_{n-1})t + C_{nn+1}^2(\Omega_{n+1}-\Omega_n)[n(\Omega_{n+1}-n(\Omega_n)]\cos[(\Omega_{n+1}-\Omega_n)t]\}\ . \tag{5.10}$$

We will define wave vectors for each n in (5.2) in the form

$$K=n\pi/L\ , \tag{5.11}$$

where L is the length of quantization ($L\to\infty$). Equation (5.10) then becomes

$$\gamma(t)=-\frac{\hbar^2 g^2}{8M_0}\theta(t)\frac{2\pi}{L}\int_0^\infty dKC^2(K,K)\left[\frac{d\Omega}{dK}\right]^2\left[\frac{dn}{d\Omega}\right]\times\cos\left[\frac{\pi}{L}\frac{d\Omega}{dK}t\right]\ , \tag{5.12}$$

where we used the limit $L\to\infty$.

It is easy to see that by (5.3)

$$\frac{d\Omega}{dK}=\frac{4\pi^2}{L^2}\frac{\omega_0}{K^3}\quad\text{as } L\to\infty \tag{5.13}$$

and by (5.9) and (5.6) that

$$C^2(K,K)=\frac{L^2K^2}{\pi^2}\quad\text{as } L\to\infty\ .$$

Now, using the fact that the frequencies approach the value ω_0 very fast when n increases, we make the following approximation:

$$\frac{dn}{d\Omega}\simeq\left.\frac{dn}{d\Omega}\right|_{\Omega=\omega_0}.$$

We shall rewrite (5.12) as

$$\gamma(t)=\frac{\hbar^2 g^2}{4M_0}\theta(t)\left[-\left.\frac{dn}{d\Omega}\right|_{\omega_0}\right]\omega_0^2\frac{16\pi^3}{L^3}\times\int_0^\infty dK\frac{\cos[(4\pi^3\omega_0 t/L^3)(1/K^3)]}{K^4}\ .$$

This integral can be easily done if we change variables, $x=\frac{4\pi^3\omega_0}{L^3}\frac{1}{K^3}$. The integral then becomes

$$\gamma(t)=\frac{\hbar^2 g^2}{4M_0}\theta(t)\left[-\left.\frac{dn}{d\Omega}\right|_{\omega_0}\right]\frac{4\omega_0}{3}\int_0^\infty dx\cos(xt)$$

and finally

$$\gamma(t)=\frac{\hbar g^2}{2M_0}\frac{\pi}{3}\frac{\hbar\omega_0}{K_BT}e^{\hbar\omega_0/K_BT}(e^{\hbar\omega_0/K_BT}-1)^{-2}\delta(t)\ , \tag{5.14}$$

which has the form (4.44).

For low temperatures, $K_BT\ll\hbar\omega_0$, we have

$$\bar{\gamma}(T)\simeq\frac{\pi}{6}\frac{\hbar g^2}{M_0}\left[\frac{\hbar\omega_0}{K_BT}\right]e^{-\hbar\omega_0/K_BT} \tag{5.15}$$

so $\bar{\gamma}(T)$ goes to zero as T goes to zero, as expected. So, for very low temperatures the mobility is extremely high and the polaron moves as a free particle. This is an expected result since at $T=0$ there are no phonons to be scattered.

For high temperatures, $K_BT\gg\hbar\omega_0$,

$$\bar{\gamma}(T)\simeq\frac{\pi}{6}\frac{\hbar g^2}{M_0}\left[\frac{K_BT}{\hbar\omega_0}\right] \tag{5.16}$$

and the mobility goes to zero at $T \to \infty$.

The diffusion parameter (4.49) can be calculated in the same way. It gives

$$\bar{D}(T)=\frac{\pi}{3}\frac{\hbar g^2}{M_0}\hbar\omega_0(e^{\hbar\omega_0/K_BT}-1)\ . \tag{5.17}$$

For low temperatures this parameter is too small, going to zero as $T\to 0$. The fluctuations are once again small due to the absence of phonons. For high temperature we see that the fluctuations also increase linearly with T.

Observe that

$$\frac{\bar{D}(T)}{\bar{\gamma}(T)}=2M_0K_BT(1-e^{-\hbar\omega_0/K_BT})\ , \tag{5.18}$$

which gives the classical result of the fluctuation-dissipation theorem[15] for the Brownian motion at low temperatures.

