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The polaron at large total momentum

Herbert Spohn

Universität München, Theoretische Physik, Theresienstrasse 37, D-8000 München, Federal Republic of Germany

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Abstract. We prove that for dimensions $d=1,2$ the polaron (with general dispersion relation and couplings) has a unique ground state for any value of the total momentum (particle + Bose field). For $d \geqslant 3$ and for sufficiently small total momentum we show the existence of a unique ground state, extending however the domain of uniqueness known previously.

1. Introduction

The polaron is an electron coupled to a polar crystal. Following Fröhlich [1] the Hamiltonian is

$$H = \frac{1}{2m} p^2 + \int \mathrm{d}^d k\, \omega(k) a^+(k) a(k) + \sqrt{\alpha} \int \mathrm{d}^d k\, \lambda(k) (\mathrm{e}^{\mathrm{i}kx} a(k) + \mathrm{e}^{-\mathrm{i}kx} a^+(k)). \tag{1.1}$$

Here m is the mass of the electron, x, p its position and momentum respectively. $\{a^+(k), a(k) | k \in \mathbb{R}^d\}$ is a Bose field representing the quantised longitudinal optical mode. As an approximation the dispersion relation is constant

$$\omega(k) = \hbar\omega_0 \tag{1.2}$$

and the couplings are

$$\sqrt{\alpha}\lambda(k) = \sqrt{\alpha}\, \hbar\omega_0 (\hbar/2m\omega_0)^{1/4} (4\pi)^{1/2} (2\pi)^{-3/2} (1/|k|). \tag{1.3}$$

Here α is the dimensionless coupling constant. As usual, we adopt units such that $\hbar = 1 = m$.

For most of our results we do not need such specific choices. Therefore we let $\omega(k)$ be arbitrary, only subject to the constraints

$$\omega(k) \geqslant \omega_0 > 0 \tag{1.4}$$

$$\omega(k_1) + \omega(k_2) - \omega(k_1 + k_2) \geqslant 0. \tag{1.5}$$

The couplings are assumed to be real with

$$\int \mathrm{d}^d k\, \lambda(k)^2 (1 + k^2)^{-1} < \infty. \tag{1.6}$$

We also impose reflection symmetry, $\omega(k) = \omega(-k)$, $\lambda(k) = \lambda(-k)$. It is of interest to understand the dimension dependence. Therefore we let d be arbitrary ($d = 1, 2, 3$, physically).

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The Hamiltonian H commutes with the total momentum

$$P = p + \int \mathrm{d}^d k \, k a^+(k) a(k). \tag{1.7}$$

By (1.7) we eliminate p from (1.1) and perform the canonical transformation $a(k) \to -\mathrm{e}^{-\mathrm{i}kx} a(k)$. Then the Hamiltonian for fixed total momentum q, where q is a c number, is given by

$$H(q) = \frac{1}{2}\left(q - \int \mathrm{d}^d k \, k a^+(k) a(k)\right)^2 + \int \mathrm{d}^d k \, \omega(k) a^+(k) a(k) - \sqrt{\alpha} \int \mathrm{d}^d k \, \lambda(k)(a^+(k) + a(k)). \tag{1.8}$$

By the further canonical transformation $a(k) \to -a(k)$ if $\lambda(k) < 0$ we can always find that

$$\lambda(k) \geqslant 0. \tag{1.9}$$

$H(q)$ is an operator on the standard boson Fock space, $\mathscr{F}$. By our assumptions on λ and ω, $H(q)$ is self-adjoint and bounded from below for all q.

Fröhlich [2] (cf also [3]) proves that if

$$|q| < \sqrt{2\omega_0} \tag{1.10}$$

then $H(q)$ has a unique ground state which is separated by a finite gap from the continuum. The ground-state energy, $E(q)$, is analytic in q and in the coupling strength α. (Note that the condition (1.10) does not depend on α.) Physically the ground state represents a dressed electron moving frictionless at constant momentum q through the polar crystal. The result quoted leaves open the question as to what happens for large $|q|$.

For states right at the continuum edge the polaron has momentum $q = 0$ and in addition there is one free phonon with momentum q. (Here $\omega(k) = \omega_0$, cf § 5 for the general case.) For small $|q|$ such a state is energetically unfavourable and a ground state with total momentum q is preferred. The polaron at $q = 0$ *binds* the extra phonon with momentum q. The problem posed is whether there is still binding at large $|q|$.

In his book on statistical mechanics [4], Feynman argues that for small coupling there is no binding provided $|q| > \sqrt{2\omega_0}$. His result is based on the observation that the expansion of the ground-state energy in α breaks down at $q = \sqrt{2\omega_0}$. (Note that the unperturbed Hamiltonian, $\alpha = 0$, has a bound state in the continuum if $|q| > \sqrt{2\omega_0}$.) Warmenbol *et al* [5] have investigated the experimental observability of $E(q)$, in particular the deviation from the quadratic behaviour $q^2/2m^*$, where m^* is the effective mass. They also reviewed the various approximate methods developed for the determination of $E(q)$. There seems to be agreement that in the physical dimension $d = 3$ there is no binding for $|q|$ sufficiently large. This is further supported by the recent results of Gerlach [6].

