WICK'S SYMBOL APPROACH TO THE FRÖHLICH POLARON PROBLEM

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Various upper bound estimates for the ground state energy of the quantized Fröhlich's model of Landau–Pekar polaron were derived by means of a variational method based on the Wick symbol formalism and the theory of coherent states. The bounds so obtained are valid for arbitrary strengths of the electron-phonon interaction. A generalization of the proposed formalism for the case of the Fröhlich polaron model in an external magnetic field is outlined as well.

1. The Polaron Concept and a Landau–Pekar–Fröhlich Polaron

It is well known that a local change in the electronic state in a crystal leads to the corresponding local changes in the interactions between individual atoms of the crystal and, hence, to the excitation of atomic oscillations, i.e. the excitation of phonons. Vice versa, any local change in the state of lattice ions alters the local electronic state. It is common in this situation to talk about 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. When an electron moves through the crystal, the state of polarization can move together with it. This combined quantum state of "moving electron + accompanying polarization"may be considered as a sort of 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 the self-localization of an 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 formation of a polaron is a consequence of the dynamic electron-lattice interaction which is also responsible for the scattering of charge carriers, phonon frequency renormalization, as well as the screening of the interaction between charge carriers in solids.

The concept of polaron was introduced first by L.D. Landau in a very short paper [1] followed by S.I. Pekar who investigated the most essential properties of a stationary polaron in the limiting case of very intense electron-phonon interaction, so that the polaron behavior could be analyzed in the so-called adiabatic approximation. Subsequently, Landau and Pekar [3] investigated the self-energy and the effective mass of a polaron for the adiabatic or strong-coupling regime. Many other famous researchers, among them H. Fröhlich, R. Feynman, and N.N. Bogolyubov, have contributed to the development of the polaron theory later on [4–9].

Despite the apparent simplicity of the formulation, the polaron problem has not yet been solved and continues to attract much attention. It plays an important role in statistical mechanics and quantum field theory, because it can be considered as the simplest example of a nonrelativistic quantum particle interacting with a quantum field. Therefore, many sophisticated mathematical techniques have been tested for the first time, using this problem as a model. Shining examples of this are Feynman's functional integration method and alternative, closely related to it, Bogolyubov's method of chronological or T-products [9] in the theory of a particle interacting with bosonic fields. These methods were applied first to the polaron problem, before becoming conventional major methods used in statistical mechanics and quantum field theory. Another example of a novel technique originated by the polaron studies and, at the same time, one of the most important contributions to polaron theory, made by N.N. Bogolyubov, is the rigorous adiabatic perturbation theory [8] created in 1950, in which the kinetic energy of the phonon field was treated as a small perturbation. The theory is translationally invariant (which is important for the development of the strong coupling theory) and reproduced, in the zeroth order, the results for large values of the interaction constant that had already been derived. Moreover, polaron theory is an expanding field of investigation in solid state physics, because polarons are not only theoretical constructs but practically observable physical objects (see, e.g., [12]).

Interest in the polaron problem is growing: in addition to the earlier fields of research dealing mostly with spatially homogeneous systems, the investigation of charged-particle interactions with elementary excitations in spatially inhomogeneous low-dimensional systems, such as quantum wells, wires, and boxes, is gaining significance. Experimental techniques have had great success in producing such systems with well-controlled parameters, thus allowing the manufacturing of structures with predictable characteristics. Electron–phonon interactions of the polaron type play a very important role in the properties of low-dimensional quantum systems.

