ABSENCE OF PHONON-INDUCED LOCALIZATION IN POLARON SYSTEMS

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We prove that the ground-state wave function of an optical polaron is delocalized for any coupling strength. This result holds true for arbitrary spatial dimensions, anisotropic coupling and certain band-structures, deviating from the parabolic case. In addition, an extension to the (Wannier) exciton-phonon problem is possible.

1. INTRODUCTION AND DISCUSSION OF THE PROBLEM

The standard polaron model is defined by a Hamiltonian H, which was firstly proposed by Fröhlich, Pelzer and Zienau [1]. Using $\hbar\omega$ and $\sqrt{\hbar/m\omega}$ as units of energy and length, m and ω being the electron mass and an arbitrary frequency, H reads as follows:

$$(\hbar\omega)^{-1} H := \frac{\vec{p}^2}{2} + \int d^3k\, \omega(\vec{k})\, a^+(\vec{k})\, a(\vec{k}) + \sqrt{\alpha} \int d^3k\, g(\vec{k}) \left[\exp(i\vec{k}\vec{r})\, a(\vec{k}) + \text{h.c.} \right] \qquad (1)$$

On the right-hand side of (1), all quantities are dimensionless. In detail, $\vec{p}$ and $\vec{q}$ are momentum operator and position of the electron; $\vec{k}$, $\omega(\vec{k})$, $a^+(\vec{k})$, $a(\vec{k})$ are wave vector, dispersion, creation- and annihilation-operator of a phonon. Finally, $g(\vec{k})$ is the electron-phonon coupling and α the coupling constant. One should notice, that H is defined on a product Hilbert-space $\mathcal{H}$, namely

$$\mathcal{H} := \mathcal{H}_{Ph} \otimes \mathcal{H}_E \qquad (2)$$

where $\mathcal{H}_{Ph}$ denotes the usual Fock-space for phonons and $\mathcal{H}_E$ the one-particle Hilbert-space.

We now turn to the localization problem. 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 $\mathcal{H}$ i.e. normalizable with respect to the electron and phonon part. In any other case, Ψ is called delocalized. Let us specifically discuss the question, whether there exists a localized ground-state Ψ_0 of H. H commutes with the operator $\vec{P}$ of total momentum, that is

$$\vec{P} := \vec{p} + \int d^3k\, a^+(\vec{k})\, a(\vec{k}) =: \vec{p} + \vec{P}_{Ph} \tag{3}$$

Consequently, there exist simultaneous eigenfunctions of $\vec{P}$ and H. Now, the general eigenfunction of $\vec{P}$ with eigenvalue $\vec{Q}$ is given by

$$\chi(\vec{Q}) := \exp\left(i\,[\,\vec{Q} - \vec{P}_{Ph}\,]\,\vec{r}\right) \Phi_{Ph} \quad , \qquad \Phi_{Ph} \in \mathcal{H}_{Ph} \tag{4}$$

As it is sufficient to solve for $H\,\chi(\vec{Q}) = E(\vec{Q})\,\chi(\vec{Q})$, we arrive at

$$H(\vec{Q})\,\chi(\vec{Q}) = E(\vec{Q})\,\chi(\vec{Q}) \quad , \tag{5}$$

$$H(\vec{Q}) := \frac{1}{2}(\vec{Q} - \vec{P}_{Ph})^2 + \int d^3k\, \omega(\vec{k})\, a^+(\vec{k})\, a(\vec{k}) + \sqrt{\alpha} \int d^3k\, g(\vec{k})\,[\, a(\vec{k}) + a^+(\vec{k})\,] \tag{6}$$

We add as a remark, that $H(\vec{Q})$ defines the momentum decomposition of the Hamiltonian $\tilde{H}$, introduced by Lee, Low, Pines [2]. In fact, replacing $\vec{Q}$ in $H(\vec{Q})$ by the momentum operator $\vec{p}$, one finds $\tilde{H}$.
In view of equ. (4) , it appears not at all clear, whether there exists a single localized eigenfunction of H - for a given value of $\vec{Q}$, $\chi(\vec{Q})$ is apparently delocalized. We discuss this point a bit more: If α is sufficiently small, we know from perturbation theory, that the ground-state Ψ_0 of H is of type $\chi(\vec{Q}=\vec{0})$. Consequently, the ground-state energy $E_0(\vec{Q})$ fulfills

$$E_0(\vec{0}) < E_0(\vec{Q} \neq \vec{0}) \tag{7}$$

in a certain surrounding of $\alpha = 0$. Let us tentatively assume, that (7) was not true for $\alpha > \alpha_c$. Then one could deduce i): The ground-state is infinitely degenerated, as $E_0(\vec{Q})$ depends only on $|\vec{Q}|$. ii): If the minimum of $E_0(\vec{Q})$ occurs for a subset of $\vec{Q}$-vectors with different length, a suitable superposition of the corresponding eigenfunctions might yield a localized state.

