Ground state of a quantum particle coupled to a scalar Bose field

Herbert Spohn

Theoretische Physik, Ludwig-Maximilians-Universität München,
Theresienstr. 37, D-80333 München, Germany
e-mail : spohn@stat.physik.uni-muenchen.de

Abstract

We use methods from functional integration to prove existence and uniqueness of the ground state of a confined quantum particle coupled to a scalar massless Bose field. For an external potential growing at infinity the ground state exists under fairly general conditions while for a decaying potential an unphysical condition on the coupling strength is still needed.

1. Introduction

We consider a quantum particle confined by an external potential such that it has a unique state of minimal energy. The problem is whether this ground state persists as the particle is coupled to a massless scalar Bose field. Physically, the particle could be an impurity and the Bose field the phonons in a solid. More fundamental, perhaps, is the coupling of a hydrogen atom to the radiation field à la Pauli-Fierz. In our note we have nothing to say on the latter topic. To set the scene let us spell out the Hamiltonian.

The particle is governed by

$$H_e = -\frac{1}{2}\,\Delta + V\,. \tag{1.1}$$

The potential $V : {}^n \to {}$ is such that H_e is defined as a self-adjoint operator on the domain $\mathcal{D}(H_e) = \mathcal{D}(-\Delta) \subset L^2({}^n)$. We have two standard examples in mind. (i) The potential decays at infinity. One choice is $V \in L^p({}^n) + L^\infty({}^n)$ with $p = 2$ for $n \leq 3$, $p = n/2$ for $n \geq 4$. Then the essential spectrum of H_e is $[\Sigma, \infty)$ with continuum edge $\Sigma \in {}$. We assume that H_e has a (unique) ground state ψ_0 with energy $E_0 < \Sigma$, $H_e\,\psi_0 = E_0\,\psi_0$, $\psi_0 \in L^2({}^n)$, and $\psi_0 > 0$. Of course, H_e could have further bound states. We refer to [1] for details. (ii) $V(x) \to \infty$ as $|x| \to \infty$, e.g. by adding to a potential from (i) a continuous potential bounded from below. Then H_e has a purely discrete spectrum and our ground state assumption is satisfied. Formally we subsume (ii) under (i) by setting $\Sigma = \infty$.

The scalar Bose field $\{a(k), a^\dagger(k),\ k \in {}^n\}$ satisfies the commutation relations $[a(k), a^\dagger(k')] = \delta(k - k')$. Its energy is

$$H_f = \int dk\,\omega(k)\ a^\dagger(k)\,a(k) \tag{1.2}$$

defined on the bosonic Fock space, $\mathcal{F}$. For a massless field the dispersion relation $\omega(k) = |k|$. In fact, our method is more general. It suffices to assume that $\omega : {}^n \to {}$ is continuous with $\omega(k) > 0$ for $k \neq 0$ and $\omega(k) \geq \omega_0 > 0$ outside the unit ball.

We couple the particle and the field in a translation invariant manner. Then

$$H = H_e \otimes 1 + 1 \otimes H_f + \int dk\,(\lambda(k)\,e^{ikx} \otimes a^\dagger(k) + \lambda(k)^*\,e^{-ikx} \otimes a(k)) \tag{1.3}$$

on $\mathcal{H} = L^2({}^n) \otimes \mathcal{F}$. We assume $\lambda(k) = \lambda(-k)^*$. Physically $\lambda(k) = \alpha\,\hat{\rho}(k)/\sqrt{2\omega(k)}$, where α is a coupling constant and ρ, the Fourier transform of $\hat{\rho}$, is the normalized real-valued "charge" distribution. In particular $\lim_{k \to 0} \hat{\rho}(k) = 1$. To avoid trivial degeneracies we assume $\lambda \neq 0$ a.s.. We also require that $\int |\lambda|^2\,(1 + \omega^{-1})\,dk < \infty$. Then H is self-adjoint on $D(H_e) \otimes D(H_f)$ and bounded from below [2].

For $\lambda = 0$ H has the unique ground state $\psi_0 \otimes \Omega$ with Ω the Fock vacuum. We would like to have conditions which guarantee that for $\lambda \neq 0$

H still has a unique ground state. In fact, for a suitable realization of Fock space, the kernel of e^{-tH} is positivity preserving and ergodic [2]. Thus the uniqueness comes from a Perron-Frobenius argument [1, Theorems XIII.44, XIII.46] and the real issue is *existence*. Note that if $\omega(0) = 0$, then for $\lambda = 0$ the continuous spectrum starts at E_0 and a perturbative argument will not work.

Physically, one argues that the coupling to the field makes the particle more heavy. This can be seen by taking $V = 0$ and considering the ground state energy $E(P)$ as a function of the total momentum, P. The effective mass is usually defined by $m = [\partial_P^2 E(0)]^{-1}$. One can prove that $m \geq 1$ in our units [3]. Approximately the particle is then governed by the effective Hamiltonian $H_{\text{eff}} = -\frac{1}{2m}\Delta + V$. If H_e has a ground state, so does H_{eff}. Thus no matter how strong the interaction the coupled system should always have a ground state.

