Analytical behavior of the ground-state energy and pinning transitions for a bound polaron

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Spectral properties of a three-dimensional optical polaron, bound in an external potential, are studied. If the associated one-particle Hamiltonian has a bound state, it is proved that the ground-state energy of the polaron and expectation values of the ground state are analytical functions of the coupling parameter α and the potential strength β. Especially in the case of a Coulomb potential, all changes in the polaron state are continuous, disproving claims of several variational calculations. If, on the other hand, the one-particle Hamiltonian has no bound state, the existence of a pinning transition is shown for the polaron. As physically relevant potentials for the pinning transition, a spherical square well and a screened Coulomb potential are considered. Their phase diagrams are given in the effective-mass approximation.

I. INTRODUCTION

An electron, bound to a defect in polar semiconductors (such as an impurity or a vacancy) and interacting with the longitudinal optical phonons, is called a bound polaron. Since the earlier papers of Buimistrov and Pekar[1] and Platzman[2] and Larsen,[3] this important problem has received considerable attention, as recent publications show (see, e.g., Adamowski[4] and the references therein, as well as Mason and Das Sarma[5] and Degani and Hipolito[6]). The present paper is concerned with analytical and spectral properties of a polaron in a generalized external potential $V(\mathbf{r})$.

The bound (three-dimensional) polaron is described by the well-known Fröhlich Hamiltonian,[7] which reads as follows:

$$H_F(\alpha,\beta) = H_{0\text{ph}} + \mathbf{p}^2/2 - \beta V(\mathbf{r}) + \alpha^{1/2} H_{\text{IF}}, \tag{1}$$

where

$$H_{0\text{ph}} = \int d^3k\, \omega(\mathbf{k}) a^+(\mathbf{k}) a(\mathbf{k}) \tag{2}$$

and

$$H_{\text{IF}} = \int d^3k\, [g(\mathbf{k}) a(\mathbf{k}) \exp(i\mathbf{k}\mathbf{r}) + \text{H.c.}]. \tag{3}$$

Here, $\mathbf{r}$ and $\mathbf{p}$ are the position and momentum operator of the electron, respectively, and $\mathbf{k}$, $\omega(\mathbf{k})$, $a^+(\mathbf{k})$, and $a(\mathbf{k})$ are the wave vector, frequency, creation, and annihilation operators of the phonons, respectively (i.e., a scalar Bose field); $g(\mathbf{k})$ denotes the electron–phonon coupling, α being the coupling parameter. Setting $m = \hbar = 1$, we keep α and β as the only parameters ($\alpha,\beta \geqslant 0$).

Henceforth, the following conditions (4)–(6) on $\omega(\mathbf{k})$ and $g(\mathbf{k})$ are assumed:

$$\inf_{\mathbf{k}} \omega(\mathbf{k}) \equiv \omega_0 > 0, \tag{4}$$

$\omega(\mathbf{k})$ being a continuous function of $\mathbf{k}$. Thus (4) implies that we are dealing with optical phonons. Furthermore we assume

$$\int d^3k \frac{|g(\mathbf{k})|^2}{1+k^2} < \infty \tag{5}$$

and reflection symmetry

$$\omega(-\mathbf{k}) = \omega(\mathbf{k}), \quad g(-\mathbf{k}) = g(\mathbf{k}). \tag{6}$$

For more UV-singular couplings $g(\mathbf{k})$ one has to renormalize by the scheme proposed by Nelson.[8] For the potential $V(\mathbf{r})$ we treat the case

$$V \in R + L_\epsilon^\infty(\mathbb{R}^3), \tag{7}$$

where R is the Rollnik class

$$V \in R \Leftrightarrow \int d^3x\, d^3y \frac{|V(\mathbf{x})|\cdot|V(\mathbf{y})|}{|\mathbf{x}-\mathbf{y}|^2} < \infty. \tag{8}$$

Statement (7) means that for any positive ϵ, V is representable as $V = f_\epsilon + g_\epsilon$, where $f_\epsilon \in R$ and $|g_\epsilon|$ is bounded by ϵ. Additionally, we assume that the associated one-particle Hamiltonian

$$H_e(\beta) = p^2/2 - \beta V(\mathbf{r}) \tag{9}$$

is essentially self-adjoint and bounded from below and has at least one bound state with strictly negative energy $E_0(\beta)$. The last assumption is abandoned in Sec. IV.

Physically most relevant cases are $\omega(\mathbf{k}) \equiv \omega_0 > 0$ (i.e., dispersionless optical phonons) and $g(\mathbf{k}) \sim 1/k$ for polar scattering or $g(\mathbf{k}) \sim \Theta(k_0 - k)$, $k_0 > 0$, for deformation potential scattering. Possible choices for the external potential $V(\mathbf{r})$ are a Coulomb potential $[V(\mathbf{r}) = 1/r]$, a screened Coulomb potential $[V(\mathbf{r}) = \exp(-k_0 r)/r, \quad k_0 > 0]$, or a spherical square well $[V(\mathbf{r}) = \Theta(a - r), \quad a > 0]$. The case of anisotropic bound polarons is included in our general assumptions (4)–(6), too.

The analytical properties of the ground-state energy of an optical polaron, subject to an external potential $V(\mathbf{r})$, are known only for a small class of potentials: In the case of free optical polarons ($V \equiv 0$) Spohn[9] recently proved the analyticity of the ground-state energy using the functional analytical work of Fröhlich[10] whereas Gerlach and the author[11,12] showed that the (formal) free energy is analytic in α and in the temperature T for $0 < T < \infty$. In Ref. 13, the methods of Fröhlich are generalized to an optical polaron, exposed to a homogeneous magnetic field or to an external potential $V(\mathbf{r})$ with $\lim_{r\to\infty} V(\mathbf{r}) = \infty$, implying the analyticity of the ground-state energy in α and β. Apparently, this is another class of potentials as the class of impurity potentials, defined by (7). We remark that a third interesting class of potentials, which is not treated in this paper, concerns periodic potentials. They are, however, well studied in connection with quantum Brownian motion (see, e.g., Fisher and Zwerger,[14] and references therein).

The aim of the present paper is twofold.

First, we prove that the ground-state energy as well as the mean number of virtual phonons and the polaron radius of a bound polaron are analytical functions of the coupling parameter and the potential strength. A crucial assumption for this result is that the associated one-particle Hamiltonian (9) has a bound state. For long-range potentials (e.g., for a Coulomb potential) such a bound ground state exists for any potential strength.

Consequently, for long-range potentials a discontinuous "phase transition" (i.e., a nonanalyticity of the ground-state energy) does not exist. From the beginning of the polaron story up to now, the question of whether or not an optical polaron, bound in a Coulomb potential, shows up a "phase transition," was controversially discussed in the literature. It was mainly studied with the help of variational calculations yielding an upper bound on the exact ground-state energy. The physical background of such a "phase transition" becomes clear in the work of Toyozawa.[15] He gets a transition from a shallow state, formed by the external potential, to a deep self-trapped state, caused by a lattice distortion. This process is called shallow–deep instability.

On the one hand, Larsen,[3,16] Tokuda, Shoji, and Yoneya,[17] and Tokuda[18] obtain a variational bound on the ground-state energy of a bound polaron that exhibits a nonanalyticity, whereas Matsuura[19] and Mason and Das Sarma,[5] on the other hand, emphasize that their results are smooth quantities. In view of our proof, we remark that the nonanalyticities quoted above are nothing more than artifacts of the approximations made, but not intrinsic properties of the Fröhlich Hamiltonian. Takegahara and Kasuya[20] describe different states of the bound polaron by different sections in the α-β plane. However, note that, in view of our result, the properties of a bound polaron cannot be described within a phase transition concept.

