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Roughening and pinning transitions for the polaron

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Abstract. In the recent literature it is claimed that the polaron exhibits a transition from a delocalised to a localised ground state as the coupling to the phonon field is increased. The statistical mechanics analogy of this transition is the roughening transition. We argue that no such roughening can occur for the polaron. We point out the possibility of a pinning transition in a suitable, fixed pinning potential.

1. Introduction

The polaron (for a review see Devreese (1972)) is an electron coupled to the longitudinal optical mode of an ionic crystal. It is described by the Fröhlich Hamiltonian

$$H = -(\hbar^2/2m)\Delta + V(x) + \hbar\omega \int \mathrm{d}^3k\, a_k^+ a_k + \hbar\omega(\hbar/2m\omega)^{1/4}(4\pi\alpha)^{1/2} \int \mathrm{d}^3k\, |k|^{-1}\, \mathrm{e}^{\mathrm{i}kx}(a_k + a_{-k}^+). \tag{1.1}$$

We use here the standard notation: m is the mass of the electron, Δ the Laplacian in three dimensions. $\{a_k^+, a_k | k \in \mathbb{R}^3\}$ is the optical part of the phonon field, ω the frequency of the optical lattice vibration and α is the dimensionless coupling constant. Henceforth we set $m = \hbar = \omega = 1$ and keep the coupling constant α as the only parameter. V is an external potential. In most treatments, $V \equiv 0$. Physically V could originate from a well isolated lattice impurity or it could represent the periodic lattice potential.

We want to study ground state expectations of the polaron, in particular its spatial distribution $\rho_\alpha(q)\,\mathrm{d}^3q$. Quantum mechanically it is defined by

$$\lim_{T\to\infty} \mathrm{Tr}\, \mathrm{e}^{-TH} f(x)/\mathrm{Tr}\, \mathrm{e}^{-TH} = \langle f(x)\rangle_0(\alpha) = \int \mathrm{d}^3q\, \rho_\alpha(q) f(q) \tag{1.2}$$

for bounded and continuous functions f. Here $\langle\cdot\rangle_0(\ldots)$ denotes ground state expectations with the dependence on the parameters indicated in the round brackets. (In the first two terms $f(x)$ is understood as a function of the position operator x.)

If $V = 0$, then $\mathrm{Tr}\, \mathrm{e}^{-TH} = \infty$ because of the delocalisation of the electron. Therefore one has to add a confining potential and remove it *after* having taken the limit $T \to \infty$, i.e. remove it in the ground state. Two natural confining potentials suggest themselves: we add a potential $\frac{1}{2}\kappa x^2$, $\kappa > 0$, or we restrict the motion of the electron to the box Λ and take in the ground state the limit $\kappa \to 0$, resp. $\Lambda \uparrow \mathbb{R}^3$.

Feynman (1955) observed that the kernel of e^{-TH} can be written as a functional integral, cf Ginibre (1971) for some mathematical details. Because of their Gaussian character the phonon degrees of freedom can be integrated. The spatial distribution of the polaron is then obtained by the following prescription. Let $P(\mathrm{d}x(\cdot))$ be the Wiener measure. In our context we think of it as standard Brownian motion starting at $x(-T)$ with the uniform distribution d^3x. Then

$$\rho_\alpha(q) = \lim_{T\to\infty} \frac{1}{Z(2T)} \int P(\mathrm{d}x(\cdot))\delta(x(-T)-x(T))\delta(q-x(0)) \exp[-S_T(x(\cdot))]. \tag{1.3}$$

$Z(2T)$ is the obvious normalisation factor. The action S_T is given by

$$S_T(x(\cdot)) = \int_{-T}^{T} \mathrm{d}t\, V(x(t)) - \frac{\alpha}{\sqrt{2}}\frac{1}{2}\int_{-T}^{T}\mathrm{d}t \int_{-T}^{T}\mathrm{d}s \frac{g_T(|t-s|)}{|x(t)-x(s)|} \tag{1.4}$$

with

$$g_T(t) = (e^{-(2T-t)} + e^{-t})/(1-e^{-2T}) \tag{1.5}$$

for $0 \leqslant t \leqslant 2T$. The first δ-function ensures that the endpoints of the path, $x(-T)$ and $x(T)$, agree. Because of periodicity we could replace $x(0)$ by $x(T)$. Then in (1.3) we would integrate over all paths starting at q at $t=-T$ and ending at q at $t=T$. In the above form the analogy with statistical mechanics is more apparent.

We want to understand whether the polaron exhibits the phenomenon of localisation. In (1.4) we choose for V the confining potential $V(x) = \frac{1}{2}\kappa x^2$. This is in complete analogy to the external magnetic field h of a statistical mechanics model with $O(N)$ symmetry, say. If the temperature $\beta^{-1} < \beta_c^{-1}$, the limit $h \to 0_+$ singles out a particular phase with broken symmetry. With the potential added the polaron has the well defined spatial density $\rho_{\alpha,\kappa}(q)$ in the ground state. If the polaron is localised, then the limiting density

$$\lim_{\kappa\to 0} \rho_{\alpha,\kappa}(q) = \rho_\alpha(q) \tag{1.6}$$

is still normalised to one, i.e. $\int \mathrm{d}^3q\, \rho_\alpha(q) = 1$. If the polaron is delocalised, then

$$\lim_{\kappa\to 0} \rho_{\alpha,\kappa}(q) = 0. \tag{1.7}$$

With an appropriate normalisation, usually, one may still define an unnormalised polaron density. A convenient, although not completely sharp, criterion is the second moment

$$D(\alpha,\kappa) = \int \mathrm{d}^3q\, q^2 \rho_{\alpha,\kappa}(q). \tag{1.8}$$

If $D(\alpha, \kappa = 0_+) < \infty$, then the polaron is localised and $D(\alpha, \kappa = 0_+) \to \infty$ as $\alpha \to \alpha_c$, the critical coupling at which the polaron delocalises.