We will prove that for dimensions $d = 1$ and 2 the polaron has a unique ground state separated by a finite gap from the continuum at any q. This result is general in λ but requires some further regularity assumptions on ω, cf § 5. For $d \geqslant 3$ we extend the domain of uniqueness beyond (1.10). The unbinding of a phonon with momentum q is a possibility provided $|q|$ is sufficiently large.

At first sight the situation resembles the one for Schrödinger operators. For $d = 1, 2$ an attractive potential always binds, whereas for $d \geqslant 3$ the potential has to be sufficiently attractive [7]. Although suggestive we cannot substantiate this analogy on a technical level.

2. A jump process perturbed by a potential

Our starting point is that

$$H_0 = \int dk\, \omega(k) a^+(k) a(k) - \int dk\, \sqrt{\alpha}\lambda(k)(a^+(k) + a(k)) \tag{2.1}$$

is the generator of a simple jump process and that

$$V = \frac{1}{2}\left(q - \int dk\, k a^+(k) a(k)\right)^2 \tag{2.2}$$

serves as a potential. We assume

$$\int dk\, \lambda(k)^2 < \infty \tag{2.3}$$

and deal with the more singular interaction (1.6) by a limiting argument. (We set $d^d k = dk$.) The coupling strength $\sqrt{\alpha}$ will be fixed throughout and is absorbed into λ. At the very end we could have avoided the use of stochastic processes but they provide such a direct intuition that the effort is worthwhile. In the appendix we describe another approach using the standard polaron functional integral at purely imaginary external 'magnetic' field q. Unfortunately this method does not seem to be technically very powerful. The use of a jump process has been advocated before [8] for a polaron in [9]. The latter author missed regarding $\frac{1}{2}(q - \int dk\, k a^+(k) a(k))^2$ as a potential.

The ground state of H_0 is the coherent state $\zeta = (\zeta_0, \zeta_1, \dots)$ with

$$\zeta_n(k_1, \dots, k_n) = \exp\left(-\frac{1}{2}\int dk (\lambda/\omega)^2(k)\right) \frac{1}{\sqrt{n!}} \prod_{j=1}^{n} (\lambda/\omega)(k_j). \tag{2.4}$$

The ground-state energy is

$$E_0 = -\int dk (\lambda^2/\omega)(k). \tag{2.5}$$

The standard transformation

$$L_0 = -\zeta^{-1}(H_0 - E_0)\zeta \tag{2.6}$$

defines the backward generator of a Markov jump process. The jump process is denoted by X_t. The state space of this process are unordered n-tuple $(k_1, \dots, k_n)$, $k_j \in \mathbb{R}^d$, n arbitrary. We speak of $(k_1, \dots, k_n)$ as a configuration of particles, although physically it represents n phonons with momenta $k_1, \dots, k_n$. $X_t = \phi$ means no particle (no phonon) is present. The state space is denoted by

$$\Gamma = \bigcup_{n \geqslant 0} \mathbb{R}^{nd}.$$

The jump process X_t is governed by the following rates. (The present configuration $(k_1, \dots, k_n)$ is given.)

(i) Birth: independently of the given configuration a $(n+1)$th particle is created at $k+\mathrm{d}k$ with rate

$$(\lambda(k)^2/\omega(k))\,\mathrm{d}k. \tag{2.7}$$

(ii) Death: independently of all the other particles, the particle at k_j disappears with rate

$$\omega(k_j). \tag{2.8}$$

By (1.4) and (2.3) the jump process is well defined. Its stationary measure is ζ^2, i.e. a Poisson distribution of particles with density $(\lambda/\omega)^2$. Since $\omega(k)\geqslant\omega_0>0$, H_0 has a gap in its spectrum and therefore X_t has exponentially fast decaying correlations. The path measure of the jump process X_t starting at $X\in\Gamma$ is denoted by $\mathbb{P}_X$.

Obviously, on Fock space the operator $\frac{1}{2}(q-\int \mathrm{d}k\, ka^+(k)a(k))^2$ is multiplication by $\frac{1}{2}(q-\Sigma_{j=1}^n k_j)^2$ and should be regarded as a potential, V_q, with

$$V_q(k_1,\ldots,k_n)=\frac{1}{2}\left(q-\sum_{j=1}^n k_j\right)^2. \tag{2.9}$$

The potential depends on q as a parameter. If we had kept the bare electron mass, then $1/m$ would provide a strength parameter.

The Feynman-Kac construction tells us that $\exp[-TH(q)]$ with $H(q)=H_0+V_q$ has the stochastic representation

$$\zeta^{-1}(X)(\mathrm{e}^{-T(H(q)-E_0)}\zeta f)(X)=\int \mathbb{P}_X \exp\left(-\int_0^T \mathrm{d}t\, V_q(X_t)\right)f(X_T). \tag{2.10}$$

The proof is identical to the one for Schrödinger operators. Since $V_q\geqslant 0$ in our case, no problem in the definition of the integral arises.