The situation becomes quite different for an attractive three-dimensional short-range potential. This is the second concern of the present paper. In this case, the potential strength must exceed a critical value, to generate a bound ground state of the one-particle Hamiltonian (9). This phenomenon is well understood in atomic physics; we refer, for instance, to Glaser *et al.*,[21] Reed and Simon,[22] and Simon.[23] As the potential strengh β increases, a bound ground state arises from the continuum edge; the ground state undergoes a localization transition, the associated ground state energy being nonanalytic in β.

It is an interesting task to study the influence of the phonon interaction on this transition. In the framework of a discrete model for an exciton, this was examined by Shinozuka and Toyozawa.[24] In the adiabatic approximation, they found a localization transition of the ground state, which they called impurity assisted self-trapping. It is connected with a nonanalyticity of the ground-state energy. Shinozuka and Toyozawa also give the phase diagram in the α-β plane [see Fig. 2(b) in Ref. 24] Note, however, that they get even a discontinuous transition for $\beta = 0$, which was shown[25] to be an artifact of their approximation.

It was Spohn[26] who described the polaron approximatively as a single particle with phonon-induced altered mass. In this so-called effective-mass approximation, it turns out that the localization transition persists for phonon coupling $\alpha > 0$. Its critical line in the α-β plane, however, does not intersect the α axis. Spohn called this transition pinning transition; we shall use this term, too. In this paper, we prove that the exact ground state undergoes a pinning transition for any $\alpha \geqslant 0$. Consequently, the effective mass approximation reflects the right qualitative behavior of the analyticity of the ground-state energy. Furthermore, we discuss the relationship of the exact critical line to the one obtained in the effective mass approximation.

The organization of the present paper is as follows: In Sec. II, we show that $H(\alpha,\beta)$ is a well-defined self-adjoint operator. If the one-particle Hamiltonian has a bound state, we prove that the ground-state energy belongs to the discrete part of the spectrum of $H(\alpha,\beta)$ and is nondegenerate. In doing so, we make use of functional analytical methods of Fröhlich,[10] which clarified spectral properties of the free optical polaron. Moreover, we determine the continuum edge of $H(\alpha,\beta)$ and show the stability of bound states under the influence of the phonon interaction. The consequences (like analyticity properties of the ground state), following from Sec. II, and extensions of our theory are pointed out in Sec. III. Section IV is devoted to a discussion on the pinning transition. Applying our methods of Sec. II, we prove the existence of a pinning transition and discuss further properties of the pinning transition and the effective-mass approximation. In particular, a spherical square well and a screened Coulomb potential are considered. In Sec. V, we conclude our results.

II. SPECTRAL PROPERTIES OF A BOUND POLARON

It will be profitable to transform the Fröhlich Hamiltonian (1) by a Lee–Low–Pines transformation. Defining the unitary operator

$$U = \exp(-i\mathbf{P}\mathbf{r}), \tag{10}$$

where

$$\mathbf{P} = \int d^3k\, \mathbf{k} a^+(\mathbf{k}) a(\mathbf{k}) \tag{11}$$

is the phonon momentum, we shall discuss hereafter the unitarily equivalent Hamiltonian

$$H(\alpha,\beta) \equiv U^{-1} H_{\mathrm{F}}(\alpha,\beta) U = H_{0\mathrm{ph}} + \tfrac{1}{2}(\mathbf{p} - \mathbf{P})^2 - \beta V(\mathbf{r}) + \alpha^{1/2} H_{\mathrm{I}}. \tag{12}$$

In (12), H_{I} is given by

$$H_{\mathrm{I}} = \int d^3k\, [g(\mathbf{k}) a(\mathbf{k}) + g^*(\mathbf{k}) a^+(\mathbf{k})]. \tag{13}$$

To begin with, we pose the Fröhlich Hamiltonian on a mathematically rigorous level. We first specify the underlying Hilbert space. It is taken to be $\mathscr{H} = F \otimes L^2(\mathbb{R}^3)$, where

$$F = \bigoplus_{m=0}^{\infty} (L^2(\mathbb{R}^3))^{ⓢ m} \tag{14}$$

is the usual Fock space for the phonons, ⓢ denoting the symmetrical tensor product.

In (13), we replace the coupling $g(\mathbf{k})$ by $g(\mathbf{k})\Theta(\rho - k)$, where $\rho < \infty$ is a UV cutoff, which makes $g(\mathbf{k})$ square integrable and which is to be removed later. Thereby we obtain the Hamiltonian $H(\alpha,\beta,\rho)$ [resp. $H_\mathrm{I}(\rho)$]. Following Nelson,[8] it is easily proved that $H_\mathrm{I}(\rho)$ is a Kato potential with respect to $H_{0\mathrm{ph}}$ with relative bound zero. Since $H_{0\mathrm{ph}} + (\mathbf{p} - \mathbf{P})^2/2 - \beta V(\mathbf{r})$ is essentially self-adjoint, the Kato–Rellich theorem assures us that $H(\alpha, \beta, \rho)$ is bounded from below and essentially self-adjoint, too.

We now construct a discrete momentum lattice Γ_d for the phonon momentum space $\mathbb{R}^3$ in analogy to Fröhlich[10] and Glimm and Jaffe[27]:

$$\Gamma_d = \{\mathbf{k}\in\mathbb{R}^3 | \mathbf{k}_j = n_j/\Lambda_d,\ n_j\in\mathbb{Z},\ \Lambda_d = 2^d\Lambda_0,$$
$$\Lambda_0\in\mathbb{R}^+,\ j = 1,2,3\}. \tag{15}$$

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

$$\mathbf{k}|_d = (n_1,n_2,n_3)/\Lambda_d, \quad n_j = [k_j\Lambda_d], \tag{16}$$

where

$$[a] \equiv \begin{cases} \text{largest integer} \leqslant a, & \text{if } a<0,\\ \text{smallest integer} > a, & \text{if } a\geqslant 0. \end{cases}$$

Furthermore, we define a subspace $S_d \subseteq L^2(\mathbb{R}^3)$ of step functions:

$$F\in S_d \Leftrightarrow f(\mathbf{k}) = f(\mathbf{k}|_d). \tag{17}$$

For $g\in L^2(\mathbb{R}^3)$ let $g|_d$ denote the orthogonal projection of g onto S_d. This notation is readily generalized for locally integrable g. Then, let

$$F_d \equiv \bigotimes_{m=0}^{\infty} S_d^{ⓢ m} \tag{18}$$

and

$$F_d^\perp \equiv \left(\bigotimes_{m=1}^{\infty} (S_d^{\perp ⓢ m}) \right) ⓢ\, F_d. \tag{19}$$

Clearly,

$$F = F_d \otimes F_d^\perp. \tag{20}$$

Now we are able to define a new d cutoff Hamiltonian

$$H_d(\alpha,\beta,\rho) = H_{0\mathrm{ph}d} + (\mathbf{p} - \mathbf{P}|_d)^2/2 - \beta V(\mathbf{r})$$
$$+ \alpha^{1/2} H_{\mathrm{I}d}(\rho), \tag{21}$$

with

$$H_{0\mathrm{ph}d} = \int d^3k\, \omega(\mathbf{k})|_d a^+(\mathbf{k}) a(\mathbf{k}), \tag{22}$$

$$\mathbf{P}|_d = \int d^3k\, \mathbf{k}|_d a^+(\mathbf{k}) a(\mathbf{k}), \tag{23}$$

and

$$H_{\mathrm{I}d}(\rho) = \int d^3k\, [g(\mathbf{k})|_d a(\mathbf{k}) + g^*(\mathbf{k})|_d a^+(\mathbf{k})]$$
$$\times \Theta(\rho - k). \tag{24}$$

Using the same methods as for $H(\alpha,\beta,\rho)$, one easily verifies that $H_0(\alpha,\beta,\rho)$ is self-adjoint and bounded from below, too.

