THE ABDUS SALAM INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

THE BOGOLUBOV REPRESENTATION OF THE POLARON MODEL
AND ITS COMPLETELY INTEGRABLE RPA-APPROXIMATION
PART 1

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Abstract

The polaron model in ionic crystal is studied in the N. Bogolubov representation using a special RPA-approximation. A new exactly solvable approximated polaron model is derived and described in detail. Its free energy at finite temperature is calculated analytically. The polaron free energy in the constant magnetic field at finite temperature is also discussed. Based on the structure of the N. Bogolubov unitary transformed polaron Hamiltonian a very important new result is stated: the full polaron model is exactly solvable.
1 Introduction

The polaron concept, first introduced by Landau \[3\], is one of the main pillars on which the theoretical analysis of materials with strong electron-phonon coupling rests. In these compounds, the coupling between the electron and the lattice leads to a lattice deformation whose potential tends to bind the electron to the deformed region of the crystal. This process, which has been called self-trapping because the potential depends on the state of the electron, does not destroy translational invariance, even if the lattice deformation is confined to a single lattice site (small polaron) \[1, 13, 2, 6\]. Quantum mechanical tunneling between different lattice sites restores this symmetry and ensures that a self-trapped electron forms an itinerant polaronic quasi-particle.

A polaron is a quasiparticle composed of a charge and its accompanying polarization field. A slow moving electron in a dielectric crystal, interacting with lattice ions through long-range forces will permanently be surrounded by a region of lattice polarization and deformation caused by the moving electron. Moving through the crystal, the electron carries the lattice distortion with it, thus one speaks of a cloud of phonons accompanying the electron.

The resulting lattice polarization acts as a potential well that hinders the movements of the charge, thus decreasing its mobility. Polarons have spin, though two close-by polarons are spinless. The latter is called a bipolaron. In materials science and chemistry, a polaron is formed when a charge within a molecular chain influences the local nuclear geometry, causing an attenuation (or even reversal) of nearby bond alternation amplitudes. This “excited state” possesses an energy level between the lower and upper bands.

As is well known \[1, 13, 9, 10\], the quantum model of the polaron in the ion crystal of volume \(\Lambda \subset \mathbb{E}^3\) can be described \[1, 13\] by means of the Hamiltonian operator

\[
\hat{H}_p = \frac{\hat{p}^2}{2m} \otimes 1 + \sum_{(f)} 1 \otimes (\hat{b}_f^+ \hat{b}_f + 1/2)\hbar \omega_f + + \frac{1}{\Lambda^{1/2}} \sum_{(f)} L_f \left( \frac{\hbar}{2\omega_f} \right)^{1/2} e^{i<f,r>} 1 \otimes (\hat{b}_f + \hat{b}_{-f}^+),
\]

acting in the Hilbert space \(L_2(\Lambda; \mathbb{C}) \otimes \Phi(\Lambda; \mathbb{C})\), where \(\Phi(\Lambda; \mathbb{C})\) is the corresponding Fock space for the phonon quasi-particle states in the crystal, \(m\) is an effective electron mass, \(\hat{p} := \frac{\hbar}{i} \nabla\) is its momentum operator, \(\hat{b}_f^+\) and \(\hat{b}_f\), \(f \in 2\pi \Lambda^{-1/3} \mathbb{Z}^3\), are, respectively, Bose-operators of creation and annihilation of phonons with energy \(\hbar \omega_f \in \mathbb{R}_+\), the coefficient \(L_f = L_{-f}\) is a parameter of the polaron bond in the crystal and \(<.,.>\) is the ordinary scalar product in the Euclidean space \(\mathbb{E}^3\).

As it was also shown in \[1, 5\], Hamiltonian (1.1) can be transformed by means of the unitary transformation

\[
U := \exp(i \sum_{(f)} <f,r> 1 \otimes \hat{b}_f^+ \hat{b}_f),
\]

acting in the Hilbert space \(L_2(\Lambda; \mathbb{C}) \otimes \Phi(\Lambda; \mathbb{C})\), where \(\Phi(\Lambda; \mathbb{C})\) is the corresponding Fock space for the phonon quasi-particle states in the crystal, \(m\) is an effective electron mass, \(\hat{p} := \frac{\hbar}{i} \nabla\) is its momentum operator, \(\hat{b}_f^+\) and \(\hat{b}_f\), \(f \in 2\pi \Lambda^{-1/3} \mathbb{Z}^3\), are, respectively, Bose-operators of creation and annihilation of phonons with energy \(\hbar \omega_f \in \mathbb{R}_+\), the coefficient \(L_f = L_{-f}\) is a parameter of the polaron bond in the crystal and \(<.,.>\) is the ordinary scalar product in the Euclidean space \(\mathbb{E}^3\).
into the following form:

\[ \hat{H}_p = \frac{1}{2m}(\hat{p} \otimes 1 - 1 \otimes \sum_{(f)} \hbar f b_f^+ b_f) + \sum_{(f)} \hbar \omega_f 1 \otimes b_f^+ b_f + \frac{1}{1!\hbar^2} \sum_{(f)} L_f(\frac{\hbar}{2\omega_f})^{1/2} 1 \otimes (b_f + b_f^+), \]  

