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# THE EFFECTIVE MASS OF A QUANTUM POPARON

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The dynamics of the Quantum Polaron (QP) is studied at zero temperature. The phonon variables are excluded and the Green function is obtained. An 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. On the contrary to the usual polaron, QP is not accompanied by any lattice displacement. The origin of self-trapping is the local suppression of the quantum fluctuations. Either adiabatic large QP or antiadiabatic small QP can arise depending on the parameters of the system. QP can be realized in the systems, where the quadratic electron-phonon interaction of the sign, corresponding to the phonons 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, interacting with the rotational modes in molecular crystals [3].

The structure of QP and the conditions for it's existence were formulated in [1]. However, a very important question about the spectrum and dynamics of such a polaron remained open. In this paper we are solving this problem using the methods of the integration over the lattice degrees of freedom. We are studying the generalized model, in which both linear and quadratic couplings are present. It should be stressed that we are confining ourselves 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 from the most interesting and complicated case of the continual adiabatic polaron. Then the Lagrangian density of the system in the "mixed" representation [5] has a form:

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

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 and $a_0$ is the lattice spacing; $Q = Q(rt)$ is a lattice displacement, $M = M_{at}a_0^2$, $M_{at}$ is an atom's mass, $\omega_0$ is the phonon frequency; $\Gamma$ and $\gamma$ 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 $\psi$ are the dimensionless variables. Everywhere $\hbar = 1$, so $t_e$, $\omega_0$, $\Gamma$, $\gamma$ and $M^{-1}$ have the dimension of energy. For the sake of simplicity we consider only the dispersionless phonons and local interaction.

After the integration over the phonon variables the electron Green function takes a form:

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

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

where $\chi_\omega(Q)$ is a ground state wave-function of an oscillator with a frequency $\omega$ and the electron-phonon interaction 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 function of an oscillator at site $\vec{r}$ with a time-dependent frequency $\omega(\vec{r}t)$ in the presence of an external force $f(\vec{r}t)$:

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

The problem of such an oscillator is exactly semiclassical [6] and its Green 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's Green function can be expressed in terms of an effective Lagrangian:

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

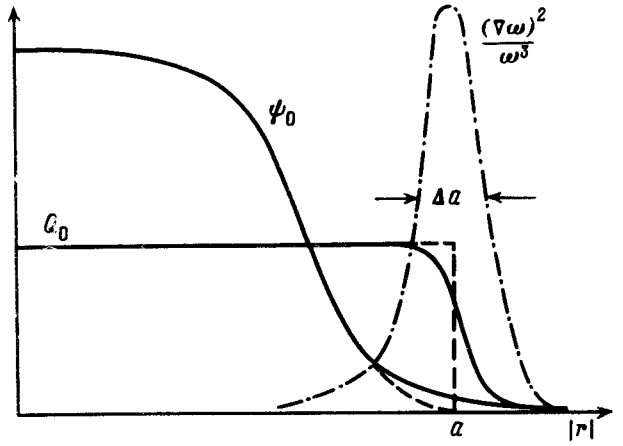
$$U = \frac{1}{2} t_e |\nabla\psi|^2 + \frac{1}{2}\omega(\rho) - \frac{1}{2} M\omega^2(\rho) Q^2(\rho), \qquad (4)$$

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

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

Here $\psi_0$ is the normalized wave-function of a stationary polaron. 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 $\gamma > 0$.




Fif.1

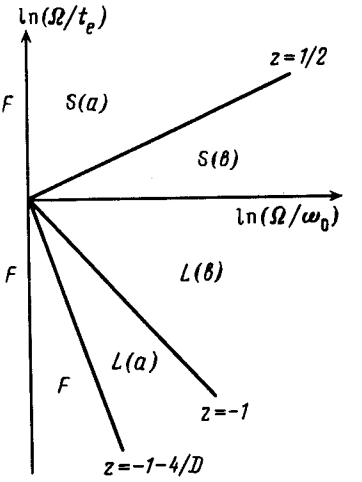



Fig.2

Fig.1. The shape of a wave-function $\psi_0$ and a lattice displacement $Q_0$ for large adiabatic $QP$ ($\psi_{rough}$ and $Q_{rough}$ are shown with broken lines). The surface $|\vec{r}| = a$ is a polaron's "core" boundary; $\Delta a$ is a thickness of a polaron's "crust". An integrand in Eq(5) for $M_{eff}$ is shown with a dash-dot line.