On the basis of variational calculations the following transition is predicted (Tokuda *et al* 1981), cf also Manka (1978), Feranchuk *et al* (1984), Tokuda and Kato (1982) Shoji and Tokuda (1981) and Jackson and Platzman (1981). The authors consider the impurity potential $V(x) = -\beta/|x|$, $\beta \geqslant 0$. The second moment (1.8) in the limit $\kappa \to 0_+$ is denoted by $D(\alpha, \beta)$. Then, if α is sufficiently large,

$$D(\alpha, \beta = 0) < \infty. \tag{1.9}$$

As α decreases the width of the spatial distribution of the polaron increases and there is a critical value α_c, $\alpha_c \simeq 8.5$, where $D(\alpha, \beta=0) \to \infty$ as $\alpha \to \alpha_c$. The dependence of $D(\alpha, \beta)$ on β is also discussed.

The occurrence of such a phase transition gains further support from the following observation. We consider the strong coupling limit $\alpha \to \infty$. Donsker and Varadhan (1983), cf also Adamowski *et al* (1980a), prove that for $V \equiv 0$ the ground state energy $E(\alpha)$ (more precisely: the bottom of the spectrum of H with the zero point energy of the phonon field subtracted) scales as $E(\alpha) \simeq \gamma\alpha^2$ and that γ is given by Pekar's variational formula

$$\gamma = \inf_{\psi, \int d^3x |\psi(x)|^2 = 1} \left(\tfrac{1}{2} \int d^3x |\mathrm{grad}\, \psi(x)|^2 - \frac{1}{\sqrt{2}} \int d^3x\, d^3x' |\psi(x)|^2 |x - x'|^{-1} \psi(x')|^2 \right). \tag{1.10}$$

Numerically $\gamma = -0.108\,5128\ldots$. Lieb (1977) shows that (1.10) has, up to translations, a unique minimum and that the minimising wavefunction ψ_0 is radial, infinitely often differentiable and has an exponential fall-off. This suggests that at infinite coupling

$$\rho_\infty(q) = \psi_0(q)^2 \tag{1.11}$$

which means that the polaron is localised. (The correct scaling limit $\alpha \to \infty$ shows that the argument is more subtle.) The problem to be answered is then whether this corresponds to a zero temperature ($\equiv$ infinite coupling) transition or whether it occurs at some finite value of the coupling constant. We will show here that the polaron is delocalised at any finite value of α in contrast to the variational calculations mentioned above. Our argument applies also to other types of polarons, cf § 4.

As will be discussed in § 3, the polaron may exhibit another type of phase transition which to the statistical mechanics community is known as the pinning transition. Physically this transition is of a very different nature to the localisation transition explained before. Basically it is the effect that a suitable *fixed* impurity potential may no longer bind the polaron if the coupling strength to the optical mode becomes too weak.

2. Absence of a roughening transition

We first want to convince the reader that the delocalised (localised) polaron corresponds to a rough (smooth) interface in statistical mechanics models and that in view of this analogy the predicted phase transition is highly implausible. We consider a two-dimensional Ising model below the critical temperature in a square box, $-N \leqslant i, j \leqslant N$. At the upper part of the boundary, i.e. $j \geqslant 0$, the spins are fixed to be $+1$ and at the lower part to be -1 ($+-$ boundary conditions). Then the region with predominantly $+$ spins will be separated by an interface from the predominantly $-$ spin region. In approximation one tries to formulate an effective statistical model for the interface. One such model is the discrete Gaussian chain. To establish the connection with the polaron we formulate it immediately in the continuum. The position of the interface relative to the line $j=0$ is denoted by $x(t) \in \mathbb{R}$, $-T \leqslant t \leqslant T$. Then $x(-T) = 0 = x(T)$, which breaks the translation symmetry. The statistical weight of the interface is assumed to be

$$(Z(2T))^{-1} P(dx(\cdot))\delta(x(-T))\delta(x(T))\, e^{-S(x(\cdot))} \tag{2.1}$$

with the action

$$S(x(\cdot)) = \beta\tfrac{1}{2}\int_{-T}^{T} \mathrm{d}t \int_{-T}^{T} \mathrm{d}s\, g_{\mathrm{I}}(|t-s|)(x(t)-x(s))^2 + \lambda \int_{-T}^{T} \mathrm{d}t \cos x(t), \tag{2.2}$$

β, $g_{\mathrm{I}} \geqslant 0$. In the usual discrete Gaussian chain g_{I} is short ranged or even zero. We consider here the general case (Kjaer and Hilhorst 1982). The action (2.2) appears also in the quantum dynamics of a superconducting tunnel junction coupled to the environment (Schmid 1983, Bulgadaev 1984, Guinea *et al* 1985). Note that although the action is quadratic it is comparable to the polaron action in the sense that paths which stay close to each other have a larger weight than those which wander about. In fact Feynman used exactly the action (2.2), without the cos term, for his variational calculation, cf also Adamowski *et al* (1980b).

