MOBILITY OF POLARON WITH STRONG COUPLING

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It has been long known that a strong interaction of an electron with phonons in a polar crystal leads to a lowering of the energy [1] and to a change in mass [2]. We calculate here the polaron mobility determined by its interaction with thermal optical phonons.

The interaction Hamiltonian corresponding to scattering of a phonon by a polaron can be separated in the strong-coupling limit with the aid of the transformations of Bogolyubov [3] and Tyablikov [4] in conjunction with the transformation of Lee, Low, and Pines [5], which describes the transition from the c.m.s. to the lab. system. In the principal order in the reciprocal coupling constant $\varepsilon = 1/\alpha\sqrt{2} << 1$, the principal role in the scattering is played by two-phonon processes. In the system of units $h = m = e^2(\varepsilon_\infty^{-1} - \varepsilon^{-1}) = 1$, the sought Hamiltonian takes the form

$$H = E_0 - \frac{1}{2\overset{*}{M}}\frac{\partial^2}{\partial \mathbf{R}^2} + \sum_{\mathbf{k}} \epsilon^2 a_{\mathbf{k}}^+ a_{\mathbf{k}} - \frac{\epsilon^2}{2}\sum_{\mathbf{k}\mathbf{k}'} B_{\mathbf{k}\mathbf{k}'}(a_{\mathbf{k}} + a_{-\mathbf{k}}^+)(a_{\mathbf{k}'} + a_{-\mathbf{k}'}^+)\, e^{i(\mathbf{k}+\mathbf{k}')\mathbf{R}} \tag{1}$$

where E_0 is the polaron shift [1], the second term is the kinetic energy of a polaron of mass $\overset{*}{M}$ [2], the third term is the energy of phonons with frequency $\omega_0 = \varepsilon^2$, and the last term describes phonon-polaron scattering with a Born amplitude

$$\epsilon^2 B_{\mathbf{k}\mathbf{k}'} = \frac{4\pi\epsilon^2}{\Omega k k'}\sum_{n\neq 0}\frac{I_{\mathbf{k}}^{on} I_{\mathbf{k}'}^{no}}{E_n - E_o}\;;\quad I_{\mathbf{k}}^{mn} = \int d^3r\, \overset{*}{\phi}_m(r)\, e^{i\mathbf{k}\mathbf{r}}\, \phi_n(\mathbf{r})\,, \tag{2}$$

where ϕ_n and E_n are the eigenfunctions and energies of the electron in the polarization well corresponding to the ground state (see [4]). In this approximation, the Hamiltonian can be obtained also by Allcock's method [6].

At temperatures T lower than the phonon energy $\omega_0 = \varepsilon^2$, Boltzmann's kinetic equation is valid by virtue of the small number of thermal phonons. Since the polaron energy is not altered by scattering from phonons without dispersion, the following expression holds for the mobility:

$$\mu = -\frac{e}{3\overset{*}{M}}\sum_{\mathbf{p}} p\frac{\partial f_o}{\partial p}\tau(\mathbf{p}),$$

$$\tau^{-1}(\mathbf{p}) = \frac{1}{2p^2}e^{-(\omega_0/T)}\sum_{\mathbf{k}\mathbf{k}'}|W_{\mathbf{k}\mathbf{k}'}^{\mathbf{p}}|^2(\mathbf{k}-\mathbf{k}')^2\,\delta\left[\frac{\mathbf{p}^2}{2\overset{*}{M}} - \frac{(\mathbf{p}+\mathbf{k}-\mathbf{k}')^2}{2\overset{*}{M}}\right]2\pi, \tag{3}$$

where $W_{kk'}^p$ is the amplitude of scattering of a phonon by a polaron with momentum p, and $f_0(p)$ is the Maxwellian distribution function.