(1.3)

wherefrom it is clearly seen the quantum nature of the polaron structure, which doesn’t depend on the force of the interaction parameter \( L_f \). This conclusion can also be made from the fact that model (1.1) possesses the conservation law of the general electron-phonon momentum:

\[ \hat{P} = \hat{p} \otimes 1 + 1 \otimes \sum_{(f)} \hbar f b_f^+ b_f, \]  

(1.4)

that is \([\hat{H}_p, \hat{P}] = 0\). It is interesting to note, that the analytical studies of the statistical properties of the model of polaron in all of the works on this problem [1, 4, 7, 9, 17], except for works [5, 6], were based on the Hamiltonian expression (1.1). But, as it was pointed out in [1], the statistical properties of the model do not depend on the unitary-equivalent representation choice for operator (1.1). In particular, expression (1.3) can be easily rewritten equivalently, making use of the normal operator ordering, as

\[ \hat{H}_p = \frac{1}{2m}(\hat{p} \otimes 1 - 1 \otimes \sum_{(f)} \hbar f b_f^+ b_f) + \sum_{(f)} \hbar \omega_f 1 \otimes b_f^+ b_f + \frac{1}{1!\hbar^2} \sum_{(f)} L_f(\frac{\hbar}{2\omega_f})^{1/2} 1 \otimes (b_f + b_f^+) = \]

\[ = \frac{1}{2m}\hat{p}^2 \otimes 1 - \frac{1}{m} \sum_{(f,g)} \langle \hat{p}_g, hf > \otimes b_g^+ b_f^+ b_f + \frac{1}{2m} \sum_{(f,g)} \langle h_f, hg > 1 \otimes b_f^+ b_f b_g^+ b_g + \frac{1}{1!\hbar^2} \sum_{(f)} L_f(\frac{\hbar}{2\omega_f})^{1/2} 1 \otimes (b_f + b_f^+) = \]

\[ = \frac{1}{2m}\hat{p}^2 \otimes 1 - \frac{1}{m} \sum_{(f,g)} \langle \hat{p}_g, hf > \otimes b_g^+ b_f^+ b_f + \frac{1}{2m} \sum_{(f,g)} \langle h_f, hg > 1 \otimes b_f^+ b_f b_g^+ b_g + \frac{1}{1!\hbar^2} \sum_{(f,g)} L_f(\frac{\hbar}{2\omega_f})^{1/2} 1 \otimes (b_f + b_f^+) = \]

(1.5)

where we made use of the tensor operator representation \( \hat{p} \otimes 1 = \sum_{(f)} \hat{p}_f \otimes b_f^+ b_f = \sum_{(f)} \hat{p} \hat{N}^{-1} \otimes b_f^+ b_f, \quad \hat{N} := \sum_{(f)} b_f^+ b_f, \) in the Fock space \( \Phi(\Lambda; \mathbb{C}) \) and of the related commutation properties: \([\hat{p}_f, \hat{p}_g] = 0 = [\hat{p}_g, b_f^+ b_f] \) for all \( f, g \in 2\pi\Lambda^{-1/3}\mathbb{Z}^{3} \). We need to mention here that this representation of the Hamiltonian operator (1.3) possesses a natural physical interpretation as a polaron model with collectively separated interaction potentials. This fact proves to become very important for our analysis that follows below.

In a series of papers on the polaron theory [1, 7] the oscillator approximation of the Hamiltonian (1.1) was analyzed. This approximation leads to the so-called “linearized” model of the polaron, when only the first member of the expansion \( \exp(i < r, f >) \simeq 1 + i < r, f > \) in (1.1) was taken into account and the quadratic compensating part \( K_0 r^2/2, \) where \( K_0^2 = \frac{1}{\Lambda} \sum_{(f)} L_f^2 f^2 \omega_f^{-2}, \) was added into the initial Hamiltonian. Under these conditions the resulting Hamiltonian persists to be translational-invariant that makes it possible to analyze its thermodynamical properties as \( N \to \infty, \Lambda \to \infty. \)
Concerning the Hamiltonian representation (1.5) one can make the following very important observation: the operator term \( H_p := \frac{1}{2m} \sum_{(f,g)} \left( < \hat{p}_f, \hbar g > + < \hat{p}_g, \hbar f > + < \hbar f, \hbar g > \right) \otimes b_f^+ b_g^+ b_g b_f \), being written in the normally ordered secondly quantized form, gives rise in an \( N \)-particle invariant Fock subspace \([13, 10, 12, 15]\) to the following effective two-particle operator expression:

