

ON LOWER BOUND ESTIMATES FOR THE ENERGY SPECTRUM OF THE FRÖHLICH POLARON MODEL

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Method of intermediate problems was applied to investigation of the energy spectrum of the Fröhlich polaron model. It was shown that various infinite sequences of nondecreasing improvable lower bound estimates for the low-lying branch of the slow-moving polaron excitation energy spectral curve adjacent to the ground state energy can be derived for arbitrary values of the electron–phonon interaction constant. These bound estimates allow for explicit numerical evaluation at all orders. In conjunction with numerous well-known upper bound estimates for the energy spectral curve of the Fröhlich polaron as a function of the interaction constant and the polaron total momentum, the aforesaid improvable lower bound estimates might provide one with virtually precise magnitude for the energy of the slow-moving polaron. Possible generalization to the case of the Fröhlich polaron in external magnetic field is outlined.

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The model to be considered is the standard quantized Fröhlich polaron [1]

$$H = \frac{\hat{\mathbf{p}}^2}{2m} + \hbar\omega \sum_{\mathbf{k}} a_{\mathbf{k}}^+ a_{\mathbf{k}} + \sum_{\mathbf{k}} (V^*(k) a_{\mathbf{k}}^+ e^{-i\mathbf{k}\mathbf{r}} + \text{h.c.}), \quad (1)$$

where $V(k) = -i \frac{\hbar\omega}{k} \left(\frac{4\pi\alpha}{V} \sqrt{\frac{\hbar}{2m\omega}} \right)^{1/2}$, and the phonon wave vector runs over a quasidiscrete set of values $\mathbf{k} = 2\pi/(La) \{n_1, n_2, n_3\}$, $n_i = 0, \pm 1, \dots, \pm(L/2 - 1), +L/2$, $i = 1, 2, 3$, 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 $V \rightarrow \infty$ assumes the rule of the transition to the continuous phonon spectrum $\lim_{V \rightarrow \infty} (1/V) \sum_{\mathbf{k}} \dots = (2\pi)^{-3} \int d\Omega_{\mathbf{k}} \int_0^{k_D} dk k^2 \dots$, where $k_D = (6\pi^2)^{1/3}/a$ is the Debye wave vector, a being the lattice constant. For any realistic, or «physical» polaron, the value of k_D is finite, whilst the limit $k_D \rightarrow \infty$ corresponds to the so-called «field-theoretical» polaron model. For the matter of convenience it is assumed further on that $\hbar = \omega = m = 1$.

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It is known that the polaron total momentum $\hat{\mathbf{P}} = \hat{\mathbf{p}} + \sum_{\mathbf{k}} \mathbf{k} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}}$ commutes with the Hamiltonian (1). Therefore, the unitary transformation $\tilde{H} = (SU)^{-1} H SU$, $SU = \exp(-i \sum_{\mathbf{k}} \mathbf{k} \hat{r} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}}) \exp\{-i \sum_{\mathbf{k}} (V(\mathbf{k}) a_{\mathbf{k}}^{\dagger} - \text{h.c.})\}$ provides us with the Hamiltonian

$$\tilde{H} = \frac{1}{2} \left(\mathbf{P} - \sum_{\mathbf{k}} \mathbf{k} (a_{\mathbf{k}}^{\dagger} - V(\mathbf{k})) (a_{\mathbf{k}} - V^{*}(\mathbf{k})) \right)^2 + \sum_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} - \sum_{\mathbf{k}} |V(\mathbf{k})|^2 \quad (2)$$

in the $\hat{\mathbf{p}}$ -representation, where $\hat{\mathbf{P}}$ becomes a quantum « c »-number \mathbf{P} , which is just the sole Hamiltonian to be treated further on. The ultimate goal is to find its lowest eigenvalue $E(P)$, i.e., the low-lying polaron energy spectral curve, for a given total polaron momentum \mathbf{P} and expand it as $E(P) = E_g + (\mathbf{P}^2/2m_{\text{eff}}) + O(P^4)$, with the coefficients E_g and m_{eff} being the polaron ground state energy and effective mass, respectively. Extensive work has already been done to evaluate $E(P)$ directly through conventional perturbational calculations or to find upper bounds to $E(P)$ by means of multitudinous variational methods. These approaches are beyond the scope of this work. It is only worth noting that, as a rule, perturbational schemes do not provide one with reliable error estimates, whilst the upper bounds can be relied upon only if they are supplemented with corresponding lower bounds to the magnitude in question. To our knowledge, lower bounds to the polaron energy spectrum have been receiving much less attention than the upper bounds throughout very long history of polaron studies. Among the most remarkable contributions, several works by E. H. Lieb should be mentioned first of all [2, 3] as well as the succeeding work by D. M. Larsen [4], who improved the result of [2], though neither of these lower bounds to the polaron ground state energy comes close to the best lowest upper bounds available so far and it is unknown how to improve them in a regular way.

