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Absence of phonon-induced localization for the free optical polaron and the corresponding Wannier exciton-phonon system

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We prove that the ground-state wave function of a free optical Fröhlich polaron is delocalized for any coupling strength, even for long-range couplings. The mathematical techniques involved are quite general and can be transferred, e.g., to the discussion of the center-of-mass motion of an exciton-phonon system. We show that this motion is delocalized, too.

I. INTRODUCTION AND BASIC NOTATIONS

The standard three-dimensional polaron model is defined by the Fröhlich Hamiltonian H_F, which describes the interaction of a single electron with one branch of phonons. Setting $\hbar = m = 1$, H_F reads as follows (see Fröhlich, Pelzer, and Zienau[1]):

$$H_F \equiv \mathbf{p}^2/2 + H_{0,\mathrm{ph}} + H_{I,F} \ , \tag{1}$$

where

$$H_{0,\mathrm{ph}} \equiv \int d^3k\, \omega(k) a^\dagger(\mathbf{k}) a(\mathbf{k}) \ , \tag{2}$$

and

$$H_{I,F} \equiv \alpha^{1/2} \int d^3k\, g(k)[\exp(i\mathbf{k}\cdot\mathbf{r}) a(\mathbf{k}) + \mathrm{H.c.}] \ . \tag{3}$$

Here, $\mathbf{r}$ is the position and $\mathbf{p}$ the momentum operator of the electron. $\mathbf{k}$, $\omega(k)$, $a(\mathbf{k})$, and $a^\dagger(\mathbf{k})$ are the wave vector, frequency, and annihilation and creation operators of phonons, $k \equiv |\mathbf{k}|$. Finally, $g(k)$ denotes the electron-phonon coupling, α being the dimensionless electron-phonon coupling parameter. Without loss of generality, $g(k)$ may be assumed to be real. H_F is defined on the Hilbert space,

$$\mathcal{H}_F \equiv F \otimes L^2(\mathbb{R}^3) \ . \tag{4}$$

$\mathcal{H}_F$ is the direct product of the usual phonon Fock space F and the one-particle Hilbert space $L^2(\mathbb{R}^3)$.

It is easily verified that the total polaron momentum is conserved: the corresponding operator $\mathbf{P}_T$, defined as

$$\mathbf{P}_T \equiv \mathbf{P}_{\mathrm{ph}} + \mathbf{p} \ , \tag{5}$$

where

$$\mathbf{P}_{\mathrm{ph}} \equiv \int d^3k\, \mathbf{k} a^\dagger(\mathbf{k}) a(\mathbf{k}) \ , \tag{6}$$

is the phonon momentum, commutes with H_F. An equivalent statement is that H_F is translational invariant. Following Lee, Low, and Pines,[2] we may use this fact to eliminate the electron coordinates from H_F. Defining the unitary operator

$$U \equiv \exp(-i\mathbf{P}_{\mathrm{ph}}\cdot\mathbf{r}) \ , \tag{7}$$

one verifies that

$$U^{-1}\mathbf{P}_T U = \mathbf{p} \tag{8}$$

and

$$\tilde{H}_F \equiv U^{-1} H_F U = \tfrac{1}{2}(\mathbf{p} - \mathbf{P}_{ph})^2 + H_{0,\mathrm{ph}} + H_I \ , \tag{9}$$

where now

$$H_I \equiv \alpha^{1/2} \int d^3k\, g(k)[a(\mathbf{k}) + a^\dagger(\mathbf{k})] \ . \tag{10}$$

Clearly, $\tilde{H}_F$ is defined on $\mathcal{H}_F$, too. One should notice, however, that $\tilde{H}_F$ does not depend on $\mathbf{r}$, i.e., $[\tilde{H}_F, \mathbf{p}] = 0$. Consequently, we arrive at the following direct integral decomposition of $\tilde{H}_F$ (see Fröhlich[3]):

$$\tilde{H}_F = \int \otimes d^3Q\, H(\mathbf{Q}) \ , \tag{11}$$

where

$$H(\mathbf{Q}) \equiv \tfrac{1}{2}(\mathbf{Q} - \mathbf{P}_{\mathrm{ph}})^2 + H_{0,\mathrm{ph}} + H_I \ . \tag{12}$$

$H(\mathbf{Q})$ is a momentum-decomposed Hamiltonian, namely the projection of $\tilde{H}_F$ onto the subspace of fixed eigenvalue $\mathbf{Q}$ of $\mathbf{P}_T$. Obviously, $H(\mathbf{Q})$ is defined on F alone.