\[
H_p^{(1)} = \frac{1}{2m} \sum_{k \neq j}^N \left( \frac{1}{N} \left< \hat{p}(y_j) \otimes \hat{\Pi}(y_k) + \hat{p}(y_k) \otimes \hat{\Pi}(y_j) \right> + \left< \hat{\Pi}(y_k), \hat{\Pi}(y_j) \right> \right),
\]

acting in the Hilbert space \( L_2(\Lambda; \mathbb{C}) \otimes L_{2,\text{sym}}(\Lambda^N; \mathbb{C}) \), where we denoted by \( \hat{\Pi}(y) \), \( y \in \Lambda \), the respectively modified momentum operator of the crystal deformations and \( \hat{p}(y) \), \( y \in \Lambda \), the uniformly distributed polaron momentum.

Taking now into account the well-known \([10, 13, 14]\) random phase approximation (RPA) for the two-particle phonon excitations in crystal, one can obtain that expression (1.6) transforms into zero, since

\[
\sum_{k \neq j=1}^N \left< \hat{\Pi}(y_k), \hat{\Pi}(y_j) \right> = 0 = \sum_{k \neq j=1}^N \frac{1}{N} \left< \hat{p}(y_j) \otimes \hat{\Pi}(y_k) + \hat{p}(y_k) \otimes \hat{\Pi}(y_j) \right> \text{ weakly in } L_{2,\text{sym}}(\Lambda^N; \mathbb{C}) \text{ owing to the stability of the crystal deformations, generated by the polaron interaction. Since we are interested in the statistical properties of our polaron model, the RPA-approximation discussed above is well fitting for this aim, because the corresponding statistical sum is calculated as the average value of the statistical operator over all of Hamiltonian (1.5) eigenstates. Thus, we can consider within the RPA-approximation a polaron model Hamiltonian in the following reduced form:

\[
\hat{\mathcal{H}}_p^{(0)} = \frac{1}{2m} \hat{\mathcal{P}}^2 \otimes (1 - \hat{\mathcal{N}}^{-1}) + \frac{1}{2m} \sum_{(f)} (\hat{p}_f - \hbar f)^2 \otimes b_f^+ b_f + \sum_{(f)} \hbar \omega_f 1 \otimes b_f^+ b_f + \frac{1}{\Lambda^{1/2}} \sum_{(f)} L_f \left( \frac{\hbar}{2\omega_f} \right)^{1/2} 1 \otimes (b_f + b_f^+),
\]

being a well defined bounded from below operator expression in the Hilbert space \( L_2(\Lambda; \mathbb{C}) \otimes \Phi(\Lambda; \mathbb{C}) \).

We believe that our model (1.7), describing the polaron properties within the RPA-approximation, is more adequate for studying its thermodynamics, remaining \( a \text{ priori } \) translation-invariant. We will study this model below in detail. Moreover, we will investigate this polaron model in the external magnetic field \( B = \text{rot}A \), where, by definition, the vector potential \( A = (0, -m\omega_c x, 0)^T \in \mathbb{R}^3 \) is directed along the axis \( Oy \) of the Euclidian space \( \mathbb{E}^3 \) and \( \omega_c \in \mathbb{R}_+ \).
denotes the corresponding “cyclotronic” frequency. In this case Hamiltonian (1.5) has the form

\[ \hat{\mathcal{H}}^{(\mu)}_p = \frac{1}{2m} (\hat{p}_f^{(\mu)} + \hat{p}_f^2) \otimes (1 - \hat{N}^{-1}) - \sum_{(f)} \frac{1}{2m} (\hat{p}_f^{(\mu)} + \hat{p}_f^2) \otimes b^+_f b_f + \]

\[ + \frac{1}{2m} \sum_{(f)} (\hat{p}_f^{(\mu)} - \hbar \bar{f})^2 \otimes b^+_f b_f + \frac{1}{2m} \sum_{(f)} (\hat{p}_f - h f_s)^2 \otimes b^+_f b_f + \]

\[ + \sum_{(f)} \hbar \omega_f 1 \otimes b^+_f b_f + \frac{1}{2} \sum_{(f)} L_f \left( \frac{\hbar}{2 \omega_f} \right)^{1/2} 1 \otimes (b_f + b^+_f), \]

where by definition \( \hat{p}_f^{(\mu)} = (\hat{p}_{f_x}, \hat{p}_{f_y}, m \omega_x x)^T, \hat{f} = (f_x, f_y)^T, \) pertaining the quadratic structure of the phonon operators.

