The effective mass of a quantum polaron

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The dynamics of the quantum polaron (QP) is studies at zero temperature. The photon variables are excluded and the Green's function is obtained. The effective mass for both large adiabatic QP and small nonadiabatic QP is calculated. In the first case the principal contribution to the mass comes from the thin "crust layer" on a polaron surface.

In our recent work[1] a new type of a self-trapped particle—quantum polaron (QP)—was proposed. In contrast with the usual polaron, QP is not accompanied by a lattice displacement. The origin of self-trapping is the local suppression of the quantum fluctuations. Either large adiabatic QP or small antiadiabatic QP can arise, depending on the parameters of the system. The quantum polaron can be realized in the systems, where the quadratic electron–phonon interaction of the sign corresponding to the phonon stiffening dominates and the linear interaction is suppressed, for example, due to the symmetry restrictions. The most interesting candidates for QP are, in our opinion, the charge carriers in La_2CuO_4 coupled to the soft orthorhombic modes,[2] and the electrons which interact with the rotational modes in molecular crystals.[3]

The structure of QP and the conditions for its existence were formulated in Ref. 1. However, a very important question about the spectrum and dynamics of such a polaron remained open. In this paper we will solve this problem by using the methods of integration over the lattice degrees of freedom. We will study the generalized model, in which both linear and quadratic couplings are present. It should be stressed that we restrict the analysis to the $T = 0$ case. It is known[4] that the quadratic coupling gives rise to unusual T-dependences even for the perturbative effects.

We will start with the most interesting and complicated case of the continual adiabatic polaron. The Lagrangian density of the system in the "mixed" representation[5] can then be written in the form

$$L = i\psi^* \partial_t \psi + \frac{1}{2} M(\partial_t Q)^2 - \frac{1}{2} t_e |\nabla \psi|^2 - \frac{1}{2} M \omega_0^2 Q^2 - \rho(\Gamma Q + \frac{1}{2}\gamma Q^2), \quad (1)$$

where $\psi = \psi(rt)$ is the electron wave function, $\rho = |\psi|^2$ is the electron density, $t_e = 1/m_e a_0^2$, m_e is the electron mass, a_0 is the lattice spacing, $Q = Q(rt)$ is a lattice displacement, $M = M_{at} a_0^2$, M_{at} is the atomic mass, ω_0 is the phonon frequency, Γ and γ are the constants of linear and quadratic electron–phonon coupling, respectively ($\gamma > 0$). All the distances are measured in the units of a_0, so r, Q, *and* ψ are the dimensionless variables. Everywhere $\hbar = 1$, so t_e, ω_0, Γ, γ, and M^{-1} have the dimension of energy. For simplicity we consider only the dispersionless phonons and the local interaction.

After the integration over the phonon variables the electron Green's function

takes a form

$$G(\vec{r}_2 t_2, \vec{r}_1 t_1) = \int D\psi^* D\psi\, \psi(\vec{r}_2 t_2)\psi^*(\vec{r}_1 t_1) \exp\{i \int d\vec{r}dt(i\psi^* \partial_t \psi - \frac{1}{2} t_e |\nabla\psi|^2)\}$$

$$\times \prod_r dQ_2 dQ_1 \chi^*_{\omega_0}(Q_2)\chi_{\omega_0}(Q_1) g[Q_2 t_2, Q_1 t_1 | \psi(\vec{r}t)], \qquad (2)$$

where $\chi_\omega(Q)$ is a ground state wave function of an oscillator with a frequency ω and the electron–phonon coupling is assumed to be adiabatically turned off at t_1 and t_2 ($t_1 \to -\infty, t_2 \to +\infty$). Note that for our single-particle problem the operator $i\partial_t$ must be determined in such a way that all the diagrams containing the electronic loops vanish.[5] In Eq. (2), g is a Green's function of an oscillator at the site $\vec{r}$ with a time-dependent frequency $\omega(\vec{r}t)$ in the presence of an external force $f(\vec{r}t)$:

$$\omega^2 = \omega_0^2 + \Omega^2 \rho(\vec{r}t), \quad f = \Gamma\rho(\vec{r}t), \quad \Omega^2 = \gamma/M. \qquad (3)$$

