Piezopolaron energy at large momenta

G. E. Volovik and V. M. Édel'shteĭn

L. D. Landau Institute of Theoretical Physics, USSR Academy of Sciences
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The energy of a piezopolaron is calculated for the case when the phonons can be described classically. It is shown that the classical phonon description is valid for arbitrary coupling constants provided that the piezopolaron momentum is sufficiently high. At such momenta the piezopolaron velocity tends asymptotically to that of sound.

We consider the "isotropic" model[1] of a piezopolaron with Hamiltonian

$$H=\frac{\mathbf{p}^2}{2m}+\left(\frac{4\pi\alpha}{\Omega}\right)^{1/2}\sum_{\mathbf{k}}\frac{s^{3/2}}{(sk)^{1/2}}(a_{\mathbf{k}}+a_{-\mathbf{k}}^{+})e^{i\mathbf{k}\mathbf{r}}+\sum_{\mathbf{k}}ska_{\mathbf{k}}^{+}a_{\mathbf{k}}, \qquad (1)$$

where α is the dimensionless coupling constant, s is the speed of sound, Ω is the volume of the crystal, and $\hbar = 1$.

We assume that the classical description of the phonon field is valid (the conditions for this will be presented below). By choosing $4\alpha^2ms^2$ and $2\alpha ms$ as the energy and momentum units we reduce the Lagrangian of the system to the form

$$\mathscr{L}(\mathbf{r},t)=\frac{i}{2}\left(\frac{\partial\psi}{\partial t}\psi^{*}-\psi\frac{\partial\psi^{*}}{\partial t}\right)-\frac{1}{2}\nabla\psi\cdot\nabla\psi^{*}-|\psi|^2\varphi+\frac{1}{8\pi}\left[\left(\frac{\partial\varphi}{c\partial t}\right)^2-(\nabla\varphi)^2\right], \qquad (2)$$

where $c = 1/2\alpha$ is the speed of sound in the chosen system of units, $\psi(\mathbf{r}, t)$ is the wave function of the electron, and $\varphi(\mathbf{r}, t)$ is the potential of the phonon field.

For the equations of motion, we seek a solution corresponding to the ground state of a piezopolaron moving with velocity $u < c$, in the form

$$\psi=\psi_0(\mathbf{r}-\mathbf{u}t)\exp[-i(W+u^2/2)t+i\mathbf{u}\mathbf{r}],\quad \varphi=\varphi_0(\mathbf{r}-\mathbf{u}t),$$

where the functions ψ_0 and φ_0 satisfy the equations

$$[-{}^1/_2\Delta+\varphi_0(\mathbf{R})]\psi_0(\mathbf{R})=W\psi_0(\mathbf{R}),$$
$$[(\mathbf{u}\nabla/c)^2-\Delta]\varphi_0(\mathbf{R})=-4\pi|\psi_0(\mathbf{R})|^2. \qquad (3)$$

It is convenient to introduce the functional $J[\psi_0, \varphi_0]$:

$$J[\psi_0,\varphi_0]=\int d^3R\left[\frac{1}{8\pi}(\nabla\varphi_0)^2-\frac{1}{8\pi}\left(\frac{\mathbf{u}\nabla}{c}\varphi_0\right)^2+\frac{1}{2}|\nabla\psi_0|^2+\varphi_0|\psi_0|^2\right], \qquad (4)$$

variation of which with respect to ψ_0 and φ_0 yields the same equations of motion. The energy of the system can be obtained from the Lagrangian (2) in standard fashion, and is equal to

$$E=J+\mathbf{p}\mathbf{u}-\frac{u^2}{2},\qquad \mathbf{p}=\mathbf{u}\left[1+\frac{1}{4\pi}\int d^3R\left(\frac{\partial\varphi_0}{c\partial z}\right)^2\right], \qquad (5)$$

where p is the average momentum of the system, while the coordinate z is directed along u.

With the aid of the second equation of the system (3), we express the Fourier components of φ_0 in terms of the Fourier components of $|\psi_0|^2$ and obtain for J an expression similar to the Pekar functional[2]:

$$J[\psi_0]=\frac{1}{2}\int d^3R(\nabla\psi_0)^2-\frac{2\pi}{\Omega}\sum_{\mathbf{k}}\frac{|(\psi_0^2)_{\mathbf{k}}|^2}{k^2-(\mathbf{k}\mathbf{u}/c)^2} \qquad (6)$$

(the functions ψ_0 are chosen to be real). From the form of this functional it follows that the longitudinal dimension of the piezopolaron decreases as the piezopolaron speed u approaches the speed of sound c. For the coordinates z and ρ parallel and perpendicular to the motion it is convenient to carry out the scale transformation

$$\tilde{z}=zL,\quad \tilde{\boldsymbol{\rho}}=\boldsymbol{\rho}L^{1/2},\quad \tilde{k}_z=k_z/L,\quad \tilde{\mathbf{k}}_\rho=\mathbf{k}_\rho/L^{1/2}$$

with a corresponding transformation of the function $\psi_0(\mathbf{R}) = L\tilde{\psi}(\tilde{\mathbf{R}})$, where L is determined from the equation

$$L(u)=-\ln[(1-u^2/c^2)L(u)].$$

Let us consider velocities u close to c, such that $L \gg 1$; then

$$J[\psi_0]=L^2(u)J^0[\tilde{\psi}]+L(u)J^1[\tilde{\psi}]+O(1-u^2/c^2), \qquad (7)$$

