Analytical properties of polaron systems or: Do polaronic phase transitions exist or not?

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For more than 40 years it was thought that polaron- and exciton-phonon systems exhibited unexpected localization properties. Particular attention was paid to the so-called phonon-induced self-trapping transition, which, it was believed, should manifest itself as a point of nonanalyticity in the ground-state energy as a function of the electron-phonon coupling parameter. It will be demonstrated for a large class of (generalized Fröhlich) models that no such transition exists. The dimensionality of space has no qualitative influence; insofar, an application of the authors' results to problems in lower dimensions (e.g., polarons in quantum wells) is straightforward. The same holds true if homogeneous external fields are involved; for example, a discontinuous mass stripping for magnetopolarons can be excluded. On the other hand, a phase-transition-like behavior will be found, if a polaron or exciton is exposed to a short-range potential, allowing a so-called pinning transition. The authors emphasize, however, that even in this case the transition is only modified, and not induced, by phonons.

CONTENTS

I. INTRODUCTION

In this review we are concerned with qualitative analytical properties of polaron systems. Studies of this type have a long history; in fact, since the introduction of the terms "polaron" and "exciton" as such, it has been a controversially discussed question whether or not the corresponding wave functions, energies, masses, etc. were analytical functions of the electron-phonon coupling parameters, the total momentum, external fields, and other variables. To the best of our knowledge, L. D. Landau was the first to argue that a polaron system might exhibit unexpected localization properties. This can be exemplified by the following quotation from his early publication on the electron motion in crystal lattices (Landau, 1933; see also 1965).

> "We can now differentiate between two essentially different cases. For, the energetically most favourable state of the system may correspond, firstly, to the undistorted lattice and the electron moving about 'freely' and, secondly, the electron trapped at a strongly distorted region."

The intention of Landau's extremely short paper was to point out the possibility of a delocalization-localization transition rather than to prove its existence; in this context, we refer to the interesting remarks of Pekar (1954) in his textbook on electrons in crystal lattices.

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Moreover, one should realize that all studies at that time were semiclassical, the lattice properties being incorporated into a classical macroscopic polarization (see Pekar 1946, 1948 and Landau and Pekar, 1948). In response to this work, Fröhlich, Pelzer, and Zienau (1950) proposed the first microscopic model; the corresponding Hamiltonian now bears Fröhlich's name.

This model soon proved to be of basic importance for various branches of solid-state physics and, until now, has attracted the attention of numerous physicists. In particular, it became clear before long that Pekar's semiclassical results could be reproduced by a variational ansatz, which was adequate in the strong-coupling regime but inadequate in the weak-coupling regime (Tjablikov, 1952a; Fröhlich, 1954). Clearly, the latter was well understood by perturbation theory. Therefore it was highly desirable to find a (variational) procedure that would give correct results in both the weak- and strong-coupling limit and that could provide an interpolation scheme. To the best of our knowledge, the first to achieve this was Buckingham (1954). Interestingly enough, his variational calculation led to a discontinuous transition in the wave function and the derivative of the ground-state energy, considered as functions of the coupling parameter. It is obvious that these results support Landau's hypothesis. It is also obvious that they cannot provide a formal proof: The analytical behavior of an exact wave function may deviate considerably from that of a variational approximation. Fröhlich (1954) stressed this aspect immediately. Analyzing the significance of variational discontinuities in connection with polaron physics, he writes,

> "These unsatisfactory features are I think largely due to some unsatisfactory properties of the method used.... The difficulty is closely connected with the fact that in this method the total wave vector is not on principal axes."

It is an apparent shortcoming of every variational calculation that a nonanalytical behavior, of, for example, adapted wave functions, may be an artifact of the approximation. Nevertheless, variational calculations are an indispensable tool for numerical work. Until now, an enormous number of publications treated polarons and polaronic excitons that way. In many of them the localization problem was studied and Buckingham's results or generalizations thereof were frequently stated (we give a representative list of references in Sec. III). After all, assertions such as "self-trapping," "delocalization-localization transition," "phonon-induced symmetry breaking," "stripping transition," etc. were so commonplace that they hardly seemed to deserve a comment. We stress explicitly that the objections of Fröhlich were occasionally rediscussed or rediscovered in a generalized context (Haken, 1955; Höhler, 1955; Toyozawa, 1961; Peeters and Devreese, 1982b). Nevertheless, there was a widespread belief (at least in the solid-state community) that nonanalyticities should occur in polaron systems under various circumstances—a "polaronic phase transition" seemed to be well established.

The contrary is true. We shall prove for the standard Fröhlich systems, namely, the free optical polaron, the magnetopolaron, and the polaronic excitation, that no phase transitions exist. It is only for the specific case of a polaron in a short-range potential that a delocalization-localization (or pinning) transition may occur.

During our studies we realized that strongly related work had been done in constructive quantum field theory. It seems to be widely unknown that a complete discussion of the ground-state energy E of a free optical polaron was available as early as 1974. We refer to the paper of Fröhlich (1974) and the detailed comments and extensions of Spohn (1987a). E was proven to be an analytical function of the coupling parameter α for all values of α. Moreover, Spohn (1986) provided analytical arguments for a polaronic pinning transition in a suitable short-range potential. A considerable part of the methods to be used in Sec. IV was directly initiated by those pioneering papers.

The organization of this review is as follows: Following the introduction, we establish the basic notations and state a formalized version of the problems with which we are concerned. Section III contains our results, combined with some comments and a compilation of references. The heading "proofs" for Section IV is self-explanatory; we hope that the clear separation of the results (Sec. III) and the technically involved proofs (Sec. IV) will facilitate reading. We close with some extensions and a short summary in Secs. V and VI, respectively.

II. BASIC NOTATIONS AND STATEMENT OF PROBLEMS

To begin with, we fix the class of models that will be discussed in this article. Consider the Hamiltonian

$$H := H_{\mathrm{P}} + H_{\mathrm{Ph}} + H_{\mathrm{I}} \; , \tag{2.1}$$

where the subscripts P, Ph, and I indicate "particles," "phonons," and "interaction." In particular, let

$$H_{\mathrm{P}} := \sum_{n=1}^{N} [\varepsilon_n(\mathbf{p}_n - q_n \mathbf{A}(\mathbf{r}_n)) + V_n(\mathbf{r}_n)] + \delta_{N,2} V(\mathbf{r}_1 - \mathbf{r}_2) \; , \tag{2.2}$$

$$H_{\mathrm{Ph}} := \sum_{m=1}^{M} \int d^D k \hbar \omega_m(\mathbf{k}) a_m^*(\mathbf{k}) a_m(\mathbf{k}) \; , \tag{2.3}$$

$$H_{\mathrm{I}} := \sum_{m=1}^{M} \sum_{n=1}^{N} \int d^D k [\tilde{g}_{mn}(\mathbf{k}) a_m(\mathbf{k}) e^{i\mathbf{k}\cdot B_n \mathbf{r}} + \mathrm{H.c.}] \; , \quad N \le 2 \; . \tag{2.4}$$

H describes a system of N distinguishable, interacting particles coupled to M branches of phonons. The spatial dimension is D. The particles have momenta $\mathbf{p}_n$, positions $\mathbf{r}_n$, and charges q_n. $\mathbf{k}$ and $\omega_m(\mathbf{k})$ denote the wave vector and dispersion of a phonon; ε_n, V_n, and V characterize the band structure, the one- and two-particle potential; $\mathbf{A}(\mathbf{r})$ is the vector potential due to a homogeneous magnetic field; $a_m(\mathbf{k})$ and $a_m^+(\mathbf{k})$ are annihilation and creation operators for phonons; $\tilde{g}_{mn}(\mathbf{k})$ is the particle-phonon coupling and B_n a D-dimensional, symmetrical, and positive-definite matrix, incorporating an eventual anisotropy of the coupling.

It is obvious that H is a generalized Fröhlich Hamiltonian, which is to exist on a Hilbert space

$$\mathcal{H}:=[L_2(\mathbb{R}^D)]^N \otimes F^M =: \mathcal{H}_{\mathrm{P}} \otimes \mathcal{H}_{\mathrm{Ph}} \ , \tag{2.5}$$

where $L^2(\mathbb{R}^D)$ is the usual one-particle Hilbert space of square-integrable functions and F the Fock space for phonons. Details will be discussed in Secs. III and IV.

In Secs. II through IV we treat a simplified version of H so that the essential steps of our approach will be made more clear. As for $\varepsilon_n(\mathbf{p})$, we assume the simplest nontrivial band structure available, namely,

$$\varepsilon_n(\mathbf{p})=\mathbf{p}^2/2m_n \ . \tag{2.6}$$

$\omega_m(\mathbf{k})$ and $\tilde{g}_{mn}(\mathbf{k})$ are to be rotational invariant. Furthermore, we put $B_n=1$. We stress that our discussion is not restricted to these cases and refer to Sec. V.

Having introduced the model, we fix the precise meaning of the heading "localized." A wave function ψ of a particle-phonon system is called localized if ψ is an element of $\mathcal{H}$, that is, normalizable with respect to the particle and phonon part; otherwise, we call ψ delocalized.

Let us now turn to specific problems.

A. The free polaron

In this case we have $N=M=1$, $A=0$, and $V_1=0$. As indicated, we discuss a quadratic band structure. Furthermore, we extract a dimensionless coupling parameter $\sqrt{\alpha}$ from $\tilde{g}(k)$. The physically relevant domain of $\sqrt{\alpha}$ is $0\le\sqrt{\alpha}<\infty$. However, from a mathematical standpoint it proves profitable to admit $-\infty<\sqrt{\alpha}<\infty$ or even $\sqrt{\alpha}$ as an arbitrary complex number. There is no technical difficulty in so doing, and we shall use this possibility in the course of Sec. IV. The total Hamiltonian has the three constituents

$$H_{\mathrm{P}}=\mathbf{p}^2/2m \ , \tag{2.7}$$

$$H_{\mathrm{Ph}}=\int d^Dk\ \hbar\omega(k)a^*(\mathbf{k})a(\mathbf{k}) \ , \tag{2.8}$$

$$H_{\mathrm{I}}=\sqrt{\alpha}\int d^Dk[g(k)a(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}}+\mathrm{H.c.}] \ . \tag{2.9}$$

Without loss of generality, we may assume $g(k)$ to be real.

The standard model, introduced by Fröhlich, Pelzer, and Zienau (1950), assumes additionally

$$\begin{aligned} &D=3, \quad \omega(k)=\omega \ , \\ &g(k)=(\hbar/2m\omega)^{1/4}\cdot\hbar\omega/(\sqrt{2}\pi k) \ . \end{aligned} \tag{2.10}$$

Our discussion, however, is not restricted to that case. Notice that for any coupling $g(k)$ the Hamiltonian commutes with the operator

$$\mathbf{P}_{\mathrm{tot}}:=\mathbf{p}+\int d^Dk\ \hbar\mathbf{k}a^*(\mathbf{k})a(\mathbf{k})=\mathbf{p}+\mathbf{P}_{\mathrm{Ph}} \tag{2.11}$$

of total momentum. Following Lee, Low, and Pines (1953), we can profitably use this fact to eliminate the electron coordinates from H; we define the unitary transformation

$$U:=\exp\left[-\frac{i}{\hbar}\mathbf{r}\cdot\mathbf{P}_{\mathrm{Ph}}\right] \tag{2.12}$$

and calculate $\mathbf{P}'_{\mathrm{tot}}:=U^{-1}\mathbf{P}_{\mathrm{tot}}U$ and $H':=U^{-1}HU$. The result is

$$P'_{\mathrm{tot}}=\mathbf{p} \ , \tag{2.13}$$

$$H'=H'_{\mathrm{P}}+H_{\mathrm{Ph}}+H'_{\mathrm{I}} \ , \tag{2.14}$$

where

$$H'_{\mathrm{P}}:=(\mathbf{p}-\mathbf{P}_{\mathrm{Ph}})^2/2m \ , \tag{2.15}$$

$$H'_{\mathrm{I}}:=\sqrt{\alpha}\int d^Dk[g(k)a(\mathbf{k})+\mathrm{H.c.}] \ . \tag{2.16}$$

Conservation of total momentum is now equivalent to $[H',\mathbf{p}]=0$ and permits us to restrict H' to the subspace of H, which is spanned by the eigenfunctions of $\mathbf{p}$ with a given eigenvalue $\hbar\mathbf{Q}$. This restriction leads to the Hamiltonian

$$H'(\mathbf{Q}):=(\hbar\mathbf{Q}-\mathbf{P}_{\mathrm{Ph}})^2/2m+H_{\mathrm{Ph}}+H'_{\mathrm{I}}=:H'_0(\mathbf{Q})+H'_{\mathrm{I}} \tag{2.17}$$

of Lee, Low, and Pines. Clearly, $H'(\mathbf{Q})$ is defined on $\mathcal{H}_{\mathrm{Ph}}=F$ alone, the electron coordinates having been eliminated. Moreover, it is sufficient to discuss $H'(\mathbf{Q})$ instead of H.

Let $E(\alpha,\mathbf{Q})$ be the ground-state energy of $H'(\mathbf{Q})$, that is, the lower limit of the spectrum of $H'(\mathbf{Q})$. The existence of $E(\alpha,\mathbf{Q})$ is directly connected with a proper mathematical definition of $H'(\mathbf{Q})$, which in turn presupposes the specification of admissible functions $\omega(k)$ and $g(k)$. We examine this point in more detail in Secs. III and IV. For the moment, we take the existence of $E(\alpha,\mathbf{Q})$ for granted. Even more, we assume $E(\alpha,\mathbf{Q})$ to be a simple eigenvalue of $H'(\mathbf{Q})$, the corresponding eigenfunction being $\psi(\alpha,\mathbf{Q})$; $\psi(\alpha,\mathbf{Q})$ has to be an element of $\mathcal{H}_{\mathrm{Ph}}$. All these properties will be proven in Sec. IV under specific circumstances. In view of our introductory discussion, we state as

Problem 1. *What is the domain of analyticity of $E(\alpha,\mathbf{Q})$ and $\psi(\alpha,\mathbf{Q})$ as functions of $\alpha,\mathbf{Q}$?*

We know from perturbation theory that for sufficiently small values of α the ground state of H is delocalized and given by

$$\begin{aligned} &\psi(\alpha):=e^{i\mathbf{Q}\cdot\mathbf{r}}U\psi(\alpha,\mathbf{Q})|_{\mathbf{Q}=0} \ , \\ &E(\alpha):=E(\alpha,\mathbf{Q})|_{\mathbf{Q}=0} \ . \end{aligned} \tag{2.18}$$

There is no *a priori* reason that this should be true for all values of α. Let us assume that $E(\alpha,\mathbf{Q}_c)<E(\alpha,\mathbf{0})$ could hold for some $\mathbf{Q}_c\neq\mathbf{0}$ and $\alpha>\alpha_c$. This would demonstrate the appearance of quantum-mechanical symmetry breaking (Gerlach and Löwen, 1988a). Moreover, because of rotational symmetry, $E(\alpha,\mathbf{Q})$ is a function of $|\mathbf{Q}|$; if the minimum of $E(\alpha,\mathbf{Q})$ should occur for a subset of $\mathbf{Q}$ vectors with different length (α being fixed), a suitable superposition of functions (2.18) might produce a localized state as ground state of H. Summarizing, we state as

Problem 2. *Does* $E(\alpha,\mathbf{0})<E(\alpha,\mathbf{Q}\neq 0)$ *hold for all values of* α *in the interval* $0\le\alpha<\infty$*?*

Our solution of Problems 1 and 2 will rely heavily on theorems of operator analysis. An alternative and, in part, complementary approach to spectral properties of Hamiltonians is possible by means of functional-integral techniques [in connection with polaron physics, we mention the marvelous paper of Feynman (1955) and the later extensions of Schultz (1963) and Adamowski, Gerlach, and Leschke (1984)]. Let us introduce the diagonal element of the reduced density operator, that is,

$$\rho(\alpha,\beta):=\mathrm{tr}_{\mathrm{Ph}}\langle\mathbf{r}|e^{-\beta H}|\mathbf{r}\rangle\ . \tag{2.19}$$

Here, $\mathrm{tr}_{\mathrm{Ph}}\langle\cdots\rangle$ indicates the trace operation concerning phonons; $\beta>0$ is a formal inverse temperature and $\mathbf{r}$ is the particle position. The right-hand side of Eq. (2.19) is independent of $\mathbf{r}$, if H is translational invariant (as in the present case). It proves useful to relate $\rho(\alpha,\beta)$ to the readily accessible expression $\rho(0,\beta)$ for an uncoupled electron-phonon system and to define a formal partition function

$$Z(\alpha,\beta):=\rho(\alpha,\beta)/\rho(0,\beta)\ . \tag{2.20}$$

On the one side, $Z(\alpha,\beta)$ can conveniently be represented as a functional integral, namely,

$$Z(\alpha,\beta)=\langle\exp(-S_{\mathrm{I}})\rangle\ , \tag{2.21}$$

where the expectation value is generally defined as

$$\langle A\rangle:=\frac{\int\delta^D R\,\exp(-S_0[\mathbf{R}])A[\mathbf{R}]}{\int\delta^D R\,\exp(-S_0[\mathbf{R}])}\ . \tag{2.22}$$

In Eq. (2.22), $\int\delta^D R\,\exp(\cdots)$ indicates Wiener-Feynman integration over all real, closed D-dimensional paths $\mathbf{R}(\tau)$ with $\mathbf{R}(0)=\mathbf{R}(\beta)=\mathbf{r}$. Moreover,

$$S_0[\mathbf{R}]:=\int_0^\beta d\tau\frac{m}{2}\dot{\mathbf{R}}^2(\tau)\ , \tag{2.23}$$

$$S_{\mathrm{I}}[\mathbf{R}]:=-\alpha\int d^Dk\,|g(k)|^2\int_0^\beta\int_0^\beta d\tau\,d\tau' G_{\omega(k)}(\tau-\tau')\times e^{i\mathbf{k}\cdot(\mathbf{R}(\tau)-\mathbf{R}(\tau'))}\ , \tag{2.24}$$

and

$$G_\omega(\tau):=\cosh(\beta\hbar\omega/2-\hbar\omega|\tau|)/[2\sinh(\beta\hbar\omega/2)]\ . \tag{2.25}$$

On the other side, $Z(\alpha,\beta)$ is connected with the formal free energy $F(\alpha,\beta)$ as follows:

$$Z(\alpha,\beta)=\exp\{-\beta[F(\alpha,\beta)-F(0,\beta)]\}\ . \tag{2.26}$$

From $F(\alpha,\beta)$ we may derive all spectral properties of H by familiar manipulations. We state as

Problem 3. *Is* $F(\alpha,\beta)-F(0,\beta)$ *a real analytic function of* α *and* β *for* $0\le\alpha<\infty$, $0<\beta<\infty$*?*

B. The magnetopolaron

In comparison with the preceding, Sec. II.A, we have to include a homogeneous, external magnetic field $\mathbf{B}$, which we choose to point into z direction. For the vector potential $\mathbf{A}(\mathbf{r})$, we use a Landau gauge, that is,

$$\mathbf{A}(\mathbf{r})=(0,Bx,0),\quad B>0\ . \tag{2.27}$$

Throughout Sec. B, we assume $D=2,3$. For $D=2$, the last component of A has to be skipped. Then, the total Hamiltonian H has the following constituents:

$$H_{\mathrm{P}}=(\mathbf{p}+|e|\,\mathbf{A}(\mathbf{r}))^2/2m\ , \tag{2.28}$$

$$H_{\mathrm{Ph}}=\int d^Dk\,\hbar\omega(k)a^*(\mathbf{k})a(\mathbf{k})\ , \tag{2.29}$$

$$H_{\mathrm{I}}=\sqrt{\alpha}\int d^Dk[g(k)a(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}}+\mathrm{H.c.}]\ . \tag{2.30}$$

As in the case of a free polaron, we carry out the unitary transformation U, defined in Eq. (2.12). Calculating $H'=U^{-1}HU$, we get

$$H'=H_{\mathrm{P}}'+H_{\mathrm{Ph}}+H_{\mathrm{I}}'\ , \tag{2.31}$$

where H_{I}' is given by Eq. (2.16) and

$$H_{\mathrm{P}}':=(\mathbf{p}+|e|\,\mathbf{A}(\mathbf{r})-\mathbf{P}_{\mathrm{Ph}})^2/2m\ . \tag{2.32}$$