There is one proviso. The coupling could be so strong that $m = \infty$. Then tunneling is suppressed and the ground state sits at one of the absolute minima of the potential. Such a phenomenon has been proved for simplified versions of (1.3) [4]. The strong reduction in fluctuations is always associated with an infinite number of bosons. Thus in our mathematical framework it would mean that there is *no* ground state for H in $\mathcal{H}$, i.e. existence is lost.

Recently Bach, Fröhlich, and Sigal [2] obtained very sharp estimates on the resonances for the Hamiltonian (1.3). As an aside, they also investigate the ground state problem by using operator methods originally developed in the context of quantum field theory. One first replaces $\omega(k) = |k|$ by $\omega_m(k) = \sqrt{k^2 + m^2}$ and proves that $H(\omega_m)$ has a ground state provided $\Sigma - E_0 - \int |\lambda|^2 \omega^{-1} dk \geq 4m > 0$. The true ground state at $m = 0$ is constructed through the weak limit $m \to 0$ of the ground states of $H(\omega_m)$. One important ingredient is an estimate on the average number of bosons in the ground state uniformly in m. Their final result reads: H has a ground state provided (i) $\Sigma - E_0 \geq \int |\lambda|^2 \omega^{-1} dk$ and (ii) $\left(\int |\lambda|^2 \omega^{-2} dk\right) \left[1 + 4(\Sigma - E_0)^{-2} \int |\lambda|^2 dk\right] < 1$. (In [2] a more general class of Hamiltonians is studied and I specialized here to the translation invariant model (1.3).) Such an approximation technique was developed independently by Arai and Hirokawa [5] and applied to a variety of related models.

In this note I use methods from functional integration. If applicable, as it happens to be the case here, functional integrals typically yield stronger results and I wanted to understand how far they reach. The use of functional integration in our context has been described elsewhere [6] and I take it for granted that certain matrix elements can be written in terms of a suitable expectation. E.g.

$$(\psi_0 \otimes \Omega, e^{-TH}\, \psi_0 \otimes \Omega) =$$

$$_{[0,T]}\, (\psi_0(x_0)\, \psi_0(x_t)\, \exp[-\int_0^T dt V(x_t) - S_{[0,T]}(x.)]) \,. \tag{1.4}$$

Here refers to the expectation in the standard Wiener measure. $t \mapsto x(t)$ is a continuous path on $[0, T]$. The first piece is the ground state process for $-\frac{1}{2}\Delta + V$. The action S originates from integrating over the Bose field. In our case it is given by

$$S_{[0,T]}(x.) = \int_0^T dt \int_0^T ds\, W(x_t - x_s, t - s)\,, \tag{1.5}$$

$$W(x,t) = -\frac{1}{2} \int |\lambda|^2\, e^{-\omega|t|} \cos kx\, dk\,. \tag{1.6}$$

By assumption $|W(x,t)| \leq \int |\lambda|^2\, dk < \infty$. Therefore the integral (1.4) is well defined.

In the form (1.4) the existence of the ground state is reduced to a problem of statistical mechanics in one dimension (i.e. the Euclidean time axis). Ground state means limit $T \to \infty$. First note that W has its minimum at $x = 0$ and that S is invariant under the global shift x_t to $x_t + a$, which reflects the translation invariance of the coupling. If $V = 0$ and if $W(\cdot, t)$ decays sufficiently fast in t we may expect that on a large scale the path measure looks effectively as Brownian motion with diffusion constant $1/m$ [3]. Since $m > 1$, the paths fluctuate less compared to $S \equiv 0$, which should improve binding. If $m = \infty$, the suppression could be so strong that in the limit $T \to \infty$ the path no longer fluctuates at all and the distribution of x_t concentrates at a single point, which means there is no ground state in $\mathcal{H}$. To have a crude estimate, one compares energy and entropy. Let me assume that $x_t = 0$ and let me study an excitation of the form $\tilde{x}_t = a$ for $|t| \leq R$ and $\tilde{x}_t = 0$ for $|t| \geq R$. The entropy of such an excitation grows as $\log R$. To be on the safe side, if the energy of this excitation remains bounded as $R \to \infty$, then the entropy will outweigh the energy and there should be sufficient fluctuations even as $T \to \infty$. This leads to the condition

$$\int_{-\infty}^0 dt \int_0^\infty ds\, (W(\tilde{x}_t - \tilde{x}_s, t - s) - W(0, t - s)) \qquad \text{essentially bounded.} \tag{1.7}$$

If we just use $|1-\cos kx| \le 2$, a sufficient condition is

$$\int |\lambda|^2\, \omega^{-2}\, dk < \infty\,, \tag{1.8}$$

which will reappear later. For $\omega(k) = |k|$ and the physical coupling the integrand of (1.8) becomes $\alpha^2\, |\hat{\rho}|^2/\omega^3$ which diverges logarithmically at $k=0$ in three dimensions ($n=3$). To improve we observe that because of the external potential $|x_t - x_s|$ should be essentially bounded. Thus we may expand at small k as $1-\cos kx = \frac{1}{2}\, k^2\, x^2$. Then (1.7) leads to the condition

$$\int |\lambda|^2\, \omega^{-2}\, k^2 (1+k^2)^{-1}\, dk < \infty\,. \tag{1.9}$$

We conjecture that if (1.9) holds then H has a unique ground state