The purpose of this study is to show that infinitely improvable lower bounds to the polaron spectral curve $E(P)$ could be derived by the method of intermediate problems in the theory of semi-bounded self-adjoint linear Hermitian operators on rigged Hilbert space, originated by H. Weyl [5] and A. Weinstein [6] and further elaborated since then by numerous contributors (see [7, 8] and refs. therein). The starting point of the method is time-independent Schrödinger equation $H\psi = E\psi$, where H is some Hermitian operator with respect to the inner product $(\phi, \psi) = \int \phi^* \psi d\tau$ in Hilbert space. It is assumed that all continuous spectrum energy levels of H are higher than the lowest discrete spectrum energy levels of one's interest. Let us assume, too, that these discrete eigenvalues of H can be ordered in a nondecreasing sequence,

$$E_1 \leq E_2 \leq \dots, \quad (3)$$

in which each degenerate eigenvalue appears the number of times of its multiplicity. The corresponding eigenstates ψ_i satisfy the equation $H\psi_i = E_i\psi_i$, and are assumed to be orthonormalized, so that $(\psi_i, \psi_j) = \delta_{ij}$, where δ_{ij} is Kronecker's delta. It is further assumed that the Hamiltonian H can be decomposed as

$$H = H^0 + H', \quad (4)$$

where H^0 has known eigenvalues and eigenstates and H' is an arbitrary Hermitian operator which is to be positive-definite in the sense that $(\psi, H'\psi) = \int \psi^* H'\psi d\tau > 0$, ($\psi \neq 0$) for every ψ in the domain of H . Hereafter, it is assumed that the lowest part of the discrete spectrum of H^0 is below its continuous spectrum and that the corresponding discrete eigenvalues can be ordered in the same manner (3) as the ones belonging to the total Hamiltonian H

$$E_1^0 \leq E_2^0 \leq \dots, \quad (5)$$

with the degenerate eigenvalues appearing the number of times of their multiplicity. The corresponding orthonormalized eigenstates ψ_i^0 satisfy the equation $H^0\psi_i^0 = E_i^0\psi_i^0$, $(\psi_i^0, \psi_j^0) = \delta_{ij}$. Because $H^0 \leq H$ in the sense of inequality $(\psi, H^0\psi) \leq (\psi, H\psi)$ for every ψ in the domain of H , it follows from the Weyl comparison theorem [5] that $E_i^0 \leq E_i$ ($i = 1, 2, \dots$). Therefore, the eigenvalues of H^0 already provide rough lower bound to the eigenvalues of H . The Hamiltonian H^0 is called the base Hamiltonian as usual. It is worth noting that the decomposition (4) is not unique and can be tailored to meet the requirements of a particular problem in question. The basic idea of the method of intermediate problems is to approximate the original Hamiltonian H from below by a non-decreasing sequence of the so-called truncated intermediate Hamiltonians $H^{l,k}$, which are to be constructed to satisfy the inequalities

$$H^{l,k} \leq H^{l+1,k} \leq H^k \leq H, \quad H^{l,k} \leq H^{l,k+1} \leq H \quad (l, k = 1, 2, \dots). \quad (6)$$

So, the Hamiltonians $H^{l,k}$ increase whatever index k or l is increased and thus must give improvable lower bounds for the lowest eigenvalues of the original Hamiltonian H . It was shown [9] that $H^{l,k}$ can be represented in a general form $H^{l,k} = H^{l,0} + H'P^k$ ($l, k = 1, 2, \dots$). Here the Hamiltonian $H^{l,0}$ is a truncation of the base Hamiltonian H^0 of the order l defined as

$$H^{l,0} = \sum_{i=1}^l E_i^0 |E_i^0\rangle \langle E_i^0| + E_{l+1}^0 \left[\hat{I} - \sum_{i=1}^l |E_i^0\rangle \langle E_i^0| \right] \quad (l = 1, 2, \dots)$$