Moreover, we define a new subspace $J \subseteq S_d$ by

$$f\in J \Leftrightarrow F(\mathbf{k}) \equiv 0, \text{ for } |\mathbf{k}|_d > \rho + 3/\Lambda_d. \tag{25}$$

Let

$$\tilde{\Gamma}_d \equiv \{\mathbf{k}\in\Gamma_d \mid |\mathbf{k}| \leqslant \rho + 3/\Lambda_d\} \tag{26}$$

and

$$W \equiv \bigoplus_{m=0}^{\infty} J^{ⓢ m}, \quad W_\perp \equiv \bigoplus_{m=0}^{\infty} J^{\perp ⓢ m},$$
$$W^\perp = W_\perp\, ⓢ\, W. \tag{27}$$

Clearly, $F_d = W \oplus W^\perp$ and $H_d(\alpha,\beta,\rho)$ as well as $H_{\mathrm{I}d}(\rho)$ leave W invariant.

We remark that there exists a canonical isomorphism between the Hamiltonian $H_d(\alpha,\beta,\rho) \restriction W \otimes L^2(\mathbb{R}^3)$ ($\restriction$ denotes, as usual, the restriction) and the Hamiltonian $H(\alpha,\beta,N)$ of the interaction of an electron with $N \equiv |\tilde{\Gamma}_d|$ phonon modes, confined to the Hilbert space $F(N) \otimes L^2(\mathbb{R}^3)$, where

$$F(N) = \bigoplus_{m=0}^{\infty} (\mathbb{C}^N)^{ⓢ m}, \tag{28}$$

which was pointed out by Glimm and Jaffe.[27] Clearly, N depends on d and ρ. Therefore, for the sake of simplicity, we consider henceforth the latter Hamiltonian

$$H(\alpha,\beta,N) = H_0(N) + \alpha^{1/2} H_\mathrm{I}(N), \tag{29}$$

with

$$H_0(N) = \sum_{j=1}^{N} \omega(\mathbf{k}_j) a^+(\mathbf{k}_j) a(\mathbf{k}_j)$$
$$+ \frac{(\mathbf{p} - \mathbf{P}(N))^2}{2} - \beta V(\mathbf{r}), \tag{30}$$

$$\mathbf{P}(N) = \sum_{j=1}^{N} \mathbf{k}_j a^+(\mathbf{k}_j) a(\mathbf{k}_j), \tag{31}$$

$$H_\mathrm{I}(N) = \sum_{j=1}^{N} [g(\mathbf{k}_j) a(\mathbf{k}_j) + g^*(\mathbf{k}_j) a^+(\mathbf{k}_j)]. \tag{32}$$

The N dependence of $H(\alpha,\beta,N)$ should not be confused with the ρ dependence of $H(\alpha,\beta,\rho)$. The quantities $H(\alpha,\beta,N)$ and $H(\alpha,\beta,\rho)$ are different Hamiltonians. In (30)–(32), $\{\mathbf{k}_j | j\in\mathbb{N}_N\} = \tilde{\Gamma}_d$. At the end of this section, we remove the discrete momentum lattice. Then we come back to our original Hamiltonians $H_d(\alpha,\beta,\rho)$ and $H(\alpha,\beta,\rho)$.

In the case $\beta \equiv 0$, the spectral properties are well understood. It has been shown[10] that $H(\alpha,0,N)$ is representable as a direct integral:

$$H(\alpha,0,N) = \int_\oplus d^3Q\, H_\mathbf{Q}(\alpha,0,N), \tag{33}$$

$\mathbf{Q}$ being the "C-number" of the conserved total momentum (see also Ref. 28). In Ref. 28, it is proved that

$$\inf_\mathbf{Q}(\inf \operatorname{spec} H_\mathbf{Q}(\alpha,0,N)) = \inf \operatorname{spec} H_{\mathbf{Q}\equiv 0}(\alpha,0,N), \tag{34}$$

and Fröhlich[10] has shown that the normalized ground state $|\Phi_0\rangle$ of $H_{\mathbf{Q}\equiv 0}(\alpha,0,N)$, lying in $F(N)$, is nondegenerate up to an arbitrary phase factor. We are now prepared to prove the following proposition.

Proposition 1:

$$\langle \Phi_0 | \mathbf{P}(N) | \Phi_0 \rangle = 0. \tag{35}$$

Proof: By Wigner's theorem, there exists a unitary operator U such that

$$Ua(\mathbf{k}_j)U^{-1} = a(-\mathbf{k}_j), \tag{36}$$

$$Ua^+(\mathbf{k}_j)U^{-1} = a^+(-\mathbf{k}_j), \tag{37}$$

for all $\mathbf{k}_j \in \widetilde{\Gamma}_d$. Then, we find

$$UH_{\mathbf{Q}\equiv 0}(\alpha,0,N)U^{-1} = H_{\mathbf{Q}\equiv 0}(\alpha,0,N) \tag{38}$$

and

$$U\mathbf{P}(N)U^{-1} = -\mathbf{P}(N). \tag{39}$$

Because of the nondegeneracy of $|\Phi_0\rangle$, (38) implies

$$\mathrm{U}|\Phi_0\rangle = \exp(i\lambda)|\Phi_0\rangle, \quad \lambda\in\mathbb{R}. \tag{40}$$

Therefore, by (39) and (40), $\langle\Phi_0|\mathbf{P}(N)|\Phi_0\rangle = -\langle\Phi_0|\mathbf{P}(N)|\Phi_0\rangle$, which implies (35). □

We now determine the essential spectrum of $H(\alpha,\beta,N)$.

Lemma 2:

$$\sigma_{\text{ess}}(H(\alpha,\beta,N)) = \sigma_{\text{ess}}(H(\alpha,0,N)). \tag{41}$$

Proof: By Weyl's theorem (see, e.g., Ref. 22), we have to prove that V is a relative form compact perturbation, i.e., that for $\zeta\notin$ spec $H(\alpha,\beta,N)\cup$ spec $H(\alpha,0,N)$,

$$(H(\alpha,\beta,N)-\zeta)^{-1} - (H_0(N)+\alpha^{1/2}H_{\mathrm{I}}(N)-\zeta)^{-1}$$
$$= \beta(H(\alpha,\beta,N)-\zeta)^{-1}V(H_0(N) + \alpha^{1/2}H_{\mathrm{I}}(N)-\zeta)^{-1} \tag{42}$$

is compact. We use the norm-convergent resolvent expansions

$$(H(\alpha,\beta,N)-\zeta)^{-1} = \sum_{n=0}^{\infty}[(H_0(N)-\beta V-\zeta)^{-1}(-\alpha^{1/2}H_{\mathrm{I}}(N))]^n \times(H_0(N)-\beta V-\zeta)^{-1}, \tag{43}$$

$$(H_0(N)+\alpha^{1/2}H_{\mathrm{I}}(N)-\zeta)^{-1} = (H_0(N)-\zeta)^{-1} \times\left(\sum_{n=0}^{\infty}[-\alpha^{1/2}H_{\mathrm{I}}(N)(H_0(N)-\zeta)^{-1}]^n\right). \tag{44}$$