If the momentum transferred in the collision is small in comparison with the thermal momentum of the polaron, it can be assumed that the phonon is scattered by a polaron moving with constant velocity $\vec{v} = \vec{p}/\overset{*}{M}$. The amplitude of this process is connected with the Born amplitude $\varepsilon^2 B_{-k,k'}$ by the equation

$$W_{\mathbf{k}\mathbf{k}'}^{\mathbf{p}} = -\epsilon^2 B_{-\mathbf{k},\mathbf{k}'} + \epsilon^2\sum_{\mathbf{k}''} B_{-\mathbf{k},\mathbf{k}''}\frac{1}{\mathbf{k}''\mathbf{v} - \mathbf{k}'\mathbf{v} + i\delta}W_{\mathbf{k}''\mathbf{k}'}^{\mathbf{p}}. \tag{4}$$

It is important that owing to the large polaron mass, $\overset{*}{M} \sim \varepsilon^{-4}m$, the integral term in (4) contains the large parameter $\varepsilon^2/v >> 1$. Taking the Fourier transform of this equation with respect to $\vec{k} - \vec{k}'$, we get

$$W^p(\mathbf{r};\mathbf{k}') = -\epsilon^2 B(\mathbf{r};\mathbf{k}') - i\frac{\epsilon^2}{v}B\left(\dot{\mathbf{r}};\mathbf{k}'-i\frac{\partial}{\partial\mathbf{r}}\right)\int_z^\infty W^p(\vec{\rho},z';\mathbf{k}')\,dz',$$

where $\vec{r} = (\vec{\rho}, z)$; the coordinate z is directed along $\vec{v}$, and the gradient in the function B does not act on the argument $\vec{r}$ of this function.

It is convenient to introduce a new function $\tilde{g}$ defined by

$$-i\int_z^\infty W^p(\vec{\rho},z';\mathbf{k}')dz' = v[1-\tilde{g}(\mathbf{r};\mathbf{k}')],$$

and satisfying the homogeneous equation

$$-i\frac{\partial}{\partial z}\tilde{g}(\mathbf{r};\mathbf{k}') = \frac{\epsilon^2}{v}B\left(\mathbf{r};\mathbf{k}'-i\frac{\partial}{\partial\mathbf{r}}\right)\tilde{g}(\mathbf{r};\mathbf{k}');\quad \tilde{g}(\vec{\rho},+\infty;\mathbf{k}')=1.$$

Here

$$\tau^{-1}(p) = \frac{v}{2p^2}e^{-(\omega_0/T)}\sum_{k'}\int d^2\rho\left|\frac{\partial}{\partial\vec{\rho}}\tilde{g}(\vec{\rho},-\infty;\mathbf{k}')\right|^2. \tag{5}$$

It will be shown that the main contribution to $\tau(p)$ is made by momenta $k' \sim (\epsilon^2/v)^{1/5} \gg 1$. It is therefore natural to seek $\tilde{g}$ in the quasiclassical form

$$\tilde{g} = a(\mathbf{r};\mathbf{k}')\exp\{ik'\chi(\mathbf{r};\mathbf{k}')\}. \tag{6}$$

In this momentum region we have

$$B\left(\mathbf{r};\mathbf{k}'-i\frac{\partial}{\partial\mathbf{r}}\right) \approx \frac{8\pi\phi_0^2(r)}{\left(k'-i\frac{\partial}{\partial\mathbf{r}}\right)^4} + 16\pi i\frac{\partial\phi_0^2(r)}{\partial\mathbf{r}}\frac{\left(\mathbf{k}'-i\frac{\partial}{\partial\mathbf{r}}\right)}{\left(\mathbf{k}'-i\frac{\partial}{\partial\mathbf{r}}\right)^6}.$$

The functions a and χ from (6) depend on k' and v/ϵ^2 only via the combination $\xi = 8\pi\epsilon^2/v(k')^5$:

$$\frac{\partial\chi}{\partial z}(\mathbf{n}+\vec{\nabla}\chi)^4 = \xi\,\phi_0^2(r),$$
$$\frac{\partial\ln a}{\partial z} = (\vec{\eta}\,\vec{\nabla})\ln a + \frac{1}{2}\operatorname{div}\vec{\eta}, \tag{7}$$

where

$$\mathbf{n} = \frac{\mathbf{k}'}{|k'|},\quad \vec{\eta} = -4\phi_0^2(r)\,\xi\,\frac{\mathbf{n}+\vec{\nabla}\chi}{(\mathbf{n}+\vec{\nabla}\chi)^6}.$$