in Dirac's bra and ket notation and \hat{I} stands for the identity operator. Truncations of H^0 satisfy the inequalities $H^{l,0} \leq H^{l+1,0} \leq H^0$ ($l = 1, 2, \dots$) proved in general case in [10]. The operator P^k defines a projection of an arbitrary

vector ϕ in the domain of H onto the subspace formed by a sequence of linearly independent vectors p_1, p_2, \dots, p_k : $P^k \phi = \sum_{i=1}^k \alpha_i p_i$, where constants α_i must satisfy the equations $[p_j, P^k \phi] = [p_j, \phi] = \sum_{i=1}^k \alpha_i [p_j, p_i]$ ($j = 1, 2, \dots, k$). Here an auxiliary inner product with respect to the metric operator H' was introduced as $[\psi, \phi] = (\psi, H' \phi) = \int \psi^* H' \phi d\tau$ for every pair of vectors ψ, ϕ for which $H' \psi$ and $H' \phi$ are defined. These vectors p_i are to be normalizable in the sense of the original inner product, i.e., $(p_i, p_i) = \mathcal{N}_i$, $\mathcal{N}_i < +\infty$ ($i = 1, 2, \dots, k$), but neither their explicit normalization nor orthonormalization are required. Projections P^k become larger with the increase of the number k of the elements p_i involved. As a consequence, the following inequality holds $0 \leq [\phi, P^k \phi] \leq [\phi, P^{k+1} \phi] \leq [\phi, \phi]$ ($k = 1, 2, \dots$). Thus, $H' P^k \leq H' P^{k+1} \leq H'$ ($k = 1, 2, \dots$), and the intermediate truncated Hamiltonians H^k defined as $H^k = H^0 + H' P^k$ ($k = 1, 2, \dots$) satisfy inequalities $H^k \leq H^{k+1} \leq H$ by construction. Hence, $H^{l,k} \leq H^{l,k+1} \leq H^{l,0} + H' \leq H$ ($l, k = 1, 2, \dots$), and, therefore, the lowest ordered eigenvalues $E_i^{l,k}$ of $H^{l,k}$ must satisfy the parallel inequalities $E_i^{l,k} \leq E_i^{l+1,k} \leq E_i^k \leq E_i$ ($i, l, k = 1, 2, \dots$), and $E_i^{l,k} \leq E_i^{l,k+1} \leq E_i$ ($i, l, k = 1, 2, \dots$), thus providing improvable lower bounds for the original eigenvalues E_i of the Hamiltonian H .

As was proved in [10], the so constructed Hamiltonian $H^{l,k}$ can have no continuous spectrum and must have E_{l+1}^0 as an eigenvalue of infinite multiplicity. Therefore, only those eigenvalues of $H^{l,k}$ that are smaller or equal to E_{l+1}^0 can be considered as lower bound estimates for the eigenvalues of the initial Hamiltonian H .

The outlined above truncation procedure can be improved significantly from the point of view of practical calculations if the original Hamiltonian H is formally decomposed as $H = H^{l,0} + (H^0 - H^{l,0}) + H' = H^{l,0} + H' + H'' = H^{l,0} + \tilde{H}'$ ($l = 1, 2, \dots$), where the operator $\tilde{H}' = H - H^{l,0}$ is obviously positive and can play the role played before by the metric operator H' . In this case, the positive contributions from the operator $H'' = H^0 - H^{l,0}$ ($l = 1, 2, \dots$) to lower bound estimates are not simply neglected at will but rather taken into consideration carefully on common grounds with the contributions stemming from H' , thus making these bounds higher than they might have been otherwise under the original truncation procedure.

The eigenvalues and eigenstates of the intermediate Hamiltonians $H^{l,k}$ of any order (i.e., for arbitrary indices l, k) can be expressed analytically and/or calculated numerically in terms of the known eigenvalues and eigenstates of H^0 and an arbitrarily chosen set of linearly independent vectors p_i ($i = 1, \dots, k$). It was proved in [9] that those eigenvalues of the Hamiltonian $H^{l,k}$ different from E_{l+1}^0 (and also from E_1^0, \dots, E_l^0 , should there be any eigenvalues of this kind in

some special cases) are the roots of the equation

$$\det \left\{ (p_j, H' p_i) + \frac{(\psi_\nu^0, H' p_i)(H' p_j, \psi_\nu^0)}{E_\nu^0 - E} + \frac{(H' p_j, H' p_i) - \sum_{\nu=1}^l (\psi_\nu^0, H' p_i)(H' p_j, \psi_\nu^0)}{E_{l+1}^0 - E} \right\} = 0. \quad (7)$$