The physics of (2.2) is partially understood. (There are no rigorous results on this model, except for the case $g_{\mathrm{I}} \equiv 0$ which is the one-dimensional sine-Gordon theory alias neutral Coulomb gas (Lenard 1961, Prager 1962, Edwards and Lenard 1962, Aizenman and Martin 1980, Aizenman and Fröhlich 1981). Duality transformation (Kjaer and Hilhorst 1982, Schmid 1983, Bulgadaev 1984, Guinea *et al* 1985), numerical simulation (Slurink and Hilhorst 1983) and renormalisation group analysis (Bulgadaev 1984, Guinea *et al* 1985) together present the following picture. If g_{I} decays faster than t^{-2}, then the interface is rough for any coupling strength β, i.e.

$$\lim_{T\to\infty} \langle x(0)^2 \rangle_T = \infty. \tag{2.3}$$

If g_{I} decays slower than t^{-2}, then the interface is smooth for any coupling strength $\beta > 0$. This means that

$$\lim_{T\to\infty} \langle x(0)^2 \rangle_T < \infty. \tag{2.4}$$

For the polaron $\langle x(0)^2 \rangle = \int \mathrm{d}q\, \rho_\alpha(q) q^2 = D(\alpha)$. Therefore (2.4) corresponds to a localised polaron. Finally if $g_{\mathrm{I}}(t)$ decays exactly as t^{-2} for large t, then a transition is expected: for small β the interface is rough and for large β it is smooth. There are predictions on the phase diagram in the (β, λ) plane (Bulgadaev 1984, Guinea *et al* 1985) and on the height-height correlations $\langle (x(t)-x(s))^2 \rangle$ (Kjaer and Hilhorst 1982).

For the occurrence of a phase transition the cos potential is crucial. If we set $\lambda = 0$, then (2.2) is a Gaussian theory. By explicit calculation one observes that for a decay slower than t^{-2} the interface is smooth (and $\rho(q)$ is Gaussian), whereas for a decay faster than t^{-2}, t^{-2} included, the interface is rough. If, however, the decay is precisely t^{-2} for large t, then the interface has logarithmic fluctuations (rather than $\sqrt{T}$ as for faster decay). In this case the periodic potential has a chance to pin the interface.

Comparing (2.2) with the polaron action we notice that the polaron action lacks the periodic external potential. This is not a severe problem. V could stand for the lattice potential which would play then the role of the cos potential. Also the polaron has three components rather than one as assumed in the above discussion. But the absolutely essential feature the polaron action is missing is the slow decay of the interaction: it decays exponentially and therefore much too fast.

For the unconvinced we present a proof that for the polaron with an action where the Coulomb singularity is smoothened (equivalently, where the coupling to the phonon field is $|k|^{-1}$ cut-off for large k) and with an external potential $V(x) = \frac{1}{2}\kappa x^2$, $\kappa > 0$,

$$\lim_{\kappa\to 0_+} \langle x^2 \rangle_0(\alpha, \kappa) = \infty \tag{2.5}$$

for any value of $\alpha \geqslant 0$.

Proposition. Let $\langle\cdot\rangle_T(\alpha,\kappa)$ refer to the expectation with respect to the probability measure (1.3) with the action

$$S_T(x(\cdot))=\tfrac{1}{2}k\int_{-T}^{T}\mathrm{d}t\,x(t)^2-\frac{\alpha}{\sqrt{2}}\frac{1}{2}\int_{-T}^{T}\mathrm{d}t\,\mathrm{d}s\,g_T(|t-s|)U(x(t)-x(s)),\tag{2.6}$$

where U is the Coulomb potential regularised as

$$U(x)=\int\mathrm{d}y\,h(y)|x-y|^{-1}.\tag{2.7}$$

h is radial, bounded, $h\geqslant 0$ and $\int\mathrm{d}y\,h(y)=1$. Then

$$\lim_{T\to\infty}\inf\langle x(0)^2\rangle_T(\alpha,\kappa)\geqslant 3M^{-1}(0,0),\tag{2.8}$$

where M is the linear operator on $L^2(\mathbb{R})$ defined by

$$M\varphi(t)=-\frac{\mathrm{d}^2}{\mathrm{d}t^2}\varphi(t)+\kappa\varphi(t)-\frac{\alpha}{3\sqrt{2}}\left(\int\mathrm{d}s\,K(t-s)\varphi(s)-\varphi(t)\int\mathrm{d}s\,K(s)\right)\tag{2.9}$$

with $K(t)=4\pi\,\mathrm{e}^{-|t|}\langle h(x(0)-x(t))\rangle(\alpha,\kappa)$. $M^{-1}(\cdot,\cdot)$ is the kernel of the inverse operator.

Proof. We discretise $[-T,T]$ in intervals of length ε, $\varepsilon N=T$ and $\varepsilon\to 0$ at the end. Then the measure (1.3) is approximated as

$$Z^{-1}\left(\prod_{j=-N}^{N-1}\mathrm{d}^3x_j\right)\exp\left(-\sum_{j=-N}^{N-1}\frac{(x_{j+1}-x_j)^2}{2\varepsilon}-\tfrac{1}{2}\kappa\varepsilon\sum_{j=-N}^{N-1}x_j^2\right.$$
$$\left.+\frac{\alpha}{\sqrt{2}}\frac{1}{2}\varepsilon^2\sum_{i,j=-N}^{N-1}g_T[\varepsilon(i-j)]\,U(x_i-x_j)\right)\tag{2.10}$$

with the convention $x_N=x_{-N}$.

