

Spectral properties of an optical polaron in a magnetic field

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(Received 30 January 1987; accepted for publication 13 January 1988)

An optical polaron, which is exposed to a homogeneous magnetic field, is considered. Making use of functional analytical methods of Fröhlich [Fortschr. Phys. **22**, 159 (1974)], it is proved that the ground-state energy, the magnetic polaron mass, and the number of virtual phonons in the ground state are analytical functions of the electron-phonon coupling parameter and the magnetic field strength. Consequently, a discontinuous stripping transition, which was claimed recently by several authors, does not exist. In fact, some authors have stated that the discontinuities they encounter might indeed be artifacts due to the approximation. The spectrum of the momentum-decomposed Fröhlich Hamiltonian is analyzed; bounds and smoothness properties of the ground state and the discrete excited states are derived. All results hold also for lower spatial dimensions.

I. INTRODUCTION AND STATEMENT OF THE PROBLEM

In the present paper we discuss spectral properties of the momentum-decomposed Fröhlich Hamiltonian of an optical polaron in a constant uniform magnetic field.

The standard (three-dimensional) polaron model is defined by the well-known Hamiltonian H_F , proposed by Fröhlich, Pelzer, and Zienau,¹

$$H_F = \frac{1}{2m} (\mathbf{p} + |e|\mathbf{A}(\mathbf{x}))^2 + \int d^3k \hbar\omega(\mathbf{k}) a_{\mathbf{k}}^+ a_{\mathbf{k}} + \int d^3k \alpha^{1/2} (g(\mathbf{k}) a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}} + \text{H.c.}) \quad (1)$$

with

$$\omega(\mathbf{k}) = \omega_0 > 0 \quad (2)$$

and

$$g(\mathbf{k}) = \hbar\omega_0 (\hbar/2m\omega_0)^{1/4} (4\pi)^{1/2} (2\pi)^{-3/2} |k|^{-1} \quad (3)$$

EL4 $\equiv \Omega |k|^{-1}$.

Here, m , \mathbf{x} , \mathbf{p} are the mass, the position, and momentum operator of the (spinless) electron; \mathbf{k} , $\omega(\mathbf{k})$ are the wave vector and frequency of the phonons (i.e., spinless bosons); $g(\mathbf{k})$ is the electron-phonon coupling, α being the dimensionless electron-phonon coupling parameter, and $|e|$ the elementary charge. As usual, we set henceforth $\hbar = \omega_0 = m = |e| = 1$ and keep α and B as the only parameters. Let the magnetic field $\mathbf{B} = (0, 0, B)$, $B > 0$, be along the x_3 axis. Then, in the Landau gauge, the vector potential \mathbf{A} may be written as $\mathbf{A}(\mathbf{x}) = (0, Bx_1, 0)$.

In the case of free optical polarons ($B = 0$), the analytical properties of the ground-state energy were unclear for a long time, until Spohn² applied the beautiful functional analytical work of Fröhlich³ directly to prove the analyticity of the ground-state energy and the polaron mass as a function of the coupling parameter. In this paper, we want to generalize this result to arbitrary magnetic fields. Making use of operator methods developed by Fröhlich,³ we do show that the ground-state energy, the ground-state wave function, and expectation values of the ground state as well as the magnetic polaron mass are analytical functions in the coupling parameter α and the magnetic field strength B ($B > 0$).

The same holds true for the energies and wave functions of the momentum-decomposed discrete excited states, i.e., the Landau levels below the one-phonon continuum.

This paper represents the first rigorous study of analytical properties in optical polaron systems for arbitrary coupling and arbitrary magnetic field strength at zero temperature. Only for very small α , Alvarez-Estrada⁴ has established analytical properties by using several perturbation approaches. We note that Gerlach and the author have proved in a previous work⁵ under rather general conditions that the (formal) free energy of an acoustical or optical polaron system, exposed to a homogeneous magnetic field, is analytic in the temperature T ($0 < T < \infty$), coupling parameter α , and magnetic field strength B ($0 < B$). But the limit $T \rightarrow 0$ was not studied there.

The most important consequence of our results concerns a so-called stripping transition, which was first studied by Peeters and Devreese.^{6,7} In a series of papers, Peeters and Devreese have calculated the ground-state energy,^{6,7} the polaron mass,^{7,8} the polaron radius⁹ as well as the number of virtual phonons in the ground state⁹ and the magnetoabsorption spectrum¹⁰ within the anisotropic Feynman approximation. They do find nonanalytical behavior of these quantities at certain critical values of α and B . They indicate that this might be an artifact of their approximation. We note that Gorshkov, Zabrodin, Rodriguez, and Fedyanin¹¹ have already questioned these discontinuous transitions. A similar nonanalytical behavior is found for a two-dimensional polaron (see the recent work of Wu Xiaoguang, Peeters, and Devreese¹²). Within the Fock approximation, Lépine and Matz¹³ and Lépine¹⁴ get discontinuous transitions, too. In fact, there may be large changes in the polaron quantities as a function of α or B , but these changes are continuous. All discontinuities reported in the references quoted above are artifacts of the the approximations rather than intrinsic properties of the Fröhlich Hamiltonian. In fact, in Refs. 6–9, Peeters and Devreese carefully stated that the discontinuities they encounter could be artifacts of their approximation.