In spite of all these efforts and unarguable achievements, there are still unsolved problems of considerable theoretical significance in the theory of polarons, especially those regarding polarons in the presence of a magnetic field. Thus, it was claimed in [23, 24] that the Feynman–Jensen inequality well-known from numerous applications of the path integral approach,

$$F \leq F^{\rm tr} + \frac{1}{\beta}\frac{\int \mathcal{D}x[S - S^{\rm tr}]e^{S^{\rm tr}}}{\int \mathcal{D}x e^{S^{\rm tr}}}, \tag{1}$$

cannot remain valid in its unmodified form unless additional constraints are imposed on the variational parameters of the trial model. Here, the action of a system reads $S = \int_0^\beta d\tau L$ with Lagrangian L, and $S^{\rm tr}$ is the action of some trial system. Both actions are real and expressed in the imaginary time variables $t \to -i\hbar\tau$. Inequality (1) is similar to the Bogolyubov inequality [26, 27] which provides the following upper bound to the free energy F of a system described by the Hamiltonian H:

$$F \leq F^{\rm tr} - \frac{1}{\beta}\frac{{\rm Tr}[H - H^{\rm tr}]e^{-\beta H^{\rm tr}}}{{\rm Tr}e^{-\beta H^{\rm tr}}}. \tag{2}$$

Not surprisingly, it was also stated in [25] that the trial-functional based version of inequality (2), elaborated in [9], is not applicable to the linearized Fröhlich polaron model in the presence of an external uniform magnetic field. Despite the abundant research work and the broad discussion on this issue (see, e.g., [23–25, 28–33] and refs. therein), the problem of the path integral approach applicability to polarons in a magnetic field has not been settled yet.

Needless to say that most of these difficulties and drawbacks of conventional methods are stipulated not in the least measure by complexities, obscurities, and sometimes ambiguities, as well as the lack of mathematical rigor, which are frequent in conventional powerful methods of mathematical physics having been routinely employed in polaron studies so far. Therefore, there always has been and will be a strong demand for simple, transparent, theoretically and mathematically well-grounded, and reliable techniques allowing one to analyze various polaron characteristics analytically and numerically. Variational approaches have always been contemplated as the ones being able to meet these requirements in the best way. Therefore, such an approach based on the Wick symbol formalism and the theory of coherent states [14–16] has been developed [17–21] primarily for the investigation of various polaron-like quantum systems. In what follows, a summary of this approach, amended and rectified, is outlined.

The model under consideration is the standard quantized Fröhlich polaron Hamiltonian introduced by H. Fröhlich [6, 13]

$$H = \frac{\hat{\mathbf{p}}^2}{2m} + \hbar\omega\sum_{\mathbf{k}} a^+_{\mathbf{k}} a_{\mathbf{k}} + \sum_{\mathbf{k}} \left(V^*(k) a^+_{\mathbf{k}} e^{-i\mathbf{k}\hat{\mathbf{r}}} + {\rm h.c.}\right), \tag{3}$$

where

$$V(k) = -i\frac{\hbar\omega}{k}\left(\frac{4\pi\alpha}{V}\sqrt{\frac{\hbar}{2m\omega}}\right)^{1/2},$$

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

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

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

$$[a_{\mathbf{k}}, a^+_{\mathbf{k}'}] = \delta_{\mathbf{k}\mathbf{k}'}, \quad [a_{\mathbf{k}}, a_{\mathbf{k}'}] = 0, \tag{4}$$

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

$$\mathbf{k} = \left\{\frac{2\pi}{La}n_1, \frac{2\pi}{La}n_2, \frac{2\pi}{La}n_3\right\},$$

$$n_i = 0, \pm 1, \pm 2, ..., \pm\frac{1}{2}(L-1), \quad i = 1, 2, 3,$$

where a^3 is the volume of an elementary crystal cell, and L^3 is the number of these cells within the volume

V of the crystal. The limit $V \to \infty$ corresponds to the transition rule from the quasidiscrete to the continuous spectrum

$$\lim_{V\to\infty} \frac{1}{V}\sum_{\mathbf{k}} ... \to \frac{1}{(2\pi)^3}\int d\mathbf{k}...$$

to be applied to all relevant expressions. For the matter of convenience, it is assumed further on that $\hbar = \omega = m = 1$.

