Condensed Matter Physics 2010, Vol. 13, No 4, 43701: 1–9

http://www.icmp.lviv.ua/journal

CONDENSED MATTER PHYSICS

Infinitely improvable upper bounds in the theory of polarons

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Received July 5, 2010

An infinite convergent sequence of improving non-increasing upper bounds to the low-lying branch of the slow-moving "physical" Fröhlich polaron ground-state energy spectral curve, adjacent to the ground state energy of the polaron at rest, was obtained by means of generalized variational method. The proposed approach is especially well-suited for massive analytical and numerical computations of experimentally measurable properties of realistic polarons, such as inverse effective mass tensor and excitation gap, and can be elaborated even further, without major alterations, to allow for treatment of multitudinous polaron-like models, those describing polarons of various sorts placed in external magnetic and electric fields among them.

Key words: *Fröhlich polaron model, upper bound estimates, variational method, ground state energy*

PACS: *71.38.-k, 71.38.Fp*

1. The polaron concept

A local change in the electronic state in a crystal leads to the excitation of crystal lattice vibrations, i.e. the excitation of phonons. And vice versa, any local change in the state of the lattice ions alters the local electronic state. This situation is commonly referred to as an "electron–phonon interaction". This interaction manifests itself even at the absolute zero of temperature, and results in a number of specific microscopic and macroscopic phenomena such as, for example, lattice polarization. When a conduction electron with band mass m moves through the crystal, this state of polarization can move together with it. This combined quantum state of the moving electron and the accompanying polarization may be considered as a quasiparticle with its own particular characteristics, such as effective mass, total momentum, energy, and maybe other quantum numbers describing the internal state of the quasiparticle in the presence of an external magnetic field or in the case of a very strong lattice polarization that causes self-localization of the electron in the polarization well with the appearance of discrete energy levels. Such a quasiparticle is usually called a "polaron state" or simply a "polaron".

The concept of the polaron was first introduced by L.D. Landau [1], followed by much more detailed work by S.I. Pekar [2] who investigated the most essential properties of stationary polaron in the limiting case of very intense electron-phonon interaction, in the so-called adiabatic approximation. Subsequently, Landau and Pekar [3] investigated the self-energy and the effective mass of the polaron for the adiabatic regime. Many other famous researchers have contributed to the development of polaron theory later on [4–9]. The polaron concept remains of interest from at least two points of view, practical and theoretical: it describes the physical properties of charge carriers in polar crystals and ionic semiconductors and, at the same time, represents a simple, but rich in content, field–theoretical model of a particle interacting with a scalar boson field.

The model under consideration is the standard quantized Fröhlich polaron Hamiltonian introduced by H. Fröhlich [6]

$$H = \frac{\hat{\mathbf{p}}^2}{2m} + \hbar\omega \sum_{\mathbf{k}} b^+_{\mathbf{k}} b_{\mathbf{k}} + \sum_{\mathbf{k}} V_k \left(b^+_{\mathbf{k}} \mathrm{e}^{-\mathrm{i}\mathbf{k}\hat{\mathbf{r}}} + b_{\mathbf{k}} \mathrm{e}^{\mathrm{i}\mathbf{k}\hat{\mathbf{r}}} \right), \tag{1}$$

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where

$$V_k = \left(\frac{4\pi\alpha}{V/r_0^3}\right)^{1/2}\frac{1}{k}, \qquad \alpha = \frac{\mathrm{e}^2}{2\hbar\omega r_0}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right), \qquad r_0 = \left(\frac{\hbar}{2m\omega}\right)^{1/2}.$$

The operators $\hat{\mathbf{p}}$ and $\hat{\mathbf{r}}$ stand for the electron momentum and position coordinate quantum operators, satisfying the usual commutation relations

$$[\hat{p}_i, \hat{r}_j] = -\mathrm{i}\hbar\delta_{ij}\,,$$

and the operators $b^+_{\mathbf{k}}$, $b_{\mathbf{k}}$, satisfying the usual commutation relations

$$[b_{\mathbf{k}}, b^+_{\mathbf{k}'}] = \delta_{\mathbf{k}\mathbf{k}'}\,, \qquad [b_{\mathbf{k}}, b_{\mathbf{k}'}] = 0,$$