The basic steps of the proof are as follows: In Sec. II, we introduce the corresponding momentum decomposed Hamiltonian $H(\mathbf{Q})$ whose spectral properties are under study. Two different cutoffs are successively introduced which

clearly have to be removed later: a UV cutoff in the coupling and a lattice cutoff which leads to a discrete phonon momentum space. Then, it is proved that the ground state energy of the momentum decomposed cutoff Hamiltonian belongs to the discrete part of the spectrum, if the momentum \mathbf{Q} fulfills a simple inequality. After that, we show that the same result is also valid if the lattice cutoff is removed. In Sec. III, it is proved that this result even holds, if the UV cutoff is removed, using a dressing transformation. After having shown that the ground state of $H(\mathbf{Q})$ is nondegenerate (see Sec. IV), we derive bounds on the ground state energy of $H(\mathbf{Q})$ (see Sec. V) that guarantee that the inequality mentioned above is fulfilled. Since this finally implies that the ground state of $H(\mathbf{Q})$ is discrete and nondegenerate, we are able to apply analytic perturbation theory in Sec. VI which establishes smoothness properties of the ground state and the discrete excited states. Finally, in Sec. VII we give other examples, to which our methods are applicable.

II. SPECTRAL PROPERTIES OF THE HAMILTONIAN WITH UV CUTOFF

First, we perform a Lee–Low–Pines transformation. Defining

$$U = \exp(-i(P_2x_2 + P_3x_3)), \quad (4)$$

where

$$\mathbf{P} = \int d^3k \mathbf{k} a_{\mathbf{k}}^+ a_{\mathbf{k}} \quad (5)$$

is the phonon momentum, we obtain

$$\tilde{H}_F := U^{-1}H_F U = \mathbf{G}^2/2 + H_{oph} + H_I \quad (6a)$$

with

$$H_{oph} = \int d^3k a_{\mathbf{k}}^+ a_{\mathbf{k}}, \quad (6b)$$

$$H_I = \alpha^{1/2} \int d^3k (g(\mathbf{k})a_{\mathbf{k}} \exp(ik_1x_1) + \text{H.c.}) \quad (6c)$$

and

$$\mathbf{G} = (p_1, Bx_1 + p_2 - P_2, p_3 - P_3). \quad (6d)$$

Furthermore,

$$U^{-1}p_i U = p_i - P_i, \quad i = 2, 3. \quad (7)$$

Clearly, \tilde{H}_F does not depend on x_2 and x_3 , i.e., p_2 and p_3 , now playing the role of the total momentum [see (7)], are conserved quantities which may be replaced by c numbers Q_2 and Q_3 . Mathematically, this means that \tilde{H}_F admits a direct integral decomposition as follows:

$$\tilde{H}_F = \int_{\mathbb{Q}} dQ_2 dQ_3 H(\mathbf{Q}), \quad \mathbf{Q} = (0, Q_2, Q_3). \quad (8)$$

Here, $H(\mathbf{Q})$, being the Hamiltonian corresponding to fixed total momentum Q_2 and Q_3 , is given by

$$H(\mathbf{Q}) = H_0(\mathbf{Q}) + H_I, \quad (9a)$$

$$H_0(\mathbf{Q}) = H_{oph} + \mathbf{G}(\mathbf{Q})^2/2, \quad (9b)$$

$$\mathbf{G}(\mathbf{Q}) = (p_1, Bx_1 + Q_2 - P_2, Q_3 - P_3). \quad (9c)$$

It is well-known that, for $B > 0$, the spectrum of $H(\mathbf{Q})$ is independent of Q_2 (see, e.g., Devreese¹⁵). Nevertheless we retain the trivial Q_2 dependence.

For the underlying Hilbert space \mathcal{H} , it is convenient to take

$$\mathcal{H} = F \otimes L^2(\mathbf{R}), \quad (10)$$

where

$$F = \bigoplus_{m=0}^{\infty} L^2(\mathbf{R}^3)^{\otimes m} \quad (11)$$

is the usual Fock space of the phonons, \bigotimes denoting the symmetrical tensor product. We define UV cutoff Hamiltonians $H_r(\mathbf{Q})$, H_{I_r} by replacing $g(\mathbf{k})$ in (9a) and (6c) by $g_r(\mathbf{k}) \equiv g(\mathbf{k}) \cdot \theta(r - k)$, $0 < r < \infty$. Then, according to a result of Nelson,¹⁶ we may state: For all $\epsilon > 0$ there exists a number $b(r, \epsilon) < \infty$ such that

$$\|H_{I_r}\psi\| \leq \epsilon \|H_{oph}\psi\| + b \|\psi\| \leq \epsilon \|H_0(\mathbf{Q})\psi\| + b \|\psi\|, \quad (12)$$

for all $|\psi\rangle \in D(H_0(\mathbf{Q}))$.

Clearly, $H_0(\mathbf{Q})$ is self-adjoint and bounded from below. Consequently, the Kato–Rellich theorem¹⁷ ensures us that $H_r(\mathbf{Q})$ is self-adjoint and bounded from below.

Now we introduce a second cutoff: We replace the phonon momentum space \mathbf{R}^3 by a momentum lattice Γ_d (see Refs. 3 and 18 for a detailed discussion),

$$\Gamma_d = \{\mathbf{k} \in \mathbf{R}^3 | k_j = n_j/\Lambda_d, n_j \in \mathbf{Z}, \Lambda_d = 2^d \Lambda_0, \Lambda_0 \in \mathbf{R}^+, j = 1, 2, 3\}. \quad (13)$$

To each $\mathbf{k} \in \mathbf{R}^3$ we associate a $\mathbf{k}|_d \in \Gamma_d$, namely,

$$\mathbf{k}|_d = (n_1, n_2, n_3)/\Lambda_d, \quad n_j = \langle k_j \Lambda_d \rangle, \quad (14)$$

where

$$\langle a \rangle \equiv \begin{cases} \text{largest integer} < a, & \text{if } a < 0, \\ \text{smallest integer} > a, & \text{if } a > 0. \end{cases}$$