We follow an idea in Brascamp *et al* (1977). Let $-H$ be the function in the exponent and let $\langle\cdot\rangle$ denote the average with respect to (2.10). Let M be the matrix with matrix elements

$$M_{i\alpha,j\beta}=\langle(\partial_{i\alpha}H)(\partial_{j\beta}H)\rangle,\tag{2.11}$$

where $\partial_{i\alpha}$ is the partial derivative with respect to the αth component of x_i, $\alpha,\beta=1,2,3$ and $i,j=-N,\ldots,N-1$. Then by partial integration and the Schwarz inequality

$$\left(\sum_{i,\alpha}\varphi_{i\alpha}\psi_{i\alpha}\right)^2=\left\langle\left(\sum_{i,\alpha}\varphi_{i\alpha}x_{i\alpha}\right)\left(\sum_{j,\beta}\psi_{j\beta}\partial_{j\beta}H\right)\right\rangle^2$$
$$\leqslant\left\langle\left(\sum_{i,\alpha}\varphi_{i\alpha}x_{i\alpha}\right)^2\right\rangle\left\langle\left(\sum_{j,\beta}\psi_{j\beta}\partial_{j\beta}H\right)^2\right\rangle.\tag{2.12}$$

Since $M\geqslant\kappa$, we may set $\psi=M^{-1}\varphi$ and obtain

$$\left\langle\left(\sum_{i,\alpha}\varphi_{i\alpha}x_{i\alpha}\right)^2\right\rangle\geqslant\sum_{i\alpha,j\beta}(M^{-1})_{i\alpha,j\beta}\varphi_{i\alpha}\varphi_{j\beta}.\tag{2.13}$$

We compute the matrix M in the form $\langle\partial_{i\alpha}\partial_{j\beta}H\rangle$. By rotation invariance $M_{i\alpha,j\beta}=\delta_{\alpha\beta}M_{ij}$ and

$$M_{ij}=-\varepsilon^{-1}\Delta_{ij}+\kappa\varepsilon\delta_{ij}-\frac{\alpha}{3\sqrt{2}}\varepsilon^2\left(K_{T,\varepsilon}(i,j)-\delta_{ij}\sum_{n=-N}^{N-1}K_{T,\varepsilon}(i,n)\right).\tag{2.14}$$

Here Δ_{ij} is the discrete Laplacian, $\Delta_{jj}=2$, $\Delta_{ij}=-1$ for $|i-j|=1$ and $\Delta_{ij}=0$ otherwise, with periodic boundary conditions and the kernel $K_{T,\varepsilon}$ is defined by

$$K_{T,\varepsilon}(i,j)=4\pi g_T(\varepsilon|i-j|)\langle h(x_i-x_j)\rangle. \tag{2.15}$$

In (2.13) we set $\varphi_{j\beta}=\varphi(\varepsilon j)$ with some smooth function φ and take the continuum limit $\varepsilon\to 0$ in the sense of quadratic forms. Then

$$\int_{-T}^{T} \mathrm{d}t\,\mathrm{d}s\,\varphi(t)\varphi(s)\langle x(t)\cdot x(s)\rangle_T(\alpha,\kappa)\geqslant 3\int_{-T}^{T}\mathrm{d}t\,\mathrm{d}s\,\varphi(t)\varphi(s)M_T^{-1}(t,s). \tag{2.16}$$

Here M_T is the linear operator

$$M_T(t)=-\frac{\mathrm{d}^2}{\mathrm{d}t^2}\varphi(t)+\kappa\varphi(t)-\frac{\alpha}{3\sqrt{2}}\left(\int \mathrm{d}s\,K_T(t,s)\varphi(s)-\varphi(t)\int \mathrm{d}s\,K_T(t,s)\right) \tag{2.17}$$

in $\mathrm{L}^2([-T,T])$ with periodic boundary conditions, where

$$K_T(t,s)=4\pi g_T(|t-s|)\langle h(x(t)-x(s))\rangle_T(\alpha,\kappa). \tag{2.18}$$

$M_T^{-1}(t,s)$ is the kernel of the inverse operator. Clearly

$$K_T(t,s)\leqslant 4\pi g_T(|t-s|)\sup h. \tag{2.19}$$

Therefore we may pass to the limit $T\to\infty$ and obtain (2.8) upon letting $\varphi(t)\to\delta(t)$.

Let

$$\hat{K}(\omega)=\int \mathrm{d}t\,\mathrm{e}^{\mathrm{i}\omega t}K(t). \tag{2.20}$$

Because of (2.19), $\hat{K}(0)-\hat{K}(\omega)\sim\omega^2$ for small ω. Therefore

$$M^{-1}(0,0)=\int \mathrm{d}\omega\left(\omega^2+\frac{\alpha}{3\sqrt{2}}(\hat{K}(0)-\hat{K}(\omega))+\kappa\right)^{-1} \tag{2.21}$$

diverges as $1/\sqrt{\kappa}$ as $\kappa\to 0$. We need a decay of $g(t)$ at least as slow as t^{-2} to be able to keep $M^{-1}(0,0)$ finite.

If the endpoints are kept fixed, i.e. $x(-T)=0=x(T)$, and $\kappa=0$, our estimate shows that $\langle x(0)^2\rangle_T\geqslant\text{constant}\times T$ and typical fluctuations are of the order $\sqrt{T}$. Therefore an external periodic potential cannot localise $x(\cdot)$.