are Bose operators of creation and annihilation of longitudinal optical phonons of energy $\hbar\omega$ and wave vector $\mathbf{k}$. It is assumed that the phonon wave vector runs over a very large but finite quasi-discrete set of values

$$\mathbf{k} = \left\{\frac{2\pi}{La}n_1, \frac{2\pi}{La}n_2, \frac{2\pi}{La}n_3\right\}, \qquad n_i = 0, \pm1, \pm2, \ldots, \pm(L/2-1), +L/2, \qquad i = 1, 2, 3,$$

where a^3 is the volume of the unit crystal cell and L^3 is the number of these cells within the volume V of the crystal, L assumed to be even. The limit $V \to \infty$ corresponds to the rule of the transition from the quasi-discrete to continuous spectrum

$$\lim_{V\to\infty}\frac{1}{V}\sum_{\mathbf{k}}\cdots \to \frac{1}{(2\pi)^3}\int \mathrm{d}\mathbf{k}\cdots = \frac{1}{(2\pi)^3}\int_0^{2\pi}\mathrm{d}\phi\int_0^{\pi}\mathrm{d}\theta\sin\theta\int_0^{k_{\mathrm{D}}}\mathrm{d}k k^2\ldots$$

to be applied to all relevant expressions. Here $k_{\mathrm{D}} = (6\pi^2)^{1/3}/a$ is the Debye wave vector, a being the lattice constant. For any realistic, or "physical", observable polaron, the value of k_{D} is finite whilst the limit $k_{\mathrm{D}} \to \infty$ corresponds to the so-called "field-theoretical" polaron model. It is important to emphasize from the very start that in this study we are mainly preoccupied with "physical" polaron model. Extensive useful discussion on various aspects of phenomenological polaron physics as well as on the derivation of physical quantum polaron model (1) and methods of its treatment can be found in [10] and refs. therein. For the matter of convenience it is assumed further on that $\hbar = \omega = 1,\ m = 1/2$.

2. Low-lying branch of the polaron energy spectrum

It is known that the polaron total momentum

$$\hat{\mathbf{P}} = \hat{\mathbf{p}} + \sum_{\mathbf{k}}\mathbf{k}b^+_{\mathbf{k}}b_{\mathbf{k}}$$

is a constant of the motion and commutes with the Hamiltonian (1). Therefore, it is possible to transform the Hamiltonian to the representation in which $\hat{\mathbf{P}}$ becomes a "c"-number by means of the unitary transformation

$$H \to \tilde{H}, \qquad \tilde{H} = S^{-1}HS, \qquad S = \exp\left(-\mathrm{i}\sum_{\mathbf{k}}\mathbf{k}\hat{\mathbf{r}}b^+_{\mathbf{k}}b_{\mathbf{k}}\right),$$

so that

$$\tilde{H} = \left(\hat{\mathbf{p}} - \sum_{\mathbf{k}}\mathbf{k}b^+_{\mathbf{k}}b_{\mathbf{k}}\right)^2 + \sum_{\mathbf{k}}b^+_{\mathbf{k}}b_{\mathbf{k}} + \sum_{\mathbf{k}}V_k\left(b^+_{\mathbf{k}} + b_{\mathbf{k}}\right),$$

or

$$\tilde{H} = \left(\mathbf{P} - \sum_{\mathbf{k}}\mathbf{k}b^+_{\mathbf{k}}b_{\mathbf{k}}\right)^2 + \sum_{\mathbf{k}}b^+_{\mathbf{k}}b_{\mathbf{k}} + \sum_{\mathbf{k}}V_k\left(b^+_{\mathbf{k}} + b_{\mathbf{k}}\right), \tag{2}$$

in the $\hat{\mathbf{p}}$-representation where $\hat{\mathbf{P}}$ becomes a quantum "c"-number $\mathbf{P}$, the value of the polaron total momentum, and the Hamiltonian (2) no longer contains the electron coordinates. Another unitary transformation

$$\tilde{H} \to \mathcal{H}(f), \qquad \mathcal{H}(f) = U^{-1}\tilde{H}U, \qquad U = \exp\left\{\sum_{\mathbf{k}} f_{\mathbf{k}}(b^{+}_{\mathbf{k}} - b_{\mathbf{k}})\right\},$$