It proves useful to repeat the transformation steps, outlined in (7) to (12), in terms of wave functions. The general eigenfunction of $\mathbf{P}_T$ with eigenvalue $\mathbf{Q}$ is given by

$$\chi_{\mathbf{Q}} \equiv \exp[i(\mathbf{Q} - \mathbf{P}_{\mathrm{ph}})\cdot\mathbf{r}]\Phi_{\mathrm{ph}} \ , \tag{13}$$

where Φ_{ph} is supposed to be an element of F. Notice that $\chi_{\mathbf{Q}}$ is not contained in $\mathcal{H}_F$; only suitable superpositions with respect to $\mathbf{Q}$ may yield a normalized state.

As H_F commutes with $\mathbf{P}_T$, it is sufficient to solve the equation

$$H_F \chi_{\mathbf{Q}} = E(\mathbf{Q})\chi_{\mathbf{Q}} \ . \tag{14}$$

Inserting in (14) H_F and $\chi_{\mathbf{Q}}$ according to Eqs. (1) and (13), we directly recover the eigenvalue problem

$$H(\mathbf{Q})\Phi_{\mathrm{ph}} = E(\mathbf{Q})\Phi_{\mathrm{ph}} \ . \tag{15}$$

In the remainder of this paper, we are entirely concerned with the ground-state energy $E_0(\mathbf{Q})$ of $H(\mathbf{Q})$. Not too surprisingly, the properties of $E_0(\mathbf{Q})$ will prove to be intimately connected with localization properties of the ground state eigenfunctions of H_F.

The paper is organized as follows. In Sec. II, we discuss the problem of localization and state our results. Then in Sec. III, we comment on previous publications related to ours. In Sec. IV, we prove our statements, excluding localization in free-optical-polaron systems, even for long-range couplings. Then, we turn to the Wannier exciton-phonon system. In Sec. V, we introduce the Hamiltonian and transfer results of Spohn to the center-of-mass motion of the exciton. Our method from Sec. IV is applied to the exciton-phonon problem too. Section VI contains some generalizations and summarizes our results.

II. THE PROBLEM OF LOCALIZATION AND STATEMENTS OF THE RESULTS

To begin with, we fix the precise meaning of the heading "localized." A polaron wave function Ψ is called localized if Ψ is an element of $\mathcal{H}_F$, i.e., it is normalizable with respect to the electron and phonon part; otherwise, we call Ψ delocalized.

In view of Eq. (13) and the considerations thereafter, it is not at all clear whether there exists a single localized polaron wave function as an eigenfunction of H_F. In fact, from the very beginning of the polaron story, it was a controversially discussed question, whether the ground-state wave function of H_F is localized for large electron-phonon coupling. The whole discussion was probably initiated by Landau's early idea of self-trapping (see, e.g., Ref. 4) and Feynman's paper[5] on Fröhlich polarons in 1955. Feynman proved that the phonon effects on the electron can exactly be incorporated into a self-energy functional. In an introductory part, he approximated this functional by a one-particle potential U, containing adjustable parameters. One may choose a variational procedure to fix these parameters, to produce upper bounds on the ground-state energy of H_F, and to get an approximate ground-state wave function. Intuitively, one expects that $U \rightarrow 0$ for $\alpha \rightarrow 0$ whereas strong binding should occur for $\alpha \rightarrow \infty$. It may even happen that the variational principle forces one to choose $U \equiv 0$ for $\alpha \leq \alpha_c$ and $U \neq 0$ for $\alpha > \alpha_c$. This would correspond to a localization transition from a delocalized ground state to a localized ground state. Calculations of this type may have caused the conjecture that the true ground-state wave function of H_F shows such a localization transition at $\alpha = \alpha_c$, too. As an immediate consequence, the ground state should be infinitely degenerate for $\alpha > \alpha_c$: Because of translational symmetry, the ground state can only be unique up to translations.