For $B\neq 0$, only the 2- and 3-components of total momentum are conserved: $[H',p_2]=[H',p_3]=0$. We denote the corresponding eigenvalues of $\hbar Q_2$ and $\hbar Q_3$ and define

$$\mathbf{Q}=(0,Q_2,Q_3)\ . \tag{2.33}$$

In analogy to Sec. II.A, it is sufficient to discuss the restriction of H' onto the subspace of $\mathcal{H}$, spanned by the eigenfunctions of p_2,p_3 with fixed eigenvalues $\hbar Q_2,\hbar Q_3$, that is,

$$H'(\mathbf{Q}):=(\mathbf{G}-\mathbf{P}_{\mathrm{Ph}})^2/2m+H_{\mathrm{Ph}}+H_{\mathrm{I}}'\ , \tag{2.34}$$

where

$$\mathbf{G}:=(p_1,|e|Bx+\hbar Q_2,\hbar Q_3)\ . \tag{2.35}$$

Let $E(\alpha,\mathbf{Q},B)$ be the ground-state energy of $H'(\mathbf{Q})$—

its existence will be proven in Sec. IV under specific conditions. Assume for the moment that $E(\alpha,\mathbf{Q},B)$ is a simple eigenvalue of $H'(\mathbf{Q})$, the corresponding eigenfunction being $\psi(\alpha,\mathbf{Q},B)$. Then we may state

Problem 4. *What is the domain of analyticity of $E(\alpha,\mathbf{Q},B)$ and $\psi(\alpha,\mathbf{Q},B)$ as functions of $\alpha,\mathbf{Q},B$?*

Functional-integral techniques can be introduced in exactly the same manner as was done in Sec. II.A [see Eqs. (2.19)–(2.26)]. Admitting B as an additional variable in the formal partition function Z and the reduced density matrix ρ, one finds

$$Z(\alpha,\beta,B):=\rho(\alpha,\beta,B)/\rho(0,\beta,0) = \langle \exp(-S_I-S_B)\rangle \ , \qquad (2.36)$$

where S_I was given in Eq. (2.24) and

$$S_B[\mathbf{R}]:=-\frac{i}{\hbar}|e|B\int_0^\beta d\tau R_1(\tau)\dot{R}_2(\tau) \ . \qquad (2.37)$$

Generalizing the formal free energy F correspondingly, we are led to

Problem 5. *Is $F(\alpha,\beta,B)-F(0,\beta,0)$ a real analytic function of α, β, B for $0\le\alpha<\infty$, $0<\beta<\infty$, $0<B<\infty$?*

C. The polaron in a potential

It is a simple task to generalize the Hamiltonian from Sec. II A. We extract a dimensionless coupling constant λ from the one-particle potential V_1 and define $V_1=:\lambda v$, $v\not\equiv 0$. If not otherwise explicitly stated, we assume $\lambda\ge 0$ and $v\le 0$ (these are technical assumptions, which can partially be removed; see Sec. IV.C). One finds

$$H_{\mathrm{P}}=\mathbf{p}^2/2m+\lambda v(\mathbf{r}) \ , \qquad (2.38)$$

$$H_{\mathrm{Ph}}=\int d^Dk\, \hbar\omega(k)a^*(\mathbf{k})a(\mathbf{k}) \ , \qquad (2.39)$$

$$H_{\mathrm{I}}=\sqrt{\alpha}\int d^Dk[g(k)a(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}}+\mathrm{H.c.}] \ . \qquad (2.40)$$

as parts of H. Once again we perform the unitary transformation, defined in Eq. (2.12). Calculating $H'=U^{-1}HU$, we arrive at

$$H'=H'_{\mathrm{P}}+H_{\mathrm{Ph}}+H'_{\mathrm{I}} \ , \qquad (2.41)$$

where H'_{I} was given in Eq. (2.16) and

$$H'_{\mathrm{P}}=(\mathbf{p}-\mathbf{P}_{\mathrm{Ph}})^2/2m+\lambda v(\mathbf{r}) \ . \qquad (2.42)$$

Let $E(\alpha,\lambda)$ be the ground-state energy of H'—its existence will be proven in Sec. IV under specific conditions. If $E(\alpha,\lambda)$ is a simple eigenvalue of H', we denote the corresponding eigenfunction by $\psi(\alpha,\lambda)$. What about the analytical properties of $E(\alpha,\lambda)$ and $\psi(\alpha,\lambda)$ in this case?

It is well known that $E(\alpha,\lambda)\le E(0,\lambda)$ is true for $\alpha\ge 0$, $E(0,\lambda)$ being the ground-state energy of H_{P}—the presence of phonons lowers the ground-state energy in any case (Adamowski, Gerlach, Leschke, 1984). Therefore we expect the analytical properties of $E(\alpha,\lambda)$ to be critically dependent on those of $E(0,\lambda)$. The latter are directly connected with the existence or nonexistence of a localized state as ground state of H_{P}; nonanalyticities can occur in this case. Summarizing, it is tempting to study

Problem 6. *What is the domain of analyticity of $E(\alpha,\lambda)$ and $\psi(\alpha,\lambda)$ as functions of α,λ, if H_p is known to have a localized ground state for any $\lambda>0$?*

Problem 7. *What is the domain of analyticity of $E(\alpha,\lambda)$ and $\psi(\alpha,\lambda)$ as functions of α,λ, if H_{P} is known to have a localized ground state only for $\lambda>\lambda_C>0$?*

Having posed the problem thus far, one realizes that it is only for $D=3$ that the existence of a localized ground state of H_{P} may be questionable (Reed and Simon, 1978). Therefore we restrict our discussion in this case to $D=3$.

Finally, we turn to functional-integral techniques. Again, they can be introduced in complete analogy to Sec. II.A. Admitting λ as an additional variable in the formal partition function Z and the reduced density matrix ρ, one finds

$$Z(\alpha,\beta,\lambda):=\rho(\alpha,\beta,\lambda)/\rho(0,\beta,0) = \langle \exp(-S_{\mathrm{I}}-S_\lambda)\rangle \ , \qquad (2.43)$$

where S_{I} was given in Eq. (2.24) and

$$S_\lambda[\mathbf{R}]:=\lambda\int_0^\beta d\tau\, v(\mathbf{R}(\tau)) \ . \qquad (2.44)$$

We notice that H is not translational invariant. Insofar, $\mathrm{tr}_{\mathrm{Ph}}\langle\mathbf{r}|\exp(-\beta H)|\mathbf{r}\rangle$ will explicitly depend on r. Nevertheless, we skip this $\mathbf{r}$ dependence, as it is irrelevant for our considerations. Generalizing the formal free energy correspondingly, we shall study

Problem 8. *Is $F(\alpha,\beta,\lambda)-F(0,\beta,0)$ a real analytic function of α,β,λ for $0\le\alpha<\infty$, $0<\beta<\infty$, $0<\lambda<\infty$?*

D. The polaronic exciton

In comparison with the cases presented in Secs. II.A–II.C, this one is more complicated and exhibits a considerably richer structure. Nevertheless, our discussion will proceed along similar lines. The total Hamiltonian can easily be abstracted from Eqs. (2.1)–(2.4). We assume as constituents of H

$$H_{\mathrm{P}}=\sum_{n=1}^{2}\mathbf{p}_n^2/2m_n+V(\mathbf{r}_1-\mathbf{r}_2) \ , \qquad (2.45)$$

$$H_{\mathrm{Ph}}=\int d^3k\, \hbar\omega(k)a^*(\mathbf{k})a(\mathbf{k}) \ , \qquad (2.46)$$

$$H_{\mathrm{I}}=\sqrt{\alpha}\sum_{n=1}^{2}(-1)^n\int d^3k[g(k)a(\mathbf{k})\exp(i\mathbf{k}\cdot\mathbf{r}_n)+\mathrm{H.c.}] \ . \qquad (2.47)$$

It is for reasons similar to those in the previous case that we choose $D=3$ again. Normally, $V(\mathbf{r}_1-\mathbf{r}_2)$ is taken to be a Coulomb potential. Our discussion is not restricted to that case. Extracting a coupling constant $\lambda>0$ from V and defining $V=\lambda U$, our only premise is that $\lambda U(r)$ is negative and binding for any $\lambda>0$. It proves useful to introduce center-of-mass and relative coordinates $\mathbf{R}$ and $\mathbf{r}$ as well as total and reduced mass M and m in the normal way. One finds

$$H_{\mathrm{P}}=\mathbf{P}^2/2M+\mathbf{p}^2/2\mu+\lambda U(\mathbf{r}) , \tag{2.48}$$

$$H_{\mathrm{I}}=\sqrt{\alpha}\sum_{n=1}^{2}(-1)^n\int d^3k[g(k)a(\mathbf{k})\exp(i\mathbf{k}\cdot\mathbf{R}+i\gamma_n\mathbf{k}\cdot\mathbf{r}) +\mathrm{H.c.}] , \tag{2.49}$$

where $\gamma_1:=m_2/M$, $\gamma_2:=-m_1/M$. Of course, H_{Ph} remains unchanged. One may verify that H commutes with the operator

$$\mathbf{P}_{\mathrm{tot}}:=\mathbf{P}+\mathbf{P}_{\mathrm{Ph}} \tag{2.50}$$

of total momentum. In complete analogy to the free-polaron case, this fact enables us to eliminate the center-of-mass coordinates from H. Performing a Lee-Low-Pines transformation, we find

$$H'=H'_{\mathrm{P}}+H_{\mathrm{Ph}}+H'_{\mathrm{I}} , \tag{2.51}$$

where

$$H'_{\mathrm{P}}=(\mathbf{P}-\mathbf{P}_{\mathrm{Ph}})^2/2M+\mathbf{p}^2/2\mu+\lambda U(\mathbf{r}) , \tag{2.52}$$

$$H'_{\mathrm{I}}=\sqrt{\alpha}\sum_{n=1}^{2}(-1)^n\int d^3k[g(k)a(\mathbf{k})\exp(i\gamma_n\mathbf{k}\cdot\mathbf{r}) +\mathrm{H.c.}] . \tag{2.53}$$

Conservation of total momentum is now equivalent to $[H',\mathbf{P}]=0$ and permits us to restrict H' to the subspace of eigenfunctions of $\mathbf{P}$ with a fixed eigenvalue $\mathbf{Q}$. So we are led to

$$H'(\mathbf{Q}):=(\hbar\mathbf{Q}-\mathbf{P}_{\mathrm{Ph}})^2/2M+\mathbf{p}^2/2\mu +\lambda U(\mathbf{r})+H_{\mathrm{Ph}}+H'_{\mathrm{I}} . \tag{2.54}$$

Introducing $\mathbf{m}$ for the two mass parameters available, we now turn to the ground-state energy $E(\mathbf{Q},\alpha,\lambda,\mathbf{m})$ of $H'(\mathbf{Q})$—its existence will be proven in Sec. IV under specific conditions. Assume for the moment that $E(\mathbf{Q},\alpha,\lambda,\mathbf{m})$ is a simple eigenvalue of $H'(\mathbf{Q})$, the corresponding eigenfunction being $\psi(\mathbf{Q},\alpha,\lambda,\mathbf{m})$. In view of our central topic, we state as

Problem 9. *What is the domain of analyticity of* $E(\mathbf{Q},\alpha,\lambda,\mathbf{m})$ *and* $\psi(\mathbf{Q},\alpha,\lambda,\mathbf{m})$ *as functions of* $\mathbf{Q},\alpha,\lambda,\mathbf{m}$*?*

Extending our localization-delocalization discussion from Sec. II.A to the present case, we shall study

Problem 10. *Does* $E(\mathbf{0},\alpha,\lambda,\mathbf{m})<E(\mathbf{Q}\neq\mathbf{0},\alpha,\lambda,\mathbf{m})$ *hold for all values of* α,λ,m_n *in the intervals* $0\le\alpha<\infty$, $0<\beta<\infty$, $0<m_n<\infty$*?*

Finally, we generalize the functional-integral concept. Introducing the diagonal element of the reduced density matrix and a formal partition function Z as functions of $\alpha,\beta,\lambda,\mathbf{m}$ and repeating the steps in Eqs. (2.19)–(2.26), we arrive at

$$\rho(\alpha,\beta,\lambda,\mathbf{m}):=\mathrm{tr}_{\mathrm{Ph}}\langle\mathbf{R}_0,\mathbf{r}_0|e^{-\beta H}|\mathbf{R}_0,\mathbf{r}_0\rangle , \tag{2.55}$$

$$Z(\alpha,\beta,\lambda,\mathbf{m}):=\rho(\alpha,\beta,\lambda,\mathbf{m})/\rho(0,\beta,0,\mathbf{m}) =\langle\exp(-S_{\mathrm{I}}-S_\lambda)\rangle , \tag{2.56}$$

where $\mathbf{R}(0)=\mathbf{R}(\beta)=\mathbf{R}_0$ and $\mathbf{r}(0)=\mathbf{r}(\beta)=\mathbf{r}_0$. Furthermore,

$$S_0[\mathbf{R},\mathbf{r}]:=\int_0^\beta d\tau[M\dot{R}^2(\tau)/2+\mu\dot{r}^2(\tau)/2] , \tag{2.57}$$

$$S_{\mathrm{I}}[\mathbf{R},\mathbf{r}]:=-\alpha\sum_{n,n'=1}^{2}(-1)^{n+n'}\int d^3k\,|g(k)|^2 \times\int_0^\beta\int_0^\beta d\tau\,d\tau' G_{\omega(k)}(\tau-\tau')\exp\{i\mathbf{k}\cdot[\mathbf{R}(\tau)-\mathbf{R}(\tau')+\gamma_n\mathbf{r}(\tau)-\gamma_{n'}\mathbf{r}(\tau')]\} , \tag{2.58}$$

$$S_\lambda[\mathbf{r}]:=\lambda\int_0^\beta d\tau U(\mathbf{r}(\tau)) . \tag{2.59}$$

Expectation values are defined as follows:

$$\langle A\rangle:=\int\delta^3R\,\delta^3r\,e^{-S_0[\mathbf{R},\mathbf{r}]}A[\mathbf{R},\mathbf{r}]/\int\delta^3R\,\delta^3r\,e^{-S_0[\mathbf{R},\mathbf{r}]} . \tag{2.60}$$

We note that $\rho(\alpha,\beta,\lambda,\mathbf{m})$ depends also on the end point $\mathbf{r}_0$ of the path $\mathbf{r}(\tau)$. We skipped this dependence in our notation, as it is irrelevant for the considerations to follow. Generalizing the free energy F correspondingly we close with

Problem 11. *Is* $F(\alpha,\beta,\lambda,\mathbf{m})-F(0,\beta,0,\mathbf{m})$ *a real analytic function of* $\alpha,\beta,\lambda,\mathbf{m}$ *for* $0\le\alpha<\infty$, $0<\beta<\infty$, $0<\lambda<\infty$, $0<m_n<\infty$*?*

III. RESULTS

In this section we present our results, compare them with previous work, and include some comments. The structure of the section is such that for any problem n to be found in Sec. II, we formulate a statement n. Moreover, the subheadings in Secs. II and III are identical.

A. The free polaron

Statement 1. *Consider the polaron Hamiltonian $H'(\mathbf{Q})$ as defined in Eq. (2.17). Assume*

$$\begin{aligned} &\omega(k)\ge\omega>0,\quad \omega(k_1)+\omega(k_2)\ge\omega(|\mathbf{k}_1+\mathbf{k}_2|)\ ,\\ &\int d^Dk|g(k)|^2/[1+(ak)^2]<\infty \end{aligned} \tag{3.1}$$

to be valid, where $a:=\sqrt{\hbar/m\omega}$ is the polaron radius. Then, the ground-state energy $E(\alpha,\mathbf{Q})$ exists and is an isolated, simple eigenvalue for $0\le\alpha<\infty$, $\hbar^2Q^2/2m<\hbar\omega$. $E(\alpha,\mathbf{Q})$ and $\psi(\alpha,\mathbf{Q})$ are real analytic functions of $\alpha,\mathbf{Q}$ in the specified domain.

We add some comments on this statement and begin with the three inequalities (3.1), the importance of which differ for our proof. $\omega(k)\ge\omega>0$ is decisive to guarantee the existence of an energy gap above the ground state: we pick up this point in Sec. V. $\omega(k_1)+\omega(k_2)\ge\omega(|\mathbf{k}_1+\mathbf{k}_2|)$ has a more technical character; this condition is needed to construct a lower bound for the energy of one- or more-phonon excitations, which will be shown to produce the continuum edge of $H'(\mathbf{Q})$. Finally, the inequality $\int d^Dk\ |g(k)|^2/[1+(ak)^2]<\infty$ ensures that $H'(\mathbf{Q})$ will be bounded from below. This condition on $g(k)$ can be weakened in the large-k domain (see, e.g., Nelson, 1964).

We now turn to applications of Statement 1. The most prominent is the qualitative analytical analysis of the standard model (2.10) for optical polarons. A more general application is the calculation of many ground-state observables as derivatives of $E(\alpha,\mathbf{Q})$ with respect to $\mathbf{Q}$ or as expectation values of type $\langle\psi(\alpha,\mathbf{Q})|X|\psi(\alpha,\mathbf{Q})\rangle$, X being an operator independent of α and $\mathbf{Q}$. As examples, we mention the polaron mass, the polaron radius, and the mean phonon number associated with $\psi(\alpha,\mathbf{Q})$. Statement 1 assures us that these observables are smooth functions of $\alpha,\mathbf{Q}$, provided $\hbar^2Q^2/2m<\hbar\omega$ is valid. Interestingly enough, the latter condition can be removed totally for $D=1,2$ and under slightly stronger conditions as (3.1); for $D=3$, the domain of Q can be extended, but Q remains finite (Spohn, 1988).

Statement 2. *Under the conditions of Statement 1, the inequality $E(\alpha,\mathbf{0})<E(\alpha,\mathbf{Q}\neq0)$ holds for $0\le\alpha<\infty$.*

Recalling the remarks concerning Problem 2, we see that the preceding statement disproves the existence of a delocalization-localization transition. The specified polaron system can show neither self-trapping nor quantum-mechanical symmetry breaking (Gerlach and Löwen, 1988a).

Statement 3. *Take the existence of $F(\alpha,\beta)-F(0,\beta)$, or, equivalently, the boundedness of $Z(\alpha,\beta)$, for granted: $0<Z(\alpha,\beta)<\infty$. Then, $F(\alpha,\beta)-F(0,\beta)$ is a real analytic function of α, β. Sufficient conditions for the existence of $F(\alpha,\beta)-F(0,\beta)$ in $0\le\alpha<\infty$, $0<\beta<\infty$ are*

$$\int d^Dk|g(k)|^2/\omega(k)<\infty\quad (\textit{short-range case})\ , \tag{3.2}$$

or

$$\omega(k)\ge\omega>0,\quad |g(k)|<\frac{\text{const}}{\sqrt{k^{D-1}}}\quad (\textit{long-range case})\ . \tag{3.3}$$

Statement 3 is surprisingly general, one reason being the simple α and β dependence of the actions S_0 and S_I; furthermore, the hard part of the proof is to establish the existence of $F(\alpha,\beta)$ (see Gerlach and Löwen, 1987a). The familiar electron-phonon couplings are of type (3.2) or (3.3); combinations of several couplings are admissible (see Sec. V).

Having established the analytical properties of the free-polaron system, we now comment in some detail on previous work that is related to ours. In view of the enormous number of relevant publications, we apologize in advance for being incomplete. We hope, however, to be representative. Let us begin with the weak-coupling case $\alpha\ll1$. Then, standard perturbation theory is applicable. We refer to Fröhlich, Pelzer, and Zienau (1950); Tjablikov (1952a); Fröhlich (1954); Krivoglaz and Pekar (1957); Höhler and Müllensiefen (1959); Grosjean (1962); Röseler (1968); Myerson (1975); Whitfield and Engineer (1975); Alvarez-Estrada (1979); Arisawa and Saitoh (1983); Peeters, Wu, and Devreese (1986a); Peeters, Warmenbol, and Devreese (1987).

