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Ground-state symmetry of a generalized polaron

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We study the structure of the ground-state wave function for a general model of a continuum polaron in d dimensions, coupled to either optical or acoustical phonons. Using a path-integral approach we derive a simple criterion which is sufficient to guarantee that the exact ground state is delocalized. This criterion applies to most polaron models studied so far and thus implies that interaction with phonons generally does not lead to a breaking of the translational symmetry, even for arbitrary strong coupling. We discuss briefly the distinction between self-trapping and localization.

Recently the problem of self-trapping of a polaron,[1–4] has gained renewed interest, both theoretically[5–8] and experimentally.[9] The self-trapping effect is usually understood to be associated with a drastic change in the polaron ground state at a certain value of the coupling strength to the phonons. Such a change may reveal itself in the ground-state energy or its derivatives[5] as a function of coupling strength. Alternatively, an appropriately defined effective mass is found to increase dramatically when the polaron becomes self-trapped. However, the clearest theoretical signature of the "self-trapping transition" is in the nature of the ground-state wave function within the adiabatic approximation, where the kinetic energy of the lattice (phonons) is ignored. It is found[4,6] that under certain conditions the *adiabatic* ground state changes sharply, at a particular value of the coupling strength, from an extended to a localized or self-trapped regime. It is the purpose of this paper to study the symmetry of the *exact* ground-state wave function, not confined to the adiabatic treatment. In particular we are interested in whether the translational symmetry present in the Hamiltonian is spontaneously broken due to the coupling to the phonon bath.[10] We derive a criterion which is sufficient to guarantee that this symmetry is not broken and the exact ground state delocalized. This criterion should be useful in evaluating the credibility of various approximations to the polaron problem. For example, it applies to most of the polaron models studied recently, thus indicating that the self-trapping transition found in the adiabatic approach must *not* be interpreted as a true localization transition.

As a model we take a generalized Fröhlich-type Hamiltonian,[11]

$$\mathscr{H}=P^2/2M+\sum_k \hbar\omega(k)a_k^\dagger a_k + \sum_k V(k)e^{ikr}(a_k+a_{-k}^\dagger)\ . \tag{1}$$

The position r and momentum p of the particle with mass M represent d-dimensional vectors. The $a_k^\dagger$ and a_k are the usual Bose creation and annihilation operators for phonons of wave vector k. In the limit of long wavelengths, $k\rightarrow 0$, the phonon frequencies $\omega(k)$ are assumed to behave as

$$\omega(k)\sim |k|^\nu,\quad k\rightarrow 0\ . \tag{2}$$

Thus the usual optical or acoustical phonons correspond to $\nu=0$ or $\nu=1$, respectively, but our model may equally well represent a coupling to other harmonic degrees of freedom with arbitrary dispersion $\omega(k)$. Similarly we assume that the coupling $V(k)$ behaves for small k as

$$V(k)\sim\sqrt{\alpha}\,|k|^{-\lambda},\quad k\rightarrow 0 \tag{3}$$

with a coupling strength α and exponent λ. In the original Fröhlich model,[11] for instance, we have $\nu=0$ and $\lambda=(d-1)/2$, whereas a deformation potential in $d=3$ corresponds to[2,6] $\nu=1$ and $\lambda=-\frac{1}{2}$. We will see below that only the small-k behavior of $\omega(k)$ and $V(k)$ is relevant in determining the symmetry of the ground-state wave function. Thus we need not specify the generally quite complicated structure of the dispersion and coupling when k becomes of the order of the inverse lattice spacing. We do, however, assume that $V(k)$ is cut off at high k.

The Hamiltonian (1) is invariant under the transformation $r\rightarrow r+r_0$, $a_k\rightarrow e^{-ikr_0}a_k$. Naively one expects that the ground-state wave function will respect this translational symmetry and be extended (delocalized) in the coordinate r. To study whether or not this symmetry can be spontaneously broken, giving a localized ground state, it is convenient to explicitly break the symmetry by adding a potential energy term of the form $Kr^2/2$ to the Hamiltonian (1), and consider the behavior in the limit $K\rightarrow 0$.[12] To this end we introduce the generating functional ($\beta=1/k_BT$)

$$G(\eta,K)=\lim_{\beta\rightarrow\infty}\mathrm{Tr}(e^{-\beta\mathscr{H}}e^{\eta r})/\mathrm{Tr}(e^{-\beta\mathscr{H}}) \tag{4}$$

which by differentiation gives equilibrium expectation values of the moments of r. The limit $\beta\rightarrow\infty$ ensures that these averages are in fact ground-state expectation values. The second moment of r

$$\langle r^2\rangle(K)=\frac{\partial^2}{\partial\eta^2}G(\eta=0,K) \quad (5)$$

is a convenient measure of the degree of spatial localization of the wave function. If the $K\to0$ limit of $\langle r^2\rangle(K)$ is finite, the translational symmetry has been broken and the ground state is localized. An infinite value indicates a delocalized ground state.[13]