Our problem has then the following abstract structure. We have a jump process with a unique smooth invariant measure and with exponentially decaying correlations. This jump process is perturbed by a decent potential V. The question is whether the perturbed process still has the same properties as the unperturbed one. Let us back up for a moment and let us assume that $\mathbb{P}_X$ is a reversible diffusion process. Then essentially

$$H_0=-\tfrac{1}{2}\Delta+W(x). \tag{2.11}$$

Δ is the Laplacian and $W(x)$ is a potential such that H_0 has a unique ground state separated by a gap from the rest of the spectrum. We add to H_0 a potential $V\geqslant 0$. Then

$$H=(-\tfrac{1}{2}\Delta+W)+V \tag{2.12}$$

may lose the ground state because V delocalises. As we will see, for our jump process the problem is not too large fluctuations, but rather too little. For a diffusion process the Brownian motion is very effective in prohibiting concentration: the Gaussian always beats the exponential. For jump processes the waiting time has an *exponential* distribution. Therefore in some parts of state space the process might have to pay too much potential energy in order to move away. For the polaron the problem is whether the perturbed process still jumps out of the subspace

$$\bigcup_{n\geqslant 1}\{k_1=q'\}\times\mathbb{R}^{(n-1)d}.$$

If not, the particle at q' stays there forever. This corresponds to the unbinding of a free phonon with momentum q'.

We deviate for a while from our subject to study this phenomenon of 'sticking' by means of a simplified example.

3. An example

We truncate the polaron Hamiltonian at $n=1$, which yields the so-called (first quantised) Lee or Friedrichs model, an exactly soluble case. The Hilbert space is $\mathscr{H}=\mathbb{C}\oplus L^2(\mathbb{R}^d, \mathrm{d}k)$. The free Hamiltonian is

$$H_0=\begin{pmatrix} 0 & -\langle\lambda| \\ -|\lambda\rangle & \omega \end{pmatrix} \qquad H_0(c,f)=(-\langle\lambda\,|f\rangle, \omega f) \tag{3.1}$$

with $\langle\cdot|\cdot\rangle$ the usual scalar product in $L^2(\mathbb{R}^d, \mathrm{d}k)$. We assume ω to be constant, $\omega>0$, and $\lambda\geqslant 0$, $\lambda>0$ close to $k=0$, $\langle\lambda\,|\lambda\rangle<\infty$. The unique ground state is

$$\psi_0=((\omega-E_0)^2+\langle\lambda\,|\lambda\rangle)^{-1/2}(\omega-E_0, \lambda) \tag{3.2}$$

with energy $E_0=[\omega-(\omega^2+4\langle\lambda\,|\lambda\rangle)^{1/2}]/2$. Stochastically a particle is created at k with rate $\lambda(k)^2/(\omega-E_0)$ and it disappears with rate $(\omega-E_0)$.

We perturb now H_0 by the potential

$$V=\begin{pmatrix} a & 0 \\ 0 & V(k) \end{pmatrix} \qquad H=H_0+V. \tag{3.3}$$

We assume $a\geqslant 0$, $V(k)\geqslant 0$, V continuous, $V(0)=0$ and $V(k)>0$ for $k\neq 0$. We imagine V to be fixed and study the ground state as a function of a. Since

$$\begin{pmatrix} 0 & \langle\lambda| \\ |\lambda\rangle & 0 \end{pmatrix}$$

is a one-dimensional perturbation, the explicit form of the resolvent, $(H-z)^{-1}$, is easily obtained. The continuum starts at ω. The implicit equation

$$a-z=\left\langle\lambda\,\middle|\,\frac{1}{V+\omega-z}\,\lambda\right\rangle \tag{3.4}$$

determines whether H has a ground state or not. If $\langle\lambda|(1/V)\lambda\rangle=\infty$ then (3.4) has always a solution $z<\omega$. z equals the ground-state energy E. The ground state is

$$\psi=\left[\left\langle\lambda\,\middle|\left(\frac{1}{V+\omega-E}\right)^2\lambda\right\rangle+1\right]^{-1/2}\left(1,\frac{1}{V+\omega-E}\,\lambda\right). \tag{3.5}$$

If $a<a_c$, H has a unique ground state, whereas for $a>a_c$, H has no ground state. The precise behaviour at a_c depends on the 'second moment'. If $\langle\lambda|(1/V)^2\lambda\rangle=\infty$ then there is no ground state at $a=a_c$. If $\langle\lambda|(1/V)^2\lambda\rangle<\infty$ then H has a ground state at the edge of the continuum.

H loses its ground state through a sharper and sharper concentration at $k=0$. If $\langle\lambda|(1/V)^2\lambda\rangle=\infty$, then

$$\psi^2\to(0,\delta(k)) \tag{3.6}$$

as $a\to a_c$.