Due to this work, analytical results for $E(\alpha,\mathbf{Q})$ and $F(\alpha,\beta)$ are available up to fourth-order perturbation theory. As important examples, we mention the explicit equations concerning $E(\alpha,\mathbf{0})$, $F(\alpha,\beta)$, and the polaron mass $m(\alpha)$ for the original Fröhlich model (2.10);

$$E(\alpha,\mathbf{0})=-[\alpha+f_1\alpha^2+O(\alpha^3)]\hbar\omega\ , \tag{3.4}$$

$$m(\alpha)=[1+\alpha/6+f_2\alpha^2+O(\alpha^3)]m\ , \tag{3.5}$$

$$F(\alpha,\beta)=F(0,\beta)-\left[\frac{\alpha\sqrt{\pi\beta\hbar\omega}I_0(\beta\hbar\omega/2)}{2\sinh(\beta\hbar\omega/2)}+O(\alpha^2)\right]\hbar\omega\ . \tag{3.6}$$

Algebraic formulas for f_1 and f_2 were given by, for example, Grosjean (1962) and Röseler (1968); in digits, one finds $f_1=0.01592\ldots$, $f_2=0.02362\ldots$.

We stated in the Introduction that in the very beginning polaron theory was a strong-coupling theory, developed by Pekar (1946) and Landau (Landau and Pekar, 1948; compare also Pekar, 1954). Later studies of the strong-coupling case $\alpha\gg1$ were usually announced as "adiabatic perturbation theory" (Bogoliubov, 1950; Tjablikov, 1951, 1952b, 1954; Allcock, 1956, 1963; Whitfield and Platzman, 1972; Hattori, 1975c; Miyake, 1975, 1976; Gross, 1976). Nonperturbative studies are due to Adamowski, Gerlach, and Leschke (1980a), Donsker and Varadhan (1983), and Spohn (1987a). Again, we include the results for Fröhlich's case (2.10):

$$\lim_{\alpha\to\infty} F(\alpha,\beta)/\alpha^2 = -\gamma\hbar\omega \ , \tag{3.7}$$

$$\gamma := -\inf_{\psi,\|\psi\|=1}\left[\tfrac{1}{2}\int d^3r\,|\nabla\psi(\mathbf{r})|^2 - \frac{1}{\sqrt{2}}\int d^3r\,d^3r'\frac{|\psi(\mathbf{r})|^2|\psi(\mathbf{r}')|^2}{|\mathbf{r}-\mathbf{r}'|}\right] = 0.108\,51\ldots\ , \tag{3.8}$$

$$\lim_{\alpha\to\infty} m(\alpha)/(m\alpha^4) = \frac{4\pi\sqrt{2}}{3}\int d^3r\,|\psi(\mathbf{r})|^4 = 0.022\,70\ldots\ . \tag{3.9}$$

The infimum $\psi(\mathbf{r})$ in Eq. (3.8) does exist (Lieb, 1977) and has to be inserted in (3.9). One should notice two peculiarities of these formulas: First, the right-hand side of (3.7) is independent of β. Secondly, admissible functions $\psi(\mathbf{r})$ of (3.8) have to be normalized; a localized ground state does exist in this case. The latter property is in marked contrast to the weak-coupling behavior and may have caused the first conjectures that a delocalization-localization transition should occur for $0<\alpha<\infty$ (Tjablikov, 1951).

The intermediate coupling regime was predominantly studied by variational techniques, providing upper bounds on $E(\alpha,\mathbf{Q})$ and $F(\alpha,\beta)$. According to their purpose, the corresponding literature can be divided into two groups.

In the first group, the main purpose was to construct bounds as low as possible. Early papers of that type are due to Lee and Pines (1952); Gurari (1953); Lee, Low, and Pines (1953); Yokota (1953; see also Osaka, 1959); and Höhler (1955), (1956). The Lee-Low-Pines procedure (see Sec. II.A) was particularly influential and became an important part of many subsequent publications. We mention Gross (1955); Haga (1955); Fulton (1956); Pines (1963); Dichtel (1966); Larsen (1966) and (1968); Röseler (1968); Barentzen (1975); Cahill (1975); Huybrechts (1976) and (1977); Tokuda (1980a, 1980b); and Bogoliubov, Kireev, and Kurbatov (1987). A significantly new development began with the advent of functional-integral methods (see the pioneering work of Feynman, 1955); in combination with refined variational procedures, they proved to be an extremely powerful tool, if not the most powerful. We refer to Osaka (1959); Schultz (1959) and (1963); Marshall and Mills (1970); Abe and Okamoto (1971); Okamoto and Abe (1972); Kochetov, Kuleshov, and Smondyrev (1975) and (1982); Sa-yakanit (1979); Adamowski, Gerlach, and Leschke (1980b); Saitoh (1980a); Saitoh and Arisawa (1980); Kochetov and Smondyrev (1981); Fedyanin and Rodriguez (1982); Kholodenko and Freed (1983); Castrigiano, Kokiantonis, and Stierstorfer (1984); Wu, Peeters, and Devreese (1985a); Fisher and Zwerger (1986); and Gerlach, Löwen, and Schliffke (1987).

In the second group of papers, the problem of phase transitions is directly addressed (Buckingham, 1954; Haga, 1954; Gross, 1959; Larsen, 1969b; Porsch, 1970; Matz and Burkey, 1971; Manka, 1978, 1979; Lépine and Matz, 1979; Luttinger and Lu, 1980; Manka and Suffczynski, 1980; Toyozawa and Shinozuka, 1980; Shoji and Tokuda, 1981; Farias, Studart, and Hipolito, 1982; Lu and Shen, 1982; Tokuda, 1982; Bodas and Hipolito, 1983; Feranchuk, Fisher, and Komarov, 1984; Das Sarma, 1985; Lépine, 1985; Mason and Das Sarma, 1986). In most cases, phase transitions were claimed to exist under condition (3.1), (3.2), or (3.3). The weak point of these assertions is that they have to rely on approximate equations for, say, the energy. Without underestimating the merits of those calculations as such, the nonanalyticities have to be classified as artifacts of the approximations made.

We close this compilation of literature with references concerning nonvariational calculations and functional analytical work. First, we mention a Padé approximation for $E(\alpha,\mathbf{0})$ and $m(\alpha)$, which was performed by Sheng and Dow (1971); the authors find strong indications that both quantities should be analytical functions of α. Secondly, there exist several Monte Carlo studies of the ground-state energy $E(\alpha,\mathbf{0})$. The starting point for these papers is formula (2.21) for the partition function $Z(\alpha,\beta)$. Reliable results for $E(\alpha,0)$ are available up to $\alpha=4$ (Gelfand and Chentsov, 1957; Sabelfeld, 1980; Becker, Gerlach, and Schliffke, 1983; Alexandrou, Fleischer, and Rosenfelder, 1990). Similar statements can be made for the polaron mass $m(\alpha)$, which was discussed by Gerlach, Löwen, and Schliffke (1987).

Last but not least we stress once more the importance of the work of J. Fröhlich (1974) and of Spohn (1986, 1987a, 1988): These authors were the first to study polaron problems by means of modern operator theory.

B. The magnetopolaron

Statement 4. *Consider the Hamiltonian* $H'(\mathbf{Q})$ *for a magnetopolaron as defined in Eq. (2.34). Assume condition (3.1) to be valid. Then, the ground-state energy* $E(\alpha,\mathbf{Q},B)$ *exists and is an isolated simple eigenvalue for* $0\le\alpha<\infty$, $\hbar^2Q_3^2/2m<\hbar\omega$, *and* $0<B<\infty$. $E(\alpha,\mathbf{Q},B)$ *and* $\Psi(\alpha,\mathbf{Q},B)$ *are real analytic functions of* $\alpha,\mathbf{Q},B$ *in the specified domain.*

Statement 5. *Take the existence of* $F(\alpha,\beta,B)-F(0,\beta,0)$, *or, equivalently, the boundedness of* $Z(\alpha,\beta,B)$, *for granted:* $0<Z(\alpha,\beta,B)<\infty$. *Then,* $F(\alpha,\beta,B)-F(0,\beta,0)$ *is a real analytic function of* α,β,B. *Sufficient conditions for the existence of* $F(\alpha,\beta,B)-F(0,\beta,0)$ *in* $0\le\alpha<\infty$, $0<\beta<\infty$, $0<B<\infty$ *are (3.2) or (3.3).*

A comparison of Statements 1,3 and 4,5 makes clear that the earlier comments can be generalized appropriately. If a physical quantity may be represented as derivative of $E(\alpha,\mathbf{Q},B)$ or $F(\alpha,\beta,B)$, it must be a smooth function of $\alpha,\mathbf{Q},B$ or α,β,B in the specified domains. An important example is the mass of a magnetopolaron, which can be defined as

$$m(\alpha,B)^{-1} := \hbar^{-2}\frac{\partial^2}{\partial Q_3^2}E(\alpha,\mathbf{Q},B)|_{\mathbf{Q}=0} \ . \qquad (3.10)$$

Statement 4 proves that a discontinuous mass stripping is impossible; $m(\alpha,B)$ is a real analytic function of α,B for $0\le\alpha<\infty$, $0<B<\infty$. The same statement can be made for the so-called cyclotron mass $m'(\alpha,\beta)$, given by

$$|e|B\hbar/m'(\alpha,B) := E'(\alpha,\mathbf{0},B)-E(\alpha,\mathbf{0},B) \ , \qquad (3.11)$$

where $E'(\alpha,\mathbf{Q},B)$ is the first excited Landau state, which we assume to be nondegenerate and below the continuum edge.

A third comment is concerned with expectation values of type $\langle\Psi(\alpha,\mathbf{Q},B)|X|\Psi(\alpha,\mathbf{Q},B)\rangle$, where X is an operator independent of $\alpha,\mathbf{Q},B$; as examples; we mention the mean phonon number and the polaron radius. Again, such quantities are analytic functions of $\alpha,\mathbf{Q},B$ in the specified domain (see Statement 4).

Finally, we turn to the previous literature on magnetopolarons related to our work. To the best of our knowledge, systematic perturbation studies for $\alpha\ll 1$ appeared only in the last few years: we mention Lindemann, Lassnig, Seidenbusch, and Gornik (1983); Das Sarma (1984); Larsen (1984) and (1986); Peeters and Devreese (1985a); Devreese and Peeters (1986); Peeters, Wu, and Devreese (1986b); and Broderix, Heldt, and Leschke (1987). An earlier semiclassical calculation is due to Bajaj (1968).

A Green's-function formulation of the strong-coupling regime $\alpha\gg 1$ was given by Porsch (1970). Unfortunately, final numerical results for $E(\alpha,\mathbf{Q},B)$ are missing.

At first glance, functional-integral methods would seem to be well suited for the discussion of magnetopolarons. In fact, magnetopolarons were discussed that way (Hellwarth and Platzman, 1962; Saitoh, 1980b, 1981, 1982; Peeters and Devreese, 1981, 1982a, 1982c, 1982d, 1983, 1985b; Gerlach and Löwen, 1987b). One runs into severe difficulties, however, when trying to combine the functional-integral approach and variational procedures: In general, Jensen's inequality does not hold for $B\neq 0$ (Gorshkov, Zabrodin, Rodriguez, and Fedyanin, 1985; Larsen, 1985; Broderix, Heldt, and Leschke, 1987; Leschke and Wonneberger, 1989). Hellwarth and Platzman, Peeters and Devreese, and Saitoh all used this inequality in their calculations, cited above. Clearly this is a shortcoming of these otherwise important papers (we refer to the corresponding remarks of Hellwarth and Platzman in their article). The same restriction must be applied to a series of publications that are based on those just listed and that discuss, for example, the optical-absorption spectrum of polarons (for an example, see Peeters and Devreese, 1986 and further references therein).

As for strictly variational calculations, we quote Larsen (1964, 1969a, 1972); Evrard, Kartheuser, and Devreese (1970); Kartheuser and Negrete (1973); and Becker, Gerlach, Hornung, and Ulbrich (1987, 1988). The results of a paper by Pfeffer and Zawadzki (1986) can be shown to be variational. Lépine and Matz (1976) claim without proof that the same holds true for their results.

In many of the aforementioned publications a discussion of the phase-transition problem is implicitly contained; direct references are Peeters and Devreese (1981, 1982a, 1982c, 1982d, 1983, 1985b), Lépine (1985), Wu, Peeters, and Devreese (1985b), and Erçelebi (1989). In all these papers phase transitions were found under conditions (3.1), (3.2), or (3.3). In view of Statements 4 and 5, these must be artifacts of the approximations made.

We close this compilation of literature with four references concerning rigorous results. Alvarez-Estrada (1979) made the first attempt to establish the existence of the perturbation series for $E(\alpha,\mathbf{Q},B)$ as a function of α, but succeeded only for $\alpha\ll 1$. Löwen (1988a) established the proof of Statement 4, and Statement 5 was shown by Gerlach and Löwen (1987b, 1988c).

C. The polaron in a potential

Before noting three statements, some remarks are necessary. Recalling the Hamiltonians under discussion, namely, H from Eqs. (2.38)–(2.40) and H' from Eqs. (2.41) and (2.42), we see that the potential $\lambda v(\mathbf{r})$ appears as an additional variable. If not explicitly stated otherwise, we choose $\lambda\ge 0$ and $v(\mathbf{r})\le 0$. As indicated in Sec. II.C, we should know about the analytical properties of the ground-state energy $E(0,\lambda)$ of $H_p=\mathbf{p}^2/2m+\lambda v(\mathbf{r})$. This is the case for the so-called Rollnik class R of potentials λv, defined by the inequality

$$\lambda^2\int d^3r\, d^3r'|v(\mathbf{r})|\,|v(\mathbf{r}')|/|\mathbf{r}-\mathbf{r}'|^2<\infty \ . \qquad (3.12)$$

The left-hand side is proportional to the Birman-Schwinger bound on the number $N(\lambda)$ of (localized) eigenfunctions of H_P. Therefore we conclude the following for $\lambda v\in R$: (i) $N(\lambda)$ is finite for $0\le\lambda<\infty$; (ii) $N(\lambda)=0$ for sufficiently small λ; and (iii) if we know that $N(\lambda)>0$ is only true for $\lambda>\lambda_c$, the ground-state energy of H_P is nonanalytic for $\lambda=\lambda_c$. As for references, we mention Glaser, Martin, Grosse, and Thirring (1976); Reed and Simon (1978); and Simon (1979).

One realizes that the familiar short-range potentials (e.g., Yukawa potential, potential well) belong to R. On the other hand, the Coulomb potential is not an element of R. To incorporate this important case, too, we consider the extension

$$R'=R+L_\varepsilon^\infty(R^3), \quad \varepsilon>0 \qquad (3.13)$$

of R. For any positive ε, an element $\lambda v\in R'$ can be represented as $\lambda v=\lambda v'+\lambda v''$, where $\lambda v'\in R$ and

$|\lambda v''| < \varepsilon$. Clearly, the Coulomb potential is contained in R'. As for a discussion of R', we refer to Simon (1971) and the references from above. Two properties are important for us: First, λv, is infinitesimally form bounded with respect to $\mathbf{p}^2/2m$; secondly, H_P is self-adjoint and bounded from below in the sense of forms. We stress that the latter addendum is mathematically important. Normally, we should demand $D(\lambda v) \supseteq D(\mathbf{p}^2/2m)$ for the domains of both operators in order to have H_P properly defined. For $\lambda v \in R'$, this is true only in the sense of forms. To avoid mathematical subtleties, we assume λv to be such that H_P is also essentially self-adjoint and bounded from below on $D(\mathbf{p}^2/2m)$. We are now prepared to note

Statement 6. *Consider the Hamiltonian H' for a polaron in a potential, as defined in Eqs. (2.41) and (2.42). For the phonon dispersion and coupling, assume (3.1) to be valid ($D=3$). The potential $\lambda v(\mathbf{r})$ is supposed to be an element of R'. H_P has to be essentially self-adjoint, bounded from below, and should have at least one bound state with a strictly negative energy for any $\lambda > 0$. Then, the ground-state energy $E(\alpha,\lambda)$ exists and is an isolated, simple eigenvalue for $0 \le \alpha < \infty$, $0 < \lambda < \infty$. $E(\alpha,\lambda)$ and $\Psi(\alpha,\lambda)$ are real analytic functions of α,λ in the specified domain.*

Statement 7. *Consider H' as defined before and assume (3.1) to be valid. Let λv be an element of R and $v \le 0$. H_R has to be essentially self-adjoint, bounded from below, and should have bound states with strictly negative energy only for $\lambda > \lambda_c > 0$. Then, $E(\alpha,\lambda)$ exists and is nonanalytic for $\lambda = \lambda_c(\alpha)$, where $\lambda_c(\alpha)$ is a unique, continuous function of α and bounded by $0 \le \lambda_c(\alpha) \le \lambda_c$.*

Statement 7 guarantees the existence of the first (and only) nonanalyticity in connection with Fröhlich models; we are concerned with the so-called pinning transition. One may notice from Statement 7 that the analytical properties of $E(0,\lambda)$ are, in fact, essential for those of $E(\alpha,\lambda)$, as was conjectured in Sec. II.C. Therefore the concept of pinning transitions should be carefully distinguished from that of phonon-induced self-trapping, which might well exist in models that are different from ours. The important ingredient for pinning to occur is the attendance of a short-range potential $\lambda v(\mathbf{r})$, which allows for a bound state only if $\lambda > \lambda_c$.

Statement 6 demonstrates that no transition can occur if polarons are exposed to a long-range potential of, for example, Coulomb type. The physically important point concerning this potential is the existence of a bound state of H_P for any $\lambda > 0$.

Statement 8. *Take the existence of $F(\alpha,\beta,\lambda) - F(0,\beta,0)$, or, equivalently, the boundedness of $Z(\alpha,\beta,\lambda)$, for granted: $0 < Z(\alpha,\beta,\lambda) < \infty$. Then, $F(\alpha,\beta,\lambda) - F(0,\beta,0)$ is a real analytic function of α,β,λ. Sufficient conditions for the existence of $F(\alpha,\beta,\lambda) - F(0,\beta,0)$ in $0 \le \alpha < \infty$, $0 < \beta < \infty$, $0 < \lambda < \infty$ are given by Eqs. (3.2) or (3.3) and (additionally)*

$$|\underline{v}(\mathbf{k})| < \frac{c}{k^2} \; . \tag{3.14}$$

where $\underline{v}(\mathbf{k})$ is the Fourier transform of $v(\mathbf{r})$ and c is a constant.

It is interesting to contrast Statements 7 and 8 directly: one may easily find potentials $v(\mathbf{r})$, which meet both assumptions. Therefore we conclude that finite temperature destroys the pinning transition.

Let us now turn to earlier publications related to this work. With only few exceptions, all authors assume $\lambda v(\mathbf{r})$ to be a Coulomb potential. Therefore we first concentrate upon this case. It is well known that second-order perturbation theory (in α) is already troublesome and was controversially discussed for some years. We quote Platzman (1962), Stoneman (1970), Sak (1971), Bajaj and Clark (1972), Engineer and Tzoar (1972) and (1973), Larsen (1974), Fedoseyev (1976), Fedoseyev and Pork (1977), Matsuura (1984), and Higashimura (1987). As for a critical comparison, we particularly refer to Matsuura's paper. Variational treatments without restriction to a certain (α,λ) domain are due to Platzman (1962); Larsen (1969b) and (1970); Matsuura (1974); Hattori (1975b); Tokuda, Shoji, and Yoneya (1981a); and Devreese, Evrard, Kartheuser, and Brosens (1982). In two papers (Larsen, 1969b; Tokuda, Shoji, and Yoneya, 1981a), phase transitions were found under condition (3.1). Statement 6 proves that these are artifacts of the approximations made.

The interest in non-Coulomb potentials in connection with a pinning transition of polarons was stimulated by papers of Toyozawa (1980) and Spohn (1986); these are directly related to Statement 7. A proof of Statements 6 and 7 as well as a numerical study of the pinning transition of a polaron in a Yukawa potential can be found in two papers by Löwen (1988b, 1988d).

D. The polaronic exciton

We remarked in Sec. II.D that this system has a more complicated structure than the previous ones. We have to clarify this point in some detail, as it is essential for the formulation and understanding of the statements that follow.