The generating functional is most conveniently analyzed in a path-integral representation. The phonon path integrals, being quadratic, can be evaluated explicitly. Using standard results it is straightforward to express G as

$$G(\eta,K)=\frac{\int Dr\, e^{\eta r(\tau=0)}e^{-S/\hbar}}{\int Dr\, e^{-S/\hbar}}\equiv\langle e^{\eta r(\tau=0)}\rangle , \quad (6)$$

with an effective action S,

$$S=\tfrac{1}{2}\int d\tau(M\dot{r}^2+Kr^2)+\tfrac{1}{2}\int d\tau d\tau'\sum_k g_k(\tau-\tau')(1-\cos\{k[r(\tau)-r(\tau')]\}) . \quad (7)$$

Here we have defined a function

$$g_k(\tau)=\frac{1}{\hbar}\,|V(k)|^2e^{-\omega(k)|\tau|} . \quad (8)$$

In (6) the path integral is over paths $r(\tau)$ with the "imaginary time" τ running from $-\infty$ to ∞. Thus (6) can be viewed[8,14] as a generating functional for a one-dimensional classical statistical mechanical system with τ playing the role of a "spatial" coordinate and r representing the classical degrees of freedom.

Due to the nonlinearities which enter the last term of the effective action (7), it is impossible to calculate the path integral for G exactly. It is, however, not difficult to give at least a *sufficient* criterion for a delocalized ground state. To this end, we first observe that the nonlocal (in τ) term in S is always positive and that $1-\cos x\le x^2/2$. Therefore the Gaussian model [denoted S_0, Eq. (10) below] which arises from S by replacing

$$1-\cos\{k[r(\tau)-r(\tau')]\}$$

with

$$\tfrac{1}{2}\{k[r(\tau)-r(\tau')]\}^2 ,$$

suppresses all paths $r(\tau)$ more strongly than the original model, except for the special paths $r(\tau)=\text{const}$. Thus, on average, the paths $r(\tau)$ will fluctuate less (with τ) in the Gaussian model. This in turn implies that the Gaussian model will be more effective at localizing the particle. In other words, the spatial extent of the ground-state wave function for the Gaussian model, $\langle r^2\rangle_0(K)$, will give a lower bound to the spatial extent of the true wave function,

$$\langle r^2\rangle_0(K)\le\langle r^2\rangle(K) . \quad (9)$$

Within the Gaussian model $\langle r^2\rangle_0(K)$ can be evaluated explicitly. If $\langle r^2\rangle_0(K)\to\infty$ as $K\to0$ we may then safely conclude that the exact ground-state wave function of the Hamiltonian (1) is spatially delocalized. If, on the other hand, $\langle r^2\rangle_0(K)$ has a finite $K\to0$ limit, the exact ground state may or may not be localized.

The action for the Gaussian model, described above, factorizes into d one-dimensional models[15]

$$S_0=\sum_{j=1}^{d}S_0(x_j)$$

of the form

$$S_0(x)=\tfrac{1}{2}\int d\tau(M\dot{x}^2+Kx^2)+\tfrac{1}{2}\int d\tau d\tau' g(\tau-\tau')[x(\tau)-x(\tau')]^2 , \quad (10)$$

with

$$g(\tau)=\frac{1}{2d\hbar}\sum_k k^2|V(k)|^2e^{-\omega(k)|\tau|} . \quad (11)$$

The function $g(\tau)$ is proportional to the coupling strength α. Its long-time behavior follows from the $k\to0$ behavior of $\omega(k)$ and $V(k)$. In particular for $\nu\ne0$, we have $g(\tau)\sim|\tau|^{-\sigma}$ as $\tau\to\infty$, with[16]

$$\sigma=\frac{d+2-2\lambda}{\nu}\quad(\nu\ne0) . \quad (12)$$

For $\nu=0$, $g(\tau)$ falls off exponentially. The ground-state expectation value of r^2 for the Gaussian model can be obtained from the generating functional (6) with S replaced by S_0. This gives

$$\langle r^2\rangle_0(K)=\left[\frac{\hbar d}{2\pi}\right]\int_{-\infty}^{\infty}\frac{d\omega}{[M+\delta M(\omega)]\omega^2+K} , \quad (13)$$

with a frequency-dependent mass enhancement defined by

$$\delta M(\omega)=\frac{4}{\omega^2}\int_0^{\infty}d\tau g(\tau)[1-\cos(\omega\tau)] . \quad (14)$$