B. The acoustical case

As we do not have exact solutions for (3.4) it will be necessary to make some approximations in the present analysis. Observe that (3.4) is a Schrödinger-like equation for a particle in a nonlocal potential

$$V(x,x')=-\frac{\partial^2 F(x,x')}{\partial x'\partial x}\ .$$

From (2.62) we observe that $V(x,x')$ goes to zero as x goes to infinity. Actually, the potential is almost zero except in the range

$$-\frac{1}{g}<x<\frac{1}{g}\ .$$

Out of this range the wave function can be well described by

$$\frac{d^2u_k}{dx^2}+k^2u_k(x)=0\ , \tag{5.19}$$

where we have used that

$$\omega=v_s|k|\ . \tag{5.20}$$

The solutions of (5.19) must be classified as even or odd. We choose

$$u_E(k,x)=\sqrt{2a/L}\cos[k|x|+\delta_E(k)]\ , \tag{5.21}$$

$$u_O(k,x)=\sqrt{2a/L}\,\mathrm{sgn}(x)\sin[k|x|+\delta_O(k)]\ , \tag{5.22}$$

where

$$\mathrm{sgn}(x)=\begin{cases}1 & \text{if } x>0\ ,\\ -1 & \text{if } x<0\ ,\end{cases}$$

and $\delta_E(k)$ and $\delta_O(k)$ are the phase shifts for the even and odd modes, respectively, which must appear due to the presence of the potential.

Another possible solution of (5.19) is

$$u_k(x)=\sqrt{2a/L}\,\{t(k)e^{ikx}\theta(x-1/g)+[e^{ikx}+r(k)e^{-ikx}]\theta(-x-1/g)\}\ . \tag{5.23}$$

This expression can be interpreted as a wave incident from the left on a potential whose $t(k)$ and $r(k)$ are the transmission and reflection amplitudes.

We can construct (5.23) from (5.21) and (5.22) as[16]

$$u_k(x)=e^{i\delta_E}u_E(k,x)+ie^{i\delta_O}u_O(k,x)$$

if

$$t(k)=\tfrac{1}{2}(e^{2i\delta_E(k)}+e^{2i\delta_O(k)})\ ,$$

$$r(k)=\tfrac{1}{2}(e^{2i\delta_E(k)}-e^{2i\delta_O(k)})\ .$$

Consequently, the transmission and reflection coefficients are given by

$$T(k)=|t(k)|^2=\cos^2[\delta_O(k)-\delta_E(k)]\ , \tag{5.24}$$

$$R(k)=|r(k)|^2=\sin^2[\delta_O(k)-\delta_E(k)]\ , \tag{5.25}$$

and $T(k)+R(k)=1$ as expected.

Once we have the phase shifts of the problem we can find the transmission and reflection probabilities using (5.24) and (5.25), or alternatively, if we have the reflection and transmission amplitudes we can obtain the phase shifts

$$\delta_E(k)=\frac{1}{2}\arctan\left[\frac{\mathrm{Im}[t(k)+r(k)]}{\mathrm{Re}[t(k)+r(k)]}\right]\ , \tag{5.26}$$

$$\delta_O(k)=\frac{1}{2}\arctan\left[\frac{\mathrm{Im}[t(k)-r(k)]}{\mathrm{Re}[t(k)-r(k)]}\right]\ . \tag{5.27}$$

Actually, Schüttler and Holstein[2] obtained these coefficients in the limit of long and short wavelengths after a rather intricate algebra (in the results of Ref. 5, R and T depend on the polaron velocity which is very small in our case and we have put it equal to zero):

(i) for $k \gg g$,

$$r(k)\simeq\frac{16\pi^2ik^3e^{-2\pi k/g}}{g^3}\ , \tag{5.28}$$

$$t(k)\simeq 1+\frac{2ig}{5k}\ , \tag{5.29}$$

(ii) for $k \ll g$,

$$r(k)\simeq-\frac{3ik}{g}-\frac{gk^2}{g^2}\ , \tag{5.30}$$

$$t(k)\simeq 1-\frac{3ik}{g}-\frac{gk^2}{g^2}\ . \tag{5.31}$$

These results allow one to compute the respective phase shifts as

(i) for $k \gg g$,

$$\delta_E(k)\simeq\delta_O(k)\simeq\frac{g}{5k}\ , \tag{5.32}$$

(ii) for $k \ll g$,

$$\delta_E(k)\simeq-\frac{3k}{g}\ ,\qquad \delta_O(k)\simeq 0\ . \tag{5.33}$$

So, the phase shifts are very small. We would say that there is a propagation of sound waves through the polaron.