where the functionals J^0 and J^1 do not depend exclusively on the velocity u:

$$J^0=\frac{1}{2}\int d^3\tilde{R}\left(\frac{\partial\tilde{\psi}}{\partial\tilde{z}}\right)^2-\frac{1}{2}\int d\tilde{z}\,d\tilde{\boldsymbol{\rho}}_1\,d\tilde{\boldsymbol{\rho}}_2\,\tilde{\psi}^2(\tilde{z},\tilde{\boldsymbol{\rho}}_1)\tilde{\psi}^2(\tilde{z},\tilde{\boldsymbol{\rho}}_2),$$

$$J^1=\frac{1}{2}\int d^3\tilde{R}\left(\frac{\partial\tilde{\psi}}{\partial\tilde{\rho}}\right)^2+\frac{1}{4\pi^2}\int d^3\tilde{k}\left[\ln\tilde{k}_z^2|(\tilde{\psi}^2)_{\tilde{k}}|^2\pi\delta(\tilde{\mathbf{k}}_\rho)+\ln\tilde{\mathbf{k}}_\rho^2\cdot\frac{\partial}{\partial\tilde{\mathbf{k}}_\rho^2}|(\tilde{\psi}^2)_{\tilde{k}}|^2\right].$$

The minimum of the functional J^0 is realized on functions of the type $\tilde{\psi} = \chi(\tilde{\rho})/2\cosh(\tilde{z}/2)$, with an arbitrary normalized function $\chi(\tilde{\rho})$, and is equal to $-{}^1/_{24}$. The function $\chi(\tilde{\rho})$ can be determined by substituting $\tilde{\psi}$ in the functional J^1 and minimizing with respect to χ. Since the functional $J^1[\chi]$ does not contain any parameters, its extremal $\chi(\tilde{\rho})$ is concentrated in the region $\tilde{\rho} \sim 1$. This means that the transverse and longitudinal dimensions of the well are $\hbar/ms\alpha L^{1/2}$ and $\hbar/ms\alpha L$, respectively. Thus, we obtain for the energy and momentum of the piezopolaron (5), as $u \to c$, the expressions

$$E\approx pu-{}^1/_{24}L^2,\quad p\approx L/6c(1-u^2/c^2),$$

so that in dimensional units the spectrum of the piezopolaron at large momenta takes the form

$$E(p)=ps-{}^1/_6\alpha^2ms^2\ln^2(p/\alpha^2ms). \qquad (8)$$

The speed of the piezopolaron approaches asymptotically the speed of sound s:

$$u=s-\frac{\alpha^2ms^2}{3p}\ln\left(\frac{p}{\alpha^2ms}\right).$$

We turn to the condition for the validity of the classical description of the phonons. To this end it is necessary[2] that the frequency of the phonons that make the main contribution to the formation of the potential well for the electron be lower than the frequencies of the motion of the electron in this well. The slowest is the transverse motion of the electron, its frequency being of the order of α^2ms^2L. The main contribution to the well comes from the phonons traveling in the direction of the velocity u ($k_z > 0$) with characteristic momenta

$$k_z\sim\alpha msL,\quad k_z(1-u^2/s^2)^{1/2}\leqslant k_\rho\leqslant\alpha msL^{1/2}$$

(it is by integration over this region of k_ρ that the logarithm of L builds up in the functional J). Their frequency, in the piezopolaran rest system, is

$$\omega=s(k_z^2+k_\rho^2)^{1/2}-k_zu\approx sk_\rho^2/2k_z<\alpha ms^2.$$

Therefore the classicality (adiabaticity) condition is the inequality

$$\alpha L\approx\alpha\ln(p/\alpha^2ms)\gg1. \qquad (9)$$

Thus, in the case of strong coupling $\alpha \gg 1$ and intermediate coupling $\alpha \sim 1$, formula (8) for the spectrum is valid at $p \gg \alpha^2 ms$. The condition (9) can be satisfied also in the case of weak coupling $\alpha \ll 1$, provided that the piezopolaron momentum is large enough. In this case, however, the state with spectrum (8) can be easily destroyed as a result of screening of the electron-phonon interaction by the free carriers. Let r_0 be the screening radius. Then the integration with respect to k_ρ in (6) is limited to the region $k_\rho > r_0^{-1}$, and in order for this region to overlap the characteristic region in which the logarithm of L is built up, it is necessary to satisfy the inequality

$$r_0^{-1}<\alpha ms(1-u^2/s^2)^{1/2}L.$$

Therefore, in the case of weak coupling the state with spectrum (8) can exist only with the following limitation on the screening radius:

$$\alpha\ln(\alpha msr_0)\gg1,$$

whereas for the intermediate and strong coupling it suffices to stipulate $\alpha msr_0 \gg 1$.

For a macroscopic analysis it is necessary that the dimensions of the piezopolaron greatly exceed the interatomic distances a, i.e., $\alpha L \ll \hbar/ms\alpha \sim 10^3$; this condition is compatible with (9).

An asymptotic approach of the piezopolaron velocity to the velocity of sound was obtained also by Rona and Whitfield[3]. They obtained, by the variational method of Lee, Low, and Pines[4], an upper bound of the ground state of the Hamiltonian (1) at a given momentum. This method did not make it possible, however, to determine the character of the asymptotic approach of u to s.

The dependence of the piezopolaron energy on the velocity at large coupling constants was considered also by Kabisov and Pokatilov[5]. However, owing to an erroneous identification of the piezopolaron energy E with the extremal value of J, the spectrum was not obtained.

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