We now analyze (13) in the $K\to0$ limit. Consider first $\sigma>3$ corresponding to a $g(\tau)$ which vanishes faster than τ^{-3}. In this case $\delta M(\omega=0)$ exists and we find

$$\langle r^2\rangle_0(K)=\frac{\hbar d}{2}\frac{1}{(KM^*)^{1/2}},\quad K\to0 \quad (15)$$

with a finite effective mass

$$M^*\equiv M+\frac{2}{d\hbar}\sum_k k^2|V(k)|^2/\omega^3(k) . \quad (16)$$

For the Gaussian model (10), this effective mass is equivalent to the one originally introduced by Feynman.[17,18] Equation (15) shows that, for $\sigma>3$, as $K\to0$ the ground-state wave function (within the Gaussian model) delocalizes as $1/\sqrt{K}$ *regardless* of the coupling strength α. For σ in the range $2<\sigma<3$ the effective mass is no longer finite. The ground state is still delocalized, however, since $\langle r^2\rangle_0(K)$ diverges as $K^{-(\sigma-2)/(\sigma-1)}$ when $K\to0$. The value $\sigma=2$ is a special marginal case. From (13) we deduce that $\langle r^2\rangle_0$ diverges as $\ln|K|$ implying a delocalized ground state. However, if an additional periodic potential is added to the action (10), then it has been shown[14,19–21] that there exists a critical coupling strength, α_c, such that for $\alpha > \alpha_c$ the ground state becomes localized. For $\sigma < 2$ the integral in (13) is finite as $K \to 0$ and the ground state is localized for arbitrary coupling strength, implying a broken translational symmetry.

The above analysis indicates that the ground state of the Gaussian model (10) is delocalized, regardless of the coupling strength, whenever

$$\sigma \equiv \frac{d+2-2\lambda}{\nu} > 2 \ . \tag{17}$$

The inequality (9) then shows that $\sigma > 2$ is a sufficient criterion to guarantee that the *exact* ground state of the Hamiltonian (1) is *delocalized.* On the other hand when $\sigma < 2$ the Gaussian model gives a localized ground state. Although we expect that in this case the exact ground state may in fact also be localized, we cannot draw any definite conclusions from the above arguments.

Applying the criterion (17) to a few particular examples of interest, we note that for the following cases the ground state is delocalized for arbitrary coupling strength, precluding any localization transitions: (i) all purely optical polaron models ($\nu \to 0$); (ii) the acoustical deformation potential coupling in $d = 3$; (iii) electrons on liquid helium,[22,23] for which $d = 2$, $\nu = 1$, and $\lambda = -\frac{1}{2}$.

It is instructive to compare our result (17) to a similar criterion recently arrived at by Spohn.[8] He finds that the ground state will be delocalized when $\sigma > 3$ in our notation. The result (17) shows, however, that this condition is, in fact, too restrictive since the ground state is delocalized regardless of the coupling strength also for $2 < \sigma \leq 3$. On the other hand, the effective mass, as defined in (16), is divergent for $\sigma \leq 3$ which suggests that the system's *dynamical* behavior may change nature[24] at $\sigma = 3$.

Finally it is interesting to contrast the criterion (17) with results from the adiabatic treatment of the self-trapping transition. According to the theory[4,6] when $\delta = d - 2\lambda - \nu - 2 \geq 0$ there is a self-trapping transition at a critical value of the coupling strength, above which the adiabatic ground state is localized. On the contrary, for $\delta < 0$ it is localized (self-trapped) for *any* coupling strength. This demonstrates clearly that the *adiabatic* ground state does not resemble, in any way, the *exact* ground state which as we have seen will in general be delocalized. In fact, we believe that the self-trapping transition found in the adiabatic approach is an artifact of the approximations used.[25] It is, however, possible that in features of the dynamical behavior, such as the polaron mobility, there are large, yet *continuous,* changes as a function of the coupling strength, which manifest themselves as a true transition within the adiabatic approximation.

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[13]It should be pointed out that a diverging $\langle r^2 \rangle$ may not necessarily imply a delocalized ground state since it is possible, in principle, to have a localized wave function falling off algebraically with distance such that $\langle r^2 \rangle$ is, in fact, infinite. Moreover we emphasize that, apart from the phonon coupling, no other mechanism is considered here which may lead to localization. Thus even if the ground state is delocalized according to the criterion (17) given below, a localization transition may still occur due to effects of a different origin like impurities or crystal imperfections producing a static random potential.
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between an infinite ($\sigma > 3$) and finite ($\sigma < 3$) zero-temperature mobility.

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