The Hamiltonians under consideration are H, H', and $H'(\mathbf{Q})$, as defined in Eqs. (2.45)–(2.49), (2.51)–(2.53), and (2.54). One can nicely deduce from H' that the exciton-phonon problem incorporates aspects of a free and a bound polaron: the center-of-mass part mimicks free-polaron motion, the relative-coordinate part bound-polaron motion, if $\lambda U(\mathbf{r})$ is properly chosen. To ensure this, we may use the conditions of Statement 6, which we abbreviate conveniently as follows:

P: $\lambda U(\mathbf{r})$ is negative and belongs to R'. $H_{\mathrm{rel}} := p^2/2\mu + \lambda U(\mathbf{r})$ is essentially self-adjoint, bounded from below, and has at least one bound state for any $\lambda > 0$, the corresponding energy being strictly negative.

Let us now turn to $H'(\mathbf{Q})$ and try to establish the existence of a localized ground-state eigenfunction $\Psi(\mathbf{Q},\alpha,\lambda,\mathbf{m})$. We proceed in two steps: first, we discuss the position of the continuum edge $E_c \equiv E_c(\mathbf{Q},\alpha,\lambda,\mathbf{m})$ of $H'(\mathbf{Q})$; second, we concern ourselves with the question of whether or not the spectrum of $H'(\mathbf{Q})$ contains points E with $E < E_c$.

Intuitively, one can imagine two paths to continuum states: On the one side, electron and hole could be separated so far that $\lambda U(\mathbf{r})$ becomes negligible. As a consequence, the energy of relative motion becomes continuous. Defining

$$E_c^1(\mathbf{Q},\alpha,\mathbf{m}) := \inf \sigma_{\mathrm{ess}}[H'(\mathbf{Q},\alpha,0,\mathbf{m})] , \qquad (3.15)$$

where $\sigma_{\mathrm{ess}}[H']$ denotes the essential part of the spectrum of H', we expect E_c^1 to be one upper bound on E_c. On the other side, a ground-state exciton of energy $E(\mathbf{Q}-\mathbf{k},\alpha,\lambda,\mathbf{m})$ might absorb a phonon of energy $\hbar\omega(k)$, thereby reaching a continuum state, too. If we define

$$E_c^2(\mathbf{Q},\alpha,\lambda,\mathbf{m}) := \inf_{\mathbf{k}}[E(\mathbf{Q}-\mathbf{k},\alpha,\lambda,\mathbf{m}) + \hbar\omega(k)] , \qquad (3.16)$$

we should obtain a second upper bound on E_c. We shall prove in Sec. IV.D that

$$E_c(\mathbf{Q},\alpha,\lambda,\mathbf{m}) \geq \min\{E_c^1(\mathbf{Q},\alpha,\mathbf{m}), E_c^2(\mathbf{Q},\alpha,\lambda,\mathbf{m})\} \qquad (3.17)$$

is true, providing us with a lower bound on E_c. Summarizing all arguments, it is highly plausible that (3.17) is an equality rather than an inequality. In any case, this inequality is sufficient to proceed with step 2 as indicated.

The right-hand side of (3.17) admits two alternatives. Let us first discuss $E_c^2 < E_c^1$. We shall prove in Sec. IV.D that in this case (3.17) becomes an equality; moreover, we demonstrate by variational arguments that $H'(\mathbf{Q})$ has eigenvalues with $E < E_c$. We are now prepared to formulate

Statement 9a. *Consider the exciton Hamiltonian $H'(\mathbf{Q})$ as defined in Eq. (2.54). Assume $\lambda U(\mathbf{r})$ to have the property P as listed above. For the phonon dispersion and coupling, (3.1) is taken for granted. Finally, let $E_c^2 < E_c^1$. Then the ground-state energy $E(\mathbf{Q},\alpha,\lambda,\mathbf{m})$ exists and is an isolated, simple eigenvalue of $H'(\mathbf{Q})$ for $0 \leq \alpha < \infty$, $0 < \lambda < \infty$, $0 < m_n < \infty$, and $\mathbf{Q}$ in a certain surrounding of $\mathbf{Q}=\mathbf{0}$. $E(\mathbf{Q},\alpha,\lambda,\mathbf{m})$ and $\Psi(\mathbf{Q},\alpha,\lambda,\mathbf{m})$ are real analytic functions of $\mathbf{Q},\alpha,\lambda,\mathbf{m}$ in the specified domain.*

We believe that this statement is true for $\hbar^2 Q^2/2M < \hbar\omega$, which would be in accordance with Statement 1. One should notice, however, that our proof in Sec. IV.D is restricted to a smaller Q regime. Apart from this fact, we can repeat the former comments (see Sec. III.A).

The second alternative in inequality (3.17) is $E_c^1 < E_c^2$. This case cannot be treated in closed form. We need further assumptions. To demonstrate this, let us choose $\mathbf{Q}=\mathbf{0}$ (this property will prove to be characteristic for the ground state of H and H'). Now, recall the functional-integral considerations summarized in Eqs. (2.55)–(2.60). It is a simple task to reformulate these in the original coordinates $\mathbf{r}_1$ and $\mathbf{r}_2$ of electron and hole. Direct inspection of Eq. (2.57) shows that the phonon-induced electron-hole interaction can be positive definite and may well overcompensate ("overscreen") $\lambda U(\mathbf{r}_1-\mathbf{r}_2)$, unless α is sufficiently small. If overscreening takes place, the localization of relative motion (which is guaranteed for $\alpha \to 0$ by property P) will disappear. To exclude such a phenomenon, one has to specify the system parameters in detail. As an interesting example, we mention

$$\omega(k) = \omega, \quad \sqrt{\alpha}\, g(k) = \sqrt{\hbar\omega d}\,/(2\pi k) , \qquad (3.18)$$

$$\lambda U(\mathbf{r}) = -\frac{\lambda}{r} . \qquad (3.19)$$

In (3.18), d is an open parameter. If we fix d as

$$d = (1-\varepsilon_\infty/\varepsilon_0)\lambda < \lambda , \qquad (3.20)$$

we recover the standard exciton-phonon problem (see, e.g., Pollmann and Büttner, 1977). Concerning this, we note

Statement 9b. *Consider the exciton Hamiltonian $H'(Q)$ as defined in Eq. (2.54), specified according to Eqs. (3.18)–(3.20) (standard exciton-phonon problem). Then, the ground-state energy $E(\mathbf{Q},\lambda,\mathbf{m})$ exists and is an isolated, simple eigenvalue for $0 < \lambda < \infty$, $0 < m_n < \infty$, and $\mathbf{Q}$ in a certain surrounding of $\mathbf{Q}=\mathbf{0}$. $E(\mathbf{Q},\lambda,\mathbf{m})$ and $\psi(\mathbf{Q},\lambda,\mathbf{m})$ are real analytic functions of $\lambda,\mathbf{m}$ and $\mathbf{Q}$ in the specified domain.*

The notation in Statements 9a and 9b is slightly different: no α dependence appears in 9b. The reason for that is obvious: In 9b we use conditions (3.18)–(3.20); consequently, the only independent coupling parameter is λ.

Statement 10. *Under the conditions of Statements 9a and 9b, the inequality $E(\mathbf{0},\alpha,\lambda,\mathbf{m}) < E(\mathbf{Q}\neq\mathbf{0},\alpha,\lambda,m)$ holds for $0 \leq \alpha < \infty$, $0 < \lambda < \infty$, $0 < m_n < \infty$.*

Statement 10 is completely analogous to Statement 2; it disproves the possibility of a delocalization-localization transition for the exciton system under consideration. We close our compilation of statements with a last one, concerning the formal free energy.

Statement 11. *Take the existence of $F(\alpha,\beta,\lambda,\mathbf{m}) - F(0,\beta,0,\mathbf{m})$, or, equivalently, the boundedness of $Z(\alpha,\beta,\lambda,\mathbf{m})$, for granted: $0 < Z(\alpha,\beta,\lambda,\mathbf{m}) < \infty$. Then, $F(\alpha,\beta,\lambda,\mathbf{m}) - F(0,\beta,0,\mathbf{m})$ is a real analytic function of $\alpha,\beta,\lambda,\mathbf{m}$. Sufficient conditions for the existence of $F(\alpha,\beta,\lambda,\mathbf{m}) - F(0,\beta,0,\mathbf{m})$ in $0 \leq \alpha < \infty$, $0 < \beta < \infty$, $0 < \lambda < \infty$, and $0 < m_n < \infty$ are given by Eqs. (3.2) or (3.3)* *and (additionally) (3.14).*

Let us now turn to the earlier literature related to this work. Most authors are concerned with the standard model, defined by Eqs. (3.18)–(3.20). Therefore we concentrate on this case. Perturbation theory of second order with respect to the exciton-phonon coupling was performed by Mahanti and Varma (1970, 1972); Sak (1972); Matsuura and Wang (1973); and Wang and Matsuura (1974). Moreover, the perturbational results can be deduced as limiting cases from most of the variational treatments, quoted below. We mention that there was a controversial discussion concerning the correct weak-coupling limit for the polaron exciton. After all, Sak's results were confirmed.

In general, the variational approach was particularly influenced by the procedure of Lee, Low, and Pines (1953) for the free polaron. Pioneering papers are due to Haken (1956a, 1956b) and Meyer (1956). These served as the basis for the refined calculations of Mahler and Schröder (1974); Barentzen (1975); Fock, Kramer, and Büttner (1975); Pollmann and Büttner (1975, 1977); Bednarek and Suffczynski (1976); Hattori (1976); Bednarek, Adamowski, and Suffczynski (1977); Behnke and Büttner (1978, 1979); Kane (1978); Bednarek (1979); Matsuura and Büttner (1980a, 1980b, 1980c, 1980d); and Iadonisi and Bassani (1983, 1987). Not too surprising, functional-integral methods gave significant results also in this case (Haken, 1957, 1959; Moskalenko, 1958; Atzmüller, 1979; Adamowski, Gerlach, and Leschke, 1981, 1983; Gerlach, Löwen, and Schmidt, 1990).

The phase-transition problem for polaronic excitons was directly addressed in the papers of Sumi (1977) and Pekar, Rashba, and Sheka (1979), as well as in those of Shimamura and Matsuura (1983a, 1983b). In all cases nonanalyticities were found, partially under the conditions of Statement 9b; these have to be classified as artifacts of the approximations made.

We close this section with three references concerning Statements 9–11: extensive discussions can be found in the publications of Löwen (1987) and Gerlach and Löwen (1988a, 1990).

IV. PROOF OF THE RESULTS

We begin this section with some general remarks. Previous analytical studies of Hamiltonians of type (2.1) utilized two different mathematical approaches: the first approach stems from functional analysis and is usually denoted as operator theory; the second approach is provided from the calculus of functional integration.

From a strictly mathematical standpoint, the Hamiltonian (2.1) is only a formal expression representing an intuitive frame for a whole class of models. It is one of the particular merits of operator theory that it furnishes specific conditions on the couplings $g(k)$, the dispersions $\omega(k)$ and $\varepsilon(\mathbf{k})$, and the potentials $V(\mathbf{r})$, which, if fulfilled, guarantee the existence of properly defined model Hamiltonians H; because of physical reasons, these should be self-adjoint and bounded from below. If this can be taken for granted, a whole functional-analytic machinery becomes available for the discussion of bound and scattering states. As for the general operator theory, we quote the well-known books of Kato (1966) and Reed and Simon (1978). Applications to special cases of (2.1) can be found in the papers of Kato (1961), Nelson (1964), Eckmann (1970), Cannon (1971), Albeverio (1972), L. Gross (1972) and (1973), J. Fröhlich (1973) and (1974), Sloan (1974a, 1974b), Blanchard and Tarski (1978), Alvarez-Estrada (1979), and Arai (1981a, 1981b, 1981c) and (1983).

Direct inspection of these publications shows that some of them, particularly those of J. Fröhlich, are highly relevant for the solution of the phase-transition problem in polaron systems. Unfortunately, up to 1987 this had not been realized by either the above protagonists of Hamiltonian strategy or those who were concerned with a realistic polaron system. The necessary link was established in a paper by Spohn (1987a).

Functional-integration methods, on the other hand, were developed in close contact with physical applications. This can easily be seen from such standard textbooks as Feynman and Hibbs (1965), Glimm and Jaffe (1981), or Schulman (1981). As far as polaron systems are concerned, there existed a special connection to functional integration, caused by Feynman's famous paper from 1955. Nevertheless, an analytical approach to the phase-transition problem is new. To the best of our knowledge, the present authors were the first to exclude phase transitions in standard polaron systems at finite temperatures (Gerlach and Löwen, 1987a, 1987b).

Before going into detail, we include some comments concerning the following, Secs. IV.A–IV.D: We shall not repeat involved proofs that were completely given in previous publications. Instead, we want to present the basic ideas and relevant theorems to be used. It will be apparent in the course of this section that all analyticity proofs to follow have a strong conceptual similarity. Therefore we decided to take the free polaron as our special example and to treat this in greater detail (Sec. IV.A). The discussion in the subsequent Secs. IV.B–IV.D will be cut short, with only the necessary modifications being given.

Throughout the whole section, we use dimensionless variables; the units of mass, charge, frequency, and angular momentum are m, $|e|$, ω, and $\hbar$. To render a quick comparison with the problems and statements in Secs. II and III, we again use the same subtitles as before.

A. The free polaron

1. Analyticity of the ground-state energy and wave function of $H'(\mathbf{Q})$

In this section, we prove Statements 1 and 2; in doing so, we resolve Problems 1 and 2 under the specific conditions (3.1). Because of technical reasons, we have to separate the discussion of ground-state and finite-temperature properties. We shall make extensive use of J. Fröhlich's work (1974). To facilitate reading of the rather technical discussion, we briefly sketch the basic steps: Firstly, we determine the position of the continuum edge E_c of the Hamiltonian H under consideration, that is, $E_c = \inf \sigma_{\text{ess}}[H]$; as usual, $\sigma_{\text{ess}}[H]$ denotes the essential part of the spectrum of H. Secondly, we must show that the ground-state energy E of H exists and is below E_c; stated otherwise, E has to be a point of the discrete spectrum of H. Thirdly, we must guarantee the nondegeneracy of E. If all this has been done, we can finally apply analytical perturbation theory to ensure the analyticity of ground-state quantities as a function of certain parameters ($\alpha, \mathbf{Q}, B$, etc.) contained in H.

Eventual nonanalyticities of a specific system may show up at some of the steps indicated above. One possibility is that $E < E_c$ may be true only in a certain parameter region, whereas $E = E_c$ occurs elsewhere; in fact, this behavior is characteristic of the pinning transition (see Secs. III.C and IV.C). Another source of nonanalytical behavior is a degeneracy of E for certain admissible parameters.

In the following three subsections a–c, we proceed along the lines indicated above.

a. On the position of the continuum edge of $H'(\mathbf{Q})$

The main result of this subsection will be an equation between E and E_c, which—if combined with later results—will prove that $E \equiv E(\alpha, \mathbf{Q})$ belongs to the discrete spectrum of $H'(\mathbf{Q})$, provided $Q^2 < 2$ (recall that from now on we use natural units; instead of $\hbar^2 Q^2/2m < \hbar\omega$, we have $Q^2/2 < 1$). To start from a well-defined Hamiltonian, we introduce a first cutoff; this is of UV type and changes the coupling $g(k)$ appropriately. Later on, we need a second, more technical (lattice) cutoff, creating a discrete lattice of wave vectors. After that, we establish the desired relation between ground-state energy and continuum edge of the cutoff Hamiltonian. Of course, the final task will be to remove these cutoffs consecutively and to show that the relation between E and E_c survives such a procedure.

Now, recall the specific form of the Hamiltonian $H'(\mathbf{Q})$ from (2.17). Furthermore, remember condition (3.1) for Statements 1 and 2. We introduce the first (UV) cutoff by defining

$$g(k,\sigma) := g(k)\Theta(\sigma - k), \quad \sigma > 0 . \tag{4.1}$$

If we insert this coupling into (2.7) instead of $g(k)$, we find a new Hamiltonian $H'(\mathbf{Q},\sigma)$ and a corresponding interaction $H_{\mathrm{I}}'(\sigma)$. According to a result by Nelson (1964), we can now state that for any $\varepsilon > 0$, there exists a number $b \equiv b(\sigma,\varepsilon) < \infty$ such that

$$\begin{aligned} \|H_{\mathrm{I}}'(\sigma)\Psi\| &\le \varepsilon \|H_{\mathrm{Ph}}\Psi\| + b\|\Psi\| \\ &\le \varepsilon \|H_0'(\mathbf{Q})\Psi\| + b\|\Psi\| \end{aligned} \tag{4.2}$$

for any Ψ in the domain D of $H_0'(\mathbf{Q})$, D being dense in F. Thus $H_{\mathrm{I}}'(\sigma)$ is bounded with respect to $H_0'(\mathbf{Q})$ with relative bound zero. $H_0'(\mathbf{Q})$, in turn is self-adjoint and bounded from below. We conclude from a theorem of Rellich and Kato (see Reed and Simon, 1975, p. 162) that $H'(\mathbf{Q},\sigma) = H_0'(\mathbf{Q}) + H_{\mathrm{I}}'(\sigma)$ is also self-adjoint and bounded from below. In summary, the cutoff (4.1) has provided us with a properly defined Hamiltonian $H'(\mathbf{Q},\sigma)$ on the Fock space F.

Now, we introduce the second (lattice) cutoff, parametrized by a positive number d. In detail, we replace the original space $\mathbb{R}^D$ of phonon momenta by a momentum lattice Γ_d, defined as

$$\begin{aligned} \Gamma_d := (\mathbf{k} \in \mathbb{R}^D | k_j = n_j/\Lambda_d, n_j \in \mathbb{Z}, \\ \Lambda_d = 2^d \Lambda_0, \Lambda_0 \rangle 0, j = 1 \ldots D) . \end{aligned} \tag{4.3}$$

Additionally, to each $\mathbf{k} \in \mathbb{R}^D$ we associate $\mathbf{k}_d \in \Gamma_d$, namely,

$$\mathbf{k}_d := (n_1, n_2, n_3)/\Lambda_d, \quad n_j = \langle k_j \Lambda_d \rangle , \tag{4.4}$$

where

$$\langle a \rangle := \begin{cases} \text{largest integer} \le a & \text{if } a < 0 \\ \text{smallest integer} > a & \text{if } a \ge 0 . \end{cases} \tag{4.5}$$

It proves useful to construct appropriate Hilbert spaces before we introduce the new cutoff Hamiltonian. To do so, we consider a subspace $S_d \underline{c} L^2(\mathbb{R}^D)$ of step functions. For $f \in L^2(\mathbb{R}^D)$ we define $f \in S_d$, if $f(\mathbf{k}) = f(\mathbf{k}_d)$. Furthermore, we build up corresponding Fock spaces:

$$F_d := \bigoplus_{m=0}^{\infty} S_d^{\circledS m}, \quad \underline{F}_d := \bigoplus_{m=1}^{\infty} S_d^{\perp \circledS m} , \tag{4.6}$$

$$F_d^{\perp} := \underline{F}_d \circledS F_d . \tag{4.7}$$

The abbreviations used are nearly self-explanatory: $\oplus$ denotes direct sum; $\circledS$ symmetrical tensor product; and $\perp$, orthogonal complement. The original Fock space F is split into

$$F = F_d \oplus F_d^{\perp} . \tag{4.8}$$

Now, we introduce the cutoff Hamiltonian:

$$H'(\mathbf{Q},\sigma,d) := H_0'(\mathbf{Q},d) + H_{\mathrm{I}}'(\sigma,d) , \tag{4.9}$$

where

$$H_0'(\mathbf{Q},d) := \tfrac{1}{2}(\mathbf{Q} - \mathbf{P}_{\mathrm{Ph}}|_d)^2 + \int d^D k\, \omega(k)|_d a^*(\mathbf{k}) a(\mathbf{k}) , \tag{4.10}$$

$$\mathbf{P}_{\mathrm{Ph}}|_d := \int d^D k\, \mathbf{k}_d a^*(\mathbf{k}) a(\mathbf{k}) , \tag{4.11}$$

$$H_{\mathrm{I}}'(\sigma,d) := \sqrt{\alpha} \int d^D k\, [g(k,\sigma)|_d a(\mathbf{k}) + \text{H.c.}] . \tag{4.12}$$

Here, $f(\mathbf{k})|_d$ denotes the orthogonal projection of $f(\mathbf{k})$

on S_d. At first, such a definition makes sense only for functions $f \in L^2(\mathbb{R}^D)$; it can be readily extended to locally integrable functions.