The problem of such an oscillator is exactly semiclassical[6] and its Green's function can be expressed in terms of a corresponding classical solution.[7] The general expression is rather cumbersome, but in this work we are interested only in the leading adiabatic approximation and in the first nonvanishing corrections to it. Then the problem is simplified and the electron Green's function can be expressed in terms of an effective Lagrangian:

$$L_{\text{eff}} = L_{\text{kin}} - U, \quad L_{\text{kin}} = i\psi^* \partial_t \psi + \frac{1}{16} \frac{[\partial_t \omega(\rho)]^2}{\omega^3(\rho)} + \frac{M}{2}[\partial_t Q(\rho)]^2, \qquad (4)$$

$$U = \frac{1}{2} t_e |\nabla\psi|^2 + \frac{1}{2}\omega(\rho) - \frac{1}{2} M\omega^2(\rho) Q^2(\rho),$$

where $Q(\rho) = \Gamma\rho/M\omega^2(\rho)$ is the shift of the oscillator's equilibrium position due to the force f. The last two terms in L_{kin} are the nonadiabatic corrections; these terms determine the polaron's mass M_{eff}. For the calculation of M_{eff} we insert $\psi = e^{-iE_0 t}\psi_0(\vec{r} - \vec{v}t)$, which corresponds to a polaron moving with a velocity $\vec{v}$, into Eqs. (3) and (4). Expanding the result in $\vec{v}$ and identifying the coefficient at v^2_{eff} with $M_{\text{eff}}/2$, we obtain

$$M_{\text{eff}} = m_e + \frac{1}{8} \int d\vec{r}(\partial_x \omega)^2/\omega^3 + M \int d\vec{r}(\partial_x Q)^2. \qquad (5)$$

Here ψ_0 is the normalized wave function of a stationary problem. It corresponds to the minimum of the energy functional $J[\psi] = \int d\vec{r}U$ [see Eq. (4)]. In the limit $\gamma = 0$ the functional J is transformed to a well-known form for a linear coupling polaron,[8] and in the limit $\Gamma = 0$ the result of Ref. 1 for QP is reproduced. Accordingly, the third term in Eq. (5) is analogous to the usual form of a linear-coupling polaron mass,[8] and the second term is a purely quantum contribution. Note that the absence of a collapse for a three-dimensional QP (see Ref. 1) is preserved even in the presence of linear coupling: the quadratic coupling suppresses the collapse for $\gamma > 0$.

All of the above considerations apply only to the large adiabatic polaron, which is realized (see Ref. 1) when the following conditions are satisfied:

$$t_e \gg \Omega \gg \omega_0;\ (\Omega/\omega_0)(\omega/t_e)^{D/(D+4)} \gg 1, \tag{6}$$

where D is the dimension of space.

It can be shown that for $(\Gamma^2\omega_0^2/M\Omega^5)(t_e/\Omega)^{D/(D+4)} \ll 1$ a linear coupling may be treated as a perturbation. The above ψ_0 will then nearly coincide with the ψ_0 of QP, obtained in Ref. 1 (see Fig. 1). In the crude approximation (totally ignoring ω_0) we have

$$\psi_0(\vec{r}) \simeq \psi_{\text{crude}}(\vec{r}) = \vartheta(a - |\vec{r}|)(\phi_0(\vec{r}) + c). \tag{7}$$

Here ϕ_0 is a spherically symmetric wave function of a free electron, and the constant c is determined by the requirement of the $\psi_0(\vec{r})$ smoothness at the polaron surface ($|\vec{r}| = a$). The correction to J due to the linear coupling is $\Delta J = -\Gamma^2/2\gamma$, and the corresponding $Q_0(\vec{r}) \simeq Q_{\text{crude}}(\vec{r}) = (\Gamma/\gamma)\vartheta(a - |\vec{r}|)$.

