Modern Physics Letters B
Vol. 30, No. 4 (2016) 1650031 (5 pages)

DOI: 10.1142/S0217984916500317

World Scientific
www.worldscientific.com

Phonon interaction of electrons in the translation-invariant strong-coupling theory

V. D. Lakhno

Institute of Mathematical Problems of Biology,
Russian Academy of Sciences, Pushchino, Moscow Region 142290, Russia
lak@impb.psn.ru

Received 27 November 2014
Revised 29 July 2015
Accepted 19 August 2015
Published 25 January 2016

A dependence of phonon interaction on the interelectronic distance is found for a translation-invariant (TI) strong-coupling bipolaron. It is shown that the charge induced by the electrons in a TI-bipolaron state is always greater than that in a bipolaron with spontaneously broken symmetry.

Keywords: Froehlich Hamiltonian; polaron; correlation length; Coulomb; quark.

Considerable attention given to the bipolaron problem in recent years centers around attempts to explain the superconductivity phenomenon with the use of the mechanism of Bose-condensation of bipolaron gas.[1–3] In this context, the study of the interaction between the electrons caused by their interaction with phonons is a vital task. In Refs. 4–6, a new concept of a translation-invariant bipolaron (TI-bipolaron) was introduced which possesses much higher coupling energy than a bipolaron with spontaneously broken symmetry (SBS-bipolaron). Of interest is to calculate the interaction energy as a function of a distance between the electrons in a TI-bipolaron and to find the value of the charge induced by the electrons in a polar medium. Note that for the case of SBS-bipolarons, these points were discussed in a lot of papers.[7–9] Following Refs. 4–6, we will proceed from Froehlich Hamiltonian for a bipolaron which in the coordinates of the center-of-mass has the form:

$$\hat{H} = -\frac{\hbar^2}{2M_e}\Delta_R - \frac{\hbar^2}{2\mu_e}\Delta_r + U(|\mathbf{r}|) + \sum_k \hbar\omega_k a_k^+ a_k + \sum_k 2\cos\frac{\mathbf{kr}}{2}(V_k e^{i\mathbf{kR}} a_k + \text{H.C.}) \tag{1}$$

where R, r are coordinates of the center-of-mass and relative motion of electrons, respectively: $M_e = 2m$, $\mu_e = m/2$, m is an electron mass, a_k^+, a_k are operators of

a phonon field; $V_k = (e/k)\sqrt{2\pi\hbar\omega/\tilde{\epsilon}V}$, $\tilde{\epsilon}^{-1} = \epsilon_\infty^{-1} - \epsilon_0^{-1}$ and $\omega_k = \omega$ are phonon frequencies, e is the electron charge, ϵ_∞^{-1}, ϵ_0^{-1} are high-frequency and static dielectric constants, V is the systems volume and $U(r) = e^2/\epsilon_\infty|\mathbf{r}|$.

After excluding the center-of-mass coordinate by means of Heisenberg transformation[10] with the use of Lee–Low–Pines (LLP) transformation,[11]

$$S_2 = \exp\left\{\sum_k f_k(a_k - a_k^+)\right\}, \tag{2}$$

the energy of electron–phonon interaction of the electrons $U_{\rm int}(r)$, according to (1), is written as

$$U_{\rm int}(r) = \left\langle 0 \left| S_2^{-1}\left(\sum_k 2V_k \cos\frac{\mathbf{kr}}{2}(a_k + a_k^+)\right) S_2 \right| 0 \right\rangle = 4\sum_k V_k f_k \cos\frac{\mathbf{kr}}{2}. \tag{3}$$

According to Ref. 6, when the LLP function f_k is chosen in the Gaussian form:

$$\begin{gathered} f_k = -NV_k \exp\left(\frac{-k^2}{2\mu}\right), \\ \bar{V}_k = 2V_k \left\langle \Psi \left| \cos\frac{\mathbf{kr}}{2} \right| \Psi \right\rangle, \quad \Psi(r) = \left(\frac{2}{\pi l^2}\right)^{3/4} \exp\left(\frac{-r^2}{l^2}\right), \end{gathered} \tag{4}$$

where N, μ and l are varying parameters, with the use of (3) $U_{\rm int}(r)$ is expressed as

$$\tilde{U}_{\rm int}(\tilde{r}) = -\sqrt{\frac{x^2+16y}{x^2+8y}}\,\frac{1}{\tilde{r}}\,F\left(\frac{2\tilde{r}}{\sqrt{16y+x^2}}\right), \quad F(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}dt, \tag{5}$$