provides us with the Hamiltonian

$$\begin{aligned}\mathcal{H}(f) &= \left(\mathbf{P} - \sum_{\mathbf{k}} \mathbf{k}(b^{+}_{\mathbf{k}} + f_{\mathbf{k}})(b_{\mathbf{k}} + f_{\mathbf{k}})\right)^2 \\ &\quad + \sum_{\mathbf{k}} b^{+}_{\mathbf{k}} b_{\mathbf{k}} + \sum_{\mathbf{k}} [f_{\mathbf{k}} + V_k](b^{+}_{\mathbf{k}} + b_{\mathbf{k}}) + 2\sum_{\mathbf{k}} V_k f_{\mathbf{k}} + \sum_{\mathbf{k}} f^2_{\mathbf{k}}, \end{aligned} \tag{3}$$

or, in a much more convenient albeit equivalent form,

$$\mathcal{H}(f) = \mathcal{H}_0(f) + \mathcal{H}_1(f),$$

where

$$\begin{aligned}\mathcal{H}_0(f) &= P^2 + \sum_{\mathbf{k}} b^{+}_{\mathbf{k}} b_{\mathbf{k}} + \left(\sum_{\mathbf{k}} \mathbf{k} b^{+}_{\mathbf{k}} b_{\mathbf{k}}\right)^2 - \alpha', \\ \mathcal{H}_1(f) &= \sum_{\mathbf{k}} [(1+k^2) f_{\mathbf{k}} + V_k](b^{+}_{\mathbf{k}} + b_{\mathbf{k}}) + 2\sum_{\mathbf{km}} (\mathbf{k}\cdot\mathbf{m}) f_{\mathbf{k}} f_{\mathbf{m}} b^{+}_{\mathbf{k}} b_{\mathbf{m}} \\ &\quad + \sum_{\mathbf{km}} (\mathbf{k}\cdot\mathbf{m}) f_{\mathbf{k}} f_{\mathbf{m}} (b^{+}_{\mathbf{k}} b^{+}_{\mathbf{m}} + b_{\mathbf{k}} b_{\mathbf{m}}) + 2\sum_{\mathbf{km}} (\mathbf{k}\cdot\mathbf{m}) f_{\mathbf{k}} (b^{+}_{\mathbf{m}} b_{\mathbf{m}} b_{\mathbf{k}} + b^{+}_{\mathbf{k}} b^{+}_{\mathbf{m}} b_{\mathbf{m}}) \\ &\quad - 2\sum_{\mathbf{k}} (\mathbf{P}\cdot\mathbf{k})(b^{+}_{\mathbf{k}} + f_{\mathbf{k}})(b_{\mathbf{k}} + f_{\mathbf{k}}), \end{aligned}$$

and

$$-\alpha' = 2\sum_{\mathbf{k}} V_k f_{\mathbf{k}} + \sum_{\mathbf{k}} \left(1 + k^2\right) f^2_{\mathbf{k}} + \left(\sum_{\mathbf{k}} f^2_{\mathbf{k}} \mathbf{k}\right)^2,$$

which is just the sole Hamiltonian to be treated further on.

The ultimate goal is to find the lowest eigenvalue $E_{\mathrm{g}}(\alpha, \mathbf{P}, k_{\mathrm{D}})$ of this Hamiltonian corresponding to the ground state energy of the slow-moving polaron for a given total polaron momentum $\mathbf{P}$. Then, the function $E_{\mathrm{g}}(\alpha, \mathbf{P}, k_{\mathrm{D}})$ could be expanded in powers of $\mathbf{P}$ as

$$E_{\mathrm{g}}(\alpha, \mathbf{P}, k_{\mathrm{D}}) = E_{\mathrm{g}}(\alpha, 0, k_{\mathrm{D}}) + \frac{P^2}{2m_{\mathrm{eff}}} + O\left(P^4\right),$$

where $E_{\mathrm{g}}(\alpha, 0, k_{\mathrm{D}})$ is the ground state energy of the polaron at rest and the coefficient m_{eff} can be interpreted as the polaron effective mass. In a general spatially anisotropic case, the so-called inverse mass tensor

$$\left(\frac{1}{m_{\mathrm{eff}}}\right)_{ij} = \left.\frac{\partial^2 E(\alpha, \mathbf{P}, k_{\mathrm{D}})}{\partial P_i \partial P_j}\right|_{\mathbf{P}=0}$$

should be introduced instead of the scalar effective mass parameter m_{eff}. Another important goal would be to evaluate the so-called excitation gap, i.e. the distance between the ground and the first excited state of the slow-moving polaron Hamiltonian (3). It is worth noticing that $P < 1$ condition is to be imposed throughout all these calculations to avoid the creation of real phonons.