For Re ζ sufficiently small and negative, the second factor of (44) as well as the first factor of (43) define bounded operators. Therefore, to establish the compactness of (42) it is sufficient to show that

$$(H_0(N)-\beta V-\zeta)^{-1}V(H_0(N)-\zeta)^{-1} \tag{45}$$

is compact. Now, we observe that the operators $a^+(\mathbf{k}_j)$ and $a(\mathbf{k}_j)$, commute with (45). Hence we can classify the spectrum of (45) by a set of natural numbers $L\equiv(n_1,\ldots,n_N)$, $n_j\in\mathbb{N}^0$, where the spectrum of (45) tends to zero as $|\mathbf{L}|\to\infty$. Therefore, all that remains to prove is that (45), restricted to a subspace with $\mathbf{L}$ fixed, is compact. Choosing new momentum and position operators

$$\mathbf{p}_n = \mathbf{p} - \sum_{j=1}^{N}\mathbf{k}_j n_j, \tag{46}$$

$$\mathbf{r}_n = \mathbf{r}, \tag{47}$$

this problem is clearly the same as studying the one-particle problem

$$\left(\sum_{j=1}^{N}\omega(\mathbf{k}_j)n_j + \frac{\mathbf{p}_n^2}{2} - \beta V(\mathbf{r}_n) - \zeta\right)^{-1} V(\mathbf{r}_n) \times\left(\sum_{j=1}^{N}\omega(\mathbf{k}_j)n_j + \frac{\mathbf{p}_n^2}{2} - \zeta\right)^{-1}. \tag{48}$$

The compactness of (48) was shown by Reed and Simon (see pp. 117–118 in Ref. 22). This implies that (42) is compact, too, and our proof of Lemma 2 is finished. □

We are now able to prove the existence and stability of bound states and state the following theorem.

Theorem 3: Let $N(H)$ denote the number of bound states of the Hamiltonian H, i.e., the number of states lying below the continuum edge. Then,

$$N(H(\alpha,\beta,N)) \geqslant N(H_e(\beta)). \tag{49}$$

Proof: The idea of the proof is to apply a generalization of the Rayleigh–Ritz principle. Let $|\varphi_n\rangle$ be the normalized eigenfunctions of the one-particle Hamiltonian (9):

$$H_e(\beta)|\varphi_n\rangle = E_n|\varphi_n\rangle,$$
$$\text{with } E_n<0, \quad n\in\mathbb{N}^0, \quad n<N(H_e(\beta)). \tag{50}$$

Consider the "trial functions" $|\varphi_n\rangle\otimes|\Phi_0\rangle\in D(H(\alpha,\beta,N))$. Because of Proposition 1, we obtain

$$\langle\varphi_n|\otimes\langle\Phi_0|H(\alpha,\beta,N)|\Phi_0\rangle\otimes|\varphi_m\rangle$$
$$= \delta_{nm}\langle\Phi_0|H_{\mathbf{Q}\equiv 0}(\alpha,0,N)|\Phi_0\rangle + \langle\varphi_n|H_e(\beta)|\varphi_m\rangle - \langle\varphi_n|\mathbf{p}|\varphi_m\rangle\langle\Phi_0|\mathbf{P}(N)|\Phi_0\rangle$$
$$= \delta_{nm}(\inf\operatorname{spec} H(\alpha,0,N) + E_n). \tag{51}$$

Hence the Rayleigh–Ritz technique tells us that we have found upper bounds on the exact bound states, which—because of Lemma 2—belong to the discrete part of spec $H(\alpha,\beta,N)$. Consequently, (49) is established. □

Returning to our original Hamiltonian $H(\alpha,\beta,\rho)$, we state the following lemma.

Lemma 4: Let $E(\alpha,\beta,\rho) = \inf\operatorname{spec} H(\alpha,\beta,\rho)$ and let f_δ be a positive C^∞ function on $\mathbb{R}$ with $f_\delta(0)=1$ and $f_\delta(x)=0$ for $x\geqslant\delta$. Then $f_\delta(H(\alpha,\beta,\rho)-E(\alpha,\beta,\rho))$ is compact, if

$$\delta<\Delta(\rho)\equiv\min(\omega_0,E(\alpha,0,\rho)-E(\alpha,\beta,\rho))>0. \tag{52}$$

Proof: First, via the isomorphism mentioned above all our spectral results for $H(\alpha,\beta,N)$ are directly transferable to the Hamiltonian $H_d(\alpha,\beta,\rho)\restriction W\otimes L^2(\mathbb{R}^3)$.

Let

$$E_d(\alpha,\beta,\rho) = \inf\operatorname{spec} H_d(\alpha,\beta,\rho)\restriction F_d\otimes L^2(\mathbb{R}^3).$$

The same calculations as in Ref. 13 (the second step of the proof of lemma 2.1 in Ref. 13) yield

$$\inf\operatorname{spec}(H_d(\alpha,\beta,\rho)\restriction W^{\perp}\otimes L^2(\mathbb{R}^3))\geqslant\omega_0+E_d(\alpha,\beta,\rho). \tag{53}$$

Since $F_d = W\oplus W^{\perp}$, it follows from Lemma 2 that

$$f_\delta(H_d(\alpha,\beta,\rho)-E_d(\alpha,\beta,\rho))\restriction F_d\otimes L^2(\mathbb{R}^3)$$

is compact, if

$$\delta<\Delta_d\equiv\min(\omega_0,E_d(\alpha,0,\rho)-E_d(\alpha,\beta,\rho)).$$

From Theorem 3 we know that $\Delta_d>0$.

We apply this argumentation once more: The same calculations as in Ref. 10 (Corollary 2.2.iii) can be used to show

$$\inf \operatorname{spec} H_d(\alpha,\beta,\rho) \restriction F_d^\perp \otimes L^2(\mathbb{R}^3) \geqslant \omega_0 + \inf \operatorname{spec} H_d(\alpha,\beta,\rho) \restriction F \otimes L^2(\mathbb{R}^3). \quad (54)$$

Since $F = F_d \oplus F_d^\perp$, it follows that

$$\inf \operatorname{spec} H_d(\alpha,\beta,\rho) \restriction F \otimes L^2(\mathbb{R}^3) = E_d(\alpha,\beta,\rho)$$

and that

$$f_\delta(H_d(\alpha,\beta,\rho) - E_d(\alpha,\beta,\rho)) \restriction F \otimes L^2(\mathbb{R}^3)$$

is compact, if $\delta < \Delta_d$. The methods used by Fröhlich (Lemma 2.1 in Ref. 10) show that $H_d(\alpha,\beta,\rho) \to H(\alpha,\beta,\rho)$ in norm resolvent convergence as $d \to \infty$. Consequently, $E_d(\alpha,\beta,\rho) \to E(\alpha,\beta,\rho)$ as $d \to \infty$ and $f_\delta(H(\alpha,\beta,\rho) - E(\alpha,\beta,\rho))$ remains compact if $\delta < \Delta(\rho)$. The same proof as in Theorem 3 results in $\Delta(\rho) > 0$, which completes the proof of Lemma 4. □

All what remains to do is to remove the UV cutoff ρ.