A polaron therefore consists roughly of a "core" of radius a and an "outer space" ($|\vec{r}| > a$), where $\psi_0 \equiv 0$ and the oscillators are free. However, in a more accurate approach, there is a thin intermediate layer—a "crust" ($||\vec{r}| - a| \lesssim \Delta a$), where the two terms in Eq. (3) for ω^2 are of the same order of magnitude and the true ψ_0 differs from ψ_{crude}. The crust thickness is

$$\Delta a \simeq (\omega_0 t_e)^{1/2}/\Omega \ll a \simeq (t_e/\Omega)^{2/(D+4)}. \tag{8}$$

In deriving Eq. (8) we have assumed for simplicity that a linear coupling is negligible both in the core and in the crust. It needs a somewhat stronger restriction on Γ: $\Gamma^2\omega_0/M\Omega^4 \ll 1$.

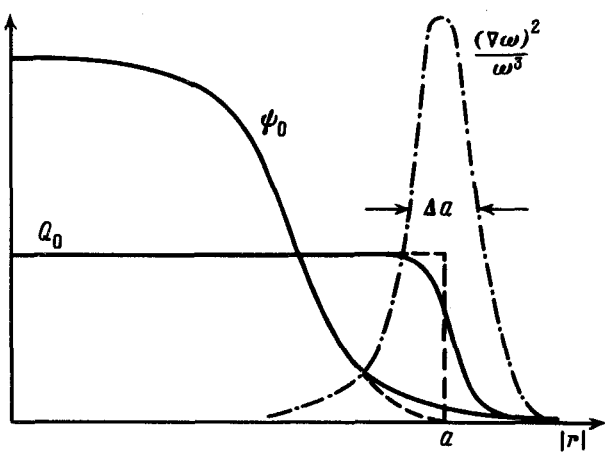

FIG. 1. The shape of a wave function ψ_0 and a lattice displacement Q_0 for large adiabatic QP (ψ_{crude} and Q_{crude} are shown by the broken lines). The surface $|\vec{r}| = a$ is a polaron's "core" boundary; Δa is a thickness of a polaron's "crust." An integrand in Eq. (5) for M_{eff} is represented by a dot-dashed line.

If the crust is ignored and M_{eff} is calculated by inserting ψ_{crude} into Eq. (5), then the result would diverge in the limit $|\vec{r}| \to a$, since $\psi_{\text{crude}}(\vec{r}) \simeq (\Omega/t_e)(|\vec{r}| - a)^2$ at $0 < a - |\vec{r}| \ll a$. This means that the main contribution to M_{eff} comes only from the crust, and that M_{eff} depends on ω_0. Simple estimates give

$$\frac{M_{\text{eff}}}{m_e} = c_1 \left(\frac{\Omega}{\omega_0}\right)^{3/2} \left(\frac{t_e}{\Omega}\right)^{5D/(2D+8)} + c_2 \frac{\Gamma^2}{M\Omega^3} \left(\frac{\Omega}{\omega_0}\right)^{1/2} \left(\frac{t_e}{\Omega}\right)^{5D/(2D+8)}, \quad (9)$$

where c_1 and c_2 are on the order of unity. The first term is due exclusively to the quadratic coupling and exists at $\Gamma = 0$. The second term is a small correction due to the linear coupling. Note that $M_{\text{eff}} \gg m_e$ in the entire domain of adiabatic polaron existence.

The principal role of the crust in the effective mass poses a nontrivial question about the adiabacity of the system's wave function within the crust. The adiabacity fails sooner or later if one goes outside the polaron center. It can be shown, however, that within the crust the adiabacity is preserved as long as $\Delta a \gg 1$, i.e., $(\omega_0 t_e)^{1/2}/\Omega \gg 1$ (Fig. 2). This means that unless the crust is macroscopically thick (thicker than the lattice spacing), the adiabatic approximation is inapplicable for the calculation of M_{eff}.