The localization problem may be viewed from another standpoint. If we choose α to be sufficiently small, we know from perturbation theory that the ground-state Ψ_0 of H_F is of type $\chi_{\mathbf{Q}=0}$ [see Eq. (13); χ_0 is an eigenstate of $\mathbf{P}_T$ with eigenvalue $\mathbf{Q}=0$]. Consequently,

$$E_0(\mathbf{0}) < E_0(\mathbf{Q} \neq \mathbf{0}) \tag{16}$$

holds in a certain surrounding of $\alpha = 0$. Let us tentatively assume that (16) was not true for $\alpha > \alpha_c$. Then we could deduce the following.

(i) The ground state is infinitely degenerated, as $E_0(\mathbf{Q})$ depends merely on $|\mathbf{Q}|$.

(ii) If the minimum of $E_0(\mathbf{Q})$ occurs for a subset of $\mathbf{Q}$ vectors with different length, a suitable superposition of the corresponding eigenfunctions might yield a localized state.

(iii) There exists Ψ_0 such that

$$\exp(i\boldsymbol{\lambda}\cdot\mathbf{P}_T)\Psi_0 \neq \Psi_0, \quad \text{for any real } \boldsymbol{\lambda} \neq \mathbf{0} . \tag{17}$$

Property (iii) would show that for $\alpha > \alpha_c$ there exists a ground-state wave function of H_F which has a lower symmetry than H_F itself. Such a phenomenon is usually denoted as quantum-mechanical symmetry breaking. If a localization transition would exist, translation symmetry was necessarily broken.

At this point, we remark that the above concept of symmetry breaking is well distinguished from the field-theoretical one (see e.g., Guralnik *et al.*[6]). In the latter case, one starts with an infinity of degenerate ground states and an associated nonseparable Hilbert space, selects one fixed ground state, and expands the equation of motion around this fixed ground state. This procedure is connected with a change of Hilbert space and is necessary in order to get a new separable Hilbert space. In this sense, symmetry breaking can only take place for acoustical-phonon dispersion, if it takes place at all. It is only in this case that the electron can generate an infinite number of (zero-energy) phonons which keep it localized. Such ground states are infinitely degenerated and do not belong to the usual Fock space. In order to get a "physical" theory, where one of these ground states is contained, one has to change the Hilbert space from the Fock space to a new "physical" Hilbert space. In the following, however, we shall restrict ourselves to optical dispersion where such problems do not occur.

Our central results, to be proven in Sec. IV, exclude the possibilities (i)–(iii). We show the following.

Statement 1: If $\omega(k) \geq \omega_0 > 0$ and $\int d^3k\, g^2(k)/(1+k^2) < \infty$, the ground state of H_F is delocalized for $0 \leq \alpha < \infty$.

Statement 2: Under the conditions of statement 1, inequality (16) holds for $0 \leq \alpha < \infty$. Consequently, no symmetry breaking occurs.

It is interesting to contrast these results to well-known properties of the infinite-coupling case ($\alpha \rightarrow \infty$). According to Allcock,[7] Adamowski, Gerlach, and Leschke,[8] and Donsker and Varadhan,[9] the ground-state energy E_0 of H_F fulfills the equation

$$\lim_{\alpha\rightarrow\infty} E_0/\alpha^2 = \inf_{\psi, \|\psi\|=1} \Big[\tfrac{1}{2}\int d^3x\, |\nabla\psi(\mathbf{x})|^2 - 2^{-1/2}\int d^3x\, d^3y\, |\psi(\mathbf{x})|^2 \times |\mathbf{x}-\mathbf{y}|^{-1} |\psi(\mathbf{y})|^2\Big] . \tag{18}$$

In addition, Lieb[10] proved that the minimizing solution of (18) is unique up to translations and exhibits an exponential falloff (see also the numerical studies of Miyake[11]). Therefore, there exists a localized ground state in this case.

III. COMPARISON WITH PREVIOUS WORK

The literature on "localization phenomena and optical polarons" is enormously extensive.