The continuum limit is obtained by taking the limit $d \rightarrow \infty$. We now define a subspace $S_d \subseteq L^2(\mathbf{R}^3)$ of step functions,

$$f \in S_d \Leftrightarrow f(\mathbf{k}) = f(\mathbf{k}|_d). \quad (15)$$

For $g \in L^2(\mathbf{R}^3)$ let $g|_d$ denote the orthogonal projection of g onto S_d . We need some further definitions,

$$F_d \equiv \bigoplus_{m=0}^{\infty} S_d^{\otimes m}, \quad (16)$$

$$F_d^\perp \equiv \left(\bigoplus_{m=1}^{\infty} S_d^{\perp \otimes m} \right) \bigotimes F_d. \quad (17)$$

Then we have

$$F = F_d \oplus F_d^\perp. \quad (18)$$

We introduce the d cutoff in the Hamiltonian in the following way:

$$H_{dr}(\mathbf{Q}) = H_{0d} + H_{I_{dr}}, \quad (19)$$

$$H_{0d} = \int d^3k a_{\mathbf{k}}^+ a_{\mathbf{k}} + \frac{p_1^2}{2} + \frac{(Bx_1 + Q_2 - P_2|_d)^2}{2} + \frac{(Q_3 - P_3|_d)^2}{2}, \quad (20)$$

$$H_{I_{dr}} = \alpha^{1/2} \int d^3k ((g_r(\mathbf{k})|_d \exp(ik_1|_d x_1) a_{\mathbf{k}} + \text{H.c.}), \quad (21)$$

where now

$$\mathbf{P}|_d = \int d^3k k|_d a_{\mathbf{k}}^+ a_{\mathbf{k}}.$$

One easily verifies that (12) remains true for the new d cutoff Hamiltonian $H_{dr}(\mathbf{Q})$. Consequently, $H_{dr}(\mathbf{Q})$ is self-adjoint and bounded from below, too. Let $E(r, \mathbf{Q})$, $E(d, r, \mathbf{Q})$ be the ground-state energy of the Hamiltonians $H_r(\mathbf{Q})$, $H_{dr}(\mathbf{Q})$.

Lemma 2.1: Suppose that the momentum \mathbf{Q} is such that

$$\inf_{\mathbf{k}} (E(r, d, \mathbf{Q} - (0, k_2, k_3)) + 1 - E(r, d, \mathbf{Q})) \equiv \Delta(r, d, \mathbf{Q}) > 0. \quad (22)$$

Then the interval $[E(r, d, \mathbf{Q}), E(r, d, \mathbf{Q}) + \Delta(r, d, \mathbf{Q})]$ belongs to the discrete part of $\text{spec}(H_{dr}(\mathbf{Q}) \upharpoonright F_d \otimes L^2(\mathbb{R}))$, where \upharpoonright denotes (as usual) the restriction.

Proof: First, we define a new subspace $J \subseteq S_d$ by

$$f \in J \Leftrightarrow f(\mathbf{k}) \equiv 0, \quad \text{for } |\mathbf{k}|_d > r + 3/\Lambda_d. \quad (23)$$

Moreover, let $\tilde{\Gamma}_d \equiv \{\mathbf{k} \in \Gamma_d \mid |\mathbf{k}| \leq r + 3/\Lambda_d\}$ and

$$W \equiv \bigoplus_{m=0}^{\infty} J^{\otimes m}, \quad W_1 \equiv \left(\bigoplus_{m=1}^{\infty} J^1 \otimes^m \right), \\ W^1 = W_1 \otimes W. \quad (24)$$

Clearly, $F_d = W \otimes W^1$ and $H_{dr}(\mathbf{Q})$, H_{Idr} leave W invariant.

We consider $(\vartheta - H_{dr})^{-1} \upharpoonright W \otimes L^2(\mathbb{R})$. Since H_{Idr} is a Kato potential with respect to H_{Od} the following von Neumann resolvent expansion converges in norm:

$$\langle \chi | H_{dr}(\mathbf{Q}) | \chi \rangle = \sum_{j=1}^N \langle \chi | \chi \rangle + \langle \varphi | H_{dr} \left(\mathbf{Q} - \sum_{j=1}^N (0, k_j^2 |_d, k_j^3 |_d) \right) | \varphi \rangle \langle \theta | \theta \rangle \\ \geq \left(1 + E \left(d, r, \mathbf{Q} - \sum_{j=1}^N (0, k_j^2 |_d, k_j^3 |_d) \right) \right) \langle \chi | \chi \rangle \geq \left(1 + \inf_{\mathbf{k}} E(d, r, \mathbf{Q} - (0, k_2, k_3)) \right) \langle \chi | \chi \rangle.$$

The same inequalities are valid for vectors which are finite linear combinations of pairwise orthogonal vectors of the form $|\theta(\tilde{k}^N)\rangle \otimes |\varphi\rangle$, $N \in \mathbb{N}$. Since these vectors are dense in $W^1 \otimes L^2(\mathbb{R})$ we conclude

$$\inf \text{spec}(H_{dr}(\mathbf{Q}) \upharpoonright W^1 \otimes L^2(\mathbb{R})) \\ > 1 + \inf_{\mathbf{k}} E(d, r, \mathbf{Q} - (0, k_2, k_3)). \quad (26)$$

Third, let f be a positive C^∞ function on \mathbb{R} such that $f(0) = 1$, $f(x) = 0$ if $x \geq \Delta(r, d, \mathbf{Q}) > 0$. Then we know from (26),

$$f(H_{dr}(\mathbf{Q}) - E(d, r, \mathbf{Q})) \upharpoonright W^1 \otimes L^2(\mathbb{R}) \equiv 0.$$

On the other hand, the compactness of $(\vartheta - H_{dr})^{-1} \upharpoonright W \otimes L^2(\mathbb{R})$ implies that $f(H_{dr}(\mathbf{Q}) - E(d, r, \mathbf{Q})) \upharpoonright W \otimes L^2(\mathbb{R})$ is compact.