Each solution of (7) provides n linear independent eigenfunctions of $H^{l,k}$, where n is the nullity of the coefficient matrix in (7). If the number of such eigenfunctions is less than $k + l$, then it is necessary to check if some of the eigenvalues $E_1^0, E_2^0, \dots, E_l^0$ of $H^{l,0}$ are also the eigenvalues of $H^{l,k}$. A verification algorithm to test this assumption was outlined in [9].

So, it is clear that $H^{l,k}$ may possess at most $l + k$ eigenvalues different from E_{l+1}^0 , which is an eigenvalue of $H^{l,k}$ of infinite multiplicity by construction and every of its corresponding eigenfunctions is orthogonal to all other eigenfunctions of the Hamiltonian $H^{l,k}$. To obtain the lower bounds to the eigenvalues E_i of the original Hamiltonian H , the so obtained eigenvalues of $H^{l,k}$ lying below E_{l+1}^0 are to be ordered in a nondecreasing sequence $E_1^{l,k} \leq E_2^{l,k} \leq \dots \leq E_t^{l,k}$, $t \leq l + k$, in which each eigenvalue is repeated according to its multiplicity. Then, the requisite lower bounds read as $E_i^{l,k} \leq E_i$ ($i = 1, 2, \dots, t$) $E_{l+1}^0 \leq E_i$ ($i = t + 1, t + 2, \dots$).

For the transformed polaron Hamiltonian (2) the Hamiltonians H^0 and H' in (4) can be identified immediately as

$$H^0 = \sum_{\mathbf{k}} a_{\mathbf{k}}^+ a_{\mathbf{k}} - \sum_{\mathbf{k}} |V(k)|^2 - \varepsilon \quad (8)$$

and

$$H' = \frac{1}{2} \left(\mathbf{P} - \sum_{\mathbf{k}} \mathbf{k} (a_{\mathbf{k}}^+ - V(k))(a_{\mathbf{k}} - V^*(k)) \right)^2 + \varepsilon, \quad (9)$$

respectively. Here an arbitrary positive parameter ε was introduced formally and identically to ensure strict positivity of the Hamiltonian H' as required by the method. However, such a straightforward partitioning is only appropriate for finite k_D , i.e., for «physical» polaron model. In general case, an alternative partitioning is to be employed with

$$H^0 = \varepsilon_2 \sum_{|\mathbf{k}| < K} a_{\mathbf{k}}^+ a_{\mathbf{k}} + \varepsilon_2 \sum_{|\mathbf{k}| \geq K} a_{\mathbf{k}}^+ a_{\mathbf{k}} + \sum_{|\mathbf{k}| < K} (V^*(k) a_{\mathbf{k}}^+ + \text{h.c.}) - \frac{3}{2}(1 - \varepsilon_2) - \varepsilon$$

explicitly soluble and

$$\begin{aligned}
 H' = & \frac{1}{2}(\mathbf{P} - \sum_{\mathbf{k}} \mathbf{k} a_{\mathbf{k}}^+ a_{\mathbf{k}})^2 + (1 - \varepsilon_2) \sum_{|\mathbf{k}| < K} a_{\mathbf{k}}^+ a_{\mathbf{k}} + \\
 & + (1 - \varepsilon_2) \sum_{|\mathbf{k}| \geq K} a_{\mathbf{k}}^+ a_{\mathbf{k}} + \sum_{|\mathbf{k}| \geq K} (V^*(k) a_{\mathbf{k}}^+ + \text{h.c.}) + \frac{3}{2}(1 - \varepsilon_2) + \varepsilon,
 \end{aligned}$$

which can be proved positive-definite for $K_{\min} < K < k_D$ following the approach outlined in [3]. Here K_{\min} is defined in such a way

$$K_{\min} = \frac{\frac{8\sqrt{2}\alpha}{3\pi(1-\varepsilon_2)}}{1 + \frac{8\sqrt{2}\alpha}{3\pi(1-\varepsilon_2)} \frac{1}{k_D}}$$

that $K_{\min} < k_D$ for any finite $\alpha > 0$ and $0 < \varepsilon_2 < 1$.