2. Wick's Symbol Approach to Fröhlich Polaron

As a result of the unitary transformation

$$\tilde{H} = U^+HU,\ \ U = \prod_{\mathbf{k}} e^{-ia^+_{\mathbf{k}}a_{\mathbf{k}}\chi(\mathbf{k})\mathbf{k}\hat{\mathbf{r}}},\ \ U^+U = 1, \tag{5}$$

the original Hamiltonian (3) can be changed into a new one

$$\tilde{H} = \frac{1}{2}\left(\hat{\mathbf{p}} - \sum_{\mathbf{k}}\chi(\mathbf{k})\mathbf{k}a^+_{\mathbf{k}}a_{\mathbf{k}}\right)^2 + \sum_{\mathbf{k}} a^+_{\mathbf{k}}a_{\mathbf{k}} +$$

$$+\sum_{\mathbf{k}}\left(V^*(k)a^+_{\mathbf{k}}e^{-i(1-\chi(\mathbf{k})\mathbf{k}\hat{\mathbf{r}}} + \text{h.c.}\right), \tag{6}$$

but possessing the same ground state energy. The components of the momentum and position operators can be represented in terms of the Bose operators

$$\hat{\mathbf{p}} = i\left(\frac{\eta}{2}\right)^{1/2}(\mathbf{b}^+ - \mathbf{b}),\ \ \hat{\mathbf{r}} = \left(\frac{1}{2\eta}\right)^{1/2}(\mathbf{b} + \mathbf{b}^+), \tag{7}$$

where

$$\mathbf{b} = (b_x, b_y, b_z),\ \ [b_i, b_j] = 0,\ \ [b_i, b_j^+] = \delta_{ij}, \tag{8}$$

and η is an arbitrary positive parameter. By means of the well-known operator identity

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}}\cdot e^{\hat{B}}\cdot e^{-\frac{1}{2}[\hat{A},\hat{B}]} \tag{9}$$

which only holds if the commutator $[\hat{A}, \hat{B}]$ is a complex number, all the exponential operator functions in Hamiltonian (6) can be disentangled, and the resulting Hamiltonian can be written as

$$\tilde{H} = \frac{1}{2}\left(i\sqrt{\frac{\eta}{2}}(\mathbf{b}^+ - \mathbf{b}) - \sum_{\mathbf{k}}\chi(\mathbf{k})\mathbf{k}a^+_{\mathbf{k}}a_{\mathbf{k}}\right)^2 + \sum_{\mathbf{k}} a^+_{\mathbf{k}}a_{\mathbf{k}} +$$

$$+\sum_{\mathbf{k}}\left(V^*(k)a^+_{\mathbf{k}}e^{-\frac{(1-\chi(\mathbf{k}))^2}{4\eta}k^2}e^{-i(1-\chi(\mathbf{k}))\sqrt{\frac{1}{2\eta}}\mathbf{k}\mathbf{b}^+}\times\right.$$

$$\left.\times e^{-i(1-\chi(\mathbf{k}))\sqrt{\frac{1}{2\eta}}\mathbf{k}\mathbf{b}} + \text{h.c.}\right). \tag{10}$$

It is known that the variational upper bound to the ground state energy

$$E_0 \le \langle\Psi|\tilde{H}|\Psi\rangle \tag{11}$$

holds for any trial state Ψ. Let us choose Ψ to be a direct product of coherent states, i.e.

$$|\Psi\rangle = \prod_{\mathbf{k}}\otimes|z_{\mathbf{k}}\rangle\otimes|\mathbf{z}\rangle,\ \ |\mathbf{z}\rangle = |z_x\rangle\otimes|z_y\rangle\otimes|z_z\rangle, \tag{12}$$

$$a_{\mathbf{k}}|z_{\mathbf{k}}\rangle = z_{\mathbf{k}}|z_{\mathbf{k}}\rangle,\ \ \mathbf{b}|\mathbf{z}\rangle = \mathbf{z}|\mathbf{z}\rangle,\ \ \mathbf{z} = (z_x, z_y, z_z), \tag{13}$$

$$b_i|z_i\rangle = z_i|z_i\rangle,\ \ i = x, y, z, \tag{14}$$

so that inequality (11) leads to the bound

$$E_0 \le \inf_{\{\mathbf{z},\mathbf{z}^*,\{z_{\mathbf{k}},z^*_{\mathbf{k}}\}\}} W(\mathbf{z}, \mathbf{z}^*, \{z_{\mathbf{k}}, z^*_{\mathbf{k}}\}, \eta, \chi(\mathbf{k})), \tag{15}$$