The variational calculations mentioned cannot distinguish between the action (1.4) and a mildly regularised one. Of course, the numerical value of α_c would change under regularisation. Our result shows then that the transition predicted is an artefact of the approximation method used.

Still, we have not ruled out the possibility of a localisation transition for the action (1.4). The difficulty is that in this case $h(y)=\delta(y)$ and therefore the simple bound (2.19) breaks down. Let us first compute the expectation

$$\langle\delta(x(t)-x(0))\rangle(0,\kappa)=[2\pi/(C(0,0)+C(t,t)-2C(0,t))]^{3/2} \tag{2.22}$$

with $C=(-\mathrm{d}^2/\mathrm{d}t^2+\kappa)^{-1}$. $[C(0,0)+C(t,t)-2C(0,t)]\sim t$ for small t and tends to $2\pi/\sqrt{\kappa}$ as $t\to\infty$. In the limit $\kappa\to 0$ this quantity grows exactly as t. Then $K(t)=\mathrm{e}^{-t}(2/t)^{3/2}$. Nevertheless $\hat{K}(0)-\hat{K}(\omega)\sim\omega^2$ for small ω and the conclusion drawn from (2.21) would still remain valid. We were not able to obtain a bound on $\langle\delta(x(t)-x(0))\rangle(\alpha,\kappa)$ for $\alpha>0$ which would guarantee that $\hat{K}(0)-\hat{K}(\omega)\sim\omega^2$ for small ω. For short 'times' $x(t)$ should look like diffusion and therefore we would expect that also

$$\langle\delta(x(t)-x(0))\rangle(\alpha,\kappa)\sim t^{-3/2} \tag{2.23}$$

for small t. For large t, even assuming localisation, $\langle\delta(x(t)-x(0))\rangle(\alpha, \kappa)$ should be bounded. If this and (2.23) are a bound on the actual behaviour, then $M^{-1}(0,0)$ would still diverge as $1/\sqrt{\kappa}$ as $\kappa \to 0$. The main technical difficulty is to exclude in (2.23) a divergence as t^{-3} or faster as $t \to 0$. In that case the lower bound in (2.8) would drop to zero.

3. The pinning transition

Abraham (1980) considered a two-dimensional ferromagnetic Ising model, $-M \leq i \leq M$, $1 \leq j \leq N$. The boundary conditions are periodic in the i direction, $\sigma_{-Mj} = \sigma_{M+1j}$, $+$ on the top, $j = N$, and $+$ on the bottom except for a stretch $-M < -T \leq i \leq T < M$ where $-$ boundary conditions are imposed. The half space limit, N, $M \to \infty$, is taken. There is a domain wall (contour) starting at $(-T-\frac{1}{2}, 1)$ and ending at $(T+\frac{1}{2}, 1)$ which separates those $-$ spins connected with the stretch of $-$ spins at the free surface from the $+$ spins. This domain wall may have overhangs. Let J_1 (J_2) be the horizontal (vertical) coupling. Now the coupling between the zeroth and first layer is weakened as aJ_2, $0 < a < 1$. Thereby domain walls closer to the free surface are energetically favoured and there is a transition associated with the pinning of the domain wall to the free surface. For temperatures $\beta^{-1} < \beta_c^{-1}(a)$ the distance of the domain wall from the surface is bounded as $T \to \infty$. The domain wall depins as $(\beta - \beta_c(a))^{-1}$ for $\beta \to \beta_c(a)$ and below β_c typical domain wall fluctuations are of the order $\sqrt{T}$.

In a simplified form (Burkhardt 1981, Kroll 1981) this pinning transition can be understood using the Onsager-Temperley solid-on-solid (SOS) model which neglects overhangs. To establish the connection with the polaron we formulate it as a continuum model for the distance $h(t)$ of the domain wall from the free surface, $h(t) \geq 0$, $-T \leq t \leq T$, and $h(-T) = 0 = h(T)$. Other versions are considered in Burkhardt (1981) and Kroll (1981). They are all in the same universality class, however. The distribution of the domain walls is given by

$$\frac{1}{Z(2T)} P(\mathrm{d}h(\cdot))\delta(h(-T))\delta(h(T)) \exp\left(-\beta \int_{-T}^{T} \mathrm{d}t\, V(h(t))\right) \tag{3.1}$$

$\beta \geq 0$. Here $V(h) = \infty$ for $h < 0$ to guarantee the restriction $h(t) \geq 0$. V has an attractive part at short distances and decays sufficiently rapidly as $h \to \infty$, e.g. V could be the attractive single well potential $V(h) = \infty$ for $h < 0$, $V(h) = -1$ for $0 \leq h \leq 1$, and $V(h) = 0$ for $h > 1$. Obviously the transfer matrix of this model is e^{-tH} with H the Schrödinger operator

$$H = -\tfrac{1}{2}\Delta + \beta V \tag{3.2}$$

on the positive half-line with Dirichlet boundary conditions at $x = 0$. Spectral properties of these operators are well understood. For β large, H has a normalised ground state $\psi_{0,\beta}(x)$ with energy $E_0(\beta) < 0$ and possible other bound states. As β increases, $E_0(\beta)$ increases and tends to zero at some critical value β_c. The ground state delocalises as

$$\int_0^\infty \mathrm{d}x\, x|\psi_{0,\beta}(x)|^2 \simeq (\beta - \beta_c)^{-1}. \tag{3.3}$$