There exists a variety of variational calculations, providing nonanalytical upper bounds for the ground-state energy. The point of nonanalyticity at $\alpha=\alpha_c$ is interpreted as localization transition. Synonymously, the terms "phase transition" and "self-trapping transition" are used. As for a compilation of literature, see Ref. 12. Without underestimating the merits of these variational approaches as such, the proposed localization transition has to be classified as an artifact of the approximation. As for the particular aspects of breaking of the translational symmetry, we additionally refer to Haga[13] [who supposed inequality (16) to be violated], as well as to Manka[14] and to Hipolito and de Bodas.[15]

On the other hand, Höhler[16] and Haken[17] stressed in early papers that a translation-symmetry breaking is impossible (without providing a proof). Toyozawa (see, e.g., Ref. 18) emphasized that the localized solution, found in adiabatic approximations, has to be superposed to yield the true delocalized state of this system. Gross[19] proved the inequality $E_0(\mathbf{0})\le E_0(\mathbf{Q})$; apparently, this is not sufficient to exclude symmetry breaking. Peeters and Devreese[20] provide a critical review of the phase-transition literature. Their work, in turn, was initiated by an earlier one of Lepine and Matz.[21]

The present authors (together with Schliffke) studied the free energy $F=F(\mathbf{Q},T)$, T denoting the temperature, and proved, in Ref. 22, that inequality (16) holds for F, if $T>0$ and if the number of (optical) phonon modes is finite.

Closely related to the present work are two recent publications of Spohn[23] and Fisher and Zwerger.[24] Spohn uses a localization criterion, which differs from ours; adding to H_F an external potential $\kappa\mathbf{r}^2/2$, $\kappa>0$, he discusses (at finite temperature T) the functional-integral representation of the expectation value $\langle\mathbf{r}^2\rangle$ for the limits $T\to 0$ and then $\kappa\to 0$. Note that in this finite-temperature approach and for acoustical dispersion, the problem of degenerate ground states outside the Fock space (described in Sec. II) does not occur. Spohn's result [see Eq. (4.5) in Ref. 23] is as follows: Let $\omega(k)\sim k^{\nu}$ and $g(k)\sim k^{-\lambda}$, and assume the space dimensionality to be d. Moreover, define $\sigma\equiv(d+2-2\lambda)/\nu$. If one introduces a large-k cutoff in $g(k)$, then $\langle\mathbf{r}^2\rangle\to\infty$ for $\kappa\to 0$ and $\sigma>3$. Consequently, the ground state of the corresponding polaron is always delocalized. Fisher and Zwerger[24] calculate $\langle r^2\rangle$ within the Gaussian approximation and obtain delocalization for $\sigma>2$.

This is in agreement with our statement 1. We add as a comment that the introduction of a large-k cutoff is more than a technical trick, if it cannot be removed. Our method (see Sec. IV) is free from such a shortcoming.

Concerning the problem of translation-symmetry breaking, Spohn[25] has recently discussed a model for polarons in a finite volume. He proves that inequality (16) holds for all couplings, if

$$\int d^3k\, g^2(k)/\omega(k)<\infty\ ,$$
$$\int d^3k\, g^2(k)k^2/\omega^m(k)<\infty,\quad m=2,3\ , \tag{19}$$

where we have written the discrete $\mathbf{k}$ summation formally as an integration (to render a direct comparison with our assumptions in statement 1). Spohn shows that

$$\lim_{\beta\to\infty}\int d^3Q\,\mathrm{tr}Q^2\exp[-\beta H(\mathbf{Q})]/\mathrm{tr}\exp(-\beta H_F)=0\ , \tag{20}$$

which implies (16). In a slightly different functional-integral representation (see Gerlach, Löwen, and Schliffke[22]) we can directly recover (20). Interestingly enough, for acoustic dispersion and a continuous $\mathbf{k}$ space, Eq. (16) cannot be proved up to now.

IV. PROOF OF STATEMENTS 1 AND 2

In this section, we are concerned with optical polarons fulfilling the conditions for statement 1. For example, the standard optical Fröhlich model [$\omega(k)=\omega_0>0$, $g(k)\sim 1/k$] is included. It has a long-ranged coupling and in contrast to acoustical models it requires no renormalization.

Our proof is based on the following two functional analytical theorems.