Since $F_d \otimes L^2(\mathbb{R}) = (W \otimes L^2(\mathbb{R})) \oplus (W^1 \otimes L^2(\mathbb{R}))$, it follows that $f(H_{dr}(\mathbf{Q}) - E(d, r, \mathbf{Q})) \upharpoonright F_d \otimes L^2(\mathbb{R})$ is compact. This immediately implies Lemma 2.1. \square

Now we can proceed along similar lines as Fröhlich does (see Theorem 2.3 in Ref. 3). The only difference is that our Hilbert space is $F_d \otimes L^2(\mathbb{R})$ (instead of F_d) and that in our case *a priori* $f(H_{dr}(\mathbf{Q}) - E(d, r, \mathbf{Q})) \upharpoonright F_d \otimes L^2(\mathbb{R})$ is compact, whereas in Ref. 3 the *total* spectrum is discrete. Nevertheless, Fröhlich's proof can directly be mimicked. As a con-

$$(\vartheta - H_{dr})^{-1} = (\vartheta - H_{Od})^{-1} \left(\sum_{n=0}^{\infty} [H_{Idr}(\vartheta - H_{Od})^{-1}]^n \right). \quad (25)$$

For $\text{Re } \vartheta$ sufficiently small, the second factor of (25) defines a bounded operator. According to Glimm and Jaffe¹⁸ there exists an isomorphism between J and the square summable complex functions of the momentum lattice $\tilde{\Gamma}_d$ consisting of a finite number of lattice vectors. Hence the eigenvalue problem of $H_{Od} \upharpoonright W \otimes L^2(\mathbb{R})$ is completely solvable and the eigenvalues E_n can be numbered by natural numbers n , where $E_n \rightarrow \infty$ as $n \rightarrow \infty$. Therefore (see, e.g. Ref. 19), $(\vartheta - H_{Od})^{-1}$ is compact and, because of (25), $(\vartheta - H_{dr})^{-1} \upharpoonright W \otimes L^2(\mathbb{R})$ is compact for all $\vartheta \in \text{spec}(H_{dr} \upharpoonright W \otimes L^2(\mathbb{R}))$.

In a second step, we estimate $\inf \text{spec}(H_{dr}(\mathbf{Q}) \upharpoonright W^1 \otimes L^2(\mathbb{R}))$. Let us consider a vector $|\chi\rangle \in W^1 \otimes L^2(\mathbb{R})$, which has the form $|\chi\rangle = |\theta\rangle \otimes |\varphi\rangle$, where $|\varphi\rangle \in W \otimes L^2(\mathbb{R})$, $|\theta\rangle \in W_1$, $|\theta\rangle \equiv |\theta(\tilde{k}^N)\rangle$, $\tilde{k}^N = (\mathbf{k}^1, \dots, \mathbf{k}^N)$. Let $|\theta\rangle$ be an eigenstate of the phonon number operator with eigenvalue $N \geq 1$ and let $|\theta\rangle$ fulfill

$$\mathbf{P}|_d |\theta\rangle = \sum_{j=1}^N \mathbf{k}^j |_d |\theta\rangle, \quad \text{where } \mathbf{k}^j |_d \in \Gamma_d \setminus \tilde{\Gamma}_d.$$

Then, $\|\chi\| = \|\theta\| \cdot \|\varphi\|$ and

$$\langle \chi | H_{Idr} | \chi \rangle = \langle \varphi | H_{Idr} | \varphi \rangle \langle \theta | \theta \rangle$$

and therefore

sequence, we arrive at the following theorem, where the d cutoff is removed and a phonon gap in the spectrum is established.

Theorem 2.2: Suppose that the momentum \mathbf{Q} is such that

$$\inf_{\mathbf{k}} E(r, \mathbf{Q} - (0, k_2, k_3)) + 1 - E(r, \mathbf{Q}) \equiv \Delta(r, \mathbf{Q}) > 0. \quad (27)$$

Then the interval $[E(r, \mathbf{Q}), E(r, \mathbf{Q}) + \Delta(r, \mathbf{Q})]$ belongs to the discrete part of $\text{spec}(H_r(\mathbf{Q}) \upharpoonright F \otimes L^2(\mathbb{R}))$.

III. REMOVING THE UV CUTOFF

To remove the UV cutoff, we use a canonical transformation, which was proposed by Gross²⁰ and mathematically studied by Nelson.¹⁶ We define

$$H_r^T(\mathbf{Q}) = e^T H_r(\mathbf{Q}) e^{-T}, \quad (28)$$

where

$$T \equiv T_{r,\Lambda} = \int d^3k (\beta_{r,\Lambda}(\mathbf{k}) a_{\mathbf{k}} \exp(ik_1 x_1) - \text{H.c.}) \quad (29)$$

and

$$\beta_{r,\Lambda}(\mathbf{k}) \equiv \beta(\mathbf{k}) = -\alpha^{1/2} 2g_r(\mathbf{k}) \theta(k - \Lambda) / (2 + k^2), \\ 1 < \Lambda < r. \quad (30)$$

A lengthy but straightforward calculation, similar to those in Refs. 16 and 20, yields

$$H_r^T(\mathbf{Q}) = H_0(\mathbf{Q}) + \alpha^{1/2} \int d^3k (g_\Lambda(\mathbf{k}) e^{ik_1 x_1} a_{\mathbf{k}} + \text{H.c.}) + (\Phi + \Phi^*)^2/2 - \mathbf{G} \cdot \Phi - \Phi^* \cdot \mathbf{G} + \Sigma, \quad (31)$$

where we have used the abbreviation

$$\Phi = \int d^3k \mathbf{k} \beta_{r\Lambda}(\mathbf{k}) \exp(ik_1 x_1) a_{\mathbf{k}}. \quad (32)$$