Translating back to the domain wall model (3.1) we obtain that, in the limit $T \to \infty$,

$$\langle h(0)\rangle(\beta) < \infty \tag{3.4}$$

for $\beta \geqslant \beta_c$ and that the average distance from the free surface diverges as

$$\langle h(0)\rangle(\beta) \simeq (\beta - \beta_c)^{-1}. \tag{3.5}$$

Exactly the same phenomenon will happen for a model with three components and the distribution

$$p^m(\mathrm{d}x(\cdot))\delta(x(-T))\delta(x(T)) \exp\left(-\int_{-T}^{T} \mathrm{d}t\, V(x(t))\right). \tag{3.6}$$

Here $x(t) \in \mathbb{R}^3$, V is a radial potential and $P^m(\mathrm{d}x(\cdot))$ refers to the Wiener measure generated by $-(1/2m)\Delta$, i.e. the path measure of a free quantum mechanical particle with mass m. In connection with the polaron we think of V as fixed and vary the mass m, $m \geqslant 1$. The transfer matrix is e^{-tH} with H the Schrödinger operator

$$H = -(1/2m)\Delta + V \tag{3.7}$$

on $\mathrm{L}^2(\mathbb{R}^3)$.

To have a pinning transition, H should have no bound state for $m = 1$ and should have bound states for m sufficiently large. This is a well understood chapter of atomic physics. We quote only one result and refer to the literature (Reed and Simon 1978, ch XIII.3 and XIII.15, Simon 1979, ch III, Lieb 1976, Glaser *et al* 1976) for a more complete discussion.

For an arbitrary, not necessarily radial, potential V let

$$\int \mathrm{d}^3x\, |V(x)|^{3/2} < \infty. \tag{3.8}$$

Let V_- be the attractive part of the potential. If

$$0.232 \int \mathrm{d}^3x\, |V_-(x)|^{3/2} < 1 \tag{3.9}$$

then, for $m = 1$, H has the spectrum $[0, \infty)$ and no bound states with negative energy whereas for m sufficiently large, H has a non-degenerate ground state with negative energy.

The ground state delocalises as

$$\int \mathrm{d}^3x\, x^2 |\psi_{0,m}(x)|^2 \simeq (m - m_c)^{-2}. \tag{3.10}$$

(We are not aware of a proof only under the assumptions (3.8) and (3.9).)

We return to the polaron. If $\alpha = 0$, then for the electron with mass m

$$\langle \exp[\mathrm{i}k(x(t) - x(0))]\rangle(\alpha = 0) = \exp[-(2m)^{-1}k^2 t], \tag{3.11}$$

$t > 0$. From a central limit type of argument we would expect that for the polaron, $V \equiv 0$,

$$\langle \exp[\mathrm{i}k(x(t) - x(0))]\rangle(\alpha) \simeq \exp[-(2m(\alpha))^{-1}k^2 t] \tag{3.12}$$

for $k \to 0$, $t \to \infty$ with $k^2 t$ fixed. Therefore it is natural to define the effective mass $m(\alpha)$ as

$$m(\alpha)^{-1} = \lim_{t\to\infty} \frac{1}{3t} \langle (x(t) - x(0))^2 \rangle(\alpha). \tag{3.13}$$

In the appendix we prove that, with a cut-off of $1/|k|$ for large k, $m(\alpha)^{-1}$ depends analytically on α. To obtain an estimate on $m(\alpha)$ the usual procedure is to use the variational action

$$\tfrac{1}{2}\int \mathrm{d}t\ \mathrm{d}s\, g(t-s)(x(t)-x(s))^2, \tag{3.14}$$

$g(t)=g(-t)$ and $g\geq 0$. For this action the effective mass is

$$m=1+\int_{-\infty}^{\infty}\mathrm{d}t\, t^2 g(t). \tag{3.15}$$

If g is chosen as in the Feynman trial action with parameters optimal for the ground state energy, then

$$m(\alpha)\simeq 1+\tfrac{1}{6}\alpha \tag{3.16}$$

for small α and

$$m(\alpha)\simeq(2\alpha/3\sqrt{\pi})^4 \tag{3.17}$$

for large α.

In analogy to the action (3.6) we expect a pinning transition for the polaron: in addition to the interactions with the polar crystal the electron moves in the external potential V satisfying (3.8) and (3.9). Then for $\alpha>\alpha_c$, $\langle x^2(0)\rangle\ (\alpha)=\int \mathrm{d}q\, q^2\rho_\alpha(q)<\infty$ and

$$\langle x^2(0)\rangle(\alpha)\simeq(\alpha-\alpha_c)^{-2} \tag{3.18}$$

as $\alpha\to\alpha_{c+}$. One could also keep α fixed and vary the strength of the potential. Then for λ sufficiently large, $\langle x^2(0)\rangle(\alpha,\lambda V)<\infty$ and

$$\langle x^2(0)\rangle(\alpha,\lambda V)\simeq(\lambda-\lambda_c)^{-2} \tag{3.19}$$

as $\lambda\to\lambda_{c+}$.

We assumed the critical exponent, -2, to be identical to the one of (3.6). Because of the exponential decay of memory the polaron attains its effective mass essentially on a 'time' of order one. On such a coarsened scale the polaron has the form (3.6) with $m=m(\alpha)$. Since this is only approximately so, the critical coupling is somewhat shifted relative to its value determined from $m_c=m(\alpha_c)$. However, the critical exponent should not change.