2 The RPA-approximated polaron model

To study the thermodynamics of the RPA-approximated polaron model (1.5), we need to calculate the statistical sum

\[ Z^{(0)}_p = Sp \exp(-\beta \hat{\mathcal{H}}^{(0)}_p), \]  

where \( \beta = 1/kT \) is the inverse temperature in the Boltzmann units. Then, taking into account that

\[ \hat{\mathcal{H}}^{(0)}_p = \frac{1}{2m} \hat{p}^2 \otimes (1 - \hat{N}^{-1}) + \sum_{(f)} \hbar \hat{\omega}_f \otimes b^+_f b_f + \frac{1}{2} \sum_{(f)} L_f \left( \frac{\hbar}{2 \omega_f} \right)^{1/2} 1 \otimes (b_f + b^+_f), \]

where the operators

\[ \hat{\omega}_f := \left[ \frac{1}{2m} (\hat{p}_f / \hbar - \hat{f})^2 + \omega_f \right], \quad \hat{n}_f := b^+_f b_f \]

commute to each other, that is \([\hat{\omega}_f, \hat{n}_f] = 0\), we can calculate expression (2.1) classically, having reduced it to the form

\[ Z^{(0)}_p = Sp(-\beta \hat{\mathcal{H}}^{(0)}_p) = Sp_{(c)} Z^{(0)}_{ph}(\hat{p}). \]

Here, by definition, we denoted the “phonon” part of the statistical sum as

\[ Z^{(0)}_{ph}(\hat{p}) = Sp_{(ph)} \exp(-\beta \hat{\mathcal{H}}^{(0)}_p). \]

Since the operator \( \hat{\mathcal{H}}^{(0)}_{ph} \) is a quadratic form with respect to the phonon operators, it is easy to calculate that the change of variables

\[ b_f = \tilde{b}_f - c_f (\hat{\omega}, \hat{N}_f), \quad b^+_f = \tilde{b}^+_f - c_f (\hat{\omega}, \hat{N}_f), \quad c_f (\hat{\omega}, \hat{N}_f) = \frac{1}{\Lambda^{1/2}} \sum_{(f)} L_f \left( \frac{\hbar}{2 \omega_f} \right)^{1/2} b_f, \]

transforms it to the canonical diagonal form

\[ \hat{\mathcal{H}}^{(0)}_{ph} = \frac{1}{2m} \tilde{p}^2 \otimes (1 - \hat{N}^{-1}) + \sum_{(f)} \hbar \omega_f \otimes \tilde{b}^+_f \tilde{b}_f + \frac{1}{\Lambda} \sum_{(f)} \frac{L_f^2}{2 \omega_f} \omega_f \otimes 1. \]
Here we need to mention that the operator $\hat{\omega}_f : L_2(\Lambda; \mathbb{C}) \to L_2(\Lambda; \mathbb{C})$ is a strongly positive defined expression. We also notice here (as it was done in [1]), that the phonon frequencies satisfy the symmetry condition $\omega_f = \omega_{-f}$ for all vectors $f \in 2\pi \Lambda^{-1/3}\mathbb{Z}^3$. A similar symmetry condition holds also for the operator quantities $\hat{\omega}_f$, that is $\hat{\omega}_f = \hat{\omega}_{-f}$ for all $f \in 2\pi \Lambda^{-1/3}\mathbb{Z}^3$. Based on representation (2.5), it is easy to find the following expression for the phonon part of statistical sum (2.3):

$$Z_{ph}^{(0)}(\hat{\rho}) = \exp\left(-\frac{\beta}{2m}\hat{p}^2\right)Sp(\hat{\rho}) \prod_{(f)} \sum_{(N_f)} \exp\left[\frac{\beta \hat{\rho}_f^2}{2m[N_f+c_f(\hat{\rho},N_f)]}\right] - \beta \hbar \tilde{N}_f \hat{\omega}_f(\hat{\rho},\tilde{N}_f) -$$

$$-\beta \hbar \tilde{N}_f \hat{\omega}_f(\hat{\rho},\tilde{N}_f) - \beta \frac{L^2}{2\Lambda \omega_f(\hat{\rho},N_f)\omega_f} = \exp\left(-\frac{\beta}{2m}\hat{p}^2\right) \exp\left\{\sum_{(f)} \sum_{(N_f \in \mathbb{Z}^3)} \exp\left[\frac{\beta \hat{\rho}_f^2}{2m[N_f+c_f(\hat{\rho},N_f)]}\right] - \beta \hbar \tilde{N}_f \hat{\omega}_f(\hat{\rho},\tilde{N}_f) - \beta \frac{L^2}{2\Lambda \omega_f(\hat{\rho},N_f)\omega_f}\right\} := \exp\left(-\frac{\beta}{2m}\hat{p}^2\right) \exp\left\{-\sum_{(f)} F_f(\hat{\rho};\beta)\right\},$$