If the interaction between the electron and the lattice is strong, the range of the potential is small. Therefore, the contribution to the integral in (3.17) due to the true solution is almost the same as the one we would have got had we used the free solutions (5.21) and (5.22).

First, we impose periodic boundary conditions which give the allowed values for k:

$$k_n=\frac{2n\pi}{L},\quad n=\pm1,\pm2,\pm3\ldots . \tag{5.34}$$

In order to classify the solutions we will use the following convention:

$$u_{2n-1}(x)=u_E(n,x) , \tag{5.35}$$

$$u_{2n}(x)=u_O(n,x) , \tag{5.36}$$

for $n=\pm1,\pm2,\pm3\ldots$.

Now we can evaluate (3.17). It yields

$$G_{2n-1,2m}=-\frac{2k_n}{L}\left\{\frac{\sin[(k_n-k_m)L/2]}{k_n-k_m}\cos[\delta_E(k_n)-\delta_O(k_m)]+\left[\frac{1-\cos[(k_n-k_m)L/2]}{k_n-k_m}\right]\sin[\delta_E(k_n)-\delta_O(k_m)]\right\} . \tag{5.37}$$

As in the optical case we have a matrix with zeros in the diagonal and with off-diagonal terms which decrease as a function of their distance to the main diagonal.

When $L\rightarrow\infty$ we will have [using (5.24)]

$$G_{kk'}=-\frac{2k}{L}\left\{\pi\delta(k-k')\sqrt{T(k)}+P\left[\frac{\sin[\delta_E(k)-\delta_O(k')]}{k-k'}\right]\right\} , \tag{5.38}$$

where P denotes the principal value. Substituting (5.38) in (4.47), transforming the summations into integrals, and using (5.20) we get

$$S(\omega,\omega')=-\frac{2L}{v_s^2}\omega^2\sqrt{T(\omega)}\delta(\omega-\omega')-\frac{1}{4\pi^2v_s^2}\frac{\omega(\omega+\omega')}{\omega'(\omega-\omega')^2}\sin^2[\delta_E(\omega)-\delta_O(\omega')] . \tag{5.39}$$

In (4.48) we will change the variables of integration and rewrite (4.47) as

$$\gamma(t)=\frac{\hbar\theta(t)}{2M_0}\int_0^{\omega_D}d\theta\int_{-\omega_D}^{\omega_D}d\Omega\, S\left[\theta+\frac{\Omega}{2},\theta-\frac{\Omega}{2}\right]\Omega\left[n\left[\theta+\frac{\Omega}{2}\right]-n\left[\theta-\frac{\Omega}{2}\right]\right]\cos(\Omega t) , \tag{5.40}$$

where

$$\Omega=\omega-\omega' ,$$

$$\theta=\frac{\omega+\omega'}{2} .$$

Observe that we have replaced the limit on the integration by the cutoff frequency, ω_D.

Actually we are interested in a time scale, τ, which is much longer than the typical phonon period or

$$\tau\gg\omega_D^{-1} .$$

With this approximation the cosine term in (5.40) oscillates rapidly, giving no contribution to the integration, except when Ω is close to zero. So we can approximate (5.40) as

$$\gamma(t)=\frac{\hbar\pi\delta(t)}{2m}\int_0^\infty d\theta f(\theta)\left[-\frac{dn}{d\theta}\right] , \tag{5.41}$$

where

$$f(\theta)=-\lim_{\epsilon\rightarrow0}\epsilon^2S\left[\theta+\frac{\epsilon}{2},\theta-\frac{\epsilon}{2}\right] . \tag{5.42}$$

Now, using (5.39) and noticing that the δ term does not contribute to (4.48), we get

$$f(\theta)=\frac{1}{4\pi^2v_s^2}\theta^2R(\theta) , \tag{5.43}$$

where we have used (5.25).