Changing over in (5) to integration with respect to ξ and the angles, we obtain an expression for the mobility

$$\mu = \frac{\gamma}{m\omega_0 a^2}\frac{T}{\omega_0}e^{\omega_0/T}, \tag{8}$$

where the numerical coefficient $\gamma \sim 1$ is given by the formula

$$\gamma^{-1} = \frac{1}{25\pi^2}\int do\frac{d\xi}{\xi^2}d^2\rho\, a^2_{\xi,\mathbf{n}}(\vec{\rho},-\infty)\left[\frac{\partial}{\partial\vec{\rho}}\chi_{\xi,\mathbf{n}}(\vec{\rho},-\infty)\right]^2, \tag{9}$$

From (7) and the corresponding boundary conditions we see that $a_{\xi,n}(\vec{\rho}, -\infty) = 1$ and the integral with respect to ξ converges at the upper and lower limits. It follows therefore that the effective ξ are those of the order of unity, thus confirming the foregoing estimate of the significant values of k'. The requirement that the thermal momentum of the polaron greatly exceed k' imposes on the temperature the condition $\epsilon^{10/3} \ll T$. Thus, the temperature interval in which formula (8) is valid is given, in dimensional units, by

$$\frac{\omega^0}{a^{4/3}} \ll T \ll \omega_0.$$

A more detailed analysis of the polaron-phonon interaction will be published later.

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LIMITATION ON THE MASSES OF SUPERCHARGED HADRONS IN THE WEINBERG MODEL

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Upper bounds on the mass of the supercharged quark, which follow from an analysis of the $K_L \to 2\mu$ decay and the $K_L - K_S$ mass difference, are obtained within the framework of a weak-interaction scheme based on hadron SU(4) symmetry.

The need for introducing supercharged hadrons is connected with the requirement that there be no weak neutral currents with $|\Delta S| = 1$ [1]. A renormalizable scheme of weak and electromagnetic hadron interactions, based on introducing a fourth p' quark, was proposed in [2, 3]. We derive below bounds on the masses of the p' quark and the ordinary p quark; these bounds follow from an analysis of the $K_L \to 2\mu$ decay and the $K_L - K_S$ mass difference. The analysis is based on the assumption $m_p \ll m_{p'} \ll \mu_W$, where m_p, $m_{p'}$, and μ_W are the masses of the p quark, the p' quark, and the W boson.

We start with a calculation of the annihilation amplitude of free quarks λ and n into a pair $\mu^+\mu^-$. This amplitude can serve as an effective Lagrangian, the matrix element of which between the states K^0 and the vacuum gives the amplitude of the sought process $K_L \to \mu^+\mu^-$.

In the calculation we have used the so-called generalized ξ-formalism [4]. It reduces to selection of a gauge in which the vector-field propagator is equal to

$$-i\,\frac{1}{q^2-\mu_W^2}\left[g_{\mu\nu} - \frac{q_\mu q_\nu(1-1/\xi)}{q^2-\mu^2/\xi}\right]. \tag{1}$$

The unphysical pole at $q^2 = \mu^2/\xi$ is cancelled by the contribution of the fictitious scalar particles with mass μ^2/ξ. The final expression for the amplitude, of course, should not depend on ξ.

We note the following curious circumstance: In the usual ξ-formalism [5], which uses the propagator (1) with subsequent transition to the limit $\xi \to 0$, there are no fictitious scalar particles. Yet the contribution made to the discussed amplitude from certain diagrams containing these particles remains finite also as $\xi \to 0$. In the usual ξ-formalism, the absence of such diagrams is compensated for by modification of the vector vertices.

One more remark concerning the calculation technique. Calculation of the $Z\lambda n$ vertex gives rise to divergent diagrams with scalar particles. Although the divergences cancel out mutually, the question is raised of the correctness of the calculation of the finite part of the amplitude. A gauge-invariant method of obtaining the answer may be the Pauli-Villars regularization, wherein one introduces an additional isodoublet of scalar particles with indefinite metric and anticommuting commutation relations. The mass of these particles plays the role of the cutoff parameter and should be allowed to go to infinity.

Another way is to use the Ward identity for the $Z\lambda n$ vertex. A nonzero vertex at a Z-boson momentum $k_\mu = 0$ is then possible only if the current j_μ^Z, the source of the field Z_μ, is not conserved.

By this method, the calculations can be performed also without using the ξ-formalism, directly in the Proca gauge. Taking into account the relation