Theorem 5: Let $E(\alpha,\beta) = \inf \operatorname{spec} H(\alpha,\beta)$ and f_δ as in Lemma 4. Then, $f_\delta(H(\alpha,\beta) - E(\alpha,\beta))$ is compact, if $\delta < \Delta$ where

$$\Delta \equiv \min(\omega_0, E(\alpha,0) - E(\alpha,\beta)) > 0. \quad (55)$$

Proof: Transforming the Hamiltonian $H(\alpha,\beta,\rho)$ with the canonical transformation e^T, where

$$T \equiv T_{\rho\Lambda} = \int d^3k \, (C_{\rho\Lambda}(\mathbf{k}) a(\mathbf{k}) - \text{H.c.}) \quad (56)$$

with

$$C_{\rho\Lambda}(\mathbf{k}) \equiv C(\mathbf{k}) = -\alpha^{1/2} g(\mathbf{k}) \Theta(g-k) \Theta(k-\Lambda)/(\omega(\mathbf{k}) + k^2/2), \quad 0 < \Lambda < \rho, \quad (57)$$

we obtain

$$e^T H(\alpha,\beta,\rho) e^{-T} \equiv H^T(\alpha,\beta,\rho) = H_0(\beta) + \alpha^{1/2} H_{\text{I}}(\rho) + (\mathbf{Z} + \mathbf{Z}^+)^2/2 - (\mathbf{p} - \mathbf{P}) \cdot \mathbf{Z} - \mathbf{Z}^+ (\mathbf{p} - \mathbf{P}) + \Sigma, \quad (58)$$

where

$$H_0(\beta) = H_{0\text{ph}} + (\mathbf{p} - \mathbf{P})^2/2 - \beta V(\mathbf{r}), \quad (59)$$

$$\mathbf{Z} = \int d^3k \, \mathbf{k} C_{\rho\Lambda}(\mathbf{k}) a(\mathbf{k}), \quad (60)$$

and

$$\Sigma = \int d^3k \, [\omega(\mathbf{k}) |C(\mathbf{k})|^2 + \alpha^{1/2} g^*(\mathbf{k}) C(\mathbf{k}) + \alpha^{1/2} g(\mathbf{k}) C^*(\mathbf{k})] < \infty. \quad (61)$$

Again we can use Fröhlich's methods (see Sec. 2.2 in Ref. 10) to prove the following facts: For all $\epsilon > 0$ there exists a $\Lambda < \infty$ such that

$$|H^T(\alpha,\beta,\rho) - H_0(\beta)| \leqslant \epsilon H_0(\beta) + b(\Lambda), \quad (62)$$

where $b(\Lambda)$ is uniform in $\rho \leqslant \infty$. Furthermore

$$\operatorname*{norm-lim}_{\rho \to \infty} (\zeta - H^T(\alpha,\beta,\rho))^{-1} = (\zeta - H^T(\alpha,\beta))^{-1} \quad (63)$$

exists, where $H^T(\alpha,\beta)$ is a unique self-adjoint operator bounded from below. Also

$$\operatorname*{s-lim}_{\rho \to \infty} \exp(T_{\rho\Lambda}) \equiv \exp(T_{\infty\Lambda})$$

exists as a unitary operator. Therefore

$$H(\alpha,\beta) \equiv \exp(-T_{\infty\Lambda}) H^T(\alpha,\beta) \exp(T_{\infty\Lambda})$$

is self-adjoint and bounded from below, too. Finally, the norm-resolvent convergence (63) together with Lemma 4 implies that $f_\delta(H(\alpha,\beta) - E(\alpha,\beta))$ remains compact for $\delta < \Delta$. □

We now determine the continuum edge of $H(\alpha,\beta)$.

Theorem 6: Let $E(\alpha,\beta) = \inf \operatorname{spec} H(\alpha,\beta)$. The continuum edge begins exactly at the point

$$\Omega \equiv \min(E(\alpha,\beta) + \omega_0, E(\alpha,0)). \quad (64)$$

Proof: This Ω is a lower bound for the continuum edge because Theorem 5 implies that all eigenvalues smaller than Ω are discrete. Furthermore, without loss of generality we may assume that the number of eigenvalues being smaller than Ω is finite. Otherwise these infinite eigenvalues have to accumulate at Ω and (64) is trivially proved.

Suppose first

$$E(\alpha,0) \leqslant E(\alpha,\beta) + \omega_0. \quad (65)$$

Since the absolute continuous spectrum of $H_e(\beta)$ begins at zero, we can always find functions $|\psi_n\rangle \in L^2(\mathbb{R}^3)$ ($n \in \mathbb{N}$) with $\langle \psi_n | \psi_m \rangle = \delta_{nm}$ and with $\langle \psi_n | H_E(\beta) | \psi_m \rangle = \delta_{nm} E_n$, where $E_n > 0$ and $E_n \to 0$ as $n \to \infty$. Choosing the trial functions $|\Phi_0\rangle \otimes |\psi_n\rangle$, where $|\Phi_0\rangle$ denotes the ground state of the free polaron Hamiltonian subjected to total momentum $\mathbf{Q} \equiv \mathbf{0}$, we calculate, as in the proof of Theorem 3,

$$\langle \psi_n | \otimes \langle \Phi_0 | \Phi_0 \rangle \otimes | \psi_m \rangle = \delta_{nm}$$

and

$$\langle \psi_n | \otimes \langle \Phi_0 | H(\alpha,\beta,) | \Phi_0 \rangle \otimes | \psi_m \rangle = \delta_{nm} (E(\alpha,0) + E_n). \quad (66)$$

Since $E_n \to 0$ as $n \to \infty$, a modification of the mini–max principle (see, e.g., Reed and Simon,[22] Theorem XIII.1) ensures us that $E(\alpha,0)$ is the bottom of the essential spectrum of $H(\alpha,\beta)$.

In the second case

$$E(\alpha,\beta) + \omega_0 < E(\alpha,0), \quad (67)$$

we again use a trial function argument, but now with different fuctions involving one-phonon states. By (4) we know that there exists a $\mathbf{q} \in \mathbb{R}^3$ with $\omega(\mathbf{k}) \to \omega_0$ as $\mathbf{k} \to \mathbf{q}$. Without loss of generality we assume $q < \infty$, the case $q = \infty$ can be treated quite similarly. We choose $\epsilon > 0$ fixed.

First, we need some definitions. Let $U(\delta,\mathbf{q})$ denote a ball around $\mathbf{q}$ with radius δ. We construct "disks" $D(n)$ as follows:

$$D(n) = U(\epsilon 2^{-n}, \mathbf{q}) \setminus U(\epsilon 2^{-n-1}, \mathbf{q}). \quad (68)$$

Let $H(\mathbf{q})$ be the Hamiltonian that results if one replaces $\mathbf{p}$ in $H(\alpha,\beta,)$ by $\mathbf{p} - \mathbf{q}$, $\mathbf{q}$ being a C-number. Obviously, $H(\mathbf{q})$ is unitarily equivalent to $H(\alpha,\beta)$. The ground state of $H(\mathbf{q})$ is denoted by $\psi(\mathbf{q}) \in \mathscr{H}$. Furthermore, we define a projection operator P_A ($A \subseteq \mathbb{R}^3$) that annihilates all phonon parts with momentum $\mathbf{k} \in A$ by

$$P_A = \sum_{n=1}^{\infty} \int d^3k_1 \cdots \int d^3k_n \, \chi_A(\mathbf{k}_1) \cdots \chi_A(\mathbf{k}_n) \times a(\mathbf{k}_1) \cdots a(\mathbf{k}_n), \quad (69)$$

where $\chi_A(\mathbf{k})$ is the characteristic function equal to 1 if $\mathbf{k} \in A$ and 0 otherwise.