So, we conclude that we have here a Markovian process with the damping parameter given by

$$\bar{\gamma}(T)=\frac{\hbar^2}{8\pi M_O v_s^2K_BT}\int_0^\infty d\omega\,\omega^2R(\omega)\frac{e^{\hbar\omega/K_BT}}{(e^{\hbar\omega/K_BT}-1)^2} . \tag{5.44}$$

Defining a new variable

$$\omega=gv_s\kappa/2$$

and a typical phonon temperature, T_c, by

$$T_c=\frac{\hbar g v_s}{2K_B} ,$$

we can evaluate (5.44) which reads

$$\bar{\gamma}(T)=\frac{\hbar g^2}{32\pi M_0}I\left[\frac{T_c}{T}\right] , \tag{5.45}$$

where

$$I(S)=S\int_0^{\infty}d\kappa\kappa^2R(\kappa)\frac{e^{S\kappa}}{(e^{S\kappa}-1)^2} \quad (5.46)$$

is exactly the result obtained by Schüttler and Holstein[2] for the polaron mobility using the kinetic theory.

For small temperatures, $T \ll T_c$, we shall use the long-wavelength reflectivity [see (5.30)] since it gives the largest contribution to the occupation number

$$R(\kappa)\simeq\tfrac{9}{4}\kappa^2 . \quad (5.47)$$

Then, using (5.46) and (5.47) we can approximate (5.43) by

$$\bar{\gamma}(T)=\frac{27\hbar g^2}{16\pi M_0}\left[\frac{T}{T_c}\right]^4 . \quad (5.48)$$

This result shows that the acoustical polaron, as the optical one, behaves as a free particle as $T\rightarrow 0$.

For high temperatures, $T \gg T_c$, we use the expression for short wavelengths [see (5.28)],

$$R(\kappa)\simeq 4\pi^4\kappa^6 e^{-2\pi\kappa} , \quad (5.49)$$

and one has

$$\bar{\gamma}(T)=\frac{315\hbar g^2}{64\pi^4 M_0}\left[\frac{T}{T_c}\right] , \quad (5.50)$$

which means that the mobility decreases for high temperatures. We can calculate the diffusion coefficient (4.49) in the same way and we get

$$\bar{D}(T)=\frac{\hbar g^2}{32\pi M_0}K_B T_c J(S) , \quad (5.51)$$

where

$$J(S)=\int_0^{\infty}d\kappa\frac{\kappa^2R(\kappa)}{e^{S_\kappa}-1} \quad (5.52)$$

and we have used the fact that the diffusion is a Markovian process.

For small temperatures, $T \ll T_c$, the diffusion coefficient is given by

$$\bar{D}(T)\simeq\frac{27g^2\hbar}{16\pi}K_B\frac{T^5}{T_c^4} \quad (5.53)$$

and the fluctuations decrease very fast as the temperature is lowered, exactly as in the optical case. So, the relation between relaxation and diffusion is the classical one for the Brownian motion:[15]

$$\frac{\bar{D}(T)}{\bar{\gamma}(T)}=M_0K_BT . \quad (5.54)$$

For high temperature, $T \gg T_c$,

$$\bar{D}(T)=\frac{315\hbar g^2}{16\pi^5}K_BT . \quad (5.55)$$

And, exactly as in the optical case, the fluctuations increase linearly with temperature, this is the classical result[15] which is expected to be valid in the high-temperature limit.

VI. CONCLUSIONS

In the foregoing sections we have shown that the semiclassical (mean-field) method enables us to visualize the polaron physics and allows us to treat the strong-coupling limit of an electron interacting with a lattice. The advantage of dealing with this method is the fact that, in terms of the coordinate and the modified phonons, we reduce the problem to a new model for treating quantum dissipation. In a sense, the nonlinear character of the electron-phonon interaction is somehow "hidden" in the solitonlike solution whose center is regarded as the polaron coordinate.

Eliminating the electron operators by perturbative techniques (that is, tracing over the electron coordinates) and using the well-known collective coordinate formalism, we get an effective Hamiltonian for the polaron in the presence of renormalized phonons. That Hamiltonian, in the approximation of small polaron velocity, is reduced to a very simple form which takes into account only processes which involve polaron-phonon collisions.

We developed a functional method to treat the Hamiltonian in the limit of the small polaron's velocity. Our method showed that the polaron moves as a Brownian particle which collides with the light particles of the environment. This method provided us with a tool for a systematic calculation of the damping parameter (and, as a consequence, the mobility) and the diffusion coefficient as function of the temperature. We have also shown that in the time scale of interest the motion is essentially Markovian, that is, it does not have memory.