where we denoted by $\tilde{N}_f := \tilde{b}_f^+ \tilde{b}_f$, $f \in 2\pi \Lambda^{-1/3}\mathbb{Z}^3$, the shifted phonon density operators and $\tilde{\omega}_f(\hat{\rho},N_f) := \left[\frac{1}{2m}\hat{p}/[(N_f + c_f(\hat{\rho},N_f)\hbar) - f^2 + \omega_f], f \in 2\pi \Lambda^{-1/3}\mathbb{Z}^3\right.$, the related shifted phonon frequencies. Substituting now (2.6) in (2.2), we obtain, as a result, the analytical expression for the complete statistical sum of our approximated polaron model:

$$Z_p^{(0)} = Sp(\hat{\rho}) \exp\left\{-\frac{\beta}{2m}\hat{p}^2 - \sum_{(f)} F_f(\hat{\rho};\beta)\right\} = \frac{\Lambda}{(2\pi)^3} \int_{\mathbb{R}^3} d^3k \exp\left\{-\frac{\beta}{2m} k^2 - \sum_{(f)} F_f(k;\beta)\right\},$$

where we used the known trick [1, 10, 9] of changing the discrete sum $\sum_{(k)}(\ldots)$ by the corresponding integral:

$$\sum_{(k)}(\ldots) = \frac{\Lambda}{(2\pi)^3} \int_{\mathbb{R}^3} (\ldots) d^3k.$$

Thus, if we calculate the internal sums $\sum_{(f)}(\ldots)$ of expression (2.7) for the given values of the phonon frequencies $\omega_f$ and the interaction parameter $L_f$ for all discrete values $f \in 2\pi \Lambda^{-1/3}\mathbb{Z}^3$, then the quasi-gaussian integral $\int_{\mathbb{R}^3} (\ldots) d^3k$ can be calculated analytically or by means of approximate and asymptotic methods. In particular, assuming that $L_f = \alpha^{1/2}/|f|$, and $\omega_f = \omega_0$ for all $f \in 2\pi \Lambda^{-1/3}\mathbb{Z}^3$, from (2.7) and (2.8) it is easy to obtain the explicit expression for the statistical sum of the polaron model (1.5), which is not going to be dealt with in this paper.

3 RPA-approximated polaron model in the static magnetic field

To study the RPA-approximated polaron model in the static magnetic field we will use the Hamiltonian operator (1.8), which persists to be quadratic in the phonon operators. Taking into account, that
\[ \hat{H}^{(\mu)}_p = \frac{1}{2m}(\hat{p}^{(\mu)}_f + \hat{p}^{(\mu)}_z) \otimes (1 - \hat{N}^{-1}) + \frac{1}{2m} \sum_{(f)} (\hat{p}^{(\mu)}_f - h \bar{f})^2 \otimes b^+_f b_f + \frac{1}{2m} \sum_{(f)} (\hat{p}_f - h f_z)^2 \otimes b^+_f b_f + \sum_{(f)} h \omega_f \mathbf{1} \otimes b^+_f b_f + \frac{1}{K \Omega^2} \sum_{(f)} L_f \left( \frac{\hbar}{2 \omega_f} \right) \frac{1}{2} \mathbf{1} \otimes (b_f + b^+_f), \] (3.1)

where the operators
\[ (\hat{p}^{(\mu)}_f - h \bar{f})^2, (\hat{p}_f - h f_z)^2, \hat{n}_f = b^+_f b_f \] (3.2)

commute to each other. Put, by definition,
\[ \hat{\omega}_f = \omega_f + \frac{1}{2m} (\hat{p}^{(\mu)}_f / h - \hat{f})^2 + \frac{1}{2m} (\hat{p}_f / h - f_z)^2, \quad \hat{\bar{f}}^{(\mu)} = (\hat{p}_f, \hat{p}_z + m \omega_f x)^T, \]

for \( \bar{f} = (f_x, f_y)^T \in \mathbb{R}^2 \), the respectively split statistical sum
\[ Z^{(\mu)}_{ph} = S_{p(h)} \exp(-\beta \hat{H}^{(\mu)}_{ph}) = S_{p(\psi)} \left[ S_{p(\psi)} \exp(-\beta \hat{H}^{(1)}_{ph}) \right] \] (3.3)

can be calculated successfully, where
\[ \hat{H}^{(\mu)}_{ph} = \frac{1}{2m} (\hat{p}^{(\mu)}_f + \hat{p}^{(\mu)}_z) \otimes (1 - \hat{N}^{-1}) + \sum_{(f)} h \hat{\omega}_f \otimes b^+_f b_f + \frac{1}{\Lambda} \sum_{(f)} L_f \left( \frac{\hbar}{2 \omega_f} \right) \frac{1}{2} \mathbf{1} \otimes (b_f + b^+_f), \] (3.4)