As $H'(\mathbf{Q},\sigma)$, the Hamiltonian $H'(\mathbf{Q},\sigma,d)$ is self-adjoint and bounded from below on F. Let $E'(\alpha,\mathbf{Q},\sigma,d)$ denote the ground-state energy of $H'(\mathbf{Q},\sigma,d)$. We are now prepared to state

Lemma 1. *Suppose* $\mathbf{Q}$ *to be such that*

$$\inf_{\mathbf{k}_d}[E(\alpha,\mathbf{Q}-\mathbf{k}_d,\sigma,d)+\omega(\mathbf{k})|_d]-E(\alpha,\mathbf{Q},\sigma,d) =:\Lambda(\alpha,\mathbf{Q},\sigma,d)>0 \ . \tag{4.13}$$

Then, the part of spec $H'(\mathbf{Q},\sigma,d) \restriction F_d$ *contained in the interval* $[E(\alpha,\mathbf{Q},\sigma,d),\ E(\alpha,\mathbf{Q},\sigma,d)+\Lambda(\alpha,\mathbf{Q},\sigma,d)[$ *is purely discrete (* $\restriction F_d$ *is to indicate the restriction on* F_d*).*

Before we give the proof of this lemma, some comments may be appropriate. Firstly, one should realize the restriction of $H'(\mathbf{Q},\sigma,d)$ to the subspace F_d of step functions, which is necessary at the moment; we remove this technical assumption in Lemma 2. Secondly, inequality (4.13) can be nicely interpreted: For a given total momentum $\mathbf{Q}$, any one-phonon excitation of the ground state has to have a higher energy than the ground state itself.

Proof of Lemma 1. Let $f_\Lambda(x)$ be a positive function from C_∞, which is defined on $\mathbb{R}$ and has the additional properties $f_\Lambda(0)=1$ and $f_\Lambda(x)=0$ for $x\geq\Lambda$. We shall demonstrate that $f_\Lambda(H'(\mathbf{Q},\sigma,d)-E(\alpha,\mathbf{Q},\sigma,\mathrm{d}))\restriction \mathrm{F_d}$ is compact for $\Lambda=\Lambda(\alpha,\mathbf{Q},\sigma,d)$. This proves Lemma 1 (as coreference, see Reed and Simon, 1978, p. 259).

In detail, we distinguish between phonons with momenta k larger and smaller than σ, the reason being that these are not intermixed by $H_\mathrm{I}'(\sigma,d)$ because of the σ-cutoff in $g(k,\sigma)$. We insert as a technical remark that for a given $\mathbf{k}$, $k<\sigma$, the associated vector $\mathbf{k}_d$ may have a length larger than σ because of definition (4.4); in any case, $|\mathbf{k}_d|<\sigma+\sqrt{D}/\Lambda_d$ is valid, if $k<\sigma$. In the following considerations, we skip this point, as it is presently irrelevant.

Let Γ_d be divided into

$$\Gamma_{d,\sigma}:=(\mathbf{k}|\mathbf{k}\in\Gamma_d,k\leq\sigma) \tag{4.14}$$

and $\Gamma_d\setminus\Gamma_{d,\sigma}$. In accordance, we split the space S_d of step functions by defining a subspace $S_{d,\sigma}$ as follows: An element $f\in S_d$ is contained in $S_{d,\sigma}$, if $f(\mathbf{k})=0$ for $k>\sigma$. The associated Fock spaces are

$$F_{d,\sigma}:=\bigoplus_{m=0}^{\infty} S_{d,\sigma}^{\circledS m},\quad \underline{F}_{d,\sigma}:=\bigoplus_{m=1}^{\infty} S_{d,\sigma}^{\perp\circledS m}\ , \tag{4.15}$$

$$F_{d,\sigma}^{\perp}:=\underline{F}_{d,\sigma}\circledS F_{d,\sigma}\ . \tag{4.16}$$

Then,

$$F_d=F_{d,\sigma}\oplus F_{d,\sigma}^{\perp}\ . \tag{4.17}$$

With Eq. (4.17) we have finished the technical preparations. Our first conclusion is that $f_\Lambda(H'(\mathbf{Q},\sigma,d)-E(\alpha,\mathbf{Q},\sigma,d))\restriction F_{d,\sigma}$ is compact. The reason is that the restriction on $F_{d,\sigma}$ admits only a finite number of phonon modes, namely, those that are characterized by $\Gamma_{d,\sigma}$.

Secondly, it is important that we can calculate a lower bound on inf spec $H'(\mathbf{Q},\sigma,d)\restriction F_{d,\sigma}^{\perp}$. To prove this, we consider an element $\chi\in F_{d,\sigma}^{\perp}$ of type $\chi=\Psi\circledS\varphi$, where $\Psi\in\underline{F}_{d,\sigma}$ and $\varphi\in F_{d,\sigma}$ [see Eq. (4.16)]. Moreover, we choose Ψ as an eigenfunction of the phonon-number operator such that

$$\mathbf{P}_{\mathrm{Ph}}|_d\Psi=\sum_{j=1}^{N}\mathbf{k}_d^j\Psi,\quad \mathbf{k}_d^j\in\Gamma_d\setminus\Gamma_{d,\sigma},\quad N\geq1\ . \tag{4.18}$$

Then, we find

$$\begin{aligned}&\|\chi\|=\|\Psi\|\cdot\|\varphi\|\ ,\\ &\langle\chi|H_\mathrm{I}'(\sigma,d)|\chi\rangle=\langle\Psi|\Psi\rangle\langle\varphi|H_\mathrm{I}'(\sigma,d)|\varphi\rangle\ ,\end{aligned} \tag{4.19}$$

and

$$\begin{aligned}\langle\chi|H'(\mathbf{Q},\sigma,d)|\chi\rangle&=\sum_{j=1}^{N}\omega(k^j)|_d\langle\chi|\chi\rangle+\langle\Psi|\Psi\rangle\langle\varphi|H'\left[\mathbf{Q}-\sum_{j=1}^{N}\mathbf{k}_d^j,\sigma,d\right]|\varphi\rangle\\ &\geq\left[\sum_{j=1}^{N}\omega(k^j)|_d+E\left[\alpha,\mathbf{Q}-\sum_{j=1}^{N}\mathbf{k}_d^j,\sigma,d)\right]\right]\langle\chi|\chi\rangle\ .\end{aligned} \tag{4.20}$$

Because of $\sum_{j=1}^{N}\omega(k^j)\geq\omega(|\sum_{j=1}^{N}\mathbf{k}_j|)$ according to Eq. (3.1), we find

$$\langle\chi|H'(\mathbf{Q},\sigma,d)|\chi\rangle \geq\inf_{\mathbf{k}_d}[\omega(k)|_d+E(\alpha,\mathbf{Q}-\mathbf{k}_d,\sigma,d)]\langle\chi|\chi\rangle\ . \tag{4.21}$$

The same inequality is true for finite linear combinations of pairwise orthogonal elements χ of the type $\Psi\circledS\varphi$. As these are complete on $F_{d,\sigma}^{\perp}$, we arrive at the inequality

$$\inf\mathrm{spec}H'(\mathbf{Q},\sigma,d)\restriction F_{d,\sigma}^{\perp} \geq\inf_{\mathbf{k}_d}[\omega(\mathbf{k})|_d+E(\alpha,\mathbf{Q}-\mathbf{k}_d,\sigma,d)]\ . \tag{4.22}$$

Consequently, $f_\Lambda(H'(\mathbf{Q},\sigma,d)-E(\alpha,\mathbf{Q}\sigma,d))\restriction F_{d,\sigma}^{\perp}=0$. Because of $F_d=F_{d,\sigma}\oplus F_{d,\sigma}^{\perp}$ and our above conclusion that the corresponding expression for $F_{d,\sigma}$ is compact, we finally find that $f_\Lambda(H'(\mathbf{Q},\sigma,d)-E(\alpha,\mathbf{Q},\sigma,d))\restriction F_d$ is compact—this proves Lemma 1.

We shall now remove the lattice-cutoff. Turning to the ground-state energy $E(\alpha,\mathbf{Q},\sigma)$ of $H'(\mathbf{Q},\sigma)$ (which is known to exist), we state

Lemma 2. *Suppose* $\mathbf{Q}$ *to be such that*

$$\inf_{\mathbf{k}}[E(\alpha,\mathbf{Q}-\mathbf{k},\sigma)+\omega(k)]-E(\alpha,\mathbf{Q},\sigma)$$

$$=:\Lambda(\alpha,\mathbf{Q},\sigma)>0 \ . \tag{4.23}$$

Then, the part of spec $H'(\mathbf{Q},\sigma)\restriction F$ *contained in the interval* $[E(\alpha,\mathbf{Q},\sigma),\ E(\alpha,\mathbf{Q},\sigma)+\Lambda(\alpha,\mathbf{Q},\sigma)[$ *is purely discrete.*

Proof of Lemma 2. For a moment, we return to $H'(\mathbf{Q},\sigma,d)$ and note that

$$\inf \operatorname{spec} H'(\mathbf{Q},\sigma,d)\restriction F_d^{\perp}$$

$$\geq \inf_{\mathbf{k}_d}[\omega(k)|_d+E(\alpha,\mathbf{Q}-\mathbf{k}_d,\sigma,d)] \ . \tag{4.24}$$

Inequality (4.24) can be proven in analogy to inequality (4.22), the only modification being that $F_{d,\sigma}$, $\underline{F}_{d,\sigma}$, and $F_{d,\sigma}^{\perp}$ have to be replaced by F_d, $\underline{F}_d$, and $F_d^{\perp}$. In terms of the function $f_\Lambda(x)$ from the proof of Lemma 1, we thus have

$$f_\Lambda(H'(\mathbf{Q},\sigma,d)-E(\alpha,\mathbf{Q},\sigma,d))\restriction F_d^{\perp}=0 \ . \tag{4.25}$$

On the other hand, we know from Lemma 1 that the corresponding expression for F_d instead of $F_d^{\perp}$ is compact. Both properties yield the following: $f_\Lambda(H'(\mathbf{Q},\sigma,d)-E(\alpha,\mathbf{Q},\sigma,d))\restriction F$ is compact.

Now, the striking point is that $H'(\mathbf{Q},\sigma,d)\to H'(\mathbf{Q},\sigma)$ on F in the norm resolvent sense, if $d\to\infty$. This can be shown directly by comparison of both resolvents; as for details, see Fröhlich (1974). Combining this property and the preceding one, we finally have demonstrated [compare also with Reed and Simon (1978), pp. 259, 260] that $f_{\Lambda'}(H'(\mathbf{Q},\sigma)-E(\alpha,\mathbf{Q},\sigma))\restriction F$ is compact; the zero $\Lambda':=\Lambda(\alpha,\mathbf{Q},\sigma)$ of $f_{\Lambda'}(x)$ is now given by Eq. (4.23) and evolves as the limiting value of $\Lambda(\alpha,\mathbf{Q},\sigma,d)$ for $d\to\infty$. Thus Lemma 2 has been proven.

The remaining task is to remove the UV-cutoff σ. To achieve this, we use a well-known unitary transformation known as "oscillator transform"; in our context, it was introduced by E. P. Gross (1962) and Nelson (1964). We define

$$T_{\sigma\lambda}:=\int d^Dk\,[\beta_{\sigma\lambda}(k)a(\mathbf{k})-\text{H.c.}] \ , \tag{4.26}$$

$$\beta_{\sigma\lambda}(k):=-\sqrt{\alpha}g(k,\sigma)\theta(k-\lambda)/(\omega(k)+k^2/2) \ ,$$

$$0<\lambda<\sigma \ . \tag{4.27}$$

Because of (3.1), $\exp(T_{\sigma\lambda})$ is a well-defined unitary operator on F for $0<\sigma\leq\infty$. Now, we consider

$$H''(\mathbf{Q},\sigma,\lambda):=\exp(T_{\sigma\lambda})H'(\mathbf{Q},\sigma)\exp(-T_{\sigma\lambda}) \ . \tag{4.28}$$

Explicit evaluation of the right-hand side yields

$$H''(\mathbf{Q},\sigma,\lambda)=H_0'(\mathbf{Q})+H_{\mathrm{I}}'(\lambda)+W(\mathbf{Q},\sigma,\lambda)+\Sigma(\sigma,\lambda)$$

$$=H'(\mathbf{Q},\lambda)+W(\mathbf{Q},\sigma,\lambda)+\Sigma(\sigma,\lambda) \ , \tag{4.29}$$

where

$$W(\mathbf{Q},\sigma,\lambda):=(\mathbf{Z}+\mathbf{Z}^*)^2/2-(\mathbf{Q}-\mathbf{P}_{\mathrm{Ph}})\cdot\mathbf{Z}$$

$$-\mathbf{Z}^*\cdot(\mathbf{Q}-\mathbf{P}_{\mathrm{Ph}}) \ , \tag{4.30}$$

$$\mathbf{Z}:=\int d^Dk\,\mathbf{k}\beta_{\sigma\lambda}(k)a(\mathbf{k}) \ , \tag{4.31}$$

$$\Sigma(\sigma,\lambda):=\int d^Dk\,\{\omega(k)|\beta_{\sigma\lambda}(k)|^2$$

$$+\sqrt{\alpha}[g(k,\sigma)\beta_{\sigma\lambda}(k)^*+\text{H.c.}]\} \ . \tag{4.32}$$

From Eqs. (4.30)–(4.32) and (3.1) we derive three important properties of $H''(\mathbf{Q},\sigma,\lambda)$, which are the basis for the removal of σ. Firstly, $\Sigma(\sigma,\lambda)$ is finite and uniformly bounded from below:

$$\Sigma(\sigma,\lambda)\geq-2\alpha\int d^Dk\,|g(k)|^2/[\omega(k)+k^2/2]$$

$$\geq-2\alpha\int d^Dk\,|g(k)|^2/(1+k^2/2) \tag{4.33}$$

(we are using natural units; $\omega(k)\geq\omega=1$). Secondly, $H_{\mathrm{I}}'(\lambda)$ appears in Eq. (4.29) instead of $H_{\mathrm{I}}'(\sigma)$. Finally, $H_{\mathrm{I}}'(\lambda)$ and $W(\mathbf{Q},\sigma,\lambda)$ are form bounded with respect to $H_0'(\mathbf{Q})$ with relative bound zero: For any $\varepsilon<0$, there exists λ_ε and $b(\lambda_\varepsilon)<\infty$ (independent of $\mathbf{Q}$ and σ) such that

$$|\langle\psi|H_{\mathrm{I}}'(\lambda)+W(\mathbf{Q},\sigma,\lambda)|\psi\rangle|$$

$$\leq\varepsilon\langle\psi|H_0'(\mathbf{Q})|\psi\rangle+b(\lambda_\varepsilon)\langle\psi|\psi\rangle \tag{4.34}$$

for any ψ in the domain of $[H_0'(\mathbf{Q})]^{1/2}$. This proves [see Nelson (1964) and J. Fröhlich (1974)].

Lemma 3. *For the resolvent* $[\zeta-H''(\mathbf{Q},\sigma,\lambda)]^{-1}$, *the limit*

$$\lim_{\sigma\to\infty}[\zeta-H''(\mathbf{Q},\sigma,\lambda)]^{-1}=:[\zeta-H''(\mathbf{Q},\lambda)]^{-1} \tag{4.35}$$

exists in the norm sense and is the resolvent of a self-adjoint Hamiltonian $H''(\mathbf{Q},\lambda)$, *bounded from below on F.*

We add as a comment that Lemma 3 provides us with a proper mathematical interpretation of the primarily formal expression $H'(\mathbf{Q})$ from Eq. (2.17). According to Eq. (4.28), we find

$$H'(\mathbf{Q})=\exp(-T_{\infty\lambda})H''(\mathbf{Q},\lambda)\exp(T_{\infty\lambda}) \ . \tag{4.36}$$

$H'(\mathbf{Q})$ is self-adjoint and bounded from below on F. Consequently, $E(\alpha,\mathbf{Q})$ exists. We are now prepared to state

Lemma 4. *Suppose* $\mathbf{Q}$ *to be such that*

$$\inf_{\mathbf{k}}[E(\alpha,\mathbf{Q}-\mathbf{k})+\omega(k)]-E(\alpha,\mathbf{Q})=:\Lambda(\alpha,\mathbf{Q})>0 \ . \tag{4.37}$$

Then, the part of the spec $H'(\mathbf{Q})$ *contained in the interval* $[E(\alpha,\mathbf{Q}),\ E(\alpha,\mathbf{Q})+\Lambda(\alpha,\mathbf{Q})[$ *is purely discrete.*

To prove this lemma, we recall from the proof of Lemma 2 that $f_{\Lambda'}(H'(\mathbf{Q},\sigma)-E(\alpha,\mathbf{Q},\sigma))\restriction F$ is compact, where $\Lambda'=\Lambda'(\alpha,\mathbf{Q},\sigma)$. The same holds true if $H'(\mathbf{Q},\sigma)$ is replaced by $H''(\mathbf{Q},\sigma,\lambda)$, being a unitary transform of $H'(\mathbf{Q},\sigma)$. Therefore we conclude from Lemma 3 that $f_{\Lambda''}(H''(\mathbf{Q},\lambda)-E(\alpha,\mathbf{Q}))\restriction F$ is compact, where $\Lambda''=\Lambda(\alpha,\mathbf{Q})$ is the limiting value of $\Lambda(\alpha,\mathbf{Q},\sigma)$ for $\sigma\to\infty$. As $H'(\mathbf{Q})$ is a unitary transform of $H''(\mathbf{Q},\lambda)$, we finally deduce that $f_{\Lambda''}(H'(\mathbf{Q})-E(\alpha,\mathbf{Q}))\restriction F$ is compact. This proves Lemma 4.

Summarizing thus far, we have found a lower bound on the continuum edge of $E_c(\alpha,\mathbf{Q})$ of $H'(\mathbf{Q})$:

$$E_c(\alpha,\mathbf{Q})\geq\inf_{\mathbf{k}}[E(\alpha,\mathbf{Q}-\mathbf{k})+\omega(k)]\ . \tag{4.38}$$

This result is nicely complemented by the following one:

Lemma 5.

$$E_c(\alpha,\mathbf{Q})\leq\inf_{\mathbf{k}}[E(\alpha,\mathbf{Q}-\mathbf{k})+\omega(k)]\ . \tag{4.39}$$

Spohn (1988) provided a proof of Lemma 5, which uses a Rayleigh-Ritz argument: For an infinite number of pairwise orthogonal trial functions, the variational bounds on the energies of $H'(\mathbf{Q})$ accumulate at the right-hand side of (4.39).

A combination of inequality (4.38) and Lemma 5 leads us to the central result of this subsection, namely,

Theorem 1. *The continuum edge of $H'(\mathbf{Q})$ is produced by one-phonon excitations and is given by*

$$E_c(\alpha,\mathbf{Q})=\inf_{\mathbf{k}}[E(\alpha,\mathbf{Q}-\mathbf{k})+\omega(k)]\ . \tag{4.40}$$

We enclose a useful inequality that can be derived from Theorem 1 in combination with $\omega(k)\geq\omega=1$ [condition (3.1)] and an earlier estimate of *L*. Gross (1972), namely, $E(\alpha,\mathbf{Q})\geq E(\alpha,\mathbf{0})$. Starting from Eq. (4.40), we find

$$E_c(\alpha,\mathbf{Q})\geq 1+E(\alpha,\mathbf{0})\ . \tag{4.41}$$

We recall that $\omega(k)=\omega$ is true for the standard Fröhlich model, defined in Eq. (2.10). In this case, (4.41) becomes an equality.

b. Uniqueness of the ground state of $H'(\mathbf{Q})$ and proof of Statement 2

To begin with, we specify an upper bound on $E(\alpha,\mathbf{Q})$:

Lemma 6.

$$E(\alpha,\mathbf{Q})\leq E(\alpha,\mathbf{0})+\mathbf{Q}^2/2\ . \tag{4.42}$$

To prove this result, it is sufficient to consider $H'(\mathbf{Q},\sigma)$ and the corresponding energy $E(\alpha,\mathbf{Q},\sigma)$ as discussed in the preceding subsection. In analogy to $E(\alpha,\mathbf{Q})$, $E(\alpha,\mathbf{Q},\sigma)$ depends merely on $|\mathbf{Q}|$. We split $H'(\mathbf{Q},\sigma)$ as follows:

$$\begin{aligned}H'(\mathbf{Q},\sigma)-\mathbf{Q}^2/2&=\tfrac{1}{2}(\mathbf{P}_{\mathrm{Ph}})^2+H_{\mathrm{Ph}}+H_{\mathrm{I}}'(\sigma)-\mathbf{Q}\cdot\mathbf{P}_{\mathrm{Ph}}\\&=:h(\sigma)-\mathbf{Q}\cdot\mathbf{P}_{\mathrm{Ph}}\ .\end{aligned} \tag{4.43}$$

$h(\sigma)$ is bounded from below, and $\mathbf{Q}\cdot\mathbf{P}_{\mathrm{Ph}}$ is form bounded with respect to $h(\sigma)$ with relative bound zero. Consequently, the ground-state energy of $H'(\mathbf{Q},\sigma)-\mathbf{Q}^2/2$ is a continuous and monotonously decreasing function of $|\mathbf{Q}|$ (as a reference, see Reed and Simon, 1978, page 98). This proves Lemma 6.