Theorem I: Let H be a Hamiltonian, defined on a Hilbert space $\mathcal{H}$ and bounded from below, the ground-state energy being E_0. Choose a fixed representation of the Hilbert space. If E_0 is an eigenvalue and $\exp(-H)$ is positivity improving with respect to the fixed representation, then E_0 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. This property clearly 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 the exponential of a Hamiltonian is positivity improving.

Theorem II: Let $H=H_0+U$ and choose a fixed representation of the Hilbert space. Suppose that U is a multiplication operator (i.e., that it is diagonal in the 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 a strong resolvent sense. Then $\exp(-H)$ is positivity improving, if $\exp(-H_0)$ is positivity improving.

For a proof of these theorems, we refer to Reed and Simon (Chap. XIII in Ref. 26). We shall use them twice to obtain a proof for statements 1 and 2.

Firstly, we turn to the localization problem and prove statement 1. We suppose that the ground state of H_F is localized and then we deduce a contradiction. Let

$\Psi_1 \in \mathcal{H}_F$ be such a localized ground state of H_F. Then, because of the translational symmetry of H_F, there exists $\boldsymbol{\lambda} \in \mathbb{R}^3$ such that $\Psi_2 \equiv \exp(i\boldsymbol{\lambda}\cdot P_T)\Psi_1$ is linearly independent of Ψ_1. Clearly, $\Psi_2 \in \mathcal{H}_F$ and Ψ_2 is a localized ground state of H_F, too.

Now, as an insertion, we show that $\exp(-H_F)$ is positivity improving. As representation, we take the Schrödinger (position) representation for the electronic coordinate and the Q representation for the phonon coordinates. The latter is obtained by rewriting the annihilation and creation operators $a(\mathbf{k})$ and $a^\dagger(\mathbf{k})$ in terms of position and momentum operators $q(\mathbf{k})$ and $p(\mathbf{k})$ (see Ginibre[27] for details), such that the $q(\mathbf{k})$'s act as multiplication operators. For an extensive mathematical discussion of the Q representation, we refer to Simon.[28]

In this chosen representation, $H_{I,F}$ acts as multiplication operator. The analysis of Fröhlich[3] makes clear that—under the conditions of statement 1—$H_{I,F}$ can be approximated by bounded multiplication operators U_n as required in theorem II. Now, in order to prove that $\exp(-H_F)$ is positivity improving, theorem II ensures us that it is sufficient to show that $\exp(-\mathbf{p}^2/2-H_{0,\mathrm{ph}})$ is positivity improving. But this follows directly from the fact that $\exp(-\mathbf{p}^2/2)$ is positivity improving with respect to the Schrödinger representation for the electron and that $\exp(-H_{0,\mathrm{ph}})$ is positivity improving in the phonon Q space (see again Simon[28]). By this, our insertion of the proof of the positivity-improving property of $\exp(-H_F)$ is finished.

Now we can continue our original proof. By theorem I, it follows that the ground-state energy of H_F is a simple eigenvalue. But this is the desired contradiction to the fact that we can construct two different localized ground states Ψ_1 and Ψ_2, if there would exist one localized ground state Ψ_1. Consequently, the ground state of H_F cannot be localized.

Secondly, we prove statement 2, that is Eq. (16). Let us consider the Hamiltonian $\tilde{H}_F$ [see (9)], defined on another, new Hilbert space

$$\mathcal{H}_c = F \otimes L^2([-a,a[^3), \quad 0<a<\infty \tag{21}$$

restricting the electronic functions to a finite cube with length a (they are periodically continued to define them on $\mathbf{R}^3$). Of course, we have to explain how the operators $\mathbf{r}$ and $\mathbf{p}$ are defined on the space $L^2([-a,a[^3)$: $\mathbf{r}$ acts as usual multiplication operator and $\mathbf{p}$ is defined as the multiplication operator in the associated discrete Fourier space. Note that $\exp(i\boldsymbol{\lambda}\cdot\mathbf{p})$ acts in such a way as to cause a translation of $\boldsymbol{\lambda}$.