We are now able to give the explicit form of our trial functions $\Phi_{n\epsilon}$, $n \in \mathbb{N}$,

$$\Phi_{n\epsilon} = [(P_{U(\epsilon,\mathbf{q})}\psi(\mathbf{q})) \circledS \varphi_{n\epsilon}]/\|(P_{U(\epsilon,\mathbf{q})}\psi(\mathbf{q})) \circledS \psi_{n\epsilon}\|, \tag{70}$$

where $\varphi_{n\epsilon}$ is a one-phonon state, $\varphi_{n\epsilon} \geqslant 0$, whose momentum distribution is explicitly given by

$$|\varphi_{n\epsilon}(\mathbf{k})|^2 d^3k = \chi_{D(n)}(\mathbf{k}) d^3k. \tag{71}$$

For ϵ sufficiently small, $\Phi_{n\epsilon} \in \mathscr{H}$ and $\Phi_{n\epsilon} \not\equiv 0$. Since $U(\epsilon,\mathbf{q}) \supseteq D(n)$ and since the $D(n)$ are pairwise disjunct, one calculates

$$\langle \Phi_{n\epsilon} | \Phi_{m\epsilon} \rangle = \delta_{nm}, \quad \langle \Phi_{n\epsilon} | H(\alpha,\beta) | \Phi_{m\epsilon} \rangle = E_n(\epsilon)\delta_{nm}. \tag{72}$$

Further inspection of E_n shows that $E_n(\epsilon) \to \omega_0 + E(\alpha,\beta,\epsilon)$ as $n \to \infty$, where $\omega_0(\epsilon) \to \omega_0$ and $E(\alpha,\beta,\epsilon) \to E(\alpha,\beta)$ as $\epsilon \to 0$. Since $\epsilon > 0$ can be chosen arbitrarily small, again the minimax principle tells us that the continuum edge has the upper bound $\omega_0 + E(\alpha,\beta)$.

Putting all facts together, we finally finish the proof of Theorem 6. □

The physical interpretation of the two possibilities (64) for the continuum edge is easily understood. In the case (67) the continuum involves scattering states with one real phonon of energy ω_0 present. On the other hand, if (65) holds, the continuum at $E(\alpha,0)$ consists of delocalized electron states.

Obviously, the Rayleigh–Ritz argument of Theorem 3 can be done for $H(\alpha,\beta)$, too. If (65) holds, this implies the existence and stability of the bound states and gives furthermore simple upper bounds on the associated energies.

Corollary 7: Let $E(\alpha,0) < E(\alpha,\beta) + \omega_0$ and let $N(H)$ be the number of states of the Hamiltonian H below the continuum edge. Then,

$$N(H(\alpha,\beta)) \geqslant N(H_e(\beta)), \quad \text{for all } \alpha \geqslant 0. \tag{73}$$

□

We know from Theorem 5 that $E(\alpha,\beta)$ is an eigenvalue. Now we prove the next lemma.

Lemma 8: The ground state of $H(\alpha,\beta)$ is nondegenerate.

Proof: We represent the underlying Hilbert space now as

$$L^2(Q,d\mu) \otimes L^2(\mathbb{R}^3,d^3x), \tag{74}$$

where $L^2(Q,d\mu)$ is the phonon Q space, which is isomorphic to the Fock space F (see Simon[29] for a detailed discussion). If one takes the Schrödinger representation ($\mathbf{r}$ representation) for the electron coordinate, the operator

$$L \equiv -\beta V(\mathbf{r}) + \alpha^{1/2} H_\mathrm{I} \tag{75}$$

acts as a multiplication operator. The operator L can be approximated by bounded multiplication operators L_n, such that $H_0 + L_n \to H(\alpha,\beta)$ and $H(\alpha,\beta) - L_n \to H_0$ in the strong resolvent sense as $n \to \infty$. This holds for arbitrary cutoff $\rho \leqslant \infty$. We know from the proof of Theorem 5 that the operators $H_0 + L_n$ and $H(\alpha,\beta) - L_n$ are uniformly bounded from below. Therefore, Theorem XIII.45 of Reed and Simon[22] is applicable (see also Ref. 28). This implies that, in order to prove Lemma 8, we have to show that $\exp(-H_{0\mathrm{ph}} - (\mathbf{p}-\mathbf{P})^2/2)$ is positivity improving in the chosen representation. We write $\exp(-(\mathbf{p}-\mathbf{P})^2/2)$ as Fourier transform

$$\exp(-(\mathbf{p}-\mathbf{P})^2/2) = (2\pi)^{-3/2}\int d^3\lambda \exp\left(-\frac{1}{2}\lambda^2\right) e^{i\lambda\mathbf{p}} e^{-i\lambda\mathbf{P}}. \tag{76}$$

Now, $\exp(-H_{0\mathrm{ph}})$ is positivity improving and $\exp(-i\lambda\mathbf{p})$ is positivity preserving with respect to the phonon Q space; $\exp(i\lambda\mathbf{p})$ acts as translational operator in the $\mathbf{r}$ representation of the electron coordinate. Since $\exp(-\frac{1}{2}\lambda^2)$ is strictly positive, we get that $\exp(-H_{0\mathrm{ph}} - \frac{1}{2}(\mathbf{p}-\mathbf{P})^2)$ is positivity improving in the chosen representation. This implies that $\exp(-H(\alpha,\beta))$ is positivity improving and consequently $E(\alpha,\beta)$ is a simple eigenvalue. □

Summarizing, we have proved in this section that the Hamiltonian $H(\alpha,\beta)$ for a bound optical polaron is a well-defined self-adjoint operator, bounded from below. If the one-particle Hamiltonian (9) has a bound ground state, then also $H(\alpha,\beta)$ has a discrete bound ground state that is nondegenerate. This ground state is separated from the continuous spectrum by a gap whose magnitude was exactly determined: It is the minimum of the phonon dispersion ω_0 or the difference $E(\alpha,0) - E(\alpha,\beta) \geqslant |E_0(\beta)|$, where $E_0(\beta)$ is the ground-state energy of the one-particle Hamiltonian (9).

III. CONSEQUENCES AND GENERALIZATIONS

To begin with, we state that the associated forms of the resolvent of Eq. (63) $(\zeta - H^T(\alpha,\beta))^{-1}$ are an analytic family of type (B) in the sense of Kato[30] in both parameters α (see Fröhlich[10]) and β (see Simon[31]) for $\alpha,\beta \geqslant 0$. Since Lemma 8 implies that $E(\alpha,\beta)$ is an isolated, simple eigenvalue for $\alpha \geqslant 0$ [β being such that $H_e(\beta)$ has a negative eigenvalue], the standard analytical perturbation theory (see Kato[30]) is applicable. It follows from Hartog's theorem that $E(\alpha,\beta)$ is jointly real analytic in α and β in the specified domain. The same is true for the discrete excited states, if they are not degenerate. Moreover, the associated wave functions are analytic in α and β, too.