A combination of this lemma and inequality (4.41) yields directly

Lemma 7. *For $Q<\sqrt{2}$, $E(\alpha,\mathbf{Q})$ belongs to the discrete part of the spectrum of $H'(\mathbf{Q})$.*

The proof is very simple: For $Q<\sqrt{2}$, a successive application of (4.41) and (4.42) shows that $E_c(\alpha,\mathbf{Q})>\mathbf{Q}^2/2+E(\alpha,\mathbf{0})\geq E(\alpha,\mathbf{Q})$ is true. This proves Lemma 7.

Summarizing thus far, we have established the existence of (normalizable) eigenfunctions of $H'(\mathbf{Q})$ for $Q<\sqrt{2}$. The admissible $\mathbf{Q}$ domain may be larger in specific cases such as Eq. (2.10). This can be easily demonstrated by perturbation theory. As for a more involved discussion, we refer to Spohn (1988). We are now prepared to give the

Proof of Statement 2.

$$E(\alpha,\mathbf{0})<E(\alpha,\mathbf{Q}\neq 0)\ . \tag{4.44}$$

The inequality (4.44) is certainly true, if $E(\alpha,\mathbf{Q})$ does not belong to the discrete part of spec $H'(\mathbf{Q})$. In that case (4.41) provides us with $E(\alpha,\mathbf{Q})\geq 1+E(\alpha,\mathbf{0})>E(\alpha,\mathbf{0})$.

Therefore it is sufficient to find a proof for the case when $E(\alpha,\mathbf{Q})$ is an eigenvalue. Let us assume that (4.44) was not true for some $Q_c\neq 0$, that is, $E(\alpha,0)\geq E(\alpha,\mathbf{Q}_c)=E(\alpha,-\mathbf{Q}_c)$. Then the ground state of H' would automatically be degenerate. Our strategy will be to reject this assumption. To achieve this, we shall use two powerful theorems from operator theory that enable one to decide whether or not a ground-state eigenvalue is simple. As an insertion, we list these theorems [proofs can be found in the book by Reed and Simon (1978, pp. 204, 205)]:

> I. Let the Hamiltonian H be self-adjoint and bounded from below on a certain Hilbert space, the ground-state energy being E. Choose a fixed representation of the Hilbert space. If E is an eigenvalue and $\exp(-tH)$ is positivity improving for all $t>0$ within the chosen representation, then E is a simple eigenvalue.

Here, an operator A is called positivity improving if for any positive $\Psi\neq 0$ the function $A\Psi$ is strictly positive. Clearly, this property depends on the representation of the Hilbert space. If $A\Psi$ is only positive and $A\Psi\neq 0$, the operator A is called positivity preserving.

The second theorem provides a manageable criterion to decide whether $\exp(-tH)$ is positivity improving.

> II. Let $H=H_0+U$ and choose a fixed representation

of the Hilbert space. Suppose that U is a multiplication operator (that is, diagonal) in the chosen representation and that there exists a sequence of bounded multiplication operators U_n such that $H_0+U_n \to H$ and $H-U_n \to H_0$ in the strong resolvent sense. Then, $\exp(-tH)$ is positivity improving, if this is true for $\exp(-tH_0)$.

To apply these theorems, we consider the Hamiltonian H' [not $H'(\mathbf{Q})$] according to Eq. (2.14). H' depends on $\mathbf{p}$, but not on $\mathbf{r}$, and is usually defined on $H:=L^2(\mathbb{R}^D)\otimes F$. An essential point of our proof is that we redefine H' on another Hilbert space $\mathcal{H}_c:=L^2([-a,a[^D)\otimes F$, $a:=\hbar/Q_c$—we restrict the electronic part of the wave function to a finite cube of length a. It is only in this way that we can apply the preceding theorems I and II, as will become clear in a moment. One should notice three facts or properties:

(i) By periodic continuation, we can define functions on $\mathbb{R}^D$ that were originally given on $[-a,a[^D$.

(ii) The momentum operator $\mathbf{p}$ works as a multiplication operator in the Fourier space, associated with $L^2([-a,a[^D)$. Application of $\exp(i\mathbf{a}\cdot\mathbf{p})$, $\mathbf{a}\in\mathbb{R}^D$ to a wave function $X(\mathbf{r})\in L^2([-a,a[^D)$ induces a translation about $\mathbf{a}$.

(iii) The existence of ground-state eigenfunction(s) of H' is guaranteed in H_c; because of $[H',\mathbf{p}]=0$, they can be parametrized as follows:

$$\phi(\alpha,\mathbf{Q}_n):=\exp(i\mathbf{Q}_n\cdot\mathbf{r})\Psi(\alpha,\mathbf{Q}_n)\ . \tag{4.45}$$

Here, $\mathbf{Q}_n$ is a discrete wave vector (by construction), and $\Psi(\alpha,\mathbf{Q}_n)$ a ground-state eigenfunction of $H'(\mathbf{Q}_n)$. Therefore $\phi(\alpha,\mathbf{Q}_n)$ has the eigenvalue $E(\alpha,\mathbf{Q}_n)$. If H_c is replaced by H, property (iii) is no longer valid.

We shall now demonstrate that $\exp(-tH')$ is positivity improving. As fixed representation, we choose the position representation for the electronic coordinates, and the so-called Q representation for the phonon coordinates. The latter is obtained by rewriting the operators $a(\mathbf{k})$ in $a^+(\mathbf{k})$ in terms of position and momentum operators $q(\mathbf{k})$ and $p(\mathbf{k})$, and by choosing once more a position representation (for details, we refer to Ginibre, 1971 and Simon, 1974). In this representation, H_I' acts as a multiplication operator. Furthermore, the analysis of J. Fröhlich (1974) makes clear that H_I' can be approximated by bounded multiplication operators as required in Theorem II. All that remains to be done is to show that $\exp(-tH_0)$ is positivity improving, where now $H_0:=\frac{1}{2}(\mathbf{p}-\mathbf{P}_{\mathrm{Ph}})^2+H_{\mathrm{Ph}}$. We proceed as follows:

$$\exp(-tH_0)=\exp(-tH_{\mathrm{Ph}})(2\pi)^{-D/2}\int d^Da\,\exp(-\mathbf{a}^2/2)\exp(i\sqrt{t}\,\mathbf{a}\mathbf{p})\exp(-i\sqrt{t}\,\mathbf{a}\cdot\mathbf{P}_{\mathrm{Ph}})\ . \tag{4.46}$$

Now, $\exp(-tH_{\mathrm{Ph}})$ is positivity improving with respect to the phonon coordinates and positivity preserving with respect to the electron coordinates; $\exp(-i\sqrt{t}\,\mathbf{a}\mathbf{P}_{\mathrm{Ph}})$ is positivity preserving in both cases. The positivity of $\exp(-\mathbf{a}^2/2)$, and the fact that $\exp(i\sqrt{t}\,\mathbf{a}\cdot\mathbf{p})$ acts as a translation operator, assures us that $\exp(-tH_0)$ is positivity improving in the chosen representation of H_c.

We can now apply Theorem I to H', defined on H_c, and conclude that the ground state has to be nondegenerate. If $E(\alpha,0)\geq E(\alpha,\mathbf{Q}_c)=E(\alpha,-\mathbf{Q}_c)$ were true for some $\mathbf{Q}_c\neq 0$, however, the ground state of H' would be degenerate. Therefore we have to reject this assumption, and Statement 2 has been proven.

We close this subsection with a remark. J. Fröhlich (1973) applied Theorems I and II to $H'(\mathbf{Q})$. Proceeding along lines similar to the above, he arrived at the following result: If $E(\alpha,\mathbf{Q})$ belongs to the discrete part of spec $H'(\mathbf{Q})$, it is a simple eigenvalue. In complete analogy, one may discuss the cutoff Hamiltonians $H'(\mathbf{Q},\sigma)$ and $H''(\mathbf{Q},\sigma,\lambda)$. We can profitably use these results in the following, final step of our analyticity proof.

c. Proof of Statement 1

Having established the existence of a nondegenerate, discrete ground state of $H'(\mathbf{Q})$ for $Q<\sqrt{2}$, we now apply analytical perturbation theory to show that $E(\alpha,\mathbf{Q})$ and $\Psi(\alpha,\mathbf{Q})$ are real analytic functions of α and $\mathbf{Q}$ for $0\leq\alpha<\infty$, $Q<\sqrt{2}$ (Statement 1).

It proves useful to start from the cutoff Hamiltonian $H''(\mathbf{Q},\sigma,\lambda)\equiv H''(\sqrt{\alpha},\mathbf{Q},\sigma,\lambda)$, which was introduced in Eq. (4.28). In this subsection, it is necessary to indicate the α dependence explicitly. In particular, we define

$$h(\sqrt{\alpha},\mathbf{Q},\sigma,\lambda):=H''(\sqrt{\alpha},\mathbf{Q},\sigma,\lambda)-\frac{Q^2}{2}\ . \tag{4.47}$$

To apply analytical perturbation theory, the basic quantity to discuss is the deviation of $h(\sqrt{\alpha},\mathbf{Q},\sigma,\lambda)$ from $h(\sqrt{\alpha_0},Q_0,\sigma,\lambda)$, where α_0,α and $\mathbf{Q}_0,\mathbf{Q}$ are admissible parameters in the specified domain and $\alpha_0,\mathbf{Q}_0$ are fixed. Direct calculation shows, for example, that

$$h(\sqrt{\alpha_0},\mathbf{Q},\sigma,\lambda)-h(\sqrt{\alpha_0},\mathbf{Q}_0,\sigma,\lambda) = -(\mathbf{Q}-\mathbf{Q}_0)\cdot[\mathbf{P}_{\mathrm{Ph}}+\mathbf{Z}+\mathbf{Z}^*] \tag{4.48}$$

is true. $\mathbf{P}_{\mathrm{Ph}}$, $\mathbf{Z}$, and $\mathbf{Z}^*$ are form bounded with respect to $h(\sqrt{\alpha_0},\mathbf{Q}_0,\sigma,\lambda)$. Consequently, the Hamiltonians $h(\sqrt{\alpha_0},\mathbf{Q},\sigma,\lambda)$—$\mathbf{Q}$ is considered as variable—form a holomorphic family of self-adjoint operators of type B (see Kato, 1966, in particular, Chapter VII, Sec. 4). Furthermore, as the form boundedness of $\mathbf{P}_{\mathrm{Ph}}$, $\mathbf{Z}$, and $\mathbf{Z}^*$ with respect to $h(\sqrt{\alpha_0},\mathbf{Q},\sigma,\lambda)$ is uniform in σ, the limit $\sigma\to\infty$ can be performed (see Lemma 3). Therefore the Hamiltonians

$$h(\sqrt{\alpha_0},\mathbf{Q},\lambda):=H''(\sqrt{\alpha_0},\mathbf{Q},\lambda)-\frac{Q^2}{2} \tag{4.49}$$

form a holomorphic family of self-adjoint operators of type B, too. If we combine this property with the nondegeneracy of the discrete ground state of $H''(\sqrt{\alpha_0},\mathbf{Q},\lambda)$ for $Q<\sqrt{2}$, we can conclude that the ground-state energy and wave function of $H''(\sqrt{\alpha_0},\mathbf{Q},\lambda)$ are real analytic functions of $\mathbf{Q}$ for $Q<\sqrt{2}$. As $H'(\mathbf{Q})\equiv H'(\sqrt{\alpha},\mathbf{Q})$ is a unitary transform of $H''(\sqrt{\alpha},\mathbf{Q},\lambda)$, the transformation operator $T_{\infty\lambda}$ being independent of $\mathbf{Q}$, we arrive at the result that $E(\alpha_0,\mathbf{Q})$ and $\Psi(\alpha_0,\mathbf{Q})$ are real analytic functions of $\mathbf{Q}$ for $Q<\sqrt{2}$ (and a given value α_0).

Proceeding along similar lines, we can prove the corresponding result for the $\sqrt{\alpha}-$ dependence of $E(\alpha,\mathbf{Q}_0)$ and $\Psi(\alpha,Q_0)$. As the perturbation series for $E(\alpha,\mathbf{Q}_0)$ and $\Psi(\alpha,\mathbf{Q}_0)$ around $\alpha=0$ contain only even powers of $\sqrt{\alpha}$, we have finally proven the real analyticity of $E(\alpha,\mathbf{Q}_0)$ and $\Psi(\alpha,\mathbf{Q}_0)$ with respect to α, even for $\alpha=0$. This completes the proof of Statement 1.

We close this subsection with a remark concerning discrete excited states (if they exist at all): If they are nondegenerate, Statement 1 will hold again.

2. Analyticity of the formal free energy of H. Proof of Statement 3

In this section we sketch the basic ideas for the proof of Statement 3. A detailed discussion can be found in two papers by the present authors (Gerlach and Löwen, 1987a, 1987b).

As a starting point, we use Eqs. (2.21) and (2.26), which relate $F(\alpha,\beta)$ and $Z(\alpha,\beta)$ to the action $S_{\rm I}\equiv S_{\rm I}(\alpha,\beta)$ as defined in (2.24):

$$Z(\alpha,\beta)=\exp\{-\beta[F(\alpha,\beta)-F(0,\beta)]\}$$
$$=\langle\exp(-S_{\rm I})\rangle\ . \tag{4.50}$$

Clearly, it is sufficient to study the analytical properties of $Z(\alpha,\beta)$. To do so, let us consider

$$Z_N(\alpha,\beta):=\left\langle\sum_{n=0}^{N}\frac{1}{n!}(-S_{\rm I})^n\right\rangle$$
$$=\sum_{n=0}^{N}\frac{1}{n!}\langle(-S_{\rm I})^n\rangle\ . \tag{4.51}$$

Now, $-S_{\rm I}$ is positive and the functional integral in $\langle(-S_{\rm I})^n\rangle$ can be evaluated for any $n\geq 0$. In fact, direct inspection of Eq. (2.24) shows that

$$\frac{1}{n!}\langle(-S_{\rm I})^n\rangle=:\alpha^n f_n(\beta) \tag{4.52}$$

is true, where $f_n(\beta)>0$ can be represented as a finite-dimensional integral. Therefore $Z_N(\alpha,\beta)$ is strictly positive and monotonically increasing as a function of N (α and β being fixed). If we can prove that $Z_N(\alpha,\beta)$ is uniformly bounded from above by some function $C(\alpha,\beta)<\infty$, we can apply the monotone-convergence theorem to assure that

$$\lim_{N\to\infty}Z_N(\alpha,\beta)=:Z_\infty(\alpha,\beta)$$

exists and

$$Z(\alpha,\beta)=\sum_{n=0}^{\infty}f_n(\beta)\alpha^n\ . \tag{4.53}$$

On the other hand, we may assume that $Z(\alpha,\beta)$ exists. Then, $Z(\alpha,\beta)>Z_N(\alpha,\beta)$ is true, and Eq. (4.53) holds again. Insofar, $Z(\alpha,\beta)$ exists if and only if this is true for $Z_\infty(\alpha,\beta)$.

Therefore we examine Eq. (4.53) in more detail. Despite its introduction as a function of positive α and β, the right-hand side of (4.53) may be discussed as an infinite series of complex α and β. This complex series converges absolutely for all α and $0<\mathrm{Re}\beta<\infty$, if (and only if) the original series (4.53) converges for $0\leq\alpha<\infty$, $0<\beta<\infty$. To prove this, one has to recall that $f_n(\beta)$ is positive, if β is positive; for complex β, one derives

$$|f_n(\beta)|\leq\left[\frac{|\beta|}{\mathrm{Re}\beta}\right]^{2n}f_n(\mathrm{Re}\beta) \tag{4.54}$$

by direct inspection.

Having in mind that $f_n(\beta)$ is an analytical function of β for $0<\mathrm{Re}\beta<\infty$, we may state the following result: (4.53) exists as a complex series for all α and $0<\mathrm{Re}\beta<\infty$ and represents an analytical function of α and β in the quoted domain, if (4.53) exists as a real series for $0\leq\alpha<\infty$, $0<\beta<\infty$. As the latter is strictly positive, we have proven the first part of Statement 3.

The remaining task is to ensure the convergence of the real series (4.53) under conditions (3.2) or (3.3). We begin with the comparatively simple case of short-range coupling. To get an upper bound on an arbitrary term in the series (4.53), we replace the exponential factor in $S_{\rm I}[R]$ by 1 [see Eq. (2.24)]. Using condition (3.2), a positive function $C(\beta)<\infty$ exists such that

$$f_n(\beta)<C(\beta)^n/n!\ . \tag{4.55}$$

Clearly, this inequality proves convergence of (4.53).

The case of long-range coupling is much more involved and was treated in detail in the quoted reference. We give the final result. Condition (3.3) leads to

$$f_n(\beta)\leq C_1(\beta)\frac{C_2(\beta)^n}{\sqrt{n!}}\ , \tag{4.56}$$

where $C_1(\beta)$ and $C_2(\beta)$ are finite positive functions of β. Therefore convergence of (4.53) is guaranteed again. This completes the proof of Statement 3.

Conditions (3.2) and (3.3) are sufficient, but not necessary, to establish convergence of (4.53). Up to now, a necessary and sufficient condition is not known.

B. The magnetopolaron

As in the preceding part, Sec. IV.A, we have to separate the discussion of ground-state and finite-temperature properties. We shall proceed along similar lines. Therefore many details can be skipped; necessary modifications, however, will be stressed. Throughout this section we assume a nonzero magnetic field pointing into z direction: $\mathbf{B}=(0,0,B)$, $B>0$.

1. Analyticity of the ground-state energy and wave function of $H'(\mathbf{Q})$

In this section we prove Statement 4, which is concerned with the ground-state energy $E(\alpha,\mathbf{Q},B)$ and the corresponding wave function $\Psi(\alpha,\mathbf{Q},B)$ of Hamiltonian $H'(\mathbf{Q})$ [see Eq. (2.34)]; as a general reference, we quote Löwen (1988a). The first component of $\mathbf{Q}$ is zero [see Eq. (2.33)]; if not stated otherwise, we suppose this property for any wave vector to follow in this section.

a. On the position of the continuum edge of $H'(\mathbf{Q})$

One key result is the generalization of Lemma 4, namely,

Lemma 8. *Suppose* $\mathbf{Q}$ *to be such that*

$$\inf_{\mathbf{k}}[E(\alpha,\mathbf{Q}-\mathbf{k},B)+\omega(k)]-E(\alpha,\mathbf{Q},B)=:\Delta(\alpha,\mathbf{Q},B)>0\ . \tag{4.57}$$

Then, the part of spec $H'(Q)$ contained in the interval $[E(\alpha,\mathbf{Q},B),\, E(\alpha,\mathbf{Q},B)+\Delta(\alpha,\mathbf{Q},B)[$ is purely discrete.

To prove this lemma, one has to introduce an UV-cutoff as well as a lattice-cutoff in complete analogy to Sec. IV.A.1.a. Following the procedure used in the proof of Lemma 1, we see that the essential difference now is that the first component of the total momentum is not conserved; the electronic variables x and p_x remain in $H'(\mathbf{Q})$. We notice, however, that x appears only in an oscillator potential of the type $(Bx+Q_2-P_{\mathrm{Ph},2})^2$. Consequently, for $B>0$ the additional electronic degree of freedom causes a purely discrete spectrum; the further conclusions in the proof of Lemma 1 are not affected.