where the expression

$$W(\mathbf{z}, \mathbf{z}^*, \{z_{\mathbf{k}}, z^*_{\mathbf{k}}\}, \eta, \chi(\mathbf{k})) =$$

$$= \frac{1}{2}\left(i\sqrt{\frac{\eta}{2}}(\mathbf{z}^* - \mathbf{z}) - \sum_{\mathbf{k}}\chi(\mathbf{k})\mathbf{k}z^*_{\mathbf{k}}z_{\mathbf{k}}\right)^2 + \frac{3\eta}{4} +$$

$$+\sum_{\mathbf{k}}\left(1 + \frac{k^2}{2}\chi^2(\mathbf{k})\right)z^*_{\mathbf{k}}z_{\mathbf{k}} + \sum_{\mathbf{k}} e^{-\frac{(1-\chi(\mathbf{k}))^2}{4\eta}k^2}\times$$

$$\times\left(V^*(k)z^*_{\mathbf{k}}e^{-i(1-\chi(\mathbf{k}))\sqrt{\frac{1}{2\eta}}\mathbf{k}(\mathbf{z}^*+\mathbf{z})} + \text{h.c.}\right). \tag{16}$$

is the so-called Wick symbol for Hamiltonian (10).

Actually, this expression represents a set of Wick symbols parametrized by $\chi(\mathbf{k})$ and η, and the infimum in inequality (15) is taken over the whole set of complex numbers $\mathbf{z}^*$, $\mathbf{z}$, $\{z^*_{\mathbf{k}}, z_{\mathbf{k}}\}$. Changing the variables

$$z_{\mathbf{k}} = z'_{\mathbf{k}}e^{-i(1-\chi(\mathbf{k}))\sqrt{\frac{1}{2\eta}}\mathbf{k}(\mathbf{z}^*+\mathbf{z})},$$

$$z^*_{\mathbf{k}} = z'^*_{\mathbf{k}}e^{+i(1-\chi(\mathbf{k}))\sqrt{\frac{1}{2\eta}}\mathbf{k}(\mathbf{z}^*+\mathbf{z})}, \tag{17}$$

and replacing, as usual, the summation over **k** by the integration over the whole range of phonon wave-vectors, one arrives at the following upper bound to the Fröhlich polaron ground state energy

$$E_0 \leq \inf_{\{\eta,\chi(k)\}} \left\{ \frac{3\eta}{4} - \frac{\alpha\sqrt{2}}{\pi} \int\limits_0^{k_D} dk \frac{e^{-\frac{(1-\chi(k))^2}{2\eta}k^2}}{1+\frac{k^2}{2}\chi^2(k)} \right\}, \quad (18)$$

where $k_D = 2^{1/3}\pi/a$ is the Debye wave-vector, a being the lattice constant. In what follows, it is assumed, as usual, that $k_D \to \infty$. Variational equations for the parameters $\chi(k)$ and η are

$$\frac{1-\chi(k)}{\eta}\left(1+\frac{k^2}{2}\chi^2(k)\right) - \chi(k) = 0, \quad (19)$$

and

$$\frac{3}{4} - \frac{\alpha}{\pi\sqrt{2}\eta^2}\int\limits_0^{\infty} dk k^2 \frac{(1-\chi(k))^2}{1+\frac{k^2}{2}\chi^2(k)} \exp\left(\frac{(1-\chi(k))^2}{2\eta}k^2\right) = 0, \quad (20)$$

respectively.