where $\tilde{U}_{\rm int}(\tilde{r}) = U_{\rm int}(r)/(4me^4/\hbar^2\tilde{\epsilon}^2)$ and $\tilde{r} = (e^2m/\hbar^2\tilde{\epsilon})r$ are dimensionless variables. The values of $x = x(\eta)$ and $y = y(\eta)$ (where $\eta = \epsilon_\infty/\epsilon_0$ is the parameter of ion coupling) for each η value are determined from the condition that the function $\Phi(x, y; \eta)$ be minimum:[6]

$$\Phi(x, y; \eta) = \frac{6}{x^2} + \frac{20,25}{x^2+16y} - \frac{16\sqrt{x^2+16y}}{\sqrt{\pi}(x^2+8y)} + 4\frac{\sqrt{2/\pi}}{x(1-\eta)}. \tag{6}$$

Relation of quantities x and y with the parameters μ and l in (4) is given by formulae $x = l\alpha$ and $y = \alpha^2/\mu$, where

$$\alpha = \left(\frac{e^2}{\hbar\tilde{\epsilon}}\right)\sqrt{m/2\hbar\omega} \tag{7}$$

is a constant of electron–phonon coupling.

Figure 1 demonstrates the dependencies $\tilde{U}_{\rm int}(\tilde{r})$ for some values of η parameter. It is seen that for small $\tilde{r}$, the interaction potential is independent of $\tilde{r}$, for intermediater has linear dependence on r, while for large $\tilde{r}$, it has a Coulomb form: $\tilde{U}_{\rm int}(\tilde{r}) \sim 1/\tilde{r}$. Figure 1 also suggests that at the point $\eta = \eta_c = 0,289$, i.e. at the point where a TI-bipolaron decays into TI-polarons,[6] interaction $U_{\rm int}(r)$ does not demonstrate any jumps and changes continuously as η increases up to the value of

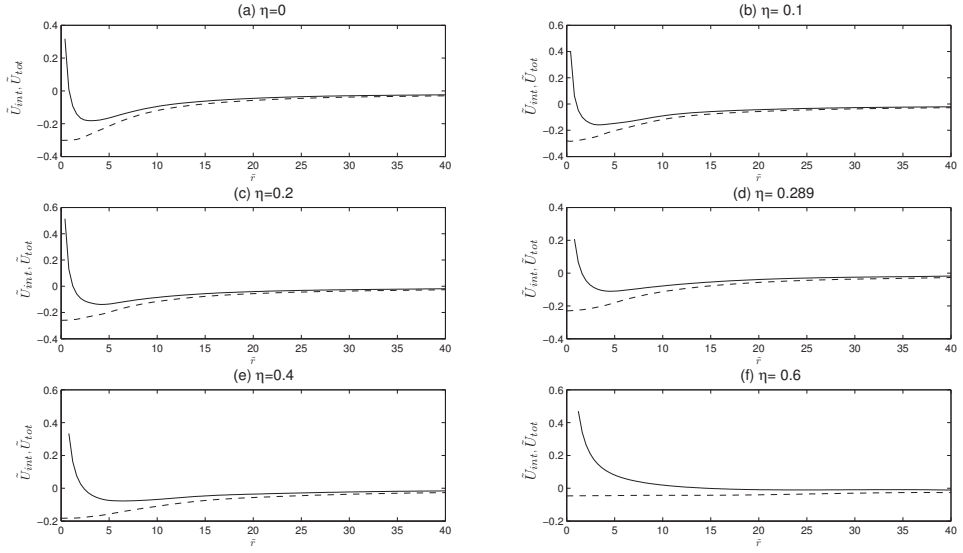

Fig. 1. The dependence of interaction potentials $\tilde{U}_{\rm int}$ (dashed) and total potential $\tilde{U}_{\rm tot}$ (solid) on η.

$\eta = 1-1/2\sqrt{2}$, at which the total energy of a TI-bipolaron $E_{bp} = \Phi\alpha^2$ vanishes. The total interaction potential $U_{\rm tot}(r)$ should include the Coulomb interaction $U(r)$:

$$U_{\rm tot}(r) = U_{\rm int}(r) + U(r) \tag{8}$$

and is shown in Fig. 1.

It looks like Coulomb interaction in the case of small r and has a near-linear shape in a certain range of r variation (this is especially clear in Fig. 1(f): $\eta = 0, 6$). This behavior reminds the interaction between quarks with repulsive instead attractive as in the case of quark Coulomb potential. (A polaron model of quarks was considered in Ref. 12.)