To understand the concentration mechanism through the jump process we transform to the backward generator by (2.6). Then, for $a < a_c$, a particle is created at k with rate $\lambda(k)^2/(V(k)+\omega-E)$ and it disappears with rate $(V(k)+\omega-E)$. As $a \to a_c$, $\omega - E \to 0$ and the state at $k=0$ becomes sticky, i.e. the rate to jump out of it tends to zero. For $a > a_c$ the transformation (2.6) no longer makes sense. The stationary jump process is then to be constructed through the rules of statistical mechanics. We choose the time interval $[-T, T]$ and require that the unperturbed process starts at $(1, 0)$ at time $-T$ and ends at $(1, 0)$ at time T. The perturbed process is

$$\frac{1}{Z(T)} \mathbb{P}_{00} \exp\left(- \int_{-T}^{T} \mathrm{d}t\, V(X_t) \right) = \mathbb{P}^{(T)} \tag{3.7}$$

with $Z(T)$ the 'partition function'

$$Z(T) = \int \mathbb{P}_{00} \exp\left(- \int_{-T}^{T} \mathrm{d}t\, V(X_t) \right).$$

For $a < a_c$, in the limit $T \to \infty$, $\mathbb{P}^{(T)}$ tends to the stationary jump process with the rates already determined. For $a > a_c$, $\mathbb{P}^{(T)}$ degenerates in the limit $T \to \infty$. The limit process is such that one particle sits at $k=0$ forever.

If $\langle \lambda | (1/V)^2 \lambda \rangle = \infty$, then the invariant measure of the perturbed process tends continuously to $(0, \delta(k))$ ('second-order transition'). If $\langle \lambda | (1/V)^2 \lambda \rangle < \infty$, then the invariant measure jumps discontinously to $(0, \delta(k))$ at a_c ('first-order transition').

4. Ground-state energy and continuum edge

A vector in Fock space is denoted by $\psi = (\psi_0, \psi_1, \ldots)$. $\Omega = (1, 0, \ldots)$ is the Fock vacuum. If unambiguous from the context, λ stands also for the vector $(0, \lambda, 0, \ldots)$. $\langle \cdot | \cdot \rangle$ denotes the inner product in Fock space, $\|\psi\| = \langle \psi | \psi \rangle^{1/2}$. We assume that $\lambda > 0$, i.e. supp $\lambda = \mathbb{R}^d$. Otherwise the allowed k have to be restricted to the set supp λ; ω is continuous; λ and ω are reflection invariant and satisfy (1.4), (1.5) and (1.6). The bottom of the spectrum is

$$E(q) = \inf_{\psi, \|\psi\|=1} \langle \psi | H(q) \psi \rangle. \tag{4.1}$$

$E(q) > -\infty$; $E_c(q)$ denotes the bottom of the continuous part of the spectrum of $H(q)$.

From [2], cf also [3], we know the following properties of $E(q)$. $E(q)$ is continuous in q and satisfies the bounds

$$0 \leq E(q) - E(0) \leq \tfrac{1}{2} q^2. \tag{4.2}$$

Let

$$\Delta_q(q') = E(q - q') + \omega(q') - E(q) \tag{4.3}$$

and let

$$\Delta_q = \inf_{q'} \Delta_q(q'). \tag{4.4}$$

If $\Delta_q > 0$, then $H(q)$ has a unique ground state $\psi_q \in \mathcal{F}$. The ground state is at least a distance Δ_q below $E_c(q)$. ψ_q is positive (up to an overall phase factor) and $\langle \Omega | \psi_q \rangle > 0$.

If $|q|<\sqrt{2\omega_0}$, then $\Delta_q>0$ because of (4.2). For $|q|<\sqrt{2\omega_0}$, $E(q)$ is analytic in q. For small q

$$E(q)-E(0)=\frac{1}{2m^*}q^2 \tag{4.5}$$

with $1<m^*<\infty$, m^* being the effective mass of the polaron.

In fact, we have more precise information about $E_c(q)$.

Proposition. The lower edge of the continuous spectrum of $H(q)$ is given by

$$E_c(q)=E(q)+\Delta_q=\inf_{q'}(E(q-q')+\omega(q')). \tag{4.6}$$

In particular, $\Delta_q \geqslant 0$.

Proof. From [2] we know already that

$$E_c(q)\geqslant E(q)+\Delta_q. \tag{4.7}$$

We choose a trial wavefunction of the form

$$\zeta_\delta=\chi_\delta \circledS \psi/\|\chi_\delta \circledS \psi\|. \tag{4.8}$$

with $\psi\in\mathcal{F}$, $\|\psi\|=1$ and

$$\chi_\delta\in L^2(\mathbb{R}^d, \mathrm{d}k) \qquad \chi_\delta(k)^2\,\mathrm{d}k\to\delta(k-q')\,\mathrm{d}k$$

as $\delta\to 0$. $\circledS$ denotes symmetrisation. Then by a straightforward computation

$$\lim_{\delta\to 0}\langle\zeta_\delta|H(q)\zeta_\delta\rangle=\langle\psi|\{\omega(q')+H(q-q')\}\psi\rangle \tag{4.9}$$

$$\lim_{\delta\to 0}\langle\zeta_\delta|H(q)^2\zeta_\delta\rangle=\langle\psi|\{\omega(q')+H(q-q')\}^2\psi\rangle. \tag{4.10}$$

Let $\mathbb{E}_q(\mathrm{d}\lambda)$ be the spectral measure of $H(q)$ and let

$$Q_\varepsilon=\mathbb{E}_q([E(q)+\Delta_q-\varepsilon, E(q)+\Delta_q+\varepsilon]).$$