In principle, an explicit expression for $\chi(k)$ as a function of k and η can be derived from Eq. (19) and substituted into Eq. 20), thus leading to a closed equation for the only unknown variational parameter η. But the resulting equation would be so cumbersome that it could be treated only numerically. Though this work is under way now, here we would like to offer a simplified analysis of the bound estimate (18) only to show that even the weaker bounds originating from bound (18) might approximate the polaron ground state energy quite well in comparison to the best upper bound estimates obtained so far by various other methods. To derive a simplified upper bound, let us assume firstly that

$$\chi(k) \equiv \chi, \;\; \chi \in [0,1] \quad (21)$$

for all wave vectors k. We also introduce new variational parameters u and v such that

$$v^2 = \frac{(1-\chi)^2}{\eta\chi^2}, \;\; v \in [0,\infty], \quad (22)$$

$$u = \frac{1}{\sqrt{\eta}}, \;\; u \in [0,\infty], \quad (23)$$

which steps yield

$$E_0 \leq \inf_{\{u,v\}} \left\{ \frac{3}{4u^2} - \alpha\frac{v+u}{u}(1-\Phi(v))e^{v^2} \right\}, \quad (24)$$

where

$$\Phi(v) = \frac{2}{\sqrt{\pi}} \int\limits_0^v dx e^{-x^2}. \quad (25)$$

The obvious limiting cases for bound (24) are

$$E_0 \leq -\alpha \quad \text{if} \quad u \to \infty, \;\; v = 0, \quad (26)$$

and

$$E_0 \leq -\frac{\alpha^2}{3\pi}, \quad \text{if} \quad v \to \infty, \quad u = \frac{3\sqrt{\pi}}{2\alpha}. \quad (27)$$

Both bounds (26) and (27) are well-known since long ago [7, 22], though they were originally derived in a much more complicated way, and hold for an arbitrary value of the electron-phonon interaction constant α. The fact that bound (26) works well in the weak coupling limit, while bound (27) performs very well just in the opposite case of the strong electron-phonon coupling, compounded with another fact that both bounds were actually generated by one and the same simplified bound (24), infers that even this simplified bound, if properly treated, might provide upper bounds on par with the existing ones. Really, for any fixed values of α and v, the optimal value of the variational parameter u is

$$u = \frac{3}{2\alpha v}\frac{e^{-v^2}}{1-\Phi(v)}. \quad (28)$$

For this particular value of u, bound (24) yields another bound

$$E_0 \leq \inf_{\{v\}} \left\{ -\alpha(1-\Phi(v))e^{v^2} - \frac{\alpha^2}{3}\left(v(1-\Phi(v))e^{v^2}\right)^2 \right\} \quad (29)$$

which holds, again, for arbitrary values of α and is remarkable on its own because two distinctive terms - the one linear in α and the other quadratic in α - are clearly visible. Bound (29) was investigated by numerical minimization over v. It was shown that $v = 0$ is the optimal value of the variational parameter v for all magnitudes of α up to $\alpha = 8.53$ approximately. Therefore, bound (26) holds as the best bound for this range of the interaction constant. For $\alpha \geq 8.53$, the second minimum of the right-hand side of inequality (29) at, approximately, $v = 2.52147$ becomes deeper than the persistent local minimum at $v = 0$. Nevertheless, such a behavior of the bound does not imply any "phase transition" in the polaron ground state, because it was rigorously proved [34] that no such transition actually exists. It is rather an artifact caused by a particular choice (21) of the function $\chi(k)$. The optimal choice (19) must yield a much better and smoother upper bound for intermediate values $1 < \alpha < 10$ of the interaction parameter, and the only objective against such a choice would be the complexity of the analytic form of the ensuing upper bound. Hence, in light of all the aforesaid and the results obtained so far, simplified choices for $\chi(k)$, for example, like this one

$$\chi(k) = \lambda e^{-\gamma k}, \quad \lambda \in [0,1], \quad \gamma \geq 0$$

with two independent variational parameters λ and γ, are undoubtedly worth considering.