Extensive work has already been done to evaluate $E(\alpha, \mathbf{P}, k_{\mathrm{D}})$ directly through conventional perturbational calculations or to find the upper bound estimates for its value by means of multitudinous variational methods. These approaches are beyond the scope of this work. It is only worth mentioning that, as a rule, perturbational schemes do not provide us with reliable error bound estimates whilst the quality of upper bounds derived by variational methods depends mostly on the choice of proper trial states in any particular case and, being this way, these bounds cannot be improved significantly, not to say infinitely, step by step, through any regular scheme of calculations.

The purpose of the present research is to show that infinitely improvable upper bounds for the low-lying branch of the "physical" polaron energy spectrum $E(\alpha, \mathbf{P}, k_{\mathrm{D}})$ can be obtained by generalized variational method formulated for the first time in [12] and later in [14] in a different context.

3. "Physical" versus "field-theoretical" polaron

Let us put $f_{\mathbf{k}} = -V_k$ in (3), so that

$$\mathcal{H}(f) = \left(\mathbf{P} - \sum_{\mathbf{k}} \mathbf{k}(b_{\mathbf{k}}^{+} - V_k)(b_{\mathbf{k}} - V_k)\right)^2 + \sum_{\mathbf{k}} b_{\mathbf{k}}^{+} b_{\mathbf{k}} - \sum_{\mathbf{k}} V_k^2 \,.$$

It is seen that

$$E_{\mathrm{g}}(\alpha, \mathbf{P}, k_{\mathrm{D}}) \geqslant -\sum_{\mathbf{k}} V_k^2 \to -\alpha \frac{2k_{\mathrm{D}}}{\pi} \qquad \text{as} \qquad V/r_0^3 \to \infty \tag{4}$$

for arbitrary values of model parameters α, $\mathbf{P}$ and k_{D}. The inequality (4) clearly shows the difference between the "physical" and "field-theoretical" polaron models. For the former, the ground state energy can only decrease no faster than linearly in α for any fixed $\mathbf{P}$ and k_{D}, while the latter, as is well-known from numerous previous studies, allows for the quadratic in the electron-phonon interaction constant upper bound

$$E_{\mathrm{g}}(\alpha, 0, k_{\mathrm{D}}) \leqslant -\frac{\alpha^2}{3\pi} \,,$$

incompatible with (4) for large enough α. Nevertheless, the "field-theoretical" limit $k_{\mathrm{D}} \to \infty$ has been routinely applied in quite a few polaron studies rather formally, mainly to facilitate analytical calculations of improper integrals arising along the way, without giving much thought to underlaying physics. Actually, for optical polarons observed so far in many practically important crystal substances, such as alkali halides, the value of dimensionless maximum wave vector k_{D} is not large but rather manifestly small. For example, $k_{\mathrm{D}} \approx 0.3551$ in units of $1/r_0$ for KCl, accompanied by $k_{\mathrm{D}} \approx 0.41$ for KBr. It is also known that hardly any practical necessity exists to carry out calculations for $\alpha > 10$ in the case of experimentally observable "physical" polarons. Hence, it seems perfectly justified and sensible to treat "physical" and "field-theoretical" polaron models in a different way from the very beginning.

4. Generalized variational method

It was proved in [12] following the ideas outlined in [13], and also found later in [14] by a different approach, that for a quantum system represented by some Hamiltonian $\hat{H}$ and any normalized trial state $|\psi\rangle$, such that $\langle\psi|\psi\rangle = 1$,

$$E_{\mathrm{g}} \leqslant \min\left(a_1^{(n)}, \ldots, a_n^{(n)}\right) \leqslant \langle\psi|\hat{H}|\psi\rangle,$$

where the ordered by increase real numbers $\left(a_1^{(n)}, \ldots, a_n^{(n)}\right)$ are the roots of the n-th order polynomial equation