Let $|\psi_0(\alpha,\beta)\rangle$ be the wave function of the ground state of $H(\alpha,\beta)$. Then the mean number of virtual phonons in the ground state is defined by

$$N(\alpha,\beta) = \langle \psi_0(\alpha,\beta) | \int d^3k \; a^+(\mathbf{k}) a(\mathbf{k}) | \psi_0(\alpha,\beta) \rangle. \tag{77}$$

Furthermore, several possibilities were proposed to define a polaron radius and a self-induced potential as quantities derived from the ground-state expectation values of H_I (see, e.g., Peeters and Devreese[32]). Clearly, $N(\alpha,\beta)$ as well as the polaron radius and the self-induced potential are analytic in α and β for $\alpha \geqslant 0$, β as above.

We conclude that all changes in the bound polaron state are not accompanied by a nonanalytical behavior, but are smooth transitions.

We now add some remarks on possible extensions of our theory. First, one may consider an optical polaron in arbitrary spatial dimension (see Peeters, Wu Xiaoguang, and Devreese[33]). The conditions (4)–(8) are readily generalized to arbitrary dimensions (see Simon[31] for an extension of the Rollnik condition). Then, the same proof is possible.

We mention two physical interesting examples. First, Sak[34] (see also Degani and Hipolito[6]) considers an electron that couples to the optical surface phonon modes and is bound in the perpendicular direction to a Coulomb potential resulting from its image charge. The associated Hamiltonian H_s can be cast into the form

$$H_s = (Q_1 - P_1)^2/2 + (Q_2 - P_2)^2/2 + p_3/2 - \beta V(r_3) + \omega_s \int d^2k\, a^+(\mathbf{k}) a(\mathbf{k}) + \alpha^{1/2} \int d^2k\, k^{-1/2} \times \exp(-k_3 r_3)[a(\mathbf{k}) + a^+(\mathbf{k})]. \quad (78)$$

The Hilbert space $\mathscr{H}_s$ belonging to H_s is

$$\mathscr{H}_s = F \otimes L^2([0,\infty[). \quad (79)$$

The parameters Q_1 and Q_2 correspond to the conserved components of the momentum. To get inf spec H_s, one may set $Q_1 = Q_2 = 0$ (see Ref. 28). For $V(r_3)$ we do not take $1/r_3$, as Sak does, but for mathematical and physical reasons (see Cole[35]) we have to take a cutoff potential:

$$V(\mathbf{z}) = \begin{cases} 1/\mathbf{z}, & \text{for } \mathbf{z} \geqslant b, \\ 1/b, & \text{for } \mathbf{z} < b, \end{cases} \quad (80)$$

where the cutoff b is a strictly positive constant. Without going into the mathematical details, we remark that our methods are applicable to H_s. In particular, the ground-state energy is analytic in α and β. This is in a marked contrast to the work of Tokuda.[18] The above model can be extended to include bulk phonon effects, which was discussed recently by Gu and Zheng.[36]

A second example concerns a quasi-two-dimensional polaron in polar quantum wells, bound to a two-dimensional Coulomb potential, which was studied by Mason and Das Sarma.[5]

IV. THE PINNING TRANSITION

Up to now, for all potentials considered, the associated ground-state energies are analytic in α or β. One may ask the question the other way around: Which potentials lead to a ground-state energy that is nonanalytic in α or β? This brings us back directly to our condition that the one-particle Hamiltonian (9) has at least one bound state. In one or two dimensions, it is well known that an attractive potential always leads to a bound state. No so in three dimensions; the question of whether or not the one-particle Hamiltonian has a bound state depends sensitively on the mass of the particle for short-range potentials. The idea of Spohn[26] is to describe the polaron problem approximately as a one-particle problem with an effective mass $m(\alpha)$ and to study then the occurrence of bound states with increasing α. For a suitable static binding potential, at a critical coupling α_c a pinning transition is obtained, i.e., by the phonon-induced mass enhancement of the electron, a new bound state suddenly arises from the continuum.

To get a connection with our results, we consider a slightly different situation: Let α be fixed and vary β ($\beta \in \mathbb{R}$). For the sake of definiteness, let V be an element of the Rollnik class R [see (8)] and let V be negative ($V \leqslant 0$). The occurrence of bound states of $H_e(\beta)$ is well understood (see Refs 21–23). The Birman–Schwinger bound shows that for all $\beta \in \mathbb{R}$ the number of bound states $N(H_e(\beta))$ is finite and that $N(H_e(\beta)) = 0$ for $\beta < \beta_c$, where $\beta_c > 0$. Therefore, inf spec $H_e(\beta)$ is nonanalytic for $\beta = \beta_c$, corresponding to a localization transition (pinning transition) of the ground state.

We prove that such a transition is obtained even if the electron–phonon coupling is nonzero and state the following.

Theorem 4.9: Let the potential V be in the Rollnik class R for spatial dimension $d = 3$ and let $V \leqslant 0$. Let the ground-state energy of the one-particle Hamiltonian $H_e(\beta)$ be nonanalytic for $\beta = \beta_c > 0$. Then the ground-state energy $E(\alpha,\beta)$ of the bound polaron is nonanalytic for $\beta = \beta_c(\alpha)$, where $\beta_c(\alpha)$ is a unique number with

$$0 \leqslant \beta_c(\alpha) \leqslant \beta_c, \quad (81)$$

and $\beta_c(\alpha)$ is continuous in α for $0 \leqslant \alpha < \infty$.

Proof: Clearly, $E(\alpha,\beta)$ is monotone decreasing (and concave) in β. From Theorem 6, it then follows that $E(\alpha,\beta) = E(\alpha,0)$, for $\beta \leqslant 0$. On the other hand, we know from Corollary 7 that $E(\alpha,\beta) < E(\alpha,0)$ for $\beta > \beta_c$ and that $E(\alpha,\beta)$ is analytic in β for $\beta > \beta_c$. Thus $E(\alpha,\beta)$ cannot be analytic in β in the total interval $[0,\beta_c]$ because the identity theorem for holomorphic functions requires that then $E(\alpha,\beta) \equiv E(\alpha,0)$. Therefore, there exists a nonanalyticity $\beta_c(\alpha)$, with $0 \leqslant \beta_c(\alpha) \leqslant \beta_c$. At $\beta = \beta_0(\alpha)$, $E(\alpha,\beta)$ abandons the continuum edge. Because of the monotonicity of $E(\alpha,\beta)$ in β, $E(\alpha,\beta)$ is separated by a gap from the continuum for all $\beta > \beta_c(\alpha)$. Analytical perturbation theory ensures us that $E(\alpha,\beta)$ is analytic in β for all $\beta > \beta_c(\alpha)$. Therefore the nonanalyticity $\beta_c(\alpha)$ is a unique number with $0 \leqslant \beta_c(\alpha) \leqslant \beta_c$. The continuity of $\beta_c(\alpha)$ in α follows directly from analytical perturbation theory and from the monotonicity of $E(\alpha,\beta)$ in β. □

We remark that the same proof can be done to show that the energy of the nth discrete excited state is nonanalytic at the point where it is pushed out of the continuum edge.

Clearly, $\beta_c(0) \equiv \beta_c$ and we conjecture that $\beta_c(\alpha)$ is monotone decreasing in α and that $\beta_c(\alpha) \to 0$ as $\alpha \to \infty$. An estimation on $\beta_c(\alpha)$, which is better than (81), however, requires a nontrivial extension of our result. We leave this as an open problem.

We summarize our results in two figures. In Fig. 1 we sketch $E(\alpha,\beta)$ for three different fixed values of α and vary β.