An important comment about our work is that it is fully quantized and the "semi-classical" argument is only used as an artifact. Furthermore, it confirms some important results for the acoustical polaron obtained by Schüttler and Holstein[2] using kinetic transport theory.

ACKNOWLEDGMENTS

We are very grateful to Professor A. J. Leggett for a critical reading of the manuscript. One of us (A.H.C.N.) would like to acknowledge FAPESP (Fundacao de Amparo a Pesquisa do Estado de Sao Paulo) while A.O.C. kindly acknowledges the partial support of CNPq (Conselho Nacional de Desenvolvimento Cientifico e Tecnologico) and FAEP (Fundo de Apoio ao Ensino e Pesquisa da UNICAMP).

APPENDIX A

In this appendix we wish to calculate the first-order correction in energy due to a many-electron wave function in (2.42) and (2.47). In the case of many electrons the ground state is the Fermi sphere with radius k_F, which is given by

$$k_F=\frac{\pi}{2a}\left[\frac{N_e}{N}\right] , \quad (A1)$$

where N_e is the number of electrons and N the number of sites.

The nonperturbed Hamiltonian is

$$H_0=E_0a_0^\dagger a_0+\sum_{n=1}^{\infty}E_na_n^\dagger a_n \tag{A2}$$

with the ground-state wave function

$$|\psi^0\rangle=|n_k=1,k\le k_F;n_k=0,k>k_F\rangle \ . \tag{A3}$$

The ground-state energy is

$$E^0=\frac{N}{\hbar}\frac{\hbar^2}{ma^2}(k_Fa)^3-\frac{\hbar^2g^2}{4m} \ , \tag{A4}$$

where we have accounted for the spin degeneracy.

The first-order correction is given from the interaction term in (2.42) or (2.47),

$$E^{(1)}=\langle\psi_0|H_I|\psi_0\rangle \ .$$

For the optical case it reads

$$E^{(1)}=\frac{D}{a}\sum_{qk}f_{qq}(k)\theta(k_F-|q|)q_k$$

or

$$E^{(1)}=\sum_k\frac{\Delta(k)}{a}q_k \ , \tag{A5}$$

where

$$\Delta(k)=\frac{D}{\pi\sqrt{N}}\left\{k_F\delta(k)-\frac{2\pi}{g}\arctan\left[\frac{2k_F}{g}\right]|k|\text{csch}\left[\frac{2|k|}{g}\right]\right\} . \tag{A6}$$

For the acoustical case,

$$E^{(1)}=i\sum_k k\Delta(k)q_k \ . \tag{A7}$$

So, at first order the ions are displaced from their equilibrium positions by

$$\frac{\Delta(-k)}{Ma\omega_0^2}$$

in the optical case and

$$\frac{ik\Delta(-k)}{M\omega_k^2}$$

in the acoustical case. This causes a change in the energy given by

$$\Delta E=-\sum_k\frac{\Delta(k)\Delta(-k)}{2a^2M\omega_0^2}$$

for the optical case, and

$$\Delta E=-\sum_k\frac{\Delta(k)\Delta(-k)}{2Mv_s^2}$$

for the acoustical case.

APPENDIX B

Let us first show how to obtain the zero-mode solution for the optical case. Making $\Omega_0=0$ in (3.3) we get

$$u_0(x)=\int dx'F(x,x')u_0(x') \ . \tag{B1}$$

Define a function $g(x,x')$

$$g(x,x')=\sum_{n=0}^{\infty}\frac{\phi_n^{*F}(x)\phi_n^F(x')}{(k_n^2+g^2/4)} \ . \tag{B2}$$

Then, from (2.31),

$$\left[-\frac{\partial^2}{\partial x^2}-\frac{g^2}{2}\text{sech}^2\left[\frac{gx}{2}\right]+\frac{g^2}{4}\right]g(x,x')=-\frac{g}{4}\text{sech}\left[\frac{gx}{2}\right]\text{sech}\left[\frac{gx'}{2}\right]+\delta(x,x') \ , \tag{B3}$$

where we have used the completeness of the adiabatic states

$$\phi_0(x)\phi_0(x')+\sum_{n=0}^{\infty}\phi_n^{F*}(x)\phi_n^F(x')=\delta(x,x') \tag{B4}$$

and the explicit form for $\phi_0(x)$.