3. Fröhlich Polaron in a Magnetic Field

In the case of a polaron in a nonzero uniform external magnetic field, the corresponding Hamiltonian is

$$H = \frac{1}{2}\left(\hat{p}_x - \frac{\omega_c}{2}\hat{y}\right)^2 + \frac{1}{2}\left(\hat{p}_y + \frac{\omega_c}{2}\hat{x}\right)^2 + \frac{1}{2}\hat{p}_z^2 +$$

$$+ \sum_{\mathbf{k}} a^+_{\mathbf{k}} a_{\mathbf{k}} + \sum_{\mathbf{k}} \left(V^*(k) a^+_{\mathbf{k}} e^{-i\mathbf{k}\hat{\mathbf{r}}} + \text{h.c.}\right), \tag{30}$$

where ω_c is the cyclotron frequency in units of the optical phonon frequency ω. A spatial anisotropy caused by the external magnetic field $\mathbf{B}$ in the direction of the z axis brings about an asymmetry in the bosonic representation (7) which now reads as

$$\hat{p}_j = i\left(\frac{\eta_j}{2}\right)^{1/2}(b_j - b_j^+), \;\; \hat{r}_j = \left(\frac{1}{2\eta_j}\right)^{1/2}(b_j + b_j^+), \tag{31}$$

$$j = x, y, z,$$

where $\eta_x = \eta_y = \eta$ and $\eta_z \neq \eta$ unlike in the totally symmetric case of zero magnetic field, where $\eta_x = \eta_y = \eta_z = \eta$. The same transformation (5) can be applied to Hamiltonian (30) accompanied by all the subsequent machinery of the corresponding Wick symbol derivation. Being similar to the above-treated case of zero magnetic field, the details of this derivation are omitted here, and only the final expression for the upper bound

$$E_0 \leq \inf_{\{\eta,\eta_z,\{\chi(\mathbf{k})\}\}}\left\{\frac{\eta}{2} + \frac{\omega_c^2}{8\eta} + \frac{\eta_z}{4} - \frac{\alpha}{\pi\sqrt{2}}\int_0^\pi d\theta \sin(\theta)\times\right.$$

$$\left.\times\int_0^\infty dk \frac{e^{-\frac{(1-\chi(\mathbf{k}))^2}{2}k^2\left(\frac{\sin^2(\theta)}{\eta} + \frac{\cos^2(\theta)}{\eta_z}\right)}}{1 + \frac{k^2}{2}\chi^2(\mathbf{k})}\right\} \tag{32}$$

is presented. For $\alpha = 0$, the right-hand side of (32) is minimized for $\eta_z = 0$, $\eta = \omega/2$, thus providing the bound

$$E_0 \leq \frac{\omega_c}{2} \tag{33}$$

which corresponds to a precise value of the ground state energy for an arbitrary cyclotron frequency ω_c. The opposite case $\omega_c = 0$, $\alpha \neq 0$, reproduces the upper bound (18) predictably.

Again, it is convenient to introduce new variational parameters

$$\chi(\mathbf{k}) \equiv \chi, \;\; \chi \in [0,1], \tag{34}$$

$$v^2 = \frac{(1-\chi)^2}{\eta\chi^2}, \;\; v \in [0,\infty], \tag{35}$$

$$u = \frac{1}{\sqrt{\eta}}, \;\; u \in [0,\infty], \tag{36}$$

$$u_z = \sqrt{\frac{\eta}{\eta_z}}, \;\; u_z \in [0,\infty], \tag{37}$$

so that

$$E_0 \leq \inf_{(u,u_z,v)}\left\{\frac{1}{2u^2} + \frac{u^2\omega_c^2}{8} + \frac{1}{4u^2u_z^2} - \alpha\frac{v+u}{2u}\int_{-1}^{1} dx\times\right.$$

$$\left.\times\left(1-\Phi\left(v(1+(u_z^2-1)x^2)^{1/2}\right)\right)e^{v^2(1+(u_z^2-1)x^2)}\right\}. \tag{38}$$