We have to show that $\dim(Q_\varepsilon)=\infty$ for any $\varepsilon>0$. Since E and ω are continuous in q, these exists a q'' such that $|\Delta_q(q'')-\Delta_q|<\varepsilon/4$. We choose $q'=q''$ in (4.9) and (4.10). For ψ we choose an approximate ground state for $H(q-q')$. Furthermore from the sequence ζ_δ we can construct a new sequence ζ_n such that $\langle\zeta_m|\zeta_n\rangle=\delta_{mn}$ and such that (4.9) and (4.10) hold as $n\to\infty$. There exists then an $N=N(\varepsilon)$ such that

$$\langle\zeta_n|(H(q)-E(q)-\Delta_q)^2\zeta_n\rangle\leqslant\varepsilon^2/2 \tag{4.11}$$

for all $n\geqslant N$. Let μ_n be the spectral measure of ζ_n. Equation (4.11) implies that

$$\mu_n([E(q)+\Delta_q-\varepsilon, E(q)+\Delta_q+\varepsilon])\geqslant\tfrac{1}{2}$$

and hence $\langle\zeta_n|Q_\varepsilon\zeta_n\rangle\geqslant\frac{1}{2}$ for all $n\geqslant N$. $\dim(Q_\varepsilon)=\infty$ follows.

If $\omega(k)=\omega_0$, then

$$E_c(q)=E(0)+\omega_0. \tag{4.12}$$

Our argument does not exclude further bound states in the half-open interval $[E(q), E_c(q)]$. Physically, such bound states are not expected.

Repeating the above construction with two phonons, the energy is

$$E(q-k_1-k_2)+\omega(k_1)+\omega(k_2)=E(q-k_1-k_2)+\omega(k_1+k_2)$$
$$+(\omega(k_1)+\omega(k_2)-\omega(k_1+k_2))\geqslant E(q)+\Delta_q. \tag{4.13}$$

A corresponding inequality holds for n phonons. Therefore assumption (1.5) ensures that n-phonon excitations do not lie below the one-phonon excitations.

The condition $\Delta_q>0$ appears in [2] through a momentum lattice approximation. An instructive reinterpretation is obtained from the study of the waiting time of the jump process. For this purpose we assume (2.3). Let the process start in the configuration $X=(q', Y)$. We want to estimate the probability that the particle at q' stays there up to time T. This survival probability is given by

$$\left[\int \mathbb{P}_{(q',Y)} \exp\left(-\int_0^T \mathrm{d}t\, V_q(X_t)\right)\right]^{-1}\int \mathbb{P}_{(q',Y)} \exp\left(-\int_0^T \mathrm{d}t\, V_q(X_t)\right)$$
$$\times\chi(\{X_t=(q', Y_t) \text{ for } 0\leqslant t\leqq T\}). \tag{4.14}$$

Here χ denotes the indicator function of the set $\{\cdot\}$. Since the particle at q' stays there for $0\leqslant t\leqslant T$ and, because of the particular structure of V_q, we have $V_q(X_t)=V_{q-q'}(Y_t)$. For the free process particles are independent and the survival probability is $\mathrm{e}^{-\omega(q')T}$. Therefore

$$(4.14)=\mathrm{e}^{-\omega(q')T}\left\{\left[\int \mathbb{P}_{(q',Y)} \exp\left(-\int_0^T \mathrm{d}t\, V_q(X_t)\right)\right]^{-1}\int \mathbb{P}_Y \exp\left(-\int_0^T \mathrm{d}t\, V_{q-q'}(Y_t)\right)\right\}. \tag{4.15}$$

For large T the ratio behaves as $\exp[(E(q-q')-E(q))T]$. Now if $\Delta_q(q')>0$, then the survival probability has an exponentially decaying bound and the particle has to jump out of q' eventually. $\Delta_q>0$ means that there are no sticky spots.

5. Binding

We try to mimic the simplified example of § 3. We start in the vacuum, i.e. no particle present, and mark the time spans the system stays in the vacuum. The waiting time in the vacuum has an exponential distribution. However, in contrast to the simplified example studied before, the waiting time in 'no vacuum' has some complicated and unknown distribution. Furthermore the particle present at the end of the last vacuum period may be at some other position than the particle to be destroyed at the beginning of the next vacuum period. Waiting times are still independent.

Let us first impose condition (2.3) and let us then write

$$H(q)=H_1(q)+P \tag{5.1}$$

with

$$P\psi=\left(-\int \mathrm{d}k\,\lambda(k)\psi_1(k), 0, 0, \ldots\right)+(0, -\psi_0\lambda(k_1), 0, \ldots). \tag{5.2}$$

P is a (non-normalised) one-dimensional projection. $H_1(q)$ commutes with the projection onto the Fock vacuum. On this subspace $H_1(q)$ is multiplication by $\frac{1}{2}q^2$. We write

$$H_1(q)=\tilde{H}(q)+\tfrac{1}{2}q^2\delta_{0,0}. \tag{5.3}$$

Note that $\tilde{H}(q)$ corresponds again to a perturbed jump process, only $|X_t| \geq 1$ ($|X|$ denotes the number of particles in the configuration X). In particular,

$$E(q) \leq \inf_{\psi, \|\psi\|=1} \langle \psi | \tilde{H}(q) \psi \rangle.$$

For z sufficiently negative

$$(H(q)-z)^{-1} = \sum_{n=0}^{\infty} (H_1(q)-z)^{-1}[-P(H_1(q)-z)^{-1}]^n \tag{5.4}$$

is a norm convergent sum. Since P is one dimensional, we have

$$\left(\left\langle \Omega \left| \frac{1}{H(q)-z} \Omega \right.\right\rangle\right)^{-1} = \tfrac{1}{2}q^2 - z - \langle \lambda | (\tilde{H}(q)-z)^{-1} \lambda \rangle. \tag{5.5}$$

Both sides are analytic for $z < E(q)$. Equation (5.5) holds then for all $z < E(q)$.