To remove the cutoffs, one uses the procedures outlined in Lemmas 2–4. As for full details, we refer to Löwen (1988a).

Summarizing so far, Lemma 8 provides us with a lower bound for the continuum edge $E_c(\alpha,\mathbf{Q},B)$ of $H'(\mathbf{Q})$, namely,

$$E_c(\alpha,\mathbf{Q},B)\geq\inf_{\mathbf{k}}[E(\alpha,\mathbf{Q}-\mathbf{k},B)+\omega(k)]\ . \tag{4.58}$$

Recalling the results from Sec. IV.A, we are not surprised to find that the above inequality can be reversed. In fact, it is comparatively simple to generalize the Rayleigh-Ritz argument of Spohn (1988) to prove

Lemma 9.

$$E_c(\alpha,\mathbf{Q},B)\leq\inf_{\mathbf{k}}[E(\alpha,\mathbf{Q}-\mathbf{k},B)+\omega(k)] \tag{4.59}$$

(see Löwen, 1988a). A combination of the inequalities (4.58) and (4.59) leads us to the central result of this subsection, namely,

Theorem 2. *The continuum edge of $H'(\mathbf{Q})$ is produced by one-phonon excitations and is given by*

$$E_c(\alpha,\mathbf{Q},B)=\inf_{\mathbf{k}}[E(\alpha,\mathbf{Q}-\mathbf{k},B)+\omega(k)]\ . \tag{4.60}$$

We include a useful inequality, which (again) generalizes our previous results for the free polaron. We mentioned in the latter case that $E(\alpha,\mathbf{Q})\geq E(\alpha,\mathbf{0})$ was proven by L. Gross (1972). Gross applied the Trotter formula and a sequence of estimates to show the inequality $\|\{\exp[-\beta H'(\mathbf{Q})]\}\Psi\|\leq\|\{\exp[-\beta H'(\mathbf{0})]\}\Psi\|$ for any $\Psi\in F$. Löwen (1988a) demonstrated that this result holds true also for $B\neq0$. In combination with $\omega(k)\geq\omega=1$, we conclude from (4.60),

$$E_c(\alpha,\mathbf{Q};B)\geq 1+E(\alpha,\mathbf{0},B)\ . \tag{4.61}$$

If $\omega(k)=\omega$, as in the case of the standard Fröhlich model, (4.61) becomes an equality. This is of particular importance for the interpretation of magneto-optical data.

b. Uniqueness of the ground state of $H'(\mathbf{Q})$ and proof of Statement 4

We begin with two introductory remarks, which are concerned with the $\mathbf{Q}$ dependence of $E(\alpha,\mathbf{Q},B)$.

First, $E(\alpha,\mathbf{Q},B)$ is independent of Q_2 for $B>0$. To understand this property, one has to recall that $H'(\mathbf{Q})$ contains Q_2 and the electronic position x only in the combined form $Bx-Q_2$. Therefore Q_2 can be eliminated by an appropriate unitary transformation of x [and $H'(\mathbf{Q})$].

Second, $E(\alpha,\mathbf{Q},B)$ depends only on $|Q_3|$. The reason for this property is that we can unitarily transform $x,p_1,a(\mathbf{k})$ and $a^*(\mathbf{k})$ into $-x,-p_1,a(-\mathbf{k})$ and $a^*(-\mathbf{k})$, proving that $H'(0,0,-Q_3)$ is unitarily equivalent to $H'(0,0,Q_3)$.

A combination of both properties yields the useful result

$$E(\alpha,\mathbf{Q},B)=E(\alpha,(0,0,|Q_3|),B)\ . \tag{4.62}$$

It demonstrates that the ground states of H [see Eqs. (2.28)–(2.30)] and H' [see Eq. (2.31)] are highly degenerate. Statement 2 cannot be transferred to the present case. Obviously, this is in marked contrast to the discussion of a free polaron. However, interesting analogies reappear, if we turn to $H'(\mathbf{Q})$. A first example is

Lemma 10.

$$E(\alpha,\mathbf{Q},B)\leq E(\alpha,\mathbf{0},B)+Q_3^2/2\ . \tag{4.63}$$

For a proof, we refer to Lemma 6; the previous consideration can be generalized directly.

A combination of Lemma 10 and inequality (4.61) yields

Lemma 11. *For* $|Q_3|<\sqrt{2}$, $E(\alpha,\mathbf{Q},B)$ *belongs to the discrete part of the spectrum of* $H'(\mathbf{Q})$.

In summary, we have established the existence of (normalizable) eigenfunctions of $H'(Q)$ for $|Q_3|<\sqrt{2}$, $0<B<\infty$, and $0\le\alpha<\infty$. According to our prevoius scheme, the next step in the analyticity proof is to ensure the uniqueness of the ground state of $H'(\mathbf{Q})$. We find

Theorem 3. *If* $E(\alpha,\mathbf{Q},B)$ *belongs to the discrete part of the spectrum of* $H'(\mathbf{Q})$, *it is a simple eigenvalue.*

Theorem 2 parallels the result of J. Fröhlich (1973) for free polarons and can be proven similarly. Again, the main difficulty is to ensure that $\exp[-tH'(\mathbf{Q})]$ is positivity improving for $t>0$. For details, see Löwen (1988a).

Having established the existence of a unique, discrete ground state of $H'(\mathbf{Q})$ for $|Q_3|<\sqrt{2}$, we finally apply analytical perturbation theory to show that $E(\alpha,\mathbf{Q},B)$ and $\Psi(\alpha,\mathbf{Q},B)$ are real analytic functions of α,Q_3,B for $0\le\alpha<\infty$, $|Q_3|<\sqrt{2}$, and $0<B<\infty$ (Statement 4). To be explicit, let us write $H'(\mathbf{Q})\equiv H'(\alpha,\mathbf{Q},B)$. In view of our discussion in Sec. IV.A.1.b, the only property to show is the relative boundedness of $H'(\alpha,\mathbf{Q},B)-H'(\alpha,\mathbf{Q},B_0)$ with respect to $H'(\alpha,\mathbf{Q},B_0)$, B_0 being a fixed value of the magnetic field. As we may assume $Q_2=0$ (see the first introductory remark in Sec. IV.B.1.b), this property can be easily demonstrated.

In summary, Statement 4 is proven.

2. Analyticity of the formal free energy of H. Proof of Statement 5.

To begin with, we recall Eqs. (2.36) and (2.37) and their relation to the formal free energy:

$$Z(\alpha,\beta,B)=\exp\{-\beta[F(\alpha,\beta,B)-F(0,\beta,0)]\}$$
$$=\langle\exp[-S_I-S_B]\rangle\ . \qquad (4.64)$$

Let us consider

$$Z_N(\alpha,\beta,B):=\sum_{n=0}^{N}\frac{1}{n!}\langle(-S_I)^n\exp[-S_B]\rangle$$
$$=:\sum_{n=0}^{N}\alpha^n f_n(\beta,B)\ . \qquad (4.65)$$

$f_n(\beta,B)$ can be represented as a finite-dimensional integral (see Gerlach and Löwen, 1987b). In particular, $f_n(\beta,B)$ is a real analytic function of β,B for $0<\beta<\infty, 0<B<\infty$. What about the convergence of $Z_N(\alpha,\beta,B)$ for $N\to\infty$? As S_B is purely imaginary, one can easily derive

$$|Z_N(\alpha,\beta,B)|\le\sum_{n=0}^{N}\frac{1}{n!}\langle(-S_I)^n\rangle=Z_N(\alpha,\beta)\ , \qquad (4.66)$$

where $Z_N(\alpha,\beta)$ is the free-polaron expression from Sec. IV.A.2 which does converge. Consequently, the dominated convergence theorem assures us that

$$\lim_{N\to\infty}Z_N(\alpha,\beta,B)=:Z_\infty(\alpha,\beta,B)$$

exists and

$$Z(\alpha,\beta,B)=Z_\infty(\alpha,\beta,B)\ . \qquad (4.67)$$

Moreover, $Z(\alpha,\beta,B)$ is a real analytic function of α,β,B for $0\le\alpha<\infty, 0<\beta<\infty, 0<B<\infty$. The results of Sec. IV.B.1 show that $Z(\alpha,\beta,B)$ is strictly positive, and Statement 5 is proven.

C. The polaron in a potential

In the first part of this section we are concerned with ground-state properties of the Hamiltonians H or H', respectively, which were defined in Eqs. (2.38)–(2.40) and in Eqs. (2.41) and (2.42). In particular, we sketch the proofs of Statements 6 and 7. In the second part we turn to the formal free energy and Statement 8.

1. Analytical properties of the ground-state energy and wave function of H. Proof of Statements 6 and 7

To begin with, we recall the specific form of $H=H_P+H_{Ph}+H_I$ and $H'=H'_P+H_{Ph}+H'_I$. Throughout this part, we assume H_P to be essentially self-adjoint and bounded from below; if not explicitly stated otherwise, λv should be an element of R' as explained in Eq. (3.13). Moreover, let $v(\mathbf{r})\le 0$ (more or less for the sake of illustration; we pick up this point at the end of this part).

For the proofs in Secs. IV.A.1 and IV.B.1, the first important step was to relate the continuum edge and the ground-state energy. Trying to establish an equation as before, we need here a specific modification. The physical reason for this can be easily found. The additional potential λv allows for a new type of continuum state: in Secs. IV.A.1 and IV.B.1, the continuum edge was formed by one-phonon excitations; in addition, we are now confronted here with the possibility of delocalized particle states. An analogous phenomenon was discussed in Sec. II.D in connection with polaronic excitons.

To be specific, let us denote $H'\equiv H'(\alpha,\lambda)$, the corresponding ground-state energy being $E(\alpha,\lambda)$. As a first step we introduce an UV-cutoff σ and a lattice-cutoff d, as before, and consider the restriction of $H'(\alpha,\lambda)$ on $F_{d,\sigma}\otimes L^2(\mathbb{R}^3)$. Effectively, we construct thereby a Hamiltonian $H'(\alpha,\lambda,N)$, which accounts for a finite number $N\equiv N(d,\sigma)$ of phonon modes. $H'(\alpha,\lambda,N)$ is properly defined and is, in particular, self-adjoint and bounded from below. By construction, its continuum edge $E_c(\alpha,\lambda,N)$ can only be caused by delocalized particle states. In fact, one finds

$$E_c(\alpha,\lambda,N)=\inf\operatorname{spec}H'(\alpha,0,N)\ . \qquad (4.68)$$

Löwen (1988b) provides a formal proof of this equation using Weyl's essential spectrum theorem (see Reed and Simon, 1978, pp. 112, 118). The basic point of this theorem is to show that the resolvent difference

$$[\zeta - H'(\alpha,\lambda,N)]^{-1} - [\zeta - H'(\alpha,0,N)]^{-1}$$

is compact.

To remove the cutoffs, one proceeds as in Sec. IV.A.1 [until now we had no proper mathematical interpretation of the primarily formal expression $H'(\alpha,\lambda)$; in particular, the existence of the ground-state energy $E(\alpha,\lambda)$ and wave function $\Psi(\alpha,\lambda)$ is guaranteed]. Since we now incorporate an infinite number of phonon modes, phonon-induced continuum states appear. In combination with Eq. (4.68), we find for the position of the continuum edge $E_c(\alpha,\lambda)$

Lemma 12.

$$E_c(\alpha,\lambda) \geq \min[E(\alpha,\lambda)+1, E(\alpha,0)] \; . \tag{4.69}$$

Interestingly enough, one can reverse this inequality—again in analogy to Secs. A.1 and B.1. Using a Rayleigh-Ritz argument (see Löwen, 1988b), one proves that the right-hand side of (4.69) is also an upper bound for $E_c(\alpha,\lambda)$. Summarizing, we arrive at

Theorem 4. *The continuum edge of $H'(\alpha,\lambda)$ is given by*

$$E_c(\alpha,\lambda) = \min[E(\alpha,\lambda)+1, E(\alpha,0)] \; . \tag{4.70}$$

Meanwhile it has become clear how to proceed: we have to discuss whether $E(\alpha,\lambda) < E_c(\alpha,\lambda)$ is true. Clearly, this inequality is fulfilled for the alternative $E_c(\alpha,\lambda) = E(\alpha,\lambda)+1$. So we turn to $E_c(\alpha,\lambda) = E(\alpha,0)$.

Lemma 13. *Let $E_c(\alpha,\lambda) = E(\alpha,0)$ and assume that H_P has n bound states φ_j with energies $e_j, j = 1 \ldots n$, and $e_1 \leq e_2 \leq \cdots \leq e_n < 0$. Then, $H'(\alpha,\lambda)$ has at least n localized eigenstates.*

To prove this lemma, we use once more a Rayleigh-Ritz argument. Consider the product states $\Psi_j := \varphi_j \otimes \Phi$, where Φ is the normalized free-polaron eigenfunction of $H'(\mathbf{Q}=0)$, $H'(\mathbf{Q})$ having been defined in Eq. (2.17). Because of $\langle \Phi | P_{\mathrm{Ph}} | \Phi \rangle = \mathbf{0}$, we derive

$$\begin{aligned} \langle \Psi_j | H'(\alpha,\lambda) | \Psi_{j'} \rangle &= \langle \varphi_j | H_P | \varphi_{j'} \rangle + \delta_{jj'} \langle \Phi | H'(\mathbf{Q}=\mathbf{0}) | \Phi \rangle \\ &= \delta_{jj'} [e_j + E(\alpha,\lambda=0)] \; . \end{aligned} \tag{4.71}$$

Equation (4.71) proves Lemma 13.

Summarizing thus far, we can state that $E(\alpha,\lambda)$ is a discrete eigenvalue of $H'(\alpha,\lambda)$ if H_P has at least one bound state with strictly negative energy. If this can be taken for granted, then $E(\alpha,\lambda)$ is a simple eigenvalue. We omit the proof, as all technical details can be transferred from Sec. IV.A.1.b (discussion of Statement 2). Therefore the final step is to apply analytical perturbation theory. As for the α dependence, we refer to Sec. IV.A.1.c. As far as the λ dependence is concerned, we recall that $v(\mathbf{r})$ is infinitesimally form bounded with respect to H_P and $H'(\alpha,\lambda=\lambda_0)$, λ_0 being fixed. Therefore $E(\alpha,\lambda)$ and $\psi(\alpha,\lambda)$ are real analytic functions of α, λ for $0 \leq \alpha < \infty$ and $0 < \lambda < \infty$. Statement 6 has been proven.

As announced before, we add a comment on the assumption $\lambda v(\mathbf{r}) \leq 0$. Reviewing our foregoing proof, one notices that all we needed with respect to H_P was the following: For the given potential $\lambda v \in R'$ and any $\lambda > 0$, H_P has to be well defined and should have at least one bound state with strictly negative energy. It is useful to add the following result: If H_P is known to have a bound state with strictly negative energy for some $\lambda = \lambda_0$, this is sufficient to guarantee the analyticity of $E(\alpha,\lambda)$ and $\psi(\alpha,\lambda)$ in a certain surrounding of $\lambda = \lambda_0$.

We now turn to Statement 7 and the phenomenon of pinning transitions. In this case we restrict $\lambda v(\mathbf{r})$ to the class of Rollnik potentials R as explained in Eq. (3.12).

As R is contained in R', we can transfer some general results from the preceding discussion. Let us start with $\lambda > \lambda_c > 0$, λ_c having been defined in Sec. II.C. We know in this case that H_P has at least one bound state with strictly negative energy, and Statement 6 assures us that $E(\alpha,\lambda)$ is a real analytic function of α and λ for $0 \leq \alpha < \infty$ and $\lambda_c < \lambda < \infty$; furthermore, we have $E(\alpha,\lambda) < E(\alpha,0)$ according to Lemma 13. Now, we consider the case $\lambda < 0$: Theorem 4 is valid and yields $E(\alpha,\lambda) \leq E(\alpha,0)$; on the other hand, $\lambda v(\mathbf{r})$ is positive and therefore $E(\alpha,\lambda) \geq E(\alpha,0)$. Consequently, we find $E(\alpha,\lambda) = E(\alpha,0)$ for $\lambda < 0$. Contrasting the results for $\lambda > \lambda_c > 0$ and $\lambda < 0$, we conclude that $E(\alpha,\lambda)$ cannot be analytic for the whole interval $0 \leq \lambda < \lambda_c$; the identity theorem for analytical functions would require $E(\alpha,\lambda) = E(\alpha,0)$ for all λ.

We can discuss this nonanalyticity in greater detail. For a given value of α, $E(\alpha,\lambda)$ is monotonically decreasing in λ. There exists a unique value $\lambda = \lambda_c(\alpha)$, $0 \leq \lambda_c(\alpha) \leq \lambda_c$, such that $E(\alpha,\lambda) = E(\alpha,0)$ for $\lambda < \lambda_c(\alpha)$ and $E(\alpha,\lambda) < E(\alpha,0)$ for $\lambda > \lambda_c(\alpha)$. In the latter case the ground-state energy is separated from the continuum edge and (repeating earlier arguments) is a simple eigenvalue. Analytical perturbation theory proves that $E(\alpha,\lambda)$ is even real analytic in λ for $\lambda > \lambda_c(\alpha)$. Now, consider different values for α. Then, $\lambda_c(\alpha)$ is a continuous function of α; one proves this property by assuming the contrary—the analyticity of $E(\alpha,\lambda)$ in λ for $\lambda > \lambda_c(\alpha)$ and the monotonicity in λ provide a contradiction. In summary, Statement 7 has been proven.

We stress that we made repeated use of $\lambda v(\mathbf{r}) \leq 0$ in the course of the last proof; in connection with Statement 7, this assumption cannot generally be abandoned.

2. Analyticity of the formal free energy of *H*. Proof of Statement 8

The quantities of interest, namely, Z and F, are related by the equations

$$Z(\alpha,\beta,\lambda)=\langle \exp(-S_{\mathrm{I}}-S_\lambda)\rangle$$
$$=\exp\{-[F(\alpha,\beta,\lambda)-F(0,\beta,0)]\} \; ; \qquad (4.72)$$

S_{I} and S_λ were defined in Eqs. (2.24) and (2.44). Both actions are negative. Let us consider

$$Z_{NM}(\alpha,\beta,\lambda):=\left\langle \sum_{n=0}^{N}\frac{1}{n!}(-S_{\mathrm{I}})^n \sum_{m=0}^{M}\frac{1}{m!}(-S_\lambda)^m\right\rangle$$
$$=:\sum_{n=0}^{N}\frac{\alpha^n}{n!}\sum_{m=0}^{M}\frac{\lambda^m}{m!}f_{nm}(\beta) \; . \qquad (4.73)$$

$f_{nm}(\beta)$ is positive for any $n,m\geq 0$ and can be represented as a finite-dimensional integral. Moreover, it is an analytic function of β for $0<\mathrm{Re}\beta<\infty$. We conclude in analogy to Sec. IV.A.2: $Z(\alpha,\beta,\lambda)$ exists as a complex series for arbitrary α, λ, and β in the interval $0<\mathrm{Re}\beta<\infty$, is of the type

$$Z(\alpha,\beta,\lambda)=Z_{\infty\infty}(\alpha,\beta,\lambda)=\sum_{n,m=0}^{\infty}\frac{\alpha^n}{n!}\frac{\lambda^m}{n!}f_{nm}(\beta) \; , \qquad (4.74)$$

and represents an analytic function in the quoted domain, if the right-hand side of Eq. (4.74) exists as a real series in α,β,λ for $0\leq\alpha$, $\lambda<\infty$, and $0<\beta<\infty$. As the latter is strictly positive, we have proven the first part of Statement 8.