For the case of the «physical» as well as «field-theoretical» Fröhlich polaron model in a magnetic field the following partitioning $H = H^0 + H'$ of the original Hamiltonian (1) in the representation of the \hat{P}_z component of the polaron total momentum will work properly:

$$\begin{aligned}
 H^0 = & \left(1 - \frac{8\sqrt{2}\alpha}{3\pi(1-\varepsilon_2)} \left(\frac{1}{K} - \frac{1}{k_D}\right)\right) \left[\frac{1}{2} \left(\hat{p}_x - \frac{\omega_c}{2} \hat{y}\right)^2 + \frac{1}{2} \left(\hat{p}_y + \frac{\omega_c}{2} \hat{x}\right)^2\right] + \\
 & + \varepsilon_1 \sum_{|\mathbf{k}| < K} a_{\mathbf{k}}^+ a_{\mathbf{k}} + \varepsilon_2 \sum_{|\mathbf{k}| \geq K} a_{\mathbf{k}}^+ a_{\mathbf{k}} - \sum_{|\mathbf{k}| < K} \frac{|V(k)|^2}{1 - \varepsilon_1} - \frac{3}{2}(1 - \varepsilon_2) - \varepsilon, \quad (10)
 \end{aligned}$$

$$\begin{aligned}
 H' = & \frac{8\sqrt{2}\alpha}{3\pi(1-\varepsilon_2)} \left(\frac{1}{K} - \frac{1}{k_D}\right) \left[\frac{1}{2} \left(\hat{p}_x - \frac{\omega_c}{2} \hat{y}\right)^2 + \frac{1}{2} \left(\hat{p}_y + \frac{\omega_c}{2} \hat{x}\right)^2\right] + \\
 & + (1 - \varepsilon_1) \sum_{|\mathbf{k}| < K} a_{\mathbf{k}}^+ a_{\mathbf{k}} + (1 - \varepsilon_2) \sum_{|\mathbf{k}| \geq K} a_{\mathbf{k}}^+ a_{\mathbf{k}} + \sum_{\mathbf{k}} \left(V^*(k) a_{\mathbf{k}}^+ e^{-i(k_x \hat{x} + k_y \hat{y})} + \text{h.c.}\right) + \\
 & + \frac{1}{2} \left(P_z - \sum_{\mathbf{k}} k_z a_{\mathbf{k}}^+ a_{\mathbf{k}}\right)^2 + \sum_{|\mathbf{k}| < K} \frac{|V(k)|^2}{1 - \varepsilon_1} + \frac{3}{2}(1 - \varepsilon_2) + \varepsilon. \quad (11)
 \end{aligned}$$

Here, again in line with [3], H' can be proved positive-definite for $K_{\min} < K < k_D$ and $0 < \varepsilon_{1,2} < 1$. Further details regarding various aspects of explicit calculation by this method of various lower bounds for the Fröhlich polaron model can be found in [11].

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REFERENCES

1. *Fröhlich H.* // *Adv. Phys.* 1954. V. 3. P. 325.
2. *Lieb E. H., Yamazaki K.* // *Phys. Rev.* 1958. V. 111. P. 728.
3. *Lieb E. H., Thomas L. E.* // *Commun. Math. Phys.* 1997. V. 183. P. 511;
Lieb E. H., Thomas L. E. // *Ibid.* V. 188. P. 499.
4. *Larsen D. M.* // *Phys. Rev.* 1968. V. 172. P. 967.
5. *Weyl H.* // *Bull. Am. Math. Soc.* 1950. V. 56. P. 115.
6. *Weinstein A.* Etude des spectres des equations aux derivees partielles. *Memorial des Sci. Math. Paris*, 1937. No. 88.
7. *Weinstein A., Stenger W.* *Intermediate Problems for Eigenvalues*. N. Y.; London: Acad. Press, 1972.
8. *Gould S. H.* *Variational Methods for Eigenvalue Problems: An Introduction to the Weinstein Method of Intermediate Problems*. 2nd ed. Univ. of Toronto Press, 1966.
9. *Bazley N. W., Fox D. W.* // *Phys. Rev.* 1961. V. 124. P. 483.
10. *Bazley N. W., Fox D. W.* // *J. Res. Nat. Bur. of Standards*. 1961. V. 65B, No. 2. P. 105.
11. *Soldatov A. V.* // *Condens. Matter Phys.* 2009. V. 12, No. 4. P. 1.