Now

$$(\tilde{H}(q)-z)^{-1} = \int_0^\infty \mathrm{d}t\, \mathrm{e}^{zt}\, \mathrm{e}^{-\tilde{H}(q)t}.$$

The kernel of $\mathrm{e}^{-\tilde{H}(q)t}$ on one-particle space is denoted by $(\mathrm{e}^{-t\tilde{H}(q)})_{11}(k, k')$. It has two contributions: (i) the particle at k sits there up to time t; (ii) the particle at k disappears before time t. Therefore

$$(\mathrm{e}^{-t\tilde{H}(q)})_{11}(k, k') = \delta(k-k')h_k(t) + R_t(k, k'). \tag{5.6}$$

Note that $R_t(k, k') \geq 0$ by construction. To determine $h_k(t)$ we use the same method as in (4.15). By definition, for $0 \leq s \leq t$, the configuration is of the form $X_s = (k, Y_s)$. Hence $V_q(X_s) = V_{q-k}(Y_s)$. Since, in the free process, particles are independent, the Y_t process is identical to the X_t process with no restriction on $|X_t|$. Therefore

$$h_k(t) = \mathrm{e}^{-\omega(k)t} \langle \Omega | \mathrm{e}^{-tH(q-k)} \Omega \rangle \tag{5.7}$$

$$\langle \lambda | (\tilde{H}(q)-z)^{-1} \lambda \rangle = \int_0^\infty \mathrm{d}t\, \mathrm{e}^{zt} \left(\int \mathrm{d}k\, \lambda(k)^2 h_k(t) + \int \mathrm{d}k \int \mathrm{d}k'\, \lambda(k)\lambda(k') R_t(k, k') \right). \tag{5.8}$$

Omitting the positive contribution from R_t yields

$$\left\langle \Omega \left| \frac{1}{H(q)-z} \Omega \right.\right\rangle \geq \left(\tfrac{1}{2}q^2 - z - \int \mathrm{d}k\, \lambda(k)^2 \left\langle \Omega \left| \frac{1}{H(q-k)+\omega(k)-z} \Omega \right.\right\rangle \right)^{-1}. \tag{5.9}$$

Suppose that

$$\tfrac{1}{2}q^2 - z = \int \mathrm{d}k\, \lambda(k)^2 \left\langle \Omega \left| \frac{1}{H(q-k)+\omega(k)-z} \Omega \right.\right\rangle \tag{5.10}$$

admits a solution $z < E_c(q)$. Then, as z increases from $-\infty$, $\langle \Omega | H(q)-z)^{-1} \Omega \rangle$ has to diverge below the continuum edge. Therefore $\Delta_q > 0$ and $H(q)$ has a unique ground state. Clearly $E(q) \leq z$. Note that the left-hand side of (5.10) increases in z. If (5.10) admits a solution at all, it has to be unique.

If $\int \mathrm{d}k\, \lambda(k)^2 = \infty$, but still $\int \mathrm{d}k\, \lambda(k)^2 (1+k^2)^{-1} < \infty$, then $H(q)$ is self-adjoint (although with a domain differing from the one of H_0) and bounded from below [2]. We choose a large k cutoff λ_δ such that $\int \mathrm{d}k\, \lambda_\delta(k)^2 < \infty$ and denote the corresponding Hamiltonian by $H_\delta(q)$. Then for $z < E(q)$

$$\lim_{\delta \to 0} (H_\delta(q)-z)^{-1} = (H(q)-z)^{-1} \tag{5.11}$$

in the strong operator norm [2]. In particular, $\lim_{\delta\to 0}\langle\Omega|(H_\delta(q)-z)^{-1}\Omega\rangle = \langle\Omega|(H(q)-z)^{-1}\Omega\rangle$. Since (5.9) holds for any δ, it remains true in the limit $\delta\to 0$.

We summarise our main result.

Theorem. Let $\omega(k)\geqslant\omega_0>0$, $\omega(k_1)+\omega(k_2)-\omega(k_1+k_2)\geqslant 0$, ω continuous. Let $\int \mathrm{d}k\lambda(k)^2(1+k^2)^{-1}<\infty$ and let λ and ω be reflection invariant. Let z be the solution of

$$\tfrac{1}{2}q^2 - z = \alpha\int \mathrm{d}k\,\lambda(k)^2\left\langle\Omega\,\middle|\,\frac{1}{H(q-k)+\omega(k)-z}\Omega\right\rangle. \tag{5.12}$$

(Here we have reintroduced the coupling constant α.) If

$$z<\inf_{q'}(E(q-q')+\omega(q')) \tag{5.13}$$

then $H(q)$ has a unique ground state ψ_q. ψ_q is positive (up to an overall phase factor) and $\langle\Omega|\Omega_q\rangle>0$. Furthermore $E(q)\leqslant z$. In a sufficiently small neighbourhood of (q,α), E is jointly analytic in both variables.