An important fact is the following: Since $\tilde{H}_F$ does not depend on $\mathbf{r}$, the ground-state wave function(s) of $\tilde{H}_F$ on $\mathcal{H}_c$ can always be written as a product, namely the ground-state wave function(s) of $H(\mathbf{Q}_n)$ times an eigenfunction of $\mathbf{p}$ with eigenvalue $\mathbf{Q}_n$; recall also Eqs. (13)–(15). The associated ground-state energy is just $E_0(\mathbf{Q}_n)$. Let $\Psi(\mathbf{Q}_n)$ be such a ground-state wave function of $\tilde{H}_F$ on $\mathcal{H}_c$. Here, since $\mathbf{p}$ has only discrete eigenvalues, belonging to the discrete Fourier space of $L^2([-q,a[^3)$, $\mathbf{Q}_n$ belongs to this discrete Fourier space. The index n at $\mathbf{Q}_n$ denotes the discreteness.

Note that true eigenfunctions of $\mathbf{p}$ exist in the new Hilbert space $\mathcal{H}_c$, in contrast to the original Hilbert space $\mathcal{H}_F$. Furthermore, the phononic part of $\Psi(\mathbf{Q}_n)$ is square summable too, if $\Psi(\mathbf{Q}_n)$ corresponds to a ground state of $\tilde{H}_F$ and if the phonon dispersion is optical, as has been shown by Fröhlich.[3] This enables us to apply theorem I, where the ground-state energy of $\tilde{H}_F$ is required to be a true eigenvalue.

Now, suppose that Eq. (16) is violated for a certain $\mathbf{Q}_c \neq \mathbf{0}$, i.e., let us assume $E_0(0) \geq E_0(\mathbf{Q}_c) = E_0(|\mathbf{Q}_c|)$. Then, we deduce a contradiction: We choose the length a fixed as $a \equiv \pi/|Q_c|$, such that $(Q_c,0,0)$ as well as $(-Q_c,0,0)$ belong to the discrete Fourier space associated to $L^2([-a,a[^3)$. Consequently, $\tilde{H}_F$ defined on $\mathcal{H}_c$ has a degenerate ground state. But, on the other hand, there exists a representation such that $\exp(-\tilde{H}_F)$ is positivity improving, which we shall show below. This is a contradiction to theorem I. Consequently Eq. (16) is proved.

We add the proof that $\exp(-\tilde{H}_F)$, defined on $\mathcal{H}_c$, is positivity improving. As representation, we choose the phonon Q space and the electronic position space $L^2([-a,a[^3)$. In this representation, H_I acts as a multiplication operator. Consequently, by theorem II, all that remains to do is to show that $\exp[-(\mathbf{p}-\mathbf{P}_{\mathrm{ph}})^2/2-H_{0,\mathrm{ph}}]$ is positivity improving. We represent $\exp[-(\mathbf{p}-\mathbf{P}_{\mathrm{ph}}]^2/2]$ as the Fourier integral

$$\exp[-\tfrac{1}{2}(\mathbf{p}-\mathbf{P}_{\mathrm{ph}})^2] = (2\pi)^{-3/2}\int d^3\lambda \exp(-\boldsymbol{\lambda}^2/2) \times \exp(i\boldsymbol{\lambda}\cdot\mathbf{p})\exp(-i\boldsymbol{\lambda}\cdot\mathbf{P}_{\mathrm{ph}}) . \tag{22}$$

Now, $\exp(-H_{0,\mathrm{ph}})$ is positivity improving with respect to the phonon coordinates and positivity preserving with respect to the electron coordinates. $\exp(-i\boldsymbol{\lambda}\cdot\mathbf{P}_{\mathrm{ph}})$ is positivity preserving with respect to both phonon and electron coordinates (see again Simon[28]). The positivity of the Fourier transform $\exp(-\lambda^2/2)$ and the fact that $\exp(i\boldsymbol{\lambda}\cdot\mathbf{p})$ acts as translation operator ensures us that $\int d^3\lambda \exp(-\boldsymbol{\lambda}^2/2)\exp(i\boldsymbol{\lambda}\cdot\mathbf{p})\exp(-i\boldsymbol{\lambda}\cdot\mathbf{P}_{\mathrm{ph}})$ is positivity improving with respect to the electron coordinates and positivity preserving with respect to the phonon coordinates. Consequently, $\exp[-(\mathbf{p}-\mathbf{P}_{\mathrm{ph}})^2/2-\mathbf{H}_{0,\mathrm{ph}}]$ is positivity improving in the chosen representation.