$$P_n(x) = \sum_{i=0}^{n} X_i x^{n-i} = 0,$$

whereby $X_0 \equiv 1$ and all the other coefficients $X_i,\ 1 \leqslant i \leqslant n$ are provided by the system of n linear equations

$$\mathcal{M}\mathbf{X} + \mathbf{Y} = 0,$$

with

$$Y_i = M_{2n-i}, \qquad \mathcal{M}_{ij} = M_{2n-(i+j)}, \qquad i,j = 1,2,\dots n,$$

and

$$M_m = \left\langle \psi | \hat{H}^m | \psi \right\rangle .$$

It is assumed that all moments M_m are finite. Moreover, it was proved that a limit exists

$$\mathcal{E}_{\mathrm{g}} = \lim_{n\to\infty} \min\left(a_1^{(n)},\dots,a_n^{(n)}\right),$$

and the following inequality holds

$$\min\left(a_1^{(n+1)},\dots,a_{n+1}^{(n+1)}\right) \leqslant \min\left(a_1^{(n)},\dots,a_n^{(n)}\right).$$

For example, at the first order

$$E_{\mathrm{g}} \leqslant a_1^{(1)}, \qquad a_1^{(1)} = \langle\psi|\hat{H}|\psi\rangle,$$

and at the second order

$$\begin{aligned}
E_{\mathrm{g}} &\leqslant \min\left(a_1^{(2)},a_2^{(2)}\right) = \langle\psi|\hat{H}|\psi\rangle + \frac{K_3}{2K_2} - \left[\left(\frac{K_3}{2K_2}\right)^2 + K_2\right]^{1/2}, \\
a_1^{(2)} &= \langle\psi|\hat{H}|\psi\rangle + \frac{K_3}{2K_2} - \left[\left(\frac{K_3}{2K_2}\right)^2 + K_2\right]^{1/2}, \\
a_2^{(2)} &= \langle\psi|\hat{H}|\psi\rangle + \frac{K_3}{2K_2} + \left[\left(\frac{K_3}{2K_2}\right)^2 + K_2\right]^{1/2},
\end{aligned} \tag{5}$$

where K_2 and K_3 are the cumulants

$$K_2 = \left\langle \psi | (\hat{H} - \langle\psi|\hat{H}|\psi\rangle)^2 | \psi \right\rangle, \qquad K_3 = \left\langle \psi | (\hat{H} - \langle\psi|\hat{H}|\psi\rangle)^3 | \psi \right\rangle .$$

It is obvious that the second order upper bound (5) would lie below the first order upper bound for most physically relevant quantum models and most reasonable choices of the trial state $|\psi\rangle$.

Moreover, if $\langle\psi|E_{\mathrm{g}}\rangle \neq 0$, then $\lim_{n\to\infty} \min\left(a_1^{(n)},\dots,a_n^{(n)}\right) = E_{\mathrm{g}}$.

Furthermore, an excitation gap, should there happen to be any discernable one in the spectrum, can be approximated at the n-th order by the difference

$$G_n = a_2^{(n)} - a_1^{(n)}.$$

5. Infinitely improvable upper bounds for “physical” polaron at rest

For $\mathbf{P} = 0$, canonically transformed Fröhlich polaron model (3) can be written down as

$$\begin{aligned}
\mathcal{H}(f) &= \sum_{\mathbf{k}} b_{\mathbf{k}}^{+} b_{\mathbf{k}} + \left(\sum_{\mathbf{k}} \mathbf{k} b_{\mathbf{k}}^{+} b_{\mathbf{k}}\right)^2 - \alpha' \\
&\quad + \sum_{\mathbf{k}} \left[\left(1+k^2\right) f_k + V_k\right] (b_{\mathbf{k}}^{+} + b_{\mathbf{k}}) + 2\sum_{\mathbf{km}} (\mathbf{k}\cdot\mathbf{m}) f_k f_m b_{\mathbf{k}}^{+} b_{\mathbf{m}} \\
&\quad + \sum_{\mathbf{km}} (\mathbf{k}\cdot\mathbf{m}) f_k f_m (b_{\mathbf{k}}^{+} b_{\mathbf{m}}^{+} + b_{\mathbf{k}} b_{\mathbf{m}}) + 2\sum_{\mathbf{km}} (\mathbf{k}\cdot\mathbf{m}) f_k (b_{\mathbf{m}}^{+} b_{\mathbf{m}} b_{\mathbf{k}} + b_{\mathbf{k}}^{+} b_{\mathbf{m}}^{+} b_{\mathbf{m}}).
\end{aligned}$$