Here Σ is a finite self-energy, given by

$$\Sigma = \int d^3k [|\beta(\mathbf{k})|^2 + \alpha^{1/2} g^*(\mathbf{k}) \beta(\mathbf{k}) + \alpha^{1/2} g(\mathbf{k}) \beta^*(\mathbf{k})]. \quad (33)$$

We have to estimate each term in (31). As an example, we discuss the term involving the magnetic field. For all $|\psi\rangle \in D(H_0^{1/2})$ we have

$$\begin{aligned} & |\langle \psi | (\mathbf{G} \cdot \Phi + \Phi^* \cdot \mathbf{G}) | \psi \rangle| \\ & \leq 2 \sum_{i=1}^3 \|G_i \psi\| \cdot \|\Phi_i \psi\| \\ & \leq \|H_0^{1/2} \psi\| \cdot C(\Lambda) \cdot \|H_{0ph}^{1/2} \psi\| \leq C(\Lambda) \|H_0^{1/2} \psi\|^2, \end{aligned}$$

where $C(\Lambda) \rightarrow 0$ as $\Lambda \rightarrow \infty$.

Hence

$$|\mathbf{G} \cdot \Phi + \Phi^* \cdot \mathbf{G}| \leq C(\Lambda) H_0. \quad (34)$$

Estimating the remaining terms in analogy to Ref. 3 (see Sec. 2.2 in Ref. 3), it follows that for all $\epsilon > 0$ there exists a $\Lambda < \infty$ such that

$$|H_r^T(\mathbf{Q}) - H_0| \leq \epsilon H_0 + b(\Lambda), \quad (35)$$

where $b(\Lambda)$ is uniform in $r < \infty$ and Q . Mimicking Fröhlich's proof (see Theorem 2.4 in Ref. 3) we get the following theorem.

Theorem 3.1: Let Λ be fixed and $r \rightarrow \infty$.

$$\text{norm-lim}_{r \rightarrow \infty} (\vartheta - H_r^T(\mathbf{Q}))^{-1} = (\vartheta - H^T(\mathbf{Q}))^{-1}$$

exists, where $(\vartheta - H^T(\mathbf{Q}))$ is the resolvent of a unique s.a. operator $H^T(\mathbf{Q})$ bounded from below. Here $H^T(\mathbf{Q})$ can be related to the Hermitian forms induced by (35) by a variant of Friedrich's extension theorem (see Nelson¹⁶).

$$\text{s-lim}_{r \rightarrow \infty} \exp(T_{r\Lambda}) \equiv \exp(T_{\infty\Lambda})$$

exists. Therefore

$$H(\mathbf{Q}) \equiv \exp(-T_{\infty\Lambda}) H^T(\mathbf{Q}) \exp(T_{\infty\Lambda})$$

is self-adjoint and bounded below. \square

Again, we follow Fröhlich (Theorem 2.7 in Ref. 3) and obtain that Theorem 2.2 is even valid in the limit $r \rightarrow \infty$, i.e., the following lemma.

Lemma 3.2: Let $E(\mathbf{Q})$ denote the ground-state energy of $H(\mathbf{Q})$. Suppose that the momentum \mathbf{Q} is such that

$$\inf_{\mathbf{k}} (E(\mathbf{Q} - (0, k_2, k_3)) + 1 - E(\mathbf{Q})) \equiv \Delta(\mathbf{Q}) > 0. \quad (36)$$

Then the interval $[E(\mathbf{Q}), E(\mathbf{Q}) + \Delta(\mathbf{Q})]$ belongs to the discrete part of spec $H(\mathbf{Q})$.

IV. NONDEGENERACY OF THE MOMENTUM DECOMPOSED GROUND STATE

Keeping in mind that we intend to apply a generalized version of the Perron-Frobenius theorem, it is useful to consider a slightly different cutoff Hamiltonian $H'_n(\mathbf{Q})$. (Of course, the cutoff is removed later.) In doing so, we now replace in (6c) and (9a) the coupling $g(\mathbf{k})$ by

$$\begin{aligned} g_n(\mathbf{k}) & \equiv -g(\mathbf{k}) \mu_n(k^\perp) \\ & \equiv -g(\mathbf{k}) (\theta(n - k^\perp) \\ & \quad + \theta(k^\perp - n) \exp(-(k^\perp - n))), \end{aligned} \quad (37)$$

where

$$k^{12} = k_2^2 + k_3^2. \quad (38)$$

Note that

$$g_n(\mathbf{k}) \in L^2(\mathbb{R}^3), \quad \text{for } n < \infty. \quad (39)$$