We now turn to the existence of the real series (4.74). Starting from Eq. (4.73), we find

$$Z_{NM}(\alpha,\beta,\lambda)\leq\frac{1}{2}\left\langle\left[\sum_{n=0}^{N}\frac{1}{n!}(-S_{\mathrm{I}})^n\right]^2+\left[\sum_{m=0}^{M}\frac{1}{m!}(-S_\lambda)^m\right]^2\right\rangle$$
$$\leq\frac{1}{2}\left[\left\langle\sum_{n=0}^{2N}\frac{1}{n!}(-2S_{\mathrm{I}})^n\right\rangle+\left\langle\sum_{m=0}^{2M}\frac{1}{m!}(-2S_\lambda)^m\right\rangle\right] \; . \qquad (4.75)$$

The first term on the right-hand side of Eq. (4.75) was discussed in Sec. IV.A.2 and proven to be uniformly bounded in N (α and β fixed) when either condition (3.2) or (3.3) was fulfilled. Interestingly enough, the second term can be treated similarly if we assume condition (3.14) to be valid (as is done in Statement 8): Explicit insertion shows that the estimation procedure for the first term can be used again. Taking this for granted, the monotone-convergence theorem completes the proof of Statement 8.

D. The polaronic exciton

In this section we complete the proofs of the statements from Sec. III. Again, we begin with the discussion of ground-state properties; this time we are concerned with the exciton Hamiltonians H, H', and $H'(\mathbf{Q})$ according to Eqs. (2.45)–(2.49), (2.51)–(2.53), and (2.54). In the first part we sketch the proofs of Statements 9a, 9b, and 10; the second part contains the discussion of the formal free energy and Statement 11. General references are Löwen (1987) and Gerlach and Löwen (1990).

1. Analytical properties of the ground-state energy and wave function of $H'(\mathbf{Q})$. Proof of Statements 9a, 9b, and 10

Our discussion will be similar to that of a polaron in a potential. To begin with, we recall the general condition P for the electron-hole potential $\lambda U(\mathbf{r})$, which we stated in Sec. III.D; it guarantees that $H_{\mathrm{rel}}:=\mathbf{p}^2/2\mu+\lambda U(\mathbf{r})$ is mathematically well defined and has at least one bound state for any $\lambda>0$. To display the relevant parameters of the system, we shall use the notation $H'(\mathbf{Q})\equiv H'(\mathbf{Q},\alpha,\lambda,\mathbf{m})$.

Let us introduce an UV-cutoff σ and a lattice-cutoff d, as before, and consider the restriction of $H'(\mathbf{Q},\alpha,\lambda,\mathbf{m})$ on $F_{d,\sigma}\otimes L^2(\mathbb{R}^3)$. In doing so, we construct a Hamiltonian $H'(\mathbf{Q},\alpha,\lambda,\mathbf{m},N)$, which accounts for a finite number $N=N(d,\sigma)$ of phonon modes. This Hamiltonian is self-adjoint and bounded from below. Making use of Weyl's essential spectrum theorem, we find for the continuum edge E_c^1 of $H'(\mathbf{Q},\alpha,\lambda,\mathbf{m},N)$

$$E_c^1(\mathbf{Q},\alpha,\mathbf{m},N)=\inf\sigma_{\mathrm{ess}}[H'(\mathbf{Q},\alpha,0,\mathbf{m},N)] \; . \qquad (4.76)$$

Removing the cutoffs consecutively as described in Sec. IV.A.1, we are led by Eq. (4.76) to an edge value $E_c^1(\mathbf{Q},\alpha,\mathbf{m})$. Moreover, the one-phonon-assisted scattering states create a second (by now familiar) species of continuum states with an energy edge E_c^2, bounded as follows:

$$E_c^2(\mathbf{Q},\alpha,\lambda,\mathbf{m})\geq\inf_{\mathbf{k}}[E(\mathbf{Q}-\mathbf{k},\alpha,\lambda,\mathbf{m})+\omega(k)] \; . \qquad (4.77)$$

In summary, we find for the continuum edge of $H'(\mathbf{Q},\alpha,\lambda,\mathbf{m})$

$$E_c(\mathbf{Q},\alpha,\lambda,\mathbf{m})\geq\min[E_c^1(\mathbf{Q},\alpha,\mathbf{m}),E_c^2(\mathbf{Q},\alpha,\lambda,\mathbf{m})] \; . \qquad (4.78)$$

We believe that (4.78) can be replaced by an equality and shall give a partial proof during our later discussion. In any case the inequality is sufficient to proceed.

For subsequent use we transfer some results from the corresponding considerations in Sec. IV.A.1:

$$E(\mathbf{Q},\alpha,\lambda,\mathbf{m})\geq E(\mathbf{0},\alpha,\lambda\mathbf{m}) \; , \qquad (4.79)$$

$$E(\mathbf{Q},\alpha,\lambda,\mathbf{m})\leq E(\mathbf{0},\alpha,\lambda,\mathbf{m})+\mathbf{Q}^2/2M \; . \qquad (4.80)$$

We mentioned earlier that the center-of-mass motion of an exciton is of free-polaron type. In fact, the $\mathbf{Q}$ dependence of the corresponding Hamiltonians is the same. Therefore the proof of, for example, Eq. (4.80) is that of

Lemma 6. Furthermore, we recall that $E(\mathbf{Q},\alpha,\lambda,\mathbf{m})$ has to be a continuous function of $\mathbf{Q}$, in analogy to the polaron energy.

Now, let us discuss the alternative $E_c^2 \leq E_c^1$ in (4.78). In this case, the inequality (4.78) can indeed be replaced by the equality $E_c = E_c^2$. To prove this, one may use a Rayleigh-Ritz procedure as in Sec. A.1. We derive from (4.77)–(4.79) and (3.1)

$$E_c(\mathbf{Q},\alpha,\lambda,\mathbf{m}) \geq E(\mathbf{0},\alpha,\lambda,\mathbf{m})+1 . \tag{4.81}$$

The comparison of (4.81) and (4.80) shows that $E(\mathbf{Q},\alpha,\lambda,\mathbf{m})$ belongs to the discrete part of the spectrum of $H'(\mathbf{Q},\alpha,\lambda,\mathbf{m})$, if $Q < \sqrt{2M}$.

In view of our general outline for analyticity proofs, the next property to be established is the nondegeneracy of $E(\mathbf{Q},\alpha,\lambda,\mathbf{m})$. Let us try to transfer the corresponding discussion from the free-polaron case. This is in fact possible up to Eq. (4.46), where we performed a Gaussian linearization of $\exp[-(\mathbf{p}-\mathbf{p}_{\mathrm{Ph}})^2]$. In the present case, we find $\exp(-[\mathbf{Q}-\mathbf{P}_{\mathrm{Ph}}]^2)$ instead; on the right-hand side of (4.46), this term produces $\exp(i\sqrt{t}\,\mathbf{aQ})$. It is only for $\mathbf{Q}=\mathbf{0}$ that we find positivity. Proceeding as in Sec. A.1, we establish the nondegeneracy of $E(\mathbf{Q}=\mathbf{0},\alpha,\lambda,\mathbf{m})$. Because of the continuity of $E(\mathbf{Q},\alpha,\lambda,\mathbf{m})$ with respect to $\mathbf{Q}$, this property will also be true in a certain surrounding of $\mathbf{Q}=\mathbf{0}$. The application of analytical perturbation theory completes the proof of Statement 9a.

We now turn to the second alternative $E_c^1 < E_c^2$ in (4.78). As indicated in connection with Statement 9b, we need additional assumptions to proceed. Firstly, let us choose $\mathbf{Q}=\mathbf{0}$; this is characteristic for the ground states of H and H', respectively. We derive from the functional-integral equations (2.56)–(2.59) for the polaronic exciton

$$E(\mathbf{0},\alpha,0,\mathbf{m}) \geq \sum_{i=1}^{2} E_i(\alpha) , \tag{4.82}$$

where $E_i(\alpha)$ is the (hypothetical) free-polaron energy of constituent i of the exciton. Consequently, we can state for the continuum edge

$$E_c(\mathbf{0},\alpha,\lambda,\mathbf{m}) \geq \sum_{i=1}^{2} E_i(\alpha) . \tag{4.83}$$

For the standard exciton-phonon problem, which is addressed in Statement 9b, variational techniques (see Adamowski, Gerlach, and Leschke, 1981, 1983) were used to prove

$$E(\mathbf{0},\lambda,\mathbf{m}) < \sum_{i=1}^{2} E_i(\alpha) \tag{4.84}$$

for $0<\lambda<\infty$, $0<m_i<\infty$. Therefore $E(\mathbf{0},\lambda,\mathbf{m})$ is an eigenvalue. Because of the continuity of $E(\mathbf{Q},\lambda,\mathbf{m})$ with respect to $\mathbf{Q}$, this property holds true in a certain surrounding of $\mathbf{Q}=\mathbf{0}$. Repeating the arguments of the above discussion for $E_c^2 \leq E_c^1$, we complete the proof of Statement 9b.

Finally, we are left with Statement 10. The inequality $E(\mathbf{Q}=\mathbf{0},\alpha,\lambda,\mathbf{m}) < E(\mathbf{Q}\neq\mathbf{0},\alpha,\lambda,\mathbf{m})$ is certainly true, if $E(\mathbf{Q},\alpha,\lambda,\mathbf{m})$ belongs to the continuous part of the spectrum of $H'(\mathbf{Q},\alpha,\lambda,\mathbf{m})$. To realize this, one has to recall the inequalities (4.81) and (4.79), (4.83)–(4.84) for the continuum edge of $H'(\mathbf{Q},\alpha,\lambda,\mathbf{m})$. Therefore it is sufficient to demonstrate Statement 10 for the case in which $E(\mathbf{Q},\alpha,\lambda,\mathbf{m})$ is an eigenvalue of $H'(\mathbf{Q},\alpha,\lambda,\mathbf{m})$. Then, however, the proof of Statement 2 can be directly transferred to the present problem (see Gerlach and Löwen, 1988a).

2. Analyticity of the formal free energy of H. Proof of Statement 11

Our treatment of the polaron in a potential (see Sec. IV.C.2) is such that we can completely transfer all results, even without a change in the notation–of course, S_{I} and S_λ have to be understood as the excitonic equations (2.57) and (2.58). We recall that the positivity of $-S_{\mathrm{I}}$ was essential in the previous discussion; in fact, this property can generally be shown for Hamiltonians of type (2.1)–(2.4) and particularly for the polaronic exciton (Adamowski, Gerlach, and Leschke, 1984). Proceeding as in Sec. C.2, the only question to answer is whether the right-hand side of Eq. (4.75) is uniformly bounded in N and M. Again, we make use of the previously solved problem: Rewriting Eq. (2.57) in the original coordinates $\mathbf{r}_1$ and $\mathbf{r}_2$, one finds

$$-S_{\mathrm{I}}[\mathbf{R},\mathbf{r}] \leq -2\sum_{i=1}^{2} S_{\mathrm{I}}[\mathbf{r}_i] , \tag{4.85}$$

where $S_{\mathrm{I}}[\mathbf{r}_i]$ is the free-polaron action of constituent i of the exciton. Using the inequality (4.85) in (4.75) and repeating the former arguments, we finally complete the proof of Statement 11.

V. EXTENSIONS

The original Hamiltonian (2.1) admits of a larger number of realistic models than we have treated in Statements 1–11. We recall that we generally assumed a parabolic band structure $\varepsilon(\mathbf{k})$ and isotropic expressions for the phonon dispersion $\omega(\mathbf{k})$ and coupling $g(\mathbf{k})$; furthermore, the particles of interest were supposed to interact with a single branch of phonons only. In connection with ground-state properties, we made extensive use of the additional condition (3.1) and restricted the potentials to one of the classes R or R', respectively. More general results could be achieved for the formal free energy: Interestingly enough, its existence as such is sufficient to guarantee a smooth behavior as a function of the coupling parameters α, λ, etc.

We can extend our previous results considerably. As in Sec. IV, we demonstrate this in detail for the example of a free polaron. The corresponding extension for the magnetopolaron, the polaron in a potential, and the polaronic exciton can easily be done (Löwen, 1987; Gerlach and Löwen, 1987a, 1987b, 1988a, 1988c).

The simplest generalization is concerned with an electronic coupling to several phonon branches. One proves by direct inspection that Statements 1–3 can be correspondingly generalized, if the quoted conditions are fulfilled for every branch.

It is also simple to remove the condition of isotropy for $\omega(\mathbf{k})$ and $g(\mathbf{k})$. For the discussion of the free energy F, one may replace the inequalities (3.2) and (3.3) by the analogous ones for $\omega(\mathbf{k})$ and $g(\mathbf{k})$ and arrive at the same analyticity results for F. As far as ground-state properties are concerned, it is sufficient to assume $\omega(-\mathbf{k})=\omega(\mathbf{k})$ (Kramers's theorem) and $g(-\mathbf{k})=g(\mathbf{k})$—of course, (3.1) must be valid, too. We mention a particularly simple example, which was extensively studied in the literature: putting $g(\mathbf{k})\propto|B\mathbf{k}|^{-1}$, where B is a real, symmetrical matrix with strictly positive eigenvalues, one can qualitatively describe optical polarons in anisotropic crystals. As for variational and Monte Carlo calculations, we refer to Kahn (1968); Pekar (1969); Pekar, Sheka, and Dmitrenko (1973); Okamoto (1974); Pekar, Khazan, and Sheka (1974); Pokatilov and Tarakanova (1974); Hattori (1975a); Sheka and Khazan (1975); Sheka, Khazan, and Mozdor (1975); and Gerlach and Schliffke (1984).

It is notable that the treatment of an anisotropic band structure $\varepsilon(\mathbf{k})$ is formally equivalent to the preceding case. What about more complicated examples? These are in fact admissible in connection with Statement 2. Recalling the proof in Sec. IV.A.1.b, one will find only one decisive step where the parabolicity $\varepsilon(\mathbf{k})\propto k^2$ was relevant: in Eq. (4.46), we introduced a Gaussian linearization of $\exp[-t\varepsilon(\mathbf{p}-\mathbf{P}_{\text{Ph}})]$. More generally, one may perform a Fourier transform,

$$\exp[-t\varepsilon(\mathbf{p}-\mathbf{P}_{\text{Ph}})]=\int d^Da\, f(\mathbf{a},t)\exp[i\mathbf{a}(\mathbf{p}-\mathbf{P}_{\text{Ph}})] \ . \tag{5.1}$$

If $f(\mathbf{a},t)$ is positive, we can proceed as in Sec. IV.A.1.b and prove an extension of Statement 2 for a band structure $\varepsilon(\mathbf{k})$. One may easily provide examples, using tables of Fourier transforms. We note that the case $\varepsilon(\mathbf{k})\propto k^2+ck^4$, $c>0$, cannot be treated this way; the corresponding Fourier transform is not positive. Nevertheless, we believe that Statement 2 is valid also in this case; probably, one can find a more adequate representation of the underlying Hilbert space.

Let us now turn to ground-state properties and particularly to condition (3.1). At the moment, it is unclear whether or not the inequality $\omega(\mathbf{k})\geq\omega>0$ is necessary to block a nonanalytical behavior; we are not aware of any analyticity proof admitting an acoustical dispersion. However, studies on the localization of the ground state do exist for this case and indicate that localization can happen only for sufficiently singular couplings and lower spatial dimensions: Assume $\omega(k)$ and $g(k)$ to be proportional to k^{ν} and $k^{-\mu}$, respectively, if $k\to0$; furthermore, let $\sigma:=(D+2-2\mu)/\nu$. Spohn (1986) proved that the ground state is delocalized for $\sigma>3$. Spohn and Dümcke (1985), as well as Fisher and Zwerger (1986), performed a Gaussian approximation of the exact polaron action and thereby found indications that (i) the ground state is delocalized, but the effective mass diverges for $2<\sigma<3$; and (ii) the ground state is localized for $\sigma<2$. We add that the localization criterion of these authors is slightly different from ours. In any case one should realize that the familiar physical examples have $\sigma>3$.

There exists a variety of numerical studies on acoustic polarons, mostly of variational type. We refer to Whitfield and Platzman (1972); Sumi and Toyozawa (1973); Whitfield and Shaw (1976); Young, Shaw, and Whitfield (1979); Tokuda (1980b); Toyozawa and Shinozuka (1980); Shoji and Tokuda (1981); Tokuda, Shoji, and Yoneya (1981b); Matsuura (1972); Tokuda and Kato (1982); Das Sarma (1985); Peeters and Devreese (1985c); Mason and Das Sarma (1986); Peeters and Devreese (1987); and Erçelebi (1988). With the exception of the early papers of Whitfield and Platzman (1972), Whitfield and Shaw (1976), Young, Shaw, and Whitfield (1979), and Tokuda (1980b), all authors describe nonanalyticities of the ground-state energy as a function of the coupling parameter. As approximation procedures were used, an artifact cannot be excluded.

We close this section with some remarks concerning applications of the previously used methods to related problems.

(i) In the involved discussion of "man-made" structures, potentials such as

$$V(\mathbf{r}):=\begin{cases}Fx & \text{for } x\geq L\\ \infty & \text{for } x<L\end{cases} \tag{5.2}$$

were used to model a quasi-two-dimensional behavior of free electrons in doped layered structures (the x-y plane is chosen as the plane of symmetry). If an optical polaron is exposed to such a potential, a relevant quantity to study is the ground-state energy $E\equiv E(\alpha,\mathbf{Q},F)$, where α is the electron-phonon coupling parameter and $\mathbf{Q}=(0,Q_2,Q_3)$ the polaron wave vector. $E(\alpha,\mathbf{Q},F)$ has to be a real analytic function of $\alpha,\mathbf{Q},F$ for $0\leq\alpha<\infty$, $0<F<\infty$, and arbitrary $\mathbf{Q}$.

(ii) Magnetopolarons in quantum wells (parallel to the x-y plane) can be qualitatively discussed by a Hamiltonian, which is the sum of the previous one for a magnetopolaron [Eq. (2.31)] plus a potential term $\lambda V(z)\not\equiv0$, where $\lambda V(z)\leq0$ and $V\in L^2(\mathbb{R})$ may be assumed. In this case we can combine our discussions from Secs. II.B and II.C and apply our results from Secs. III.B and III.C. Incorporating the translation symmetry into y direction, we start from

$$H'(Q_2):=\frac{1}{2m}(\mathbf{G}-\mathbf{P}_{\text{Ph}})^2+H_{\text{Ph}}+H'_{\text{I}}+\lambda V \ , \tag{5.3}$$

where $\mathbf{G}:=(p_1,|e|Bx+\hbar Q_2,p_3)$. Let, for example, $Q_2=0$; the ground-state energy $E(\alpha,B,\lambda)$ will be a real analytic function of α,B,λ for $0\leq\alpha<\infty$, $0<B<\infty$, and $0<\lambda<\infty$.

(iii) In connection with small polarons, many authors have studied discrete models: the electron is restricted to a discrete lattice of sites and couples to a discrete phonon system. We are not going to analyze the corresponding literature (that is definitely beyond the scope of this article), but remark that a similar analysis of analytical properties can be performed. We refer to Spohn and Dümcke (1985); Leggett, Chakravarty, Dorsey, Fisher, Garg, and Zwerger (1987); and Löwen (1987, 1988c, 1988e).

VI. SUMMARY

The main purpose of this article is to clarify the qualitative analytical properties of a polaron system of Fröhlich type being characterized by parameters such as total momentum, coupling constants, and homogeneous external field strengths. The basic question to answer is whether or not the ground-state energy and wave function or the formal free energy and related observables are real analytic functions of the quoted parameters. Our results are

(1) If the formal free energy F exists at all, it is a real analytic function of the coupling parameters, the external field strength, and the inverse formal temperature β for $0<\beta<\infty$. Sufficient conditions for the existence of F can be specified [see Eqs. (3.2), (3.3), and (3.14)]; they cover the familiar physical cases.

(2) If the ground state of the momentum-decomposed Hamiltonian is simple and energetically separated from the rest of the spectrum (at least in a certain domain D of the parameters), the ground-state energy and wave function are real analytic functions of the parameters, if these belong to D.

(3) For the case of optical polarons, the domain D of analyticity can be specified (see Statements 1, 4, 6, 9a, and 9b). In particular, no phonon-induced localization transition exists; the ground state is always delocalized.

(4) If a polaron is exposed to a short-range potential of coupling strength λ, a pinning transition is known to exist: for a certain critical parameter λ_c, the ground-state energy splits off from the continuum edge of the Hamiltonian under consideration. Although this transition cannot be induced by the electron-phonon interaction, the actual value of λ_c is governed by the corresponding coupling strength α; λ_c is a continuous function of α.

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