Thus, we have excluded the possibility of spontaneous symmetry breaking in free-polaron systems.

We remark that this result also implies that the ground state of H_F is nondegenerate (in the distributional sense) and delocalized, as it belongs to zero total momentum. Nevertheless, we have given an extra proof for delocalization of the polaron ground-state wave function in the first part to illustrate the applicability of theorems I and II.

V. THE WANNIER EXCITON-PHONON SYSTEM

The Wannier exciton-phonon system can be treated in a similar way as the free polaron. We first recall the Hamilton H_E; the reader will easily recover the analogy with the corresponding parts in Sec. I. According to Haken,[29] H_E is given in the center-of-mass and relative coordinates $\mathbf{R}$ and $\mathbf{r}$ for electron and the hole, the associated momenta being $\mathbf{P}$ and $\mathbf{p}$ ($\hbar=1$):

$$H_E=\mathbf{P}^2/(2M)+H_h+H_{0,\mathrm{ph}}+H_{I,E} \ , \tag{23}$$

where

$$H_h=\mathbf{p}^2/(2\mu)-Z/r, \quad Z>0 \tag{24}$$

and

$$H_{I,E}=\int d^3k\, g(k)[\rho(\mathbf{k},\mathbf{r})\exp(i\mathbf{k}\cdot\mathbf{R})a(\mathbf{k})+\mathrm{H.c.}] \ . \tag{25}$$

Here,

$$\rho(\mathbf{k},\mathbf{r})=\exp(i\mathbf{k}\cdot\mathbf{r}m_2/M)-\exp(-i\mathbf{k}\cdot\mathbf{r}m_1/M) \ , \tag{26}$$

and $M=m_1+m_2$ and $\mu=m_1m_2/M$ are the total and the reduced mass, respectively, where m_1 is the electron, m_2 the hole mass. $g(k)$ is assumed to be real. The associated Hilbert space is now

$$\mathcal{H}_E=F\otimes L^2(\mathbb{R}^3)\otimes L^2(\mathbb{R}^3) \ . \tag{27}$$

With a Lee-Low-Pines transformation, defined by $U_E=\exp(-i\mathbf{P}_{\mathrm{ph}}\cdot\mathbf{R})$, one finds

$$\tilde{H}_E\equiv U_E^{-1}H_E U=(\mathbf{P}-\mathbf{P}_{\mathrm{ph}})^2/(2M)+H_h+H_{0,\mathrm{ph}}+H_{I,E} \ , \tag{28}$$

where

$$\tilde{H}_{I,E}=\int d^3k\, g(k)[\delta(\mathbf{k},\mathbf{r})a(\mathbf{k})+\mathrm{H.c.}] \ . \tag{29}$$

$\tilde{H}_E$ does not depend on $\mathbf{R}$. Therefore, $\mathbf{P}$ may be replaced by a c number $\mathbf{Q}$. Let $H_E(\mathbf{Q})$ be the associated total-momentum decomposed Hamiltonian with ground-state energy $E_0(\mathbf{Q})$.

In the case of an exciton-phonon system, the phonon-induced localization concerns the center-of-mass coordinates (see Toyozawa,[30] and Adamowski, Gerlach, and Leschke[31]); the translational invariance of H_E is connected with this variable. As for the relative coordinate, the wave function is assumed to be localized. For physical interesting cases (e.g., the Fröhlich model) this can definitively be proven; for general $\omega(k)$ and $g(k)$, fulfilling the assumptions of statement 1, this cannot be taken for granted; we refer to Ref. 32. The aspect of symmetry breaking may be introduced as in Sec. II. In particular, the absence of symmetry breaking may again be demonstrated by proving inequality (16) for the ground-state energy $E_0(\mathbf{Q})$ of the exciton.

In the remainder of this section, we generalize statements 1 and 2 as well as the proof of Spohn[23] (mentioned in Sec. III) to the case of an exciton-phonon system.