Let us, first, find the statistical sum
\[ Z^{(\mu)}_p = S_{p(\psi)} Z^{(\mu)}_{ph}, \] (3.5)

for which, using (3.3) and (3.5), we obtain
\[ Z^{(\mu)} = S_{p(\psi)} Z^{(\mu)}_{ph}. \] (3.6)

Using now the fact that Hamiltonian (3.2) is quadratic in the phonon variables and making transformation (2.4), we obtain
\[ \hat{\tilde{H}}^{(\mu)}_{ph} = \frac{1}{2m} (\hat{p}^{(\mu)}_f + \hat{p}^{(\mu)}_z) \otimes (1 - \hat{N}^{-1}) + \sum_{(f)} h \hat{\omega}_f \tilde{b}^+_f \tilde{b}_f + \frac{1}{\Lambda} \sum_{(f)} \frac{L^2_f}{2 \omega_f \omega_f}, \] (3.7)

Thus, from (3.7) and (3.5), one obtains that
\[ Z^{(\mu)} = \exp[-\beta \frac{1}{2m} (\hat{p}^{(\mu)}_z + \hat{p}^{(\mu)}_z)^2] \exp\left[ \sum_{(f)} \frac{\beta \hat{\omega}_f \tilde{b}^+_f \tilde{b}_f}{2 m [N_f + \frac{1}{2} (\hat{p}^{(\mu)}_f k_z; N_f)]} \right] - \beta h \hat{N}_f \hat{\omega}_f (\hat{p}^{(\mu)}_f, \hat{p}^{(\mu)}_z; \hat{N}_f) - \frac{\beta L^2_f}{2 \omega_f [\hat{p}^{(\mu)}_f \hat{p}^{(\mu)}_z; N_f \omega_f]} = \exp\left[ \frac{1}{2m} (\hat{p}^{(\mu)}_z + \hat{p}^{(\mu)}_z)^2 \right] \exp\left[ \sum_{(f)} \frac{\beta \hat{\omega}_f \tilde{b}^+_f \tilde{b}_f}{2 m [N_f + \frac{1}{2} (\hat{p}^{(\mu)}_f k_z; N_f)]} - \beta h \hat{N}_f \hat{\omega}_f (\hat{p}^{(\mu)}_f, \hat{p}^{(\mu)}_z; N_f) - \frac{\beta L^2_f}{2 \omega_f [\hat{p}^{(\mu)}_f \hat{p}^{(\mu)}_z; N_f \omega_f]} \right] := \exp \left\{ -\beta \frac{1}{2m} (\hat{p}^{(\mu)}_z + \hat{p}^{(\mu)}_z)^2 - \sum_{(f)} F_f (\hat{p}^{(\mu)}_f, \hat{p}^{(\mu)}_z; \beta) \right\}, \] (3.8)
where $\bar{\omega}_f(\hat{p}(\mu), k_z; \beta) = \omega_f + \frac{1}{2m}(\hat{p}(\mu)/[h(N_f + c_f^2)] - \bar{f})^2 + \frac{1}{2m}(k_z - f_z)^2$. Substituting (3.8) into (3.6), we obtain the expression for the statistical sum of RPA-approximated polaron model in the magnetic field:

$$Z_p^{(\mu)} = S_{p(e)} \exp \left\{ -\frac{\beta}{2m}(\hat{p}(\mu)^2 + \hat{p}_z^2) - \sum_{(f)} F_f(\hat{p}(\mu), \hat{p}_z; \beta) \right\} = S_{p(e)} \exp(-\beta \bar{H}_e^{(\mu)}). \quad (3.9)$$

Here, by definition, we have put

$$\bar{H}_e^{(\mu)} (\beta) := \frac{1}{2m} \hat{p}(\mu)^2 + \bar{V}_e^{(\mu)}(\hat{p}(\mu); \beta) \quad (3.10)$$

as an effective polaron Hamiltonian with the operator potential, defined by the expression

$$\exp[-\beta V_e^{(\mu)}(\hat{p}(\mu); \beta)] = \Lambda^{1/3} \int d\k_z \exp \left\{ -\sum_{(f)} F_f(\hat{p}(\mu), \k_z; \beta) \right\}, \quad (3.11)$$

