

BOUND POLARON AND PHONON STATES

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Besides the ground state of the polaron, there are presently known excited states corresponding to the electron excitation in the polarization well [1, 2]. As regards phonon excitations of the system, it has been assumed that their spectrum begins with the polarization frequency ω .

It will be shown below that actually, under conditions of adiabatic coupling, the lowest states of the polaron are states of polaron-phonon complexes corresponding to bound states of these two quasiparticles; naturally, the excitation energy of the complexes is $\Omega < \omega$. It turns out that there exist complexes with all values of the angular momentum, and the relative binding energy $(\omega - \Omega)/\omega$ does not depend on the Frohlich coupling constant α (if $\alpha \gg 1$). An estimate shows that at the lower values of the angular momentum we get $(\omega - \Omega)/\omega \approx 0.10 - 0.15$, which is experimentally observable. We hope that these complexes can be observed in experiments on the absorption and scattering of light by free polarons, on the structure of the intrinsic absorption near its edge, etc.

A distinguishing feature of the problem is that the first term in the polaron energy, according to Pekar [3], is close to $0.1 \alpha^2 \omega \gg \omega$, and the binding energy $(\omega - \Omega)$ of the complex is obviously less than ω . We must therefore calculate $(\omega - \Omega)$ directly, and not as a difference of large energies. The solution of this problem is facilitated by the fact that in the calculation of the vibrational frequencies the ions can be described classically. The formation of the complexes appears in this case as a manifestation of local oscillations near the polaron.

If we define the potential ϕ of the polarization $\vec{P}(\vec{r})$ by $\nabla\phi = 4\pi\vec{P}$, then the Lagrangian of the polaron is

$$L = \frac{1}{2\mu} \int |\nabla\psi|^2 d\vec{r} - e \int |\psi|^2 \phi d\vec{r} + \frac{1}{8\pi c} \int \left[\frac{1}{\omega^2} \left(\frac{\partial}{\partial t} \nabla\phi \right)^2 - (\nabla\phi)^2 \right] d\vec{r}, \quad (1)$$

where $c = \epsilon_\infty^{-1} - \epsilon_0^{-1}$, and $\hbar = 1$. From (1) we get the equations of motion

$$i \frac{\partial \psi}{\partial t} = \left(-\frac{1}{2\mu} \Delta + e\phi \right) \psi, \quad (2a)$$

$$\left(\frac{\partial^2}{\partial t^2} + \omega^2 \right) \Delta\phi = 4\pi e c \omega^2 |\psi|^2 \quad (2b)$$

For a polaron moving with velocity \vec{v} we put

$$\psi = \{ \psi_0(\mathbf{R}) \exp(-iE_0 t) + \tilde{\psi}(\mathbf{R}, t) \} \exp(i\mu\vec{v}\vec{r}), \quad \phi = \phi_0(\mathbf{R}) + \tilde{\phi}(\mathbf{R}, t), \quad (3)$$

where $\vec{R} = \vec{r} - \vec{v}t$ and $\tilde{\psi}$ and $\tilde{\phi}$ are small. In the zeroth approximation

$$H_0(\mathbf{R}, \mathbf{v}) \psi_0(\mathbf{R}) = E_0 \psi_0(\mathbf{R}), \quad H_0(\mathbf{R}, \mathbf{v}) = -\frac{1}{2\mu} \Delta_{\mathbf{R}} + e\phi_0(\mathbf{R}) + \frac{1}{2} \mu v^2 \quad (4a)$$

$$[\omega^2 + (v \nabla_R)^2] \Delta_R \psi_0(\mathbf{R}) = 4\pi e c \omega^2 \psi_0^2(\mathbf{R}). \quad (4b)$$

Equation (4a) determines the wave function ψ_0 and the energy E_0 of the ground state of the moving polaron. We choose ψ_0 real, and denote the other eigenfunctions and eigenvalues of H_0 by ψ_n and E_n ($n > 0$).

We now write the first-approximation equations for the oscillations of the ions in the presence of a moving polaron

$$[i \frac{\partial}{\partial t} - H_0(\mathbf{R}, \mathbf{v})] \tilde{\psi}(\mathbf{R}, t) = e \psi_0(\mathbf{R}) \tilde{\phi}(\mathbf{R}, t) \exp(-iE_0 t), \quad (5a)$$

$$[(\frac{\partial}{\partial t} - v \nabla_R)^2 + \omega^2] \Delta_R \tilde{\phi}(\mathbf{R}, t) = 4\pi e c \omega^2 \psi_0(\mathbf{R}) \{ \tilde{\psi}(\mathbf{R}, t) \exp(iE_0 t) + c.c. \}. \quad (5b)$$