Let us choose phonon vacuum state $|0\rangle$ as a trial state $|\psi\rangle$ for $\mathcal{H}(f)$, so that inequality

$$E_{\mathrm{g}}(\alpha,0,k_{\mathrm{D}}) \leqslant \langle 0|\mathcal{H}(f)|0\rangle = 2\sum_{\mathbf{k}} V_k f_k + \sum_{\mathbf{k}} (1+k^2) f_k^2$$

holds, the right-hand side of which is minimized by

$$f_k = -V_k/(1+k^2),$$

and, eventually,

$$E_{\mathrm{g}}(\alpha,0,k_{\mathrm{D}}) \leqslant -\alpha\cdot\frac{2}{\pi}\mathrm{arctg}(k_{\mathrm{D}}), \qquad E_{\mathrm{g}}(\alpha) \leqslant -\alpha \quad \text{if} \quad k_{\mathrm{D}} \to \infty. \tag{6}$$

The bound (6) is precisely the upper bound derived in [11] for finite k_{D}. In order to better calculate the upper bounds at higher orders of generalized variational method it is only necessary to calculate moments $\langle 0|\mathcal{H}^m(f)|0\rangle$ for sufficiently large integer exponents m. This can be easily accomplished by means of the Wick theorem. The resulting multitudinous products of integrals of the kind

$$\int_0^{k_{\mathrm{D}}} \frac{k^p \mathrm{d}k}{(1+k^2)^q}\,, \qquad p, q - \text{non-negative integers}, \tag{7}$$

can be evaluated analytically wherever necessary as well as all the concomitant integrals over the angular variables of the corresponding wave vectors.

At the second order variational approximation (5)

$$\begin{aligned}
E_{\mathrm{g}}(\alpha,0,k_{\mathrm{D}}) &\leqslant \min\left(a_1^{(2)}, a_2^{(2)}\right) = -\alpha\frac{2}{\pi}\mathrm{arctg}(k_{\mathrm{D}}) + \frac{K_3}{2K_2} - \left[\left(\frac{K_3}{2K_2}\right)^2 + K_2\right]^{1/2}, \\
K_2 &= \alpha^2\frac{2}{3\pi^2}\left(\mathrm{arctg}(k_{\mathrm{D}}) - \frac{k_{\mathrm{D}}}{1+k_{\mathrm{D}}^2}\right)^2, \\
K_3 &= \alpha^2\frac{4}{3\pi^2}\left(\mathrm{arctg}(k_{\mathrm{D}}) - \frac{k_{\mathrm{D}}}{1+k_{\mathrm{D}}^2}\right)^2 \\
&\quad + \alpha^2\frac{8}{3\pi^2}\left(k_{\mathrm{D}} - \frac{3}{2}\mathrm{arctg}(k_{\mathrm{D}}) + \frac{1}{2}\frac{k_{\mathrm{D}}}{1+k_{\mathrm{D}}^2}\right)\left(\mathrm{arctg}(k_{\mathrm{D}}) - \frac{k_{\mathrm{D}}}{1+k_{\mathrm{D}}^2}\right) \\
&\quad + \alpha^3\frac{8}{9\pi^3}\left(\mathrm{arctg}(k_{\mathrm{D}}) - \frac{k_{\mathrm{D}}}{1+k_{\mathrm{D}}^2}\right)^3,
\end{aligned} \tag{8}$$

$$\lim_{\alpha\to\infty}\frac{E_{\mathrm{g}}(\alpha,0,k_{\mathrm{D}})}{\alpha} \leqslant -\frac{2}{\pi}\mathrm{arctg}(k_{\mathrm{D}}) - \frac{2}{3\pi}\left(\mathrm{arctg}(k_{\mathrm{D}}) - \frac{k_{\mathrm{D}}}{1+k_{\mathrm{D}}^2}\right),$$

while

$$\lim_{k_{\mathrm{D}}\to\infty} E_{\mathrm{g}}(\alpha,0,k_{\mathrm{D}}) \leqslant -\alpha.$$

The excitation gap is approximated at the second order as

$$G_2(\alpha,0,k_{\mathrm{D}}) = a_2^{(2)} - a_1^{(2)} = 2\left[\left(\frac{K_3}{2K_2}\right)^2 + K_2\right]^{1/2}$$

with

$$\lim_{\alpha\to 0} G_2(\alpha,0,k_{\mathrm{D}}) = 0 \qquad \text{and} \qquad \lim_{k_{\mathrm{D}}\to\infty} G_2(\alpha,0,k_{\mathrm{D}}) = \infty$$

correspondingly.