Because $1/k^2$ is not integrable near zero in dimensions $d=1,2$, we conclude that for $d=1,2$ the polaron always has a unique ground state.

Corollary. Let ω be twice continuously differentiable. Let

$$\omega(k_1)+\omega(k_2)-\omega(k_1+k_2)\geqslant c>0$$

and let there exist a k_0 such that

$$E(q-k_0)+\omega(k_0)=\inf_k(E(q-k)+\omega(k)). \tag{5.14}$$

Then for dimensions $d=1,2$, $H(q)$ has a unique ground state. (Equation (5.12) has a solution $z<E_c(q)$.)

Proof. By assumption there is a k_0 at which the function $k\to E(q-k)+\omega(k)$ takes its minimum. Therefore $E(q-k_0)+\omega(k_0)\leqslant E(q-k')+\omega(k')$ for any k'. We choose $k'=k_0+q'$. Then

$$0<c\leqslant\omega(k_0)+\omega(q')-\omega(k_0+q')\leqslant E(q-k_0-q')+\omega(q')-E(q-k_0). \tag{5.15}$$

Hence $\Delta_{q-k_0}>0$ and $H(q-k_0)$ has a unique ground state. By continuity this still holds in a ball of radius ε around $q-k_0$ with ε sufficiently small.

If in (5.12) the right-hand side is replaced by some lower bound, all assertions remain true. Let $\mu_q(\mathrm{d}\gamma)$ be the spectral measure of $H(q)$ with vector Ω. Then the right-hand side of (5.12) equals

$$\alpha\int\mathrm{d}k\,\lambda(k)^2\int_0^\infty\mu_{q-k}(\mathrm{d}\gamma)(\gamma+E(q-k)+\omega(k)-z)^{-1}$$
$$\geqslant\alpha\int_{\{|k-k_0|<\varepsilon\}}\mathrm{d}k\,\lambda(k)^2\langle\Omega|\psi_{q-k}\rangle^2(E(q-k)+\omega(k)-z)^{-1}. \tag{5.16}$$

Close to $k=k_0$, $E(q-k)$ is analytic and ω is twice differentiable. Therefore, by (5.14) and (4.6)

$$E(q-k)+\omega(k)=E_c(q)+\frac{1}{2}\sum_{i,j=1}^{d}a_{ij}(k-k_0)_i(k-k_0)_j \tag{5.17}$$

with $a \geqslant 0$ as a matrix. Since $\lambda(k) > 0$ and $\langle\Omega|\psi_{q-k}\rangle > 0$ close to k_0, the right-hand side of (5.16) diverges as $z \to E_c(q)$. Therefore the equation $\frac{1}{2}q^2 - z =$ (right-hand side of (5.16)) has a solution z with $z < E_c(q)$.

We have too little *a priori* knowledge about $E(q)$ to verify (5.14) for general ω. If ω takes its maximum 'at infinity', then $E(0) + \omega(q) \leqslant E(\infty) + \omega(\infty)$, since $E(0) \leqslant E(q')$ for any q'. By continuity the infinum of $E(q - \cdot) - \omega(\cdot)$ has to be taken at some finite value and (5.14) holds. To improve our condition we use (1.10): for $|k| < \sqrt{2\omega_0}$ the dispersion relation is arbitrary and for $|k| > \sqrt{2\omega_0}$, ω takes its maximum 'at infinity'. In particular, if $\omega(k) = \omega_0$, then (5.14) holds with $k_0 = q$.

For dimensions $d \geqslant 3$, $1/k^2$ is integrable near zero and in general the lower bound (5.9) does not diverge as $z \to E_c(q)_-$. Let us discuss the particular case $\omega(k) = \omega_0$, λ rotation invariant, $d = 3$, Then using the lower bound as in (5.16) yields

$$\tfrac{1}{2}q^2 - z = \alpha \int_{\{|k| \leqslant \sqrt{2\omega_0}\}} \mathrm{d}^3k\, \lambda(k)^2 \langle\Omega|\psi_k\rangle^2 ((E(k) - E(0)) + E(0) + \omega_0 - z)^{-1}. \tag{5.18}$$

For small k, $E(k) - E(0) = k^2/2m^*$. If still a good approximation for the ball $|k| \leqslant \sqrt{2\omega_0}$, we can ensure a unique ground state whenever $|q| < q_c$ with

$$\tfrac{1}{2}q_c^2 - E(0) - \omega_0 = 2m^*\alpha \int_{\{|k| \leqslant \sqrt{2\omega_0}\}} \mathrm{d}^3k\, \lambda(k)^2 \langle\Omega|\psi_k\rangle^2 k^{-2}. \tag{5.19}$$

For large coupling $E(0) \simeq -\alpha$ ($\simeq -\alpha^2$ for the Fröhlich polaron) and $m^*(\alpha) \simeq \alpha^2$ ($\simeq \alpha^4$ for the Fröhlich polaron). Therefore the right-hand side dominates and $q_c \simeq$ constant $\times \sqrt{m^*}$ for large α.