Let us rewrite (1) as

$$u_0(x)=g^2\text{sech}\left[\frac{gx}{2}\right]f(x) \ , \tag{B5}$$

where

$$f(x)=\int dx'g(x,x')\text{sech}\left[\frac{gx'}{2}\right]u_0(x') \ . \tag{B6}$$

Then, from (3),

$$\left\{\frac{d^2}{dx^2}+\frac{g^2}{4}\left[2\text{sech}^2\left[\frac{gx}{2}\right]-1\right]\right\}f(x)=\text{sech}\left[\frac{gx}{2}\right]\left[-u_0(x)+\frac{g}{4}\int dx'\text{sech}^2\left[\frac{gx'}{2}\right]u_0(x')\right] \ . \tag{B7}$$

The last term in (B7) must vanish because $u_O(x)$ is odd. Using (B5) we get

$$\left\{\frac{d^2}{dx^2}+\frac{g^2}{4}\left[6\text{sech}^2\left[\frac{gx}{2}\right]-1\right]\right\}f(x)=0 \ . \tag{B8}$$

The solution is easily obtained[5] and reads

$$f(x)=\text{sech}\left[\frac{gx}{2}\right]\tanh\left[\frac{gx}{2}\right] \ . \tag{B9}$$

Substituting (B9) and (B5) and normalizing it, we get

$$u_0(x)=\sqrt{15ag/2}\tanh\left[\frac{gx}{2}\right]\mathrm{sech}^2\left[\frac{gx}{2}\right] . \qquad (B10)$$

For the acoustical case we must use (3.4) with $\Omega_0=0$, which reads

$$\frac{d^2u_0}{dx^2}=\frac{d}{dx}\int dx'F(x,x')\frac{du_0}{dx'}(x') . \qquad (B11)$$

Now, using (B2) we should define

$$h(x)=\int dx'g(x,x')\mathrm{sech}\left[\frac{gx'}{2}\right]\frac{du_0}{dx'}(x') \qquad (B12)$$

and rewrite (B11) as

$$\frac{d^2u_0}{dx^2}=g^2\frac{d}{dx}\left\{\mathrm{sech}\left[\frac{gx}{2}\right]h(x)\right\} .$$

This can be easily integrated yielding

$$u_0(x)=g^2\int_{-\infty}^{x}dx'\mathrm{sech}\left[\frac{gx'}{2}\right]h(x') , \qquad (B13)$$

where

$$u_0(-\infty)=0 .$$

Observe that $h(x)$ also obeys Eq. (8), so

$$h(x)=\tanh\left[\frac{gx}{2}\right]\mathrm{sech}\left[\frac{gx}{2}\right] . \qquad (B14)$$

Substituting (B14) in (B13) we get, after normalization,

$$u_0(x)=\sqrt{3ag/8}\,\mathrm{sech}^2\left[\frac{gx}{2}\right] . \qquad (B15)$$

APPENDIX C

We shall evaluate here the functional form for the superpropagator, J. From (3.26) we see that the Hamiltonian can be put in the form

$$H=H_S+H_R+H_I , \qquad (C1)$$

where

$$H_S=P^2/2M_0 , \qquad (C2)$$

$$H_R=\sum_{n=1}^{\infty}\hbar\Omega_n b_n^\dagger b_n+\left[\sum_{n,m=1}^{\infty}\hbar g_{nm}b_m^\dagger b_n\right]^2\Big/2M_0 , \qquad (C3)$$

$$H_I=-P\sum_{n,m=1}^{\infty}\hbar g_{nm}b_m^\dagger b_n/M_0 . \qquad (C4)$$

From (4.6) we get

$$\langle x|\hat{\rho}_s(t)|y\rangle=\int\cdots\int\left[\prod_{k=1}^{N}\frac{d^2\alpha_k}{\pi^N}\right]\langle x\boldsymbol{\alpha}|\hat{\rho}(t)|y\boldsymbol{\alpha}\rangle$$

or using the completeness relations (4.10) and (4.11) we can, with the help of (4.2), write

$$\rho_s(x,y,t)=\int dx'\int dy'\rho_s(x',y',0)J(x,y,t;x',y',0) , \qquad (C5)$$

where

$$J=\int\frac{d^2\boldsymbol{\alpha}}{\pi^N}\int\frac{d^2\boldsymbol{\beta}}{\pi^N}\int\frac{d^2\boldsymbol{\beta}'}{\pi^N}\rho_R(\boldsymbol{\beta}^*,\boldsymbol{\beta}',0)K(x\boldsymbol{\alpha}^*x'\boldsymbol{\beta},t)\times K^*(y\boldsymbol{\alpha}y'\boldsymbol{\beta}'^*t) \qquad (C6)$$

with

$$K(x\boldsymbol{\alpha}^*x'\boldsymbol{\beta}t)=\langle x\boldsymbol{\alpha}|e^{-i\hat{H}t/\hbar}|x'\boldsymbol{\beta}\rangle . \qquad (C7)$$