Fig.2. An analysis of the model Eq(1). $z$ is the tangent of a corresponding line's slope. The domain $F$ - a free electron ($M_{eff} = m_e$); The domain $L$ - large adiabatic QP; in the region $L(a)$ an adiabatic approximation is valid also 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 succeed in obtaining $M_{eff}$. It requires an information about subtle details of a wave-function in the polaron's tail.

All the above considerations make sense only for the adiabatic large polaron, which is realized (see Ref. [1]) under the conditions:

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

where $D$ is the space dimension.

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. Then the above $\psi_0$ almost coincide with $\psi_0$ of QP, obtained in Ref. [1] (see Fig.1). In the rough approximation (totally neglecting $\omega_0$) we have:

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

Here $\phi_0$ is a spherically symmetric wave-function of a free electron and a constant $c$ is determined by a 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 $Q_0(\vec{r}) \simeq Q_{rough}(\vec{r}) = (\Gamma/\gamma)\vartheta(a - |\vec{r}|)$.

So, a polaron 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 some thin intermediate layer - "a crust" ($||\vec{r}| - a| \lesssim \Delta a$) where the two terms in Eq(3) for $\omega^2$ are of the same order and the true $\psi_0$ differs from $\psi_{rough}$. The crust thickness is

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

When deriving Eq(8) we have supposed for simplicity that a linear coupling is negligible not only in the core, but also within the crust. It needs a somewhat stronger restriction on $\Gamma$: $\Gamma^2\omega_0/M\Omega^4 \ll 1$.

If to ignore the crust and calculate $M_{eff}$ inserting $\psi_{rough}$ into Eq(5) then the result would diverge at $|\vec{r}| \to a$ since $\psi_{rough}(\vec{r}) \simeq (\Omega/t_e)(|\vec{r}| - a)^2$ at $0 < a - |\vec{r}| \ll a$. It means that the main contribution to $M_{eff}$ comes just from the crust and $M_{eff}$ is $\omega_0$-dependent. The simple estimates give:

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

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

The principal role of the crust in the effective mass poses a nontrivial question about the adiabacity of a system's wave-function within the crust. Of cause the adiabacity fails sooner or later if one goes outwards the polaron center. However, it can be shown that within the crust the adiabacity is still preserved as long as $\Delta a \gg 1$, i.e., $(\omega_0 t_e)^{1/2}/\Omega \gg 1$ (See Fig.2). It 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 s switch now to 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 on a single lattice site, while the neighboring oscillators are not disturbed. Then to find a polaron bandwidth one has to calculate a matrix element of a kinetic energy between the two degenerate states, centered at the neighboring sites:

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

So $M_{eff}/m_e$ for small QP is large due to the mismatch of the oscillator frequencies corresponding to an occupied state ($\Omega$) and to an empty one ($\omega_0$). Note, that the influence of quadratic coupling on the transition amplitudes for 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 $\omega_0$ is too small. Indeed, although at $t_e \ll \Omega$ the electron visits the neighboring sites very rarely, it still may disturb the oscillators' states if they are soft enough.

So we were able to find $M_{eff}$ for both large adiabatic QP and small antiadiabatic one, but for not too small $\omega_0$ (Fig.2). Such a restriction on $\omega_0$ does not appear if one is interested only in the static characteristics of QP (polaronic shift etc.), which are determined by the core. On the contrary, $M_{eff}$ is governed by "exotic" parts of a polaron, where the system's wave-function can not be factorized and all the methods known fail.

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