2. RESULTS AND INDICATION OF THEIR PROOF

Our central statement excludes the above speculations i) and ii). We show: Let $\omega(\vec{k}) \geq \omega_0 > 0$ and $\int d^3k\, |g(\vec{k})|^2 / (1+k^2) < \infty$. Then, inequality (7) holds for $0 \leq \alpha < \infty$. Consequently, the ground-state Ψ_0 of H is nondegenerate and delocalized for any coupling strength.

The proof of this statement is based on the following two theorems:
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 $\mathcal{H}$. If E_0 is an eigenvalue and $\exp(-H)$ is positivity improving in this representation, then E_0 is a simple eigenvalue.
ii) Let $H = H_0 + V$ and choose a fixed representation of $\mathcal{H}$. Suppose that V is a multiplication operator and that there exists a sequence of bounded multiplication operators V_n such that $H_0 + V_n \to H$ and $H - V_n \to H_0$ in a strong resolvent sense. Then $\exp(-H)$ is positivity improving, if this is true for $\exp(-H_0)$. As for proofs, see ref. [3].
We apply these theorems to the Hamiltonian $\tilde{H}$ of Lee, Low and Pines (see equ. (6) and the remarks thereafter) and start with theorem i). Our assumptions guarantee the boundedness of $\tilde{H}$ from below. To assure that E_0 is an eigenvalue, we confine the electron to a box of finite volume - as for this technical point we refer to [4]. Finally, we have to establish the positivity-improving property. This will be done by means of theorem ii): If we choose the Fröhlich interaction term to be V, it is well known that V is a multiplication operator in the position-representation of $\mathcal{H}_{Ph}$; so we use this representation. Moreover, the existence of operators V_n was proven by J. Fröhlich in [5]. Turning to $\exp(-H_0)$, where $H_0 := \tilde{H} - V$, we realize that the free phonon part is positivity improving with respect to the phonon and positivity preserving with respect to the electron coordinates. In a final step we use a Gaussian linearization for the remaining term in H_0, involving $[\vec{p} - \vec{P}_{Ph}]^2$:

$$\exp\left(-\frac{1}{2}[\vec{p} - \vec{P}_{Ph}]^2\right) = (2\pi)^{-\frac{3}{2}} \int d^3\lambda \exp(-\lambda^2/2) \exp(i\vec{\lambda}\vec{p}) \exp(-i\vec{\lambda}\vec{P}_{Ph}) \qquad (8)$$

We choose a position representation also for $\mathcal{H}_E$. Then the right-hand side of (8) is positivity improving with respect to the electron- and positivity preserving with respect to the phonon coordinates.

In summary, exp(-H) is positivity improving. Consequently, the ground-state eigenvalue of H is simple and belongs to $\vec{Q} = \vec{0}$.

3. EXTENSIONS

To begin with, we mention that the above proof is valid for arbitrary spatial dimensions as well as for anisotropic electron-phonon coupling, provided the conditions on $\omega(\vec{k})$ and $g(\vec{k})$ from section two are fulfilled. Moreover, a coupling of the electron to several phonon branches is admissible. A (Wannier) exciton-phonon system can be treated in a similar manner as a free polaron. In this case, we have instead of equ. (2): $\mathcal{H} = \mathcal{H}_{Ph} \otimes \mathcal{H}_E \otimes \mathcal{H}_H$ where "H" is to indicate the hole. Choosing a position representation for $\mathcal{H}_H$, the proof from section two can be transferred. We stress the particularly interesting result that the center-of-mass part of the wave function is always delocalized; no self-trapping occurs. As for details see [4].
Very interesting problems (far from being solved) are connected with the discussion of a nonparabolic band-structure $\varepsilon(\vec{p})$. Mimicking the above proof, equation (8) would contain the Fourier-transform $f(\vec{\lambda})$ of $\exp(-\varepsilon(\vec{p}))$ instead of $\exp(-\lambda^2/2)$. If $f(\vec{\lambda})$ was positive, all conclusions would be unchanged. This is true for

$$\varepsilon(\vec{p}) = a\,p^{\nu} \quad , \quad a > 0 \quad , \quad 0 < \nu \leq 2 \tag{9}$$

(see Montroll, Shlesinger in [6]). The case $\nu > 2$ cannot be included. Unfortunately, the same holds true for the physically appealing example $\varepsilon(\vec{p}) = a\,p^2 + b\,p^4$, $a > 0$, $b > 0$ (see Simon in [7]) and many other cases $\varepsilon = \varepsilon(|\vec{p}|)$, which can be found by direct inspection of tables of Fourier sine transforms.

4. REFERENCES

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