The knowledge of $U_{\rm int}(r)$ enables us to calculate the density distribution of a charge $\rho_{\rm ind}(r)$ induced by electrons in a polar medium. Assuming

$$U_{\rm int}(r) = -2e\varphi_{\rm ind}(r)\,, \tag{9}$$

where $\varphi_{\rm ind}(r)$ is a potential induced by the electrons, we will write for $\rho_{\rm ind}(r)$:

$$\Delta_r \varphi_{\rm ind}(r) = 4\pi\rho_{\rm ind}(r)\,. \tag{10}$$

With the use of (5), (9) and (10), we express $\rho_{\rm ind}(r)$ as

$$\begin{aligned} \rho_{\rm ind}(r) &= \frac{32}{\pi}\sqrt{\frac{2}{\pi}}\frac{e}{\epsilon}\left(\frac{me^2}{\hbar^2\tilde{\epsilon}}\right)^3 \tilde{\rho}(\tilde{r})\,, \\ \tilde{\rho}(\tilde{r}) &= \frac{1}{(x^2+16y)\sqrt{x^2+8y}}\exp\left(-\frac{8\tilde{r}}{(16y+x^2)}\right). \end{aligned} \tag{11}$$

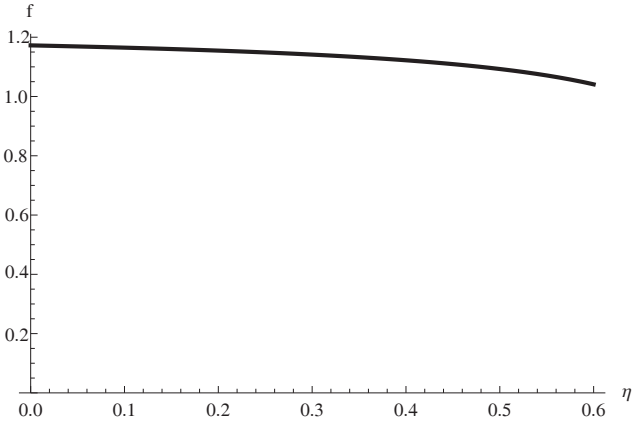

Fig. 2. The dependence of function $f = \sqrt{(16y + x^2)/(8y + x^2)}$ on η.

The total charge Q induced by a TI-bipolaron,

$$Q = \int \rho_{\text{ind}}(r) dV \,, \tag{12}$$

is equal to

$$Q = \sqrt{\frac{16y + x^2}{8y + x^2}} \; \frac{2e}{\tilde{\epsilon}} \,. \tag{13}$$

Figure 2 shows the dependence of $f = \sqrt{(16y + x^2)/(8y + x^2)}$ as a function of the parameter η. It also suggests that the value of a charge Q induced by the electrons in a TI-bipolaron state is always greater than that of a charge $2e/\tilde{\epsilon}$ induced by the electrons in a SBS-bipolaron state. These values coincide only for $\eta \to 1 - 1/2\sqrt{2}$ — value, when the effective distance between the electrons in a TI-bipolaron (correlation length) is equal to infinity. This result suggests that the adiabatic approximation in this limit holds for a TI-polaron too.

In conclusion, it may be said that the frequently introduced concept of inter-polaronic interaction[2,7–9] in the case of a TI-bipolaron is objectless, since even for large r, a TI-bipolaron cannot be presented as the one consisting of two individual polarons (here an analogy with confinement of quarks is appropriate).

This presentation, however, can be sensible, if for a certain value ($\eta = \eta_c$) a decay of a TI-bipolaron into two individual TI-polarons is possible. For this case, the dependence of the polarons interaction on the distance was calculated in Ref. 9.

Acknowledgment

The work was supported by RFBR, Project No. 13-07-00256.

References

1. A. S. Alexandrov and N. Mott, *Polarons and Bipolarons* (World Scientific, Singapore, 1996).
2. N. I. Kashirina and V. D. Lakhno, *Usp. Fiz. Nauk* **180** (2010) 449.
3. D. Emin, *Polarons* (Cambridge University Press, Cambridge, UK, 2013).
4. V. D. Lakhno, *J. Exp. Theor. Phys.* **137** (2010) 926.
5. V. D. Lakhno, *Solid State Commun.* **152** (2012) 621.
6. V. D. Lakhno, *J. Exp. Theor. Phys.* **143** (2013) 1033.
7. J. Adamowski, *Phys. Rev. B* **39** (1989) 3649.
8. D. M. Larsen, *Phys. Rev. B* **23** (1981) 628.
9. A. V. Tulub, *J. Exp. Theor. Phys.* **34** (1958) 1642.
10. V. D. Lakhno, *Phys.-Usp.* **58** (2015) 295.
11. T. D. Lee, F. Low and D. Pines, *Phys. Rev.* **90** (1953) 297.
12. S. Iwao, *Lett. Nuovo Cimento* **15** (1976) 331.