Additionally, for the first component of the phonon Fock space we now choose the q representation (Schrödinger representation) instead of the momentum representation. In this new representation the Hamiltonians read

$$H'_n(\mathbf{Q}) = H'_0 + H'_{iN}, \quad H'_0 = \int d^3l b_l^\dagger + b_l + \mathbf{G}'^2/2, \quad (40)$$

$$\begin{aligned} H'_{iN} & = \left(\frac{2\alpha}{\pi}\right)^{1/2} \Omega \int d^3l \mu_n(k^\perp) \\ & \quad \times K_0(k^\perp(x_1 - q))(b_l + b_l^\dagger), \end{aligned} \quad (41)$$

where now

$$\begin{aligned} \mathbf{G}' & = (p_1, Bx_1 + Q_2 - P'_2, Q_3 - P'_3), \\ b_l & = (2\pi)^{-1/2} \int dk_1 a_{\mathbf{k}} \exp(ik_1 q), \end{aligned} \quad (42)$$

and

$$P'_i = \int d^3l k_i b_l^\dagger + b_l, \quad i = 2, 3, \quad l = (q, k_2, k_3), \quad (43)$$

and where $K_0(x)$ denotes a strictly positive Bessel function of imaginary argument. By a canonical transformation, analogous to that in Sec. III, one proves for all $|\varphi\rangle, |\Phi\rangle \in D(H'_0)$ and for $\vartheta < \inf \text{spec } H(\mathbf{Q})$,

$$\lim_{n \rightarrow \infty} \langle \varphi | (H'_n(\mathbf{Q}) - \vartheta)^{-1} | \Phi \rangle = \langle \varphi | (H'(\mathbf{Q}) - \xi)^{-1} | \Phi \rangle, \quad (44)$$

where $H'(\mathbf{Q})$ is s.a., bounded below, and has the same spectrum as $H(\mathbf{Q})$. Because of (39) the following expansion converges in norm:

$$\begin{aligned} & (H'_n(\mathbf{Q}) - \vartheta)^{-1} \\ & = (H'_0 - \vartheta)^{-1} \sum_{m=0}^{\infty} [(-1) H'_{iN} (H'_0 - \vartheta)^{-1}]^m. \end{aligned} \quad (45)$$

Computing the kernel

$$\begin{aligned} & \langle y | \otimes \langle 0 | b_{l_1} \cdots b_{l_n} | (H'_n(\mathbf{Q}) - \vartheta)^{-1} | b_{l_1}^\dagger \cdots b_{l_n}^\dagger | 0 \rangle \otimes | x \rangle, \\ & \quad u, u' \in IN_0, \end{aligned} \quad (46)$$

we see by inspection of (45) that (46) is strictly positive for $\alpha > 0$: With respect to the electron coordinate in the Schrö-

dinger representation (i.e., with fixed positive phonon wave function), $(H'_0 - \vartheta)^{-1}$ is positivity improving as resolvent of a harmonic oscillator. With respect to the phonon coordinate, $(H'_0 - \vartheta)^{-1}$ is positivity preserving and it preserves the support. Furthermore, H'_{in} is positivity preserving with respect to the electron coordinate because of the positivity of K_0 . Moreover, for a suitable choice of m in (45) it can be achieved that

$$\langle y | \otimes \langle 0 | b_{1_i} \cdots b_{1_u} | (-H'_{in} (H'_0 - \vartheta)^{-1})^m | b_{1_i}^+ \cdots b_{1_u}^+ | 0 \rangle \otimes | x \rangle > 0. \quad (47)$$

Consequently, $(H'_n(\mathbf{Q}) - \vartheta)^{-1}$ is positivity improving in the chosen representation. Since (46) is monotonically increasing with n , we get with (44) that $(H' - \vartheta)^{-1}$ is positivity improving. From Sec. III we know that under condition (36) $\inf \text{spec } H'(\mathbf{Q}) = E(\mathbf{Q})$ is an eigenvalue of $H'(\mathbf{Q})$. Therefore (see, e.g., Ref. 19) $E(\mathbf{Q})$ is a simple eigenvalue, or, equivalently, the ground state is nondegenerate.

V. BOUNDS ON THE GROUND-STATE ENERGY

Lemma 5.1: For the ground-state energy $E(\mathbf{Q})$ we have the bounds

$$(i) E(\mathbf{Q}) \leq E(0) + Q_3^2/2, \quad (48)$$

$$(ii) E(\mathbf{Q}) \geq E(0). \quad (49)$$

Proof: (i) follows from the fact that $E(\mathbf{Q}) - Q_3^2/2$ is a concave symmetrical function of Q_3 , since the Hamiltonian $H(\mathbf{Q}) - Q_3^2/2$ couples linear to Q_3 . (ii) We use the same procedure as in (37) and (40)–(43) transforming now the third component of the phonon coordinate into the Schrödinger representation, i.e.,

$$k^{12} = k_1^2 + k_2^2, \quad \mathbf{l} = (k_1, k_2, q).$$

Thereby we obtain new Hamiltonians $\tilde{H}_n(\mathbf{Q})$, \tilde{H}_{oph} , $\tilde{G}(\mathbf{Q})^2/2$, \tilde{H}_{in} , and the phonon momentum operator \tilde{P} . Because of Theorem 3.1, it suffices to show (49) for $n < \infty$. One easily sees (e.g., by a Dyson expansion) that

$$\exp(-tL) \equiv \exp(-t(\tilde{H}_{oph} + \tilde{H}_{in} + \tilde{G}_1^2/2 + \tilde{G}_2^2/2)) \quad (50)$$

is positivity preserving for $t > 0$. Now, we follow an idea of Gross²¹ and write

$$\exp\left(-\frac{t(Q_3 - \tilde{P}_3)^2}{2}\right) = (2\pi t)^{-1/2} \int dy \exp\left(-\frac{y^2}{2t}\right) \exp(iy(Q_3 - \tilde{P}_3)). \quad (51)$$

Hence, we have, since $\exp(-iy\tilde{P}_3)$ preserves positivity,

$$\begin{aligned} & |\exp(-t\tilde{G}_3(\mathbf{Q})^2/2) \exp(-tL) |\varphi\rangle| \\ & \leq (2\pi t)^{-1/2} \int dy \exp\left(-\frac{y^2}{2t}\right) \\ & \quad \times \exp(iy\tilde{P}_3) \exp(-tL) \|\varphi\| \\ & \leq \exp(-t\tilde{G}_3(\mathbf{0})^2/2) \exp(-tL) \|\varphi\|, \\ & \quad \text{for } |\varphi\rangle \in D(\tilde{H}_n). \end{aligned} \quad (52)$$

One proceeds by induction to obtain

$$\begin{aligned} & |(\exp(-t\tilde{G}_3(\mathbf{Q})^2/(2k)) \exp(-tL/k))^k |\varphi\rangle| \\ & \leq (\exp(-t\tilde{G}_3(\mathbf{0})^2/(2k)) \exp(-tL/k))^k \|\varphi\|, \end{aligned} \quad (53)$$

which—because of the Trotter product formula—implies finally

$$\|\exp(-t\tilde{H}_n(\mathbf{Q})) |\varphi\rangle\| \leq \|\exp(-t\tilde{H}_n(\mathbf{0}))\| \|\varphi\|. \quad (54)$$

Hence (49) is established.