Inequality (38) can also be written down as

$$E_0 \leq \inf_{(u,u_z,v)}\left\{\frac{1}{2u^2} + \frac{u^2\omega_c^2}{8} + \frac{1}{4u^2u_z^2} - \alpha\frac{v+u}{u\sqrt{\pi}}\int_{-1}^{1} dx\times\right.$$

$$\left.\times\int_0^\infty dt \frac{te^{-t^2}}{\sqrt{t^2 + v^2 + v^2(u_z^2-1)x^2}}\right\}, \tag{39}$$

whose form allows for the explicit integration over x because

$$\int_{-1}^{1} \frac{dx}{\sqrt{t^2 + v^2(1 + (u_z^2-1)x^2)}} =$$

$$\frac{1}{v\sqrt{u_z^2-1}}\ln\left(\frac{\sqrt{t^2+v^2u_z^2}+v\sqrt{u_z^2-1}}{\sqrt{t^2+v^2u_z^2}-v\sqrt{u_z^2-1}}\right) \quad \text{if} \quad u_z^2>1,$$

and

$$\int_{-1}^{1}\frac{dx}{\sqrt{t^2+v^2(1+(u_z^2-1)x^2)}}=$$

$$\frac{2}{v\sqrt{1-u_z^2}}\arcsin\left(v\sqrt{\frac{1-u_z^2}{t^2+v^2}}\right) \quad \text{if} \quad 0\le u_z^2<1.$$

Being complicated and tractable only numerically, the general upper bound (32) is, nevertheless, a source of various useful simplified bounds applicable in limiting cases. Thus, the choice of the parameters

$$\chi(\mathbf{k})\equiv 1, \quad \eta=\frac{\omega_c}{2}, \quad \eta_z=0,$$

provides the upper bound in the weak electron-phonon coupling limit $\alpha\le 1$ for an arbitrary cyclotron frequency ω_c

$$E_0\le -\alpha+\frac{\omega_c}{2}, \tag{40}$$

while the opposite choice

$$\chi(\mathbf{k})\equiv 0, \quad \eta=\eta_z=\frac{4}{9\pi}\alpha,$$

corresponds to the limit of the strong electron-phonon coupling $\alpha\gg 1$ with a fixed cyclotron frequency ω_c

$$E_0\le -\frac{\alpha^2}{3\pi}+\frac{9\pi}{32}\left(\frac{\omega_c}{\alpha}\right)^2, \tag{41}$$

wherefrom it is seen that the influence of a magnetic field is negligible for

$$\frac{27}{32}\left(\frac{\pi\omega_c}{\alpha^2}\right)^2\ll 1.$$

Now let us put

$$\chi(\mathbf{k})\equiv 0, \quad \eta=\eta_z=\tilde\eta\omega_c,$$

in inequality (32). Thus, we obtain the inequality

$$E_0\le\omega_c\left(\frac14\left(3\tilde\eta+\frac{1}{2\tilde\eta}\right)-\alpha\sqrt{\frac{\tilde\eta}{\pi\omega_c}}\right) \tag{42}$$

which is anticipated to perform reasonably well in the limit of large $\alpha\gg 1$ and arbitrary ω_c if its right-hand side is minimized with respect to the new variational parameter $\tilde\eta$. The optimal value of $\tilde\eta$ is determined by the equation

$$6\tilde\eta^2-4\theta\tilde\eta^{3/2}-1=0, \qquad \theta=\frac{\alpha}{\sqrt{\pi\omega_c}} \tag{43}$$

which has the unique solution

$$\tilde\eta=\frac{\Delta^2}{36}\left(1+\frac{1}{\sqrt\Delta}\left(\Delta+\frac{2\sqrt3}{|u+v|^{1/2}}\right)^{1/2}\right)^2, \tag{44}$$

where

$$\Delta=\theta+6\sqrt3|u+v|^{3/2}, \quad u=\frac16\left((\theta^4+8)^{1/2}-\theta^2\right)^{1/3},$$

$$v=-\frac16\left((\theta^4+8)^{1/2}+\theta^2\right)^{1/3}.$$

Finally, for large $\alpha\gg 1$ and commensurable ω_c, i.e.