Thus, the statistical sum (3.9) is determined completely by means of the spectrum of the one-particle two-dimensional self-adjoint problem

$$\bar{H}_e^{(\mu)}(\beta) \psi_n = \varepsilon_n(\beta) \psi_n, \quad (3.12)$$

where the eigenvalues $\varepsilon_n(\beta) \in \mathbb{R}_+$, $n \in \mathbb{Z}_+$, compile the corresponding modified Landau’s spectrum [8, 9, 10] and $\psi_n \in L_\infty(\mathbb{E}^2; \mathbb{C}), n \in \mathbb{Z}_+$, are the eigenfunctions of the suitable two-dimensional operator with the periodic boundary conditions:

$$\psi_n(x, y) = \psi_n(x + l_x \Lambda^{-1/3}, y + l_y \Lambda^{-1/3})$$

for all $(l_x, l_y)^T \in \mathbb{Z}^2, (x, y)^T \in \mathbb{E}^2$. Then from (3.9) and (3.11) it is easy to obtain that

$$Z_p^{(\mu)} = \sum_{n \in \mathbb{Z}_+} \exp[-\beta \varepsilon_n(\beta)] \quad (3.13)$$

where the quantities of the Landau spectrum $\varepsilon_n(\beta) \in \mathbb{R}, n \in \mathbb{Z}_+$, can be found by means of appropriate quantum-mechanical methods, being already another problem to deal with. The energy of the ground state for the reduced polaron model at zero temperature (as $\beta \to \infty$) can be calculated [1, 9] as the limit $E_0 = -\lim_{\beta \to \infty} \ln Z_p^{(\mu)}$, and is also a very interesting and important problem.

4 The polaron mass

It is important to mention that the description of our polaron system, by means of the Bogolubov canonical transformation (1.2), gives rise to a direct possibility of calculating the polaron mass in magnetic field within our RPA-approximation both at zero and non-zero temperatures. Namely, based on the considerations of [20], one can consider at zero temperature the least energy state
\[ |p^{(\mu)} > \in L_2(\Lambda; \mathbb{C}) \otimes \Phi(\Lambda; \mathbb{C}) \] at a small fixed momentum \( p^{(\mu)} \in \mathbb{E}^2 \), if the interaction constant \( L_f = \sqrt{\alpha} f^{-1} \), \( f \in 2\pi \Lambda^{-1/3} \mathbb{Z}^3 \) and \( \alpha \in \mathbb{R}_+ \) is the corresponding dimensionless intensity parameter. Then the polaron energy could be defined as

\[ E(\alpha; p^{(\mu)}) = E_0(\alpha) + \frac{|p^{(\mu)}|^2}{2m^*(\alpha)} + \alpha(|p^{(\mu)}|^2), \tag{4.1} \]

where \( E_0(\alpha) \) satisfies the eigenvalue equation

\[ \mathcal{H}_p^{(\mu)} |p^{(\mu)} > = E(\alpha; p^{(\mu)}) |p^{(\mu)} > \]

under the conditions \( p^{(\mu)} |p^{(\mu)} > = p^{(\mu)} |p^{(\mu)} > \) for small vector \( p^{(\mu)} \in \mathbb{E}^2 \).

In the case of a non-zero temperature \( T > 0 \) the polaron free energy is determined by means of the following expression:

\[ F(\alpha; \beta) = -\beta^{-1} \ln \left( \frac{Z_p^{(\mu)}}{Z_{\text{ph}}^{(can)}} \right), \tag{4.2} \]

where, by definition, \( Z_{\text{ph}}^{(can)} = S_{\text{ph}} \exp(-\beta \mathcal{H}_{\text{ph}}^{(can)}) \) is the pure statistical sum of the phonon field, and \( \mathcal{H}_{\text{ph}}^{(can)} = \sum_p (b^+_p b_p + 1/2) / \hbar \omega p, \beta = 1/kT \). Making use of the result (4.2) obtained above one can calculate the average polaron energy as

\[ U(\alpha; \beta) = \frac{\partial}{\partial \beta} [\beta F(\alpha; \beta)], \tag{4.3} \]

and the proper polaron energy as

\[ E(\alpha; \beta) = U(\alpha; \beta) - 3/(2\beta). \]

At zero temperature one has:

\[ E(\alpha) = \lim_{\beta \to \infty} E(\alpha; \beta). \]

5 Conclusion

The a one-particle RPA-approximated polaron model in ion crystal described above can be applied [10], in particular, to analyze the results of de Haas-van Alfven type experiments. We would also like to mention a polaron gas model, having many interesting applications, which can be similarly investigated by means of powerful methods of the many-particle quantum theory [1, 9, 10, 18], in particular, by means of the methods of the quantum current algebra [11] and its representations, as it was recently demonstrated in [16]. Concerning our polaron model and the used RPA-approximation, it is important to mention the following: the resulting Hamiltonian operator upon the canonical Bogolubov transformation (1.2) was presented in the canonical normal ordered form as a sum of an exactly solvable operator part and of a part responsible for the maniparticle correlation interaction. The latter appeared to be exactly of the RPA-approximated form, what enable us to neglect it.
This approximation can be used either the crystal temperature is high enough or the intensity parameter \( \alpha \in \mathbb{R}_+ \) is not relatively small, being \( \alpha > 5,8 \), when there is realized \([20, 19]\) the transition of the polaron from a non-localized state to a self-localized state.