In Fig. 2, we give a qualitative picture of the phase diagram of the pinning transition in the α-β plane describing the

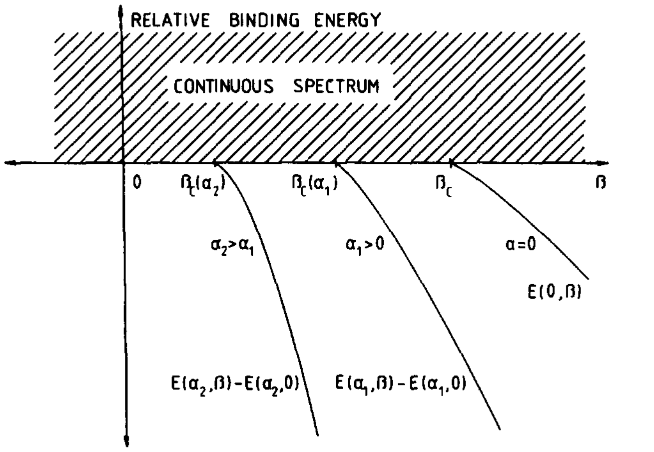

FIG. 1. Qualitative picture of the pinning transition: relative binding energy versus potential strength β for different values of the coupling α.

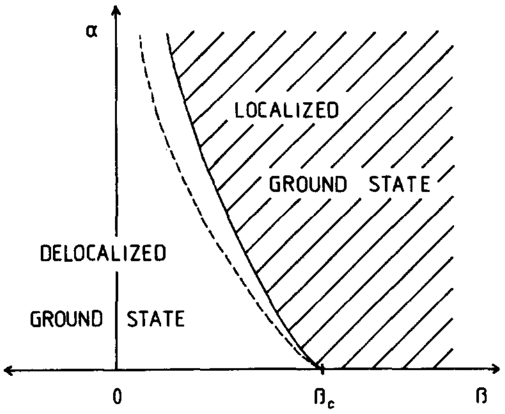

FIG. 2. Phase diagram of the pinning transition (qualitative picture). The solid line represents the exact solution, the dashed line the effective-mass approximation.

pinning transition from a delocalized to a localized state.

Let us now discuss the effective-mass approximation [i.e., the approximation of the polaron as a single-particle with mass $m(\alpha)$] in some more detail. For a Coulomb potential, Mason and Das Sarma[5] compare the ground-state energy shifts for fixed small α and varied β between the "exact" (variational) solution and the effective-mass approximation. It turns out that the effective-mass approximation yields an overestimation of the energy shift, being asymptotically correct for small β but becoming worse for intermediate and large β. Transferring this result to a short-range potential the situation is quite the same. One may conjecture that the one-particle approximation leads to a value of $\beta_c(\alpha)$ that is too small. This belief is based on the intuitive argument that a bound electron cannot use all phonons in such a way to raise its effective mass as a free electron. The one-particle approximation should only work for small α, β being small, too.

By a simple scaling argument, one finds the critical coupling strength in the effective-mass approximation by $\beta_c(\alpha)_{\text{eff}}$,

$$\beta_c(\alpha)_{\text{eff}} = \beta_c/m(\alpha), \tag{82}$$

if $m(0) = m = 1$. Therefore, critical lines for different potentials, but for the same dispersion and coupling function, are proportional in the effective-mass approximation, the potential merely determines the prefactor β_c. We have also indicated the qualitative behavior of the critical line for the effective-mass approximation in Fig. 2 (dashed line).

A finite temperature $T>0$ destroys the pinning transition. This can be seen considering the (formal) free energy (instead of the ground-state energy) in the path integral representation. The free energy is analytic in all parameters $\alpha \geqslant 0$, $\beta \geqslant 0$, and $T>0$, if the potential $V(\mathbf{r})$ is short range or if $V(\mathbf{r})$ is a long-range Coulomb potential. As for details, we refer to Ref. 25.

Finally, we give the phase diagram in the effective mass approximation for an optical Fröhlich polaron for two concrete examples: First a spherical square well

$$V(\mathbf{r}) = \Theta(1-r), \tag{83}$$

and, second, a screened Coulomb potential

$$V(\mathbf{r}) = \exp(-r)/r. \tag{84}$$

In the case of a spherical square well the eigenvalues and eigenfunctions are well-known (see, e.g., Messiah[37]). In particular, the critical potential strength turns out to be

$$\beta_c = \beta_c(0) = \pi^2/8 = 1.233\,7005\ldots . \tag{85}$$

For a screened Coulomb potential, β_c is not known analytically. Kesarwani and Varshni[38] determine β_c numerically as

$$0.839\,9032 \leqslant \beta_c \leqslant 0.839\,9039. \tag{86}$$

For the usual Fröhlich model

$$\omega(\mathbf{k}) = 1, \quad g(\mathbf{k}) = (8\pi^2)^{1/4}/k, \tag{87}$$

the polaron mass $m(\alpha)$ was calculated in Ref. 39. Consequently, all variables of (82) are known. The limiting cases (see, again, Ref. 39) are

$$\beta_c(\alpha)_{\text{eff}} = \beta_c \cdot (1-\alpha/6) + O(\alpha^2), \quad \text{as } \alpha \to 0, \tag{88}$$

$$\beta_c(\alpha)_{\text{eff}} = 44.05 \cdot \beta_c \cdot \alpha^{-4}, \quad \text{as } \alpha \to \infty. \tag{89}$$

The effective-mass approximation of the phase diagrams for the Fröhlich polaron and a spherical square well (resp. a screened Coulomb potential) are shown in Fig. 3.

A variational calculation of $\beta_c(\alpha)$ is in progress and will be published elsewhere.

Concerning experimental consequences, we finally state that first experimental evidences of the pinning transition were observed by Dmochowski *et al.*[40] They found bound polaron states very close in energy and differing strongly in localization. Such a situation just occurs in the neighborhood of the pinning transition.

V. CONCLUSIONS

Summarizing, we have proved the analyticity of polaron quantities in the coupling parameter and the potential strength, if the potential is long range (e.g., for a Coulomb potential) or if the one-particle Hamiltonian has a bound

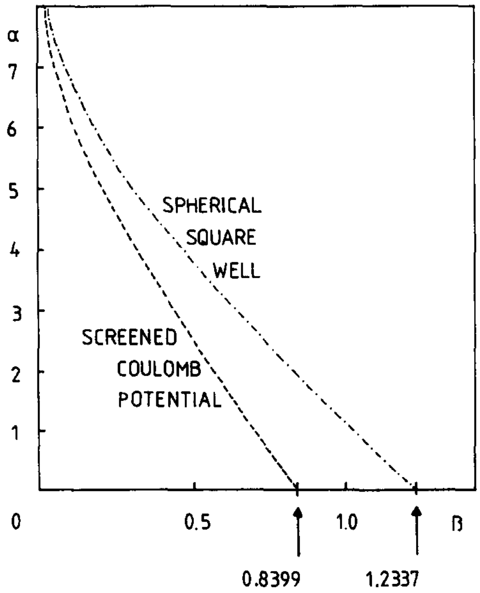

FIG. 3. Critical lines of the pinning transition in the α-β plane in the effective-mass approximation for a spherical square well and a screened Coulomb potential for a Fröhlich polaron.

state. Consequently, no "phase transitions" occur and the shallow–deep instability is continuous in this case.

For a short-range attractive potential we have shown the existence of a pinning transition, which depends on the electron–phonon coupling. This pinning transition is connected with a nonanalyticity of the ground-state energy and with a potential assisted localization transition of the ground state from a delocalized to a localized state as the potential strength increases. We have discussed this pinning transition for a spherical square well and a screened Coulomb potential, giving the phase diagram in the effective-mass approximation.

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