From Lemma 5.1 it follows immediately that (36) is fulfilled, if

$$Q_3^2 < 2. \quad (55)$$

We note that we can prove, using a new functional integral method developed by Gerlach *et al.*,²² that the continuum edge of $H(\mathbf{Q})$ begins exactly at the point $E(0) + 1$ involving scattering states with one real phonon (see Devreese²³ for a review). This yields the bound

$$E(\mathbf{Q}) \leq E(0) + 1. \quad (56)$$

VI. ANALYTICAL PERTURBATION THEORY

To establish analytical properties in \mathbf{Q} , α , and B , we start from the canonically transformed Hamiltonian $H_r^T(\mathbf{Q}) \equiv H_r^T(Q, \sqrt{\alpha}, B)$, see (28). Let now \mathbf{Q}, α, B be fixed, where $Q_3 < 2$, $\alpha > 0$, $B > 0$. We consider small deviations around these fixed parameters. The Q_2 dependence is trivial. Concerning the Q_3 dependence we have

$$\begin{aligned} & H_r^T((0, Q_2, Q_3 + \kappa), \sqrt{\alpha}, B) \\ & = H_r^T(Q, \sqrt{\alpha}, B) + \kappa(Q_3 - P_3 - \Phi_3 - \Phi_3^*) + \kappa^2/2. \end{aligned} \quad (57)$$

It is easily seen that P_3 is form bounded:

$$|P_3| \leq a H_r^T(Q, \sqrt{\alpha}, B) + b, \quad \text{for } r \leq \infty. \quad (58)$$

Therefore, the associated operators $H^T((0, Q_2, Q_3 + \kappa), \sqrt{\alpha}, B)$ are a holomorphic family of s.a. operators of type (B) in κ in the sense of Kato.¹⁷ The α dependence can be treated in a similar way:

$$H_r^T(Q, \sqrt{\alpha} + \gamma, B) = H_r^T(Q, \sqrt{\alpha}, B) + \gamma H''_r. \quad (59)$$

The estimations in Ref. 3 used in Sec. III show that H''_r is form bounded with constants independent of r ($r \leq \infty$). Hence $H^T(Q, \sqrt{\alpha} + \gamma, B)$ forms a holomorphic family of type (B) in the sense of Kato in γ , too.

The dependence on the magnetic field strength B is more difficult. We use a scaling transformation

$$\tilde{x} \equiv B^{1/2} x_1, \quad \tilde{p} \equiv B^{-1/2} p_1, \quad (60)$$

$$\tilde{a}_k \equiv B^{3/4} a_{B^{1/2}k}, \quad \tilde{a}_k^+ \equiv B^{3/4} a_{B^{1/2}k}^+. \quad (61)$$

Written in these new operators the resulting Hamiltonian $\tilde{H}_r^T(\mathbf{Q})$ has the form

$$\begin{aligned} \tilde{H}_r^T(\mathbf{Q}) & = \frac{B\tilde{G}^2}{2} + \int d^3k \tilde{a}_k^+ \tilde{a}_k + B^{1/2} \alpha^{1/2} \\ & \quad \times \int d^3k g_{\tilde{\lambda}}(\mathbf{k}) (\exp(ik_1 \tilde{x}) \tilde{a}_k + \text{H.c.}) \\ & \quad + B^{3/2} (\tilde{\Phi} + \tilde{\Phi}^+)^2/2 \\ & \quad - B^{5/4} (\tilde{G} \cdot \tilde{\Phi} + \tilde{\Phi}^+ \cdot \tilde{G}) + \Sigma, \end{aligned} \quad (62)$$

where $\tilde{\mathbf{G}}$ and $\tilde{\Phi}$ are given as in (8), (32) replacing the old operators with the new ones and the old quantities $\beta(\mathbf{k})$, Λ , r , \mathbf{Q} with

$$\tilde{\beta}(\mathbf{k}) = -2\alpha^{1/2}g_r(\mathbf{k})\theta(k - \tilde{\Lambda})/(2 + Bk^2), \quad (63)$$

$$\tilde{\Lambda} = B^{-1/2}\Lambda, \quad \tilde{r} = B^{-1/2}r, \quad \tilde{\mathbf{Q}} = B^{-1/2}\mathbf{Q}. \quad (64)$$