As is well known the temperature dependence of the effective polaron mass is of great interest for physical applications, in particular, with its relation to the interpretation of experiments of cyclotronic resonance in polar crystals \([5, 6, 7]\). Measurements fulfilled in the crystals CdTe and AgBr in weak magnetic fields at small cyclotronic frequencies demonstrate clearly enough that the corresponding cyclotronic polaron mass grows with temperature at its low values. Thereby, one can expect that the calculation of the magnetic polaron mass based on our results within the RPA-approximation can explain this effect and determine bounds of the applied method. Moreover, one can expect that our results will confirm a prediction of the existence \([9, 17, 18]\) of the first kind of phase transition of a polaron state from its self-localized state to a free state under action of the strong enough magnetic field. We plan to discuss these intriguing problems in a forthcoming paper.

### 6 Supplement

The Bogolubov unitary transformed Hamiltonian operator (1.5) can be formally written as

\[
\hat{\mathcal{H}}_p := \hat{\mathcal{H}}_p^{(0)} + \hat{\mathcal{V}}_p^{(1)},
\]

where the operator

\[
\hat{\mathcal{V}}_p^{(1)} := \frac{1}{2m} \sum_{(f,g)} (\hat{p}_f, \hbar g > + \hat{p}_g, \hbar f > + \hbar f, \hbar g > 1) \otimes b_f^+ b_g^+ b_f b_g,
\]

is responsible for the potential energy of crystal deformations caused by a polaron motion. The following proposition is crucial for our further analyzing the statistical properties of the polaron model in the Bogolubov representation (6.1).

**Proposition 6.1** The RPA-approximated polaron operator \( \hat{\mathcal{H}}_p^{(0)} : L_2(\Lambda; \mathbb{C}) \otimes \Phi(\Lambda; \mathbb{C}) \) and the crystal deformation energy operator \( \hat{\mathcal{V}}_p^{(1)} : L_2(\Lambda; \mathbb{C}) \otimes \Phi(\Lambda; \mathbb{C}) \) are commuting to each other, that is

\[
[\hat{\mathcal{H}}_p^{(0)}, \hat{\mathcal{V}}_p^{(1)}] = 0
\]

identically.

As a corollary from Proposition 6.1, the operators \( \hat{\mathcal{H}}_p^{(0)}, \hat{\mathcal{V}}_p^{(1)} : L_2(\Lambda; \mathbb{C}) \otimes \Phi(\Lambda; \mathbb{C}) \), being self-adjoint, possess the common set of eigenstates, being thereby suitably degenerate. The latter can be used for more exact calculations of the full statistical sum

\[
Z_p = Sp \exp[-\beta (\hat{\mathcal{H}}_p^{(0)} + \hat{\mathcal{V}}_p^{(1)})],
\]
if we take into account the stability condition imposed on the ion crystal deformations. Namely, we can assume that the following compatible selection conditions

\[ < (k; \alpha(k)) | \hat{V}_p^{(1)} | (k; \alpha(k)) > = 0, \quad \hat{H}_p^{(0)} | (k; \alpha(k)) > = \alpha(k) | (k; \alpha(k)) >, \]

hold for all physically permitted polaron eigenstates \(|(k; \alpha(k)) > \in L_2(\Lambda; \mathbb{C}) \otimes \Phi(\Lambda; \mathbb{C})\) of the RPA-approximated polaron operator \(\hat{H}_p^{(0)} : L_2(\Lambda; \mathbb{C}) \otimes \Phi(\Lambda; \mathbb{C})\).

The corresponding statistical sum (6.4) then reduces, owing to constraints (6.5), to

\[ Z_{p,red} = Sp_{(red)} \left( \exp(-\beta \hat{H}_p^{(0)}) \exp(-\beta \hat{V}_p^{(1)}) \right) = Sp_{(red)} \left( \exp(-\beta \hat{H}_p^{(0)}) \right), \]

where the operation \(Sp_{(red)}(\ldots)\) means the trace taken over the above selected states \(|(k; \alpha(k)) > \in L_2(\Lambda; \mathbb{C}) \otimes \Phi(\Lambda; \mathbb{C})\).

This problem, being important for suitable applications of the polaron model under regard, is planned to be treated in detail in a work under preparation.

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