6. Infinitely improvable upper bounds for slow-moving "physical" polaron

The same trial state $|0\rangle$ can be employed in general case $\mathbf{P} \neq 0$ leading to inequality

$$E_{\mathrm{g}}(\alpha, \mathbf{P}, k_{\mathrm{D}}) \leqslant \langle 0|\mathcal{H}(f)|0\rangle = P^2 + 2\sum_{\mathbf{k}} V_k f_{\mathbf{k}} + \sum_{\mathbf{k}} \left(1+k^2\right) f_{\mathbf{k}}^2 - 2\sum_{\mathbf{k}} (\mathbf{P}\cdot\mathbf{k}) f_{\mathbf{k}}^2 + \left(\sum_{\mathbf{k}} f_{\mathbf{k}}^2 \mathbf{k}\right)^2 ,$$

the right-hand side of which is minimized by

$$f_{\mathbf{k}} = -V_k / \left[1 - 2\mathbf{k}\cdot\mathbf{P}(1-\eta) + k^2\right] ,$$

where η is defined self-consistently by the equation

$$\eta \mathbf{P} = \sum_{\mathbf{k}} f_{\mathbf{k}}^2 \mathbf{k} = \sum_{\mathbf{k}} V_k^2 \mathbf{k} / \left[1 - 2\mathbf{k}\cdot\mathbf{P}(1-\eta) + k^2\right] ,$$

or, alternatively, by

$$\eta P^2 = \sum_{\mathbf{k}} V_k^2 \mathbf{k}\cdot\mathbf{P} / \left[1 - 2\mathbf{k}\cdot\mathbf{P}(1-\eta) + k^2\right] ,$$

as was done in [11]. A compromise choice

$$f_{\mathbf{k}} = -V_k / \left[1 - 2\mathbf{k}\cdot\mathbf{P} + k^2\right] ,$$

eliminating all terms linear in Bose operators $b_{\mathbf{k}}^{+}$, $b_{\mathbf{k}}$ in (3), is equally possible too, while the simplest choice

$$f_k = -V_k/(1+k^2)$$

seems to be the choice of preference, especially if the persistent no-real-phonons condition $|\mathbf{P}| < 1$ is kept in mind and accounted for, because the technicalities of calculation of arbitrary order moments $\langle 0|\mathcal{H}^m(f)|0\rangle$ for this choice are exactly the same as they were in the case $\mathbf{P} = 0$, i.e. based on the Wick theorem exclusively and without involvement of any integrations over wave vectors more complicated and laborious than the integration (7).

7. Summary

It was shown that ground-state energy function $E_{\mathrm{g}}(\alpha, \mathbf{P}, k_{\mathrm{D}})$ of the slow-moving "physical" Fröhlich polaron can be approximated from above by infinite convergent sequence of upper bounds applicable for arbitrary values of the electron-phonon interaction strength α, polaron total momentum $\mathbf{P}$ and limiting wave vector k_{D}. These bounds are provided by the generalized variational method. Then, various experimentally observable polaron characteristics of practical interest can be derived from these bounds. The proposed algorithm for the construction of the upper bounds is well suited for implementation by means of modern programming and computational environments destined for seamless fusion of analytical and numerical computation within the same application, such as, for example, *Mathematica* or *Maple*. The usage of the parallel computing techniques is advisable and would be highly advantageous, too, due to the intrinsic nature of the algorithm heavily relying on the Wick theorem and recursion relations for massive analytic integrations over wave vectors.

The proposed approach is in no way limited to the Fröhlich polaron model considered above. It is rather universal and, being so, applicable without any major alterations to a broad range of polaron models of all sorts, including those ones concerned with manifestations of various polaron-like phenomena in quantum systems of lowered dimensions, such as quantum wells, wires and dots, with or without external electric and/or magnetic fields.