A physically realistic impurity potential is the screened Coulomb potential $V(x)=-(Q/|x|)\exp(-k_0|x|)$ with $Q, k_0>0$. Relation (3.9) is satisfied provided $(Q/k_0)<0.8$. The Coulomb potential has always an infinite number of bound states and therefore does not satisfy our condition.

4. Other polarons

From the two transitions described, physically, the roughening transition is the more interesting one. Since it cannot be achieved for an electron interacting with the longitudinal optical mode of an ionic crystal, we should understand whether a roughening transition may occur for other types of polarons. The Fröhlich Hamiltonian is generalised to

$$H=-\tfrac{1}{2}\Delta+V+\int \mathrm{d}^3k\,\omega(k)a_k^+a_k+\sqrt{\alpha}\int \mathrm{d}^3k\,\lambda(k)\,\mathrm{e}^{ikx}(a_k+a_{-k}^+). \tag{4.1}$$

Here ω, $\omega(k) \geq 0$, is the dispersion relation of the phonon field and $\sqrt{\alpha}$, $\alpha > 0$, the coupling constant. We impose rotational invariance by $\omega(k) = \omega(|k|)$ and $\lambda(k) = \lambda(|k|)$. The action is given by

$$S(x(\cdot)) = \int \mathrm{d}t\, V(x(t)) - \alpha\tfrac{1}{2} \int \mathrm{d}t \int \mathrm{d}s\, G(|t-s|, x(t) - x(s)) \tag{4.2}$$

with, in the limit $T \to \infty$,

$$G(t, x) = \int \mathrm{d}^3k\, |\lambda(k)|^2\, \mathrm{e}^{-\omega(k)|t|}\, \mathrm{e}^{\mathrm{i}kx}. \tag{4.3}$$

If we apply the method of the proposition to the action (4.2) with a general G, then the kernel $K(t, s) = K(t-s)$ is given by

$$K(t) = -\tfrac{1}{3}\langle \Delta_x G(t, x(t) - x(0))\rangle(\alpha, \kappa), \tag{4.4}$$

where Δ_x is the Laplacian with respect to the second argument of G and $\langle\cdot\rangle\,(\alpha, \kappa)$ is the average with respect to $Z(2T)^{-1} \exp[-S_T(x(\cdot))]$, with $V = \frac{1}{2}\kappa x^2$, in the limit $T \to \infty$. To conclude that the lower bound diverges as $\kappa \to 0$ we need that $K(t)$ has a finite second moment. This yields the following. If $\int \mathrm{d}^3k\, \lambda(k)^2 < \infty$ and

$$\int \mathrm{d}^3k\, \lambda(k)^2 k^2 / \omega(k)^3 < \infty, \tag{4.5}$$

then the polaron with Hamiltonian (4.1) is delocalised for any coupling strength α. This criterion holds in arbitrary spatial dimension.

The criterion (4.5) applies to the acoustical and optical polaron by the deformation potential (Toyozawa 1961, Sumi and Toyozawa 1973, Gross 1976) for which $\omega(k) = |k|$ (resp. $= 1$) and $\lambda(k) = \sqrt{|k|}$ (resp. $= 1$) for small k. It also applies to the acoustic polaron by the deformation potential in one dimension (Tokuda and Kato 1982) for which $\omega(k) = |k|$, $\lambda(k) = \sqrt{|k|}$. An interesting proposal is to consider electrons on a film of liquid helium (Jackson and Platzman 1981). The authors obtain, setting all constants equal to one, $\omega(k)^2 = (k + k^3) \tanh k$ and $\lambda(k)^2 = k \tanh k / \omega(k)$ and the k integration is two-dimensional. Again (4.5) excludes a roughening transition.

Another proposal is the piezoelectric polaron (Mahan and Hopfield 1964) with $\omega(k) = |k|$, $\lambda(k) = 1/\sqrt{|k|}$ and a cut-off for large k. This yields in (4.5) a small-k behaviour as $1/k^2$ which is integrable in three dimensions.

On a formal level the only natural candidate for a roughening transition is $\omega(k) = |k|$ and $\lambda(k) = |k|^{-3/2}$. Heuristically one expects logarithmic fluctuations which may be localised by the periodic lattice potential, if the coupling is strong enough.

It is not understood for which class of couplings $\lambda(k)$ and dispersions $\omega(k)$ the polaron exhibits a roughening transition. But (4.5) sets rather severe limits on its observability.

5. Conclusions

We have shown that the polaron does not undergo a localisation transition in contrast to what has been suggested by some variational calculations. Physically this is quite obvious once the analogy to the roughening transition is understood. We support our argument also on a rigorous level. If a cut-off for large k (i.e. a smoothening of the Coulomb singularity) is introduced in the polaron action, then a lower bound proves delocalisation at any coupling strength. In addition the ground state energy and the effective mass are analytic functions of the coupling constant α. We expect these properties to remain true when the cut-off is removed. A proof, however, requires a non-trivial extension of our results.

Our lower bound on the second moment applies also to other polarons, ruling out a localisation transition there. As an effect of a physically distinct nature the polaron should undergo a pinning transition in a suitable, fixed pinning potential.

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Appendix. Effective mass and its analytic dependence on the coupling constant

The proof below was explained to the author by R L Dobrushin. We consider the general polaron (4.1) and assume

$$\int \mathrm{d}^3k\,\lambda(k)^2 < \infty \tag{A1}$$

and the existence of two constants c_1, $c_2 > 0$ such that

$$\int \mathrm{d}^3k\,\lambda(k)^2\,\mathrm{e}^{-\omega(k)|t|} \leqslant c_1 \exp(-c_2|t|). \tag{A2}$$

Note that the Fröhlich polaron with $\lambda(k) = |k|^{-1}$ and a cut-off for large k such that $\lambda(k)^2$ becomes integrable satisfies (A1) and (A2).