Note that the operators $\tilde{x}, \tilde{p}, \tilde{a}_k, \tilde{a}_k^+$ fulfill the same commutator relations as x, p, a_k, a_k^+ . Therefore, $\tilde{H}_r^T(\mathbf{Q})$ has the same spectrum as $H_r^T(\mathbf{Q})$. More properly, the Hamiltonian $\tilde{H}_r^T(\mathbf{Q})$ is obtained from $H_r^T(\mathbf{Q})$ by a canonical transformation, what is easily seen using Wigner's theorem (see Bargmann²⁴). Now, the B dependence manifests itself mainly as simple prefactors before the single parts of the Hamiltonian $\tilde{H}_r^T(\mathbf{Q})$. It is easily seen by developing (63) in its power series that

$$\begin{aligned} \tilde{H}_r^T(\mathbf{Q}, \sqrt{\alpha}, B + \epsilon) \\ = \tilde{H}_r^T(\mathbf{Q}, \sqrt{\alpha}, B) + \sum_{n=1}^{\infty} \epsilon^n G_r^{(n)}(\mathbf{Q}, \sqrt{\alpha}, B), \quad |\epsilon| < B, \end{aligned} \quad (65)$$

where in the sense of forms

$$|G_r^{(n)}(\mathbf{Q}, \sqrt{\alpha}, B)| < c^n (a' \tilde{H}_r^T(\mathbf{Q}, \sqrt{\alpha}, B) + b'), \quad \text{for } r < \infty. \quad (66)$$

Therefore we can repeat our statement that we are dealing with a holomorphic family of type (B) in ϵ . It now follows from standard perturbation theory (see Kato¹⁷) and from the fact that $E(\mathbf{Q})$ is an isolated simple eigenvalue that the ground-state energy $E(\mathbf{Q})$ is jointly real analytic in α ,²⁵ B , and \mathbf{Q} for $\alpha > 0$, $B > 0$, $Q_3^2 < 2$. The same holds true for the energies of the discrete excited states lying in the spectral interval $[E(\mathbf{0}), E(\mathbf{0}) + 1[$, where we have to exclude possible degenerate points.²⁶ Furthermore, the associated wave functions are analytic in α , B , and \mathbf{Q} . This, in turn, has immediate consequences on expectation values of operators which are independent of α , B , \mathbf{Q} like the number of virtual phonons or the polaron radius, etc. (see Peeters and Devreese⁹). Again, all these quantities are analytic in α , B , and \mathbf{Q} . From Lemma 5.1 we know that the ground-state energy $E_F(\alpha, B)$ of the original Hamiltonian H_F is obtained by taking $E(\mathbf{0})$. Especially, $E_F(\alpha, B)$ is analytic in α and B .

Another quantity, which is of interest, is the magnetic polaron mass. Peeters and Devreese⁷ have defined parallel and perpendicular magnetic polaron masses in the anisotropic Feynman approximation. One way to define a parallel magnetic polaron mass m'' a priori without using any approximation is

$$\frac{1}{m''} \equiv \left. \frac{\partial^2 E(\mathbf{Q})}{\partial Q_3^2} \right|_{\mathbf{Q}=\mathbf{0}}. \quad (67)$$

Another possibility to define a cyclotron mass m^* (depending on α and B) at weak or intermediate magnetic fields is

$$E_1(\mathbf{0}) - E(\mathbf{0}) = B/(2m^*), \quad (68)$$

where $E_1(\mathbf{Q})$ is the energy of the first excited state, i.e., the second Landau level. It follows immediately that both masses m'' and m^* are analytic in α and B .

VII. EXTENSION TO OTHER PROBLEMS

First, the dispersions and the coupling can be generalized to

$$\omega(\mathbf{k}) = \omega(k) > \omega_0 > 0, \quad (69)$$

$$g(\mathbf{k}) = g(k), \quad \int d^3k \frac{|g(k)|^2}{c + k^2} < \infty, \quad c > 0. \quad (70)$$

Additionally, performing the scaling transformation (60), (61), we have to assume that $g(k)$ is representable as a finite or infinite linear combination of powers k^p ($p \in \mathbb{R}$) in a domain of \mathbb{R}^3 . Then, the same proof goes through with two exceptions: The uniqueness proof of the ground state and Lemma 5.1 (ii) have to be modified. The condition $\omega_0 > 0$ cannot be weakened with our methods, since the gap in the spectrum, which makes perturbation theory possible, does not remain. For more singular couplings $g(\mathbf{k})$ one has to renormalize in a well-known way (see Nelson¹⁶).

Furthermore, the space dimension d is not relevant for our proof, if we take

$$|g(\mathbf{k})|^2 \sim k^{1-d}. \quad (71)$$

Several branches of optical phonons can easily be included in the proof. Whether or not we consider a discrete \mathbf{k} summation or a \mathbf{k} integration has no influence on the phase transition problem. The methods worked out in Secs. II and III are applicable, if the unperturbed Hamiltonian with discrete, cutoff \mathbf{k} sums has a compact resolvent, where conserved components of the total momentum are replaced by C numbers. For example, the problem of a polaron in an external potential $V(\mathbf{x})$, where $V(\mathbf{x}) \rightarrow \infty$ as $|\mathbf{x}| \rightarrow \infty$ is tractable. Another example concerns the polaron in an external uniform electric field. Since the resulting Hamiltonian is unbounded, it has to be renormalized. We cut off the potential as follows:

$$V(\mathbf{x}) = \begin{cases} |e|Ex_1, & \text{for } x_1 \geq L, \\ \infty, & \text{for } x_1 < L. \end{cases} \quad (72)$$

Then, all results concerning the ground-state energy, etc., hold. Especially, the ground-state energy is analytic in the coupling parameter α and the electric field strength E ($E > 0$).

ACKNOWLEDGMENTS

I am most grateful to Professor H. Spohn for valuable discussions, which have initiated this work, and for helpful information concerning Secs. IV and V. Furthermore, I thank Professor B. Gerlach for numerous clarifying discussions and Professor K. Veselic and Professor W. Hazod for explanation of some mathematical details. Moreover, I am indebted to Professor J. Fröhlich for sending me a detailed manuscript of his methods.

Financial support for this part of my thesis by the Studienstiftung des deutschen Volkes is gratefully acknowledged, too.

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