$$\frac{27}{32}\left(\frac{\pi\omega_c}{\alpha^2}\right)^2\approx 1,$$

it seems justified to assume that

$$\eta=\frac{\omega_c}{2}, \quad \eta_z=\omega_c\eta.$$

For this choice, the upper bounds would be

$$E_0\le\omega_c\inf_{\{\tilde\eta\}}\left\{\frac{\tilde\eta+4}{8}-\frac{\theta}{\sqrt2}\sqrt{\frac{\tilde\eta}{1-\tilde\eta}}\operatorname{arcsh}\left(\sqrt{\frac{1-\tilde\eta}{\tilde\eta}}\right)\right\}$$

for $0\le\tilde\eta\le 1$ and

$$E_0\le\omega_c\inf_{\{\tilde\eta\}}\left\{\frac{\tilde\eta+4}{8}-\frac{\theta}{\sqrt2}\sqrt{\frac{\tilde\eta}{\tilde\eta-1}}\arcsin\left(\sqrt{\frac{\tilde\eta-1}{\tilde\eta}}\right)\right\}$$

for $1\le\tilde\eta\le\infty$. Here, $\theta=\alpha/\sqrt{\pi\omega_c}$, and the only variational parameter $\tilde\eta$ is determined by the extremality conditions

$$1-\frac{2\sqrt2\theta}{\sqrt{\tilde\eta(1-\tilde\eta)^3}}\left(\operatorname{arcsh}\left(\sqrt{\frac{1-\tilde\eta}{\tilde\eta}}\right)-(1-\tilde\eta)^{1/2}\right)$$

for $0\le\tilde\eta\le 1$ and

$$1-\frac{2\sqrt2\theta}{\sqrt{\tilde\eta(\tilde\eta-1)^3}}\left((\tilde\eta-1)^{1/2}-\arcsin\left(\sqrt{\frac{\tilde\eta-1}{\tilde\eta}}\right)\right)$$

for $1\le\tilde\eta\le\infty$.

4. Summary

It is shown that a comprehensive and flexible variational approach to the investigation of various polaron-like quantum models can be developed on the basis of the Wick symbol formalism and the theory of coherent states. The approach is theoretically well-grounded and mathematically transparent and allows for analytical, as well as numerical, calculations of important physical characteristics of polarons, including polarons in the presence of an external magnetic field. It is important to stress that, due to its variational nature, all the upper bounds to the polaron ground state energy, yielded within the frame of this approach, hold for arbitrary values of the polaron model parameters. The upper bounds, outlined in the present paper, are pliable to further improvements by analytical and numerical methods. The proposed approach can be straightforwardly generalized for the investigation of the low-lying branch of the polaron excitation energy spectral curve adjacent to the ground state energy of a polaron at rest, thus providing the upper bound estimates for the energy spectral curve of a slowly moving polaron as a function of the electron-phonon interaction constant and the total momentum of a polaron.

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МЕТОД СИМВОЛІВ ВІКА В ЗАСТОСУВАННІ
ДО ПРОБЛЕМИ ПОЛЯРОНА ФРЬОЛІХА

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Р е з ю м е

Показано, що гнучкий варіаційний підхід до дослідження різноманітних квантових моделей поляронного типу може бути розвинений на основі формалізму символів Віка та теорії когерентних станів. Цей підхід добре обґрунтовано теоретично, прозорий з математичної точки зору і дозволяє обчислювати як аналітично, так і за допомогою числових методів важливі фізичні характеристики поляронних систем, також поляронів у зовнішньому магнітному полі. Важливо відзначити, що, завдяки варіаційній природі запропонованого підходу, усі наведені вище верхні оцінки для енергії основного стану полярона, одержані за його допомогою, справедливі для довільних значень параметрів, що фігурують у моделі полярона. Оцінки зверху, які наведено в цій роботі, можуть бути поліпшені за допомогою як аналітичних, так і числових методів. Запропонований підхід допускає безпосереднє пряме узагальнення для дослідження низьколежачої гілки спектра збуджених станів полярона, що примикає до енергії основного стану полярона, який перебуває у спокої, це узагальнення дозволяє одержати оцінки зверху для енергетичного спектра полярона, що повільно рухається, які функціонально залежать від константи електрон-фононної взаємодії і повного імпульсу полярона, що рухається.