The heuristic idea behind the proof is simple. Instead of $x(t)$ we consider its increments $\dot{x}(t)$. Then $x(t) - x(0) = \int_0^t \mathrm{d}\tau\,\dot{x}(\tau)$ and the effective mass is

$$m(\alpha)^{-1} = \tfrac{1}{3} \int \mathrm{d}t \langle \dot{x}(t) \cdot \dot{x}(0) \rangle. \tag{A3}$$

The distribution of increments is

$$Z(2T)^{-1} P(\mathrm{d}\dot{x}(\,\cdot\,)) \exp\left[\alpha \int_{-T}^{T} \mathrm{d}t \int_{-T}^{t} \mathrm{d}s\, G\left(t-s, \int_s^t \mathrm{d}\tau\,\dot{x}(\tau)\right)\right]. \tag{A4}$$

$P(\mathrm{d}\dot{x}(\,\cdot\,))$ is white noise, the derivative of Brownian motion. If we define the free energy, an 'external magnetic field' included, as

$$f(\alpha, h) = \lim_{T\to\infty} \frac{1}{2T} \log \int P(\mathrm{d}\dot{x}(\,\cdot\,)) \times \exp\left[\alpha \int_{-T}^{T} \mathrm{d}t \int_{-T}^{t} \mathrm{d}s\, G\left(t-s, \int_s^t \mathrm{d}\tau\,\dot{x}(\tau)\right) - h \int_{-T}^{T} \mathrm{d}\tau\,\dot{x}(\tau)\right], \tag{A5}$$

then

$$m(\alpha)^{-1} = \tfrac{1}{3} \sum_{j=1}^{3} \frac{\partial^2}{\partial h_j^2} f(\alpha, h)\bigg|_{h=0}. \tag{A6}$$

Now $\dot{x}(t)$ forms a one-dimensional statistical mechanics system with three components whose interaction, though many-body, decreases rapidly. Therefore the free energy is expected to be analytic.

To apply the theory in Dobrushin (1973, 1974) properly, we divide $[-T, T]$ into intervals of unit length, say, T integer. In each interval $[j, j+1)$, $j=-T, \ldots, T-1$, the path $x(t)$ is shifted by the amount $x(j)$. Let $y_j(\cdot)$ be the shifted path in the jth interval. $t \to y_j(t)$, $0 \leq t \leq 1$, is continuous and $y_j(0)=0$. The $\{t \to y_j(t), 0 \leq t \leq 1\}$ are the 'spins'. Therefore the single site space is $C([0,1], \mathbb{R}^3)$. The single site measure $P_{[0,1]}$ is Brownian motion starting at zero over the time interval $[0, 1]$. Because Brownian motion has independent increments, the single site measures are independent. Rewriting the action in terms of the $y_j(\cdot)$, the Hamiltonian of the spin system becomes

$$H = -\sum_{j=-T}^{T-1} \alpha \tfrac{1}{2} \int_j^{j+1} \mathrm{d}s \int_j^{j+1} \mathrm{d}t\, G(t-s, y_j(t)-y_j(s))$$
$$- \sum_{-T \leq i<j \leq T-1} \alpha \int_i^{i+1} \mathrm{d}s \int_j^{j+1} \mathrm{d}t\, G\left(t-s, y_j(t)+\sum_{m=i}^{j-1} y_m(1)-y_i(s)\right)$$
$$+h \sum_{j=-T}^{T-1} y_j(1). \tag{A7}$$

The free energy is

$$f(\alpha, h) = \lim_{T\to\infty} \frac{1}{2T} \log \int \prod_{j=-T}^{T-1} P_{[0,1]}(\mathrm{d}y_j(\cdot))\, \mathrm{e}^{-H}. \tag{A8}$$

We have

$$|G(t,x)| \leq \int \mathrm{d}^3k\, \lambda(k)^2\, \mathrm{e}^{-\omega(k)|t|}. \tag{A9}$$

Therefore B) and C_1) of Dobrushin (1973, 1974) are satisfied. Because of (A2) also D_2) of Dobrushin (1973, 1974) holds. Therefore we conclude that the free energy is analytic in α and h in a small complex neighbourhood of the real (α, h) plane.

In fact as stated the potential $hy_0(1)$ does not satisfy the conditions of Dobrushin (1973, theorem 3), because $y_0(1)$ is unbounded. We circumvent this difficulty by including $\exp[-hy_0(1)]$ in the single site measure.

We conclude that

$$3m(\alpha)^{-1} = \sum_j \langle y_j(1) \cdot y_0(1)\rangle = \sum_{j=1}^{3} \frac{\partial}{\partial h_j^2} f(\alpha, h)|_{h=0} \tag{A10}$$

is analytic in α. Furthermore $m(\alpha)^{-1} > 0$ by the lower bound of the proposition extended to the general polaron.

The decay condition (A2) is fairly strong. On the basis of the proposition, extended to the general polaron, we conjecture that $m(\alpha)^{-1}$ is analytic under the weaker conditions $\int \mathrm{d}^3k\, \lambda(k)^2 < \infty$ and $\int \mathrm{d}^3k\, \lambda(k)^2 k^2/\omega(k)^3 < \infty$. We leave this as an open problem.

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