Concerning the work of Spohn, we remark that the finite-temperature expectation value of $\mathbf{R}^2$ can be represented as a functional-integral expression (Ref. 23), the action S now being given by

$$S=\tfrac{1}{2}\int_0^\beta[M\dot{\mathbf{R}}^2(\tau)+u\dot{\mathbf{r}}^2(\tau) -2Z/|\mathbf{r}(\tau)|+\kappa\mathbf{R}^2(\tau)]d\tau+S_I \ . \tag{30}$$

As for S_I see, e.g., Adamowski, Gerlach, and Leschke.[33] A comparison with the action of the free polaron shows that now two three-dimensional Wiener integrations have to be done; the one concerning $\mathbf{R}(\tau)$ corresponds to the polaron case. Moreover, we have four similar interaction terms. The theory of Spohn[23] is directly applicable to this case. The result is delocalization in the center-of-mass coordinates, i.e., $\langle\mathbf{R}^2\rangle\to\infty$ as $\kappa\to 0$ for $\sigma>3$.

Furthermore, we remark that the proof of (16) of Spohn[25] for discrete $\mathbf{k}$ space is easily done for excitons, too (see Schmidt[34] for the path-integral formula and the brief discussion of Gerlach, Löwen, and Schliffke[22]).

We have formulated our proof of Sec. IV in such a way that it is directly transferable to the exciton-phonon system. As for $\omega(k)$ and $g(k)$, we need the assumptions of statement 1. In fact, in the Q representation of the phonon coordinates and the Schrödinger representation of the center-of-mass and relative coordinates, $H_{I,E}$ as well as $\tilde{H}_{I,E}$ act as multiplication operators. The rest of the Hamiltonians are positivity improving; this can be seen in the same way as in Sec. IV. Consequently, we can apply twice our theorems I and II to demonstrate that a simultaneous localization in the relative, center-of-mass, and phonon coordinates cannot take place for any coupling strength and to exclude spontaneous symmetry breaking, i.e., to show (16).

VI. GENERALIZATIONS AND CONCLUSIONS

Firstly, we mention some generalizations. Our proof is also valid for several branches of phonons, for arbitrary spatial dimension and for anisotropic cases. An interesting question is whether a general band structure $\varepsilon(\mathbf{p})$ instead of $\mathbf{p}^2/2$ in Eq. (1) can change the result. Our proof holds for such a band structure $\varepsilon(\mathbf{p})$, if the Fourier transform of $\exp[-\varepsilon(\mathbf{p})]$ is strictly positive. Then the crucial step (22) of the proof can be done in an analogous manner. This condition is fulfilled for $\varepsilon(\mathbf{p})=ap^\nu$, $a>0$, if $0<\nu\leq 2$ (see Montroll and Shlesinger[35]). Unfortunately, the physical interesting case $\varepsilon(\mathbf{p})=\lambda p^2+\mu p^4$, $\lambda,\ \mu>0$, is not included (see theorem 5 of Simon[36]).

The same proof is possible if the Fourier transform of $\varepsilon(\mathbf{p})$ exists and is a nonpositive bounded function, $g(k)$ being square integrable and $\omega(k)$ optical. Then, the positivity-improving property of $\exp[-\varepsilon(\mathbf{p})]$ is shown by developing the exponential in its power series. This is possible, since $\varepsilon(\mathbf{p})$ is defined anywhere.

Another generalization is concerned with a polaron exposed to an additional potential V. V may be caused by defects, external fields, etc. If this potential is of short-range type, the system may indeed show a localization transition (see Löwen[32]). Further details will be given in a forthcoming publication.

Finally, we remark that our discussion of symmetry breaking can also be done for a small optical polaron. Even in this case we can prove Eq. (16) with our methods, $\mathbf{Q}$ now belonging to the first Brillouin zone of the lattice. The result is that a small polaron cannot be localized over the lattice sites and that the translational symmetry cannot be broken. As for details we refer to Ref. 32.

In conclusion, we have shown the absence of phonon-induced localization in free-polaron and exciton-phonon systems for two cases: firstly, for acoustical disperson and short-range couplings (this was the result of Spohn[23]) and secondly for optical dispersion and arbitrarily ranged couplings.

The absence of spontaneous symmetry breaking was demonstrated for both polaron and exciton-phonon systems and optical dispersion. For the acoustical case there exists no proof up to now, although the result (20), obtained in a discrete **k** space, seems to indicate that the ground state respects the translational symmetry in the acoustical case and for a continuous **k** space, too.

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