It would be highly desirable to complement convergent non-increasing upper bounds to the ground state energy $E_{\mathrm{g}}(\alpha, \mathbf{P}, k_{\mathrm{D}})$ with a sequence of infinitely improving non-decreasing lower bounds derived, for example, by means of the method of intermediate problems in the theory of linear semi-bounded self-adjoint operators on rigged Hilbert space, because, under favorable conditions, this combined set of two-side bounds might provide us with virtually precise magnitude for the energy of the slow-moving polaron. An algorithm for the construction of the lower bounds of this kind was proposed in [15, 16].

It is essential to stress once again that the method of the upper bounds, as presented above, was shown to be applicable to the so-called “physical” polaron model where k_{D} is finite, which property has been consistently employed throughout all calculations. Nevertheless, this does not mean at all that no generalization of the method to the case of the “field-theoretical” polaron model is possible. Actually, the main formal obstacle to such a generalization stems from the fact that the moments $\langle 0|\mathcal{H}^m(f)|0\rangle$ and, consequently, the cumulants, of higher orders diverge for $k_{\mathrm{D}} \to \infty$, as illustrated, for example, by equation (8) showing linear divergence in k_{D} of the third order cumulant K_3. The appearance of divergencies of this type is not the flaw of the method itself. It is rather incurred by improper choice of the phonon vacuum state $|0\rangle$ as the trial state $|\psi\rangle$, which choice is well-suited for extensive “physical” polaron calculations but inappropriate for the analysis of the properties of “field-theoretical” polaron. A research on upper bounds to the “field-theoretical” polaron ground state energy derived by generalized variational method with properly designed trial states will be published elsewhere.

A plain-style approach to the “field-theoretical” polaron problem is always feasible strictly within the framework of the “physical” polaron studies already undertaken, which would mean limiting the range of the interaction constant magnitude $0 < \alpha < \alpha_{\max}$ and choosing large enough k_{D} and large enough order n of the variational approximation scheme. Then, the ground state energy function $E_{\mathrm{g}}(\alpha, k_{\mathrm{D}}, \mathbf{P})$ of the “physical” polaron and, consequently, its upper bounds, will approximate the corresponding function $E_{\mathrm{g}}(\alpha, k_{\mathrm{D}} \to \infty, \mathbf{P})$ of the “field-theoretical” polaron from above for this restricted domain of α. An alternative option going along the same pattern of reasoning would be to majorize initial Hamiltonian (3) from above by modifying the electron-phonon interaction as $V_k \to V_k \mathrm{e}^{-\varepsilon k^2}$, $\varepsilon \geqslant 0$. This measure ensures finiteness of all moments and cumulants under the passage to the limit $k_{\mathrm{D}} \to \infty$ which could be undertaken now immediately at the beginning of the calculations. Then, to obtain reasonable upper bounds to the ground state energy of the “field-theoretical” polaron for any value of α belonging to the restricted domain $0 < \alpha < \alpha_{\max}$, one has to choose small enough ε and carry out calculations at large enough order n of the generalized variational method. Exemplary calculations of this kind will be published elsewhere too.

Acknowledgements

This work was supported by the RAS research program “Mathematical Methods in Nonlinear Dynamics” and by the RFBR grant No. 09–01–00086–a.

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Нескінченнопокращені верхні границі в теорії поляронів

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За допомогою узагальненого варіаційного методу було отримано нескінченнозбіжну послідовність покращених незростаючих верхніх границь до низьколежачої гілки спектральної кривої “фізичного” полярона Фроліха в основному енергетичному стані, що повільно рухається, і яка є прилеглою до основного енергетичного стану полярона в спокої. Запропонований підхід особливо підходить для громіздких аналітичних і числових обчислень експериментально вимірюваних властивостей реалістичних поляронів, таких як тензор оберненої ефективної маси і щілина збуджень, він може бути розвинутий навіть далі, без значних змін, для опису численних поляроноподібних моделей, зокрема таких, які описують полярони різних сортів, розміщених у зовнішніх магнітних та електричних полях.

Ключові слова: *модель полярона Фроліха, оцінки верхніх границь, варіаційний метод, енергія основного стану*