Let us now consider the case of a small antiadiabatic polaron which is realized for $\omega_0 \ll t_e \ll \Omega$. If t_e is small enough, then the electron is expected to be localized at a single lattice site, while the neighboring oscillators are not disturbed. Then, to find the polaron bandwidth, one must calculate the matrix element of the kinetic energy between the two degenerate states which are centered at the neighboring sites:

$$t_{eff} = (M_{\text{eff}} a_0^2)^{-1} = t_e | < \chi_{\omega_0} | \chi_{(\omega_0^2+\Omega_0^2)^{1/2}} > |^2 \sim t_e(\omega_0/\Omega)^{1/2}. \quad (10)$$

Accordingly, M_{eff}/m_e for small QP is large due to the mismatch of the oscillator frequencies which correspond to the occupied state (Ω) and to the empty state (ω_0).

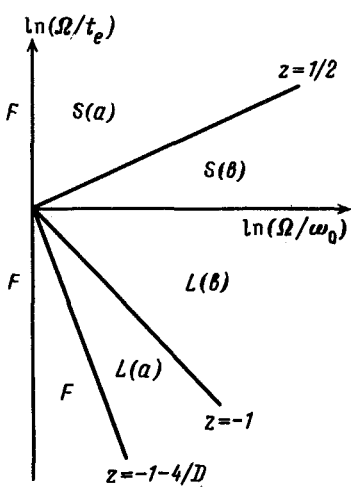

FIG. 2. An analysis of the model Eq. (1). z is the tangent of the corresponding slope of the curve. The domain F—a free electron ($M_{\text{eff}} = m_e$); The domain L—large adiabatic QP; in the region $L(a)$ an adiabatic approximation is valid for the calculation of M_{eff}. The domain S—small QP; in the region $S(a)$ for the calculation of M_{eff} the electron's kinetic energy can be treated as a perturbation. In the regions $L(b)$ and $S(b)$ we did not obtain M_{eff}. It requires information about the fine details of a wave function in the polaron's tail.

Note that the effect of quadratic coupling on the transition amplitudes of the molecular excitons was discussed in Ref. 9.

It can be shown that the above calculation is correct only for $t_e^2/\omega_0\Omega \ll 1$, i.e., it fails if ω_0 is too small. Although at $t_e \ll \Omega$ the electron visits the neighboring sites very rarely, it still could disturb the states of the oscillator if they are soft enough.

In summary, we were able to find M_{eff} for a large adiabatic QP and a small antiadiabatic QP, for not too small ω_0 (Fig. 2). Such a restriction on ω_0 does not appear if one is interested only in the static characteristics of QP (polaronic shift, etc.), which are determined by the core. In contrast, M_{eff} is governed by "exotic" parts of a polaron, where the system's wave function cannot be factorized, and where all the known methods fail.

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[1]A. O. Gogolin and A. S. Ioselevich, Pis'ma Zh. Eksp. Teor. Fiz. **53**, 456 (1991).
[2]T. R. Thurston *et al.*, Phys. Rev. B **39**, 4327 (1989).
[3]H. Gutfreund and M. Weger, Phys. Rev. B **16**, 1753 (1977).
[4]Yu. Kagan and N. V. Prokofiev, Zh. Eksp. Teor. Fiz. **96**, 2209 (1989) [Sov. Phys. JETP. **69**, 1250 (1989)].
[5]A. S. Ioselevich, Zh. Eksp. Teor. Fiz., **81**, 1508 (1981) [Sov. Phys. JETP **54**, 800 (1981)]; A. G. Aronov and A. S. Ioselevich, Pis'ma Zh. Eksp. Teor. Fiz. **41**, 71 (1985) [JETP Lett. **41**, 84, (1985)].
[6]R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw Hill, N.Y.), 1965.
[7]A. I. Baz', Ya. B. Zeldovich, and A. M. Perelomov, *Scattering, Reactions and Decays in Nonrelativistic Quantum Mechanics* (Nauka, Moscow), 1971.
[8]S. I. Pekar, *Untersuchungen über die Elektronentheorie-Kristalle* (Akademie-Verlag, Berlin), 1954.
[9]V. L. Broude, E. I. Rashba, and E. F. Sheka, *Spectroscopy of Molecular Excitons* (Springer, Berlin, Heidelberg), 1985.