In order to transform (C7) into a functional integral we must divide t in $(M-1)$ subintervals of length ϵ and use $(M-1)$ completeness relations between the $(M-1)$ exponentials in (C7). Then

$$\langle x\boldsymbol{\alpha}|e^{-i\hat{H}t/\hbar}|x'\boldsymbol{\beta}\rangle=\int dq_{N-1}\cdots\int dq_1\int\frac{d^2\boldsymbol{\alpha}_{N-1}}{\pi^N}\cdots\int\frac{d^2\boldsymbol{\alpha}_1}{\pi^N}\langle q_M\boldsymbol{\alpha}_M|e^{i\hat{H}\epsilon/\hbar}|q_{M-1}\boldsymbol{\alpha}_{M-1}\rangle\cdots\langle q_1\boldsymbol{\alpha}_1|e^{-i\hat{H}\epsilon/\hbar}|q_0\boldsymbol{\beta}_0\rangle , \qquad (C8)$$

where

$$q_M=x,\quad \boldsymbol{\alpha}_M^*=\boldsymbol{\alpha}^*,\quad q_0=x',\quad \boldsymbol{\alpha}_0=\boldsymbol{\beta} . \qquad (C9)$$

Now insert M completeness relations in the momentum representation

$$\int dp\,|p\rangle\langle p|=1$$

in (C8) in order to obtain

$$K=\prod_{k=1}^{M-1}\left\{\int dq_k\frac{d^2\boldsymbol{\alpha}_k}{\pi}\right\}\prod_{k=1}^{M}\left\{\int dP_k\right\}\langle q_N\boldsymbol{\alpha}_N|e^{-iH\epsilon/\hbar}|P_N\boldsymbol{\alpha}_{N-1}\rangle\langle P_N|q_{N-1}\rangle\cdots\langle q_1\boldsymbol{\alpha}_1|e^{-iH\epsilon/\hbar}|P_1\boldsymbol{\alpha}_0\rangle\langle P_1|q_0\rangle . \qquad (C10)$$

Now we will take the limit that $M\to\infty$, $\epsilon\to 0$ but with $t=(M-1)\epsilon$ being finite.

For small ϵ we should expand the exponential in (C10) to first order in ϵ and write

$$\langle q_k \alpha_k | e^{-iH\epsilon/\hbar} | P_k \alpha_{k-1} \rangle \simeq \langle q_k | P_k \rangle \langle \alpha_k | \alpha_{k-1} \rangle \exp\left\{ -\frac{i}{\hbar} \epsilon H(q_k, P_k, \alpha_k^*, \alpha_{k-1}) \right\} , \tag{C11}$$

where

$$H(q_k P_k \alpha_k^* \alpha_{k-1}) = \frac{\langle q_k \alpha_k | \hat{H} | P_k \alpha_{k-1} \rangle}{\langle \alpha | \alpha_{k-1} \rangle} . \tag{C12}$$

Using the overlapping relations

$$\langle \alpha | \beta \rangle = \exp\left\{ \alpha^* \cdot \beta - \frac{|\alpha|^2}{2} - \frac{|\beta|^2}{2} \right\}, \quad \langle P | q \rangle = \frac{1}{2\pi\hbar} \exp\left\{ -\frac{i}{\hbar} Pq \right\} ,$$

one obtains

$$K = \int \frac{dP_M}{2\pi\hbar} \prod_{k=1}^{M-1} \left\{ \int \frac{dq_k dP_k}{2\pi\hbar} \frac{d^2\alpha_k}{\pi^N} \right\} \exp\left\{ \sum_{k=1}^{M} \tfrac{1}{2} [\alpha_{k-1}(\alpha_k^* - \alpha_{k-1}^*) - \alpha_k^*(\alpha_k - \alpha_{k-1})] + \frac{i}{\hbar} [P_k(q_k - q_{k-1}) - \epsilon H(P_k q_k \alpha_k^* \alpha_{k-1})] \right\} . \tag{C13}$$

Now one has to integrate over P_k. So, using (C1) we must evaluate

$$\int \frac{dP_k}{2\pi\hbar} \exp\left\{ -\frac{i\epsilon}{\hbar} \left[\frac{P_k^2}{2M_0} - P_k \left[h + \frac{(q_k - q_{k-1})}{\epsilon} \right] \right] \right\} , \tag{C14}$$

where

$$h = \sum_{n,m=1}^{\infty} \frac{\hbar}{M_0} g_{nm} \alpha_n^* \alpha_m . \tag{C15}$$

This allows one to rewrite (14) in the standard form[17]

$$\left[\frac{M_0}{2\pi i \hbar \epsilon} \right]^{1/2} \exp\left\{ \frac{iM_0 \epsilon}{2\hbar} \left[h + \frac{(q_k - q_{k-1})}{\epsilon} \right]^2 \right\} . \tag{C16}$$

Now, substituting (C16) in (C13) and taking the limit of $M \to \infty$ and $\epsilon \to 0$, we get[11]

$$K = \int_{x'}^{x} Dq \int_{\beta}^{\alpha^*} D^2\alpha e^{-\frac{|\alpha|^2}{2} - \frac{|\beta|^2}{2}} \exp\{S[q,\alpha]\} , \tag{C17}$$

where

$$Dq = \lim_{M \to \infty, \epsilon \to 0} \left\{ \left[\frac{M_0}{2\pi i \hbar \epsilon} \right]^{M/2} \prod_{k=1}^{M-1} dq_k \right\} , \tag{C18}$$

$$D^2\alpha = \lim_{M \to \infty} \prod_{k=1}^{M-1} \left[\frac{d^2\alpha_k}{\pi^N} \right] , \tag{C19}$$

with

$$S = \int_0^t dt' \left\{ \frac{iM_0}{\hbar 2} [\dot{q} + h(\alpha^*, \alpha)]^2 + \frac{1}{2}(\alpha\dot{\alpha}^* - \alpha^*\dot{\alpha}) - \frac{i}{\hbar} H_R(\alpha^*, \alpha) \right\} . \tag{C20}$$

Finally, using (C3) and (C15) one reaches

$$S = \int_0^t dt' \left\{ \frac{1}{2}(\alpha\dot{\alpha}^* - \alpha^*\dot{\alpha}) + \frac{i}{\hbar} \left[\frac{M_0 \dot{q}^2}{2} + M_0 \dot{q} h \right] - i \sum_{n,m=1}^{\infty} \Omega_n \alpha_n^* \alpha_n \right\} . \tag{C21}$$

Now, substituting (C21) in (C17) and (C16) we get the result (4.12).

[1] A. S. Davidov, Phys. Rep. **190**, 191 (1990), and references therein.
[2] H. B. Schüttler and T. Holstein, Ann. Phys. (NY) **166**, 93 (1986).
[3] H. Fröhlich, Proc. R. Soc. **223**, 296 (1954).
[4] C. Kittel, *Quantum Theory of Solids* (Wiley, New York, 1963).
[5] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953).
[6] P. B. Shaw and E. W. Young, Phys. Rev. B **24**, 714 (1981).
[7] T. Holstein, Mol. Cryst. Liq. Cryst. **77**, 235 (1981).
[8] T. D. Holstein and L. A. Turkevich, Phys. Rev. B **38**, 1901 (1988).
[9] L. A. Turkevich and T. D. Holstein, Phys. Rev. B **35**, 7474 (1987).
[10] R. Rajaraman, *Solitons and Instantons: An Introduction to Solitons and Instantons in Quantum Field Theory* (North-Holland, Amsterdam, 1982).
[11] R. P. Feynman and F. L. Vernon, Ann. Phys. (NY) **24**, 118 (1963).
[12] A. H. Castro Neto and A. O. Caldeira, Phys. Rev. Lett. **67**,

1960 (1991).
[13]A. H. Castro Neto and A. O. Caldeira, Phys. Rev. A **42**, 6884 (1990).
[14]A. O. Caldeira and A. J. Leggett, Physica A **121**, 587 (1983).
[15]R. Kubo, Rep. Prog. Phys. **XXIX**, 253 (1966).
[16]H. J. Lipkin, *Quantum Mechanics: New Approaches to Selected Topics* (North-Holland, Amsterdam, 1973).
[17]R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).