The lower bound (5.9) has the physically expected dependence on the coupling constant. Suppose that we have verified that the lower bound diverges at $z < E_c(q)$ for some α_0. Then the same property holds for all $\alpha > \alpha_0$. The reason is that $\langle\Omega|(H(q-k) + \omega(k) - z)^{-1}\Omega\rangle$ is increasing in α and so is the right-hand side of (5.12).

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Appendix. The polaron functional integral at purely imaginary external field

We want to represent $\langle\Omega|\mathrm{e}^{-TH(q)}\Omega\rangle$ through the standard polaron functional integral. The Hamiltonian H of (1.1) lives on $\mathscr{H} = L^2(\mathbb{R}^d, \mathrm{d}x) \otimes \mathscr{F}$. A vector in $\mathscr{H}$ is decomposed according to the total momentum as $\zeta = \int \mathrm{d}q\, g(q)\psi_q$. Then

$$\langle\zeta|\mathrm{e}^{-TH}\, \mathrm{e}^{-\mathrm{i}\xi P}\zeta\rangle = \int \mathrm{d}q\, g(q)^* g(q)\, \mathrm{e}^{-\mathrm{i}\xi q} \langle\psi_q|\mathrm{e}^{-TH(q)}\psi_q\rangle. \tag{A1}$$

We choose $\zeta = \delta(x) \otimes \Omega$, i.e. $g = (2\pi)^{-d/2}$, $\psi_q = (2\pi)^{-d/2}\, \mathrm{e}^{\mathrm{i}qx}\, \Omega$. Now

$$\mathrm{e}^{-\mathrm{i}\xi P}\zeta = \delta(x - \xi) \otimes \Omega \tag{A2}$$

since $\int \mathrm{d}k\, k a^+(k) a(k)\Omega = 0$. Therefore, inverting the Fourier transform,

$$\langle \Omega | \mathrm{e}^{-TH(q)}\Omega \rangle = \int \mathrm{d}\xi\, \mathrm{e}^{\mathrm{i}\xi q} \langle \delta(x) \otimes \Omega | \mathrm{e}^{-TH} \delta(x-\xi) \otimes \Omega \rangle. \tag{A3}$$

By the Feynman–Kac formula, integrating out the bosons, we find

$$\langle \Omega | \mathrm{e}^{-TH(q)}\Omega \rangle = \int \mathbb{P}_0(\mathrm{d}x(\cdot)) \times \exp\left(\tfrac{1}{2}\alpha \int_0^T \mathrm{d}t \int_0^T \mathrm{d}s\, W(t-s, x(t)-x(s)) \right) \exp(\mathrm{i}qx(T)). \tag{A4}$$

Here $\mathbb{P}_0$ is the Brownian motion starting at the origin and

$$W(t,x) = \int \mathrm{d}k\, \lambda(k)^2\, \mathrm{e}^{-\omega(k)|t|} \cos kx. \tag{A5}$$

Let us substitute $\mathrm{i}q$ by q. Then $\mathbb{P}_0 \exp(qx(T) - \frac{1}{2}q^2 T)$ is the path measure of Brownian motion with a constant drift q. We define the free energy per unit length, as a function of the drift q, by

$$f(q) = -\lim_{T\to\infty} \frac{1}{T} \log \int \mathbb{P}_0(\mathrm{d}x(\cdot)) \exp\left(\tfrac{1}{2}\alpha \int_0^T \mathrm{d}t \int_0^T \mathrm{d}s\, W(t-s, x(t)-x(s)) + qx(T) \right). \tag{A6}$$

Then $f(q)$ analytically continued to the purely imaginary axis equals the ground-state energy $E(q)$. This observation could be useful numerically. For a strip around the real axis f is analytic. In general, it is difficult to show from (A6) that f is analytic in the entire complex q plane (and presumably not true for $d \geq 3$).

To push the analogy with the external field a little bit further we go over to the increments, $(\mathrm{d}/\mathrm{d}t)q(t) = v(t)$. Then (A4) becomes

$$\int \tilde{\mathbb{P}}(\mathrm{d}v(\cdot)) \exp\left[\alpha \int_{\{s \leq t\}} \mathrm{d}t \int \mathrm{d}s\, W\left(t-s, \int_s^t \mathrm{d}\tau\, v(\tau) \right) + \mathrm{i}q \int \mathrm{d}t\, v(t) \right]. \tag{A7}$$

$\tilde{\mathbb{P}}$ is white noise. Discretising the integral (A7) we obtain a one-dimensional d-component 'spin' system with a many-body interaction and a purely imaginary external field.

Also other matrix elements can be represented through the functional integral. Particularly convenient are the coherent state matrix elements

$$\langle W(f)\Omega | \mathrm{e}^{-TH(q)}\, W(f)\Omega \rangle$$

where

$$W(f) = \exp\left(\int \mathrm{d}k (f(k)a(k) - f^*(k)a^+(k)) \right)$$

is the Weyl operator.

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