Putting $\tilde{\phi}(\mathbf{R}, t) = \tilde{\phi}(\vec{R}) \exp(-i\Omega t) + c.c.$, solving (5a) in first order of perturbation theory, substituting the result in (5b), and taking $|E_0| \gg \omega$ into account, we obtain ultimately

$$[\omega^2 - (\Omega - iv \nabla_R)^2] \Delta_R \tilde{\phi}(\mathbf{R}) = -8\pi e c^2 \omega^2 \sum_{n>0} \frac{\psi_0(\mathbf{R}) \psi_n(\mathbf{R}) \psi_n^*(\mathbf{R}_1) \psi_0(\mathbf{R}_1) \tilde{\phi}(\mathbf{R}_1) d\mathbf{R}_1}{E_n - E_0}. \quad (6)$$

For an approximate determination of Ω it is convenient to change over from (6) to an equivalent variational principle. We confine ourselves to the case $v = 0$ and change over to dimensionless quantities, choosing as the energy units and length $\mu e^4 c^2 / \hbar^2$ and $\hbar^2 / \mu e^2 c$, which are the characteristic scales in the theory of adiabatic coupling. Then

$$\frac{\omega^2 - \Omega^2}{8\pi\omega^2} = \max_{\phi} \left\{ \sum_{n>0} \frac{|\int \psi_n^*(\mathbf{R}) \psi_0(\mathbf{R}) \tilde{\phi}(\mathbf{R}) d\mathbf{R}|^2}{E_n - E_0} / \int |\nabla \tilde{\phi}|^2 d\mathbf{R} \right\}. \quad (7)$$

The extremum of the right-hand side of (7) cannot be determined directly, for this would call for the knowledge of all the ψ_n and E_n . We make the substitution

$$\psi_0 \tilde{\phi} = (H_0 - E_0) \psi_0 f; \quad (8)$$

it is admissible, since $\tilde{\phi}$ is defined, in accord with (6), accurate to an additive constant. Then, after simple transformations, with (4a) taken into account, formula (7) is transformed into

$$\frac{\omega^2 - \Omega^2}{8\pi\omega^2} = \max_f \left\{ \int d\mathbf{R} \psi_0^2 (\nabla f)^2 / \int d\mathbf{R} [\nabla(\Delta f + 2 \nabla f \cdot \nabla \ln \psi_0)] \right\}. \quad (9)$$

The right side of (9) contains a single quantity characterizing the polaron - the electronic wave function of the ground state. It can be found by a variational method [3] with practically arbitrary accuracy. The function f and the frequency Ω can then be determined from (9).

Since all the parameters of the Hamiltonian (μ , ω , and c) have dropped out of the right side of (9), the relative binding energies of the complexes, $(\omega - \Omega)/\omega$, have universal values in the limit of the adiabatic coupling.

The kernel in the right side of (6) is spherically symmetrical, so that $\tilde{\phi}$ and ψ correspond to definite values of the angular momentum. Since the right side of (9) is also positive definite, bound state with all values of the angular momentum should exist at $\alpha \rightarrow \infty$.

If we estimate the right side of (9) by using single-parameter approximations with the aid of the functions of the three-dimensional oscillator (1s for ψ_0 and 1s and 2p for f), then the binding energy turns out to be 0.13ω and 0.11ω for the s- and p-states of the complex, respectively. This should be observable experimentally; we note that nearly equal values of the binding energy of exciton-phonon complexes were recently measured experimentally in [4].

$$\Sigma = \text{[diagram 1]} + \text{[diagram 2]} + \text{[diagram 3]} + \dots$$

In the case of weak coupling ($\alpha \ll 1$) the main contribution to the proper energy part at energies close to ω is made by the infinite set of diagrams shown in the figure. An analysis of the equation for the vertex part shows that in this case there are no bound states, but in a strong magnetic field, when the cyclotron frequency ω_c is nearly equal to ω , the complexes are produced. This is precisely the nature of the "magneto-optic anomaly" [5]. The mechanism whereby it occurs, due to the resonance polarizability, is close to that considered in [6].

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- [6] Sh. M. Kogan and R. A. Suris, Zh. Eksp. Teor. Fiz. 50, 1279 (1966) [Sov. Phys.-JETP 23, 850 (1966)].

E R R A T U M

In the article by V. I. Mel'nikov and E. I. Rashba, Vol. 10, No. 2, p. 61, formula (9) should read:

$$\frac{\omega^2 - \Omega^2}{16\pi\omega^2} = \max_f \left\{ \int d\mathbf{R} \psi_0^2 (\nabla f)^2 / \int d\mathbf{R} [\nabla(\Delta f + 2\nabla f \nabla \ln \psi_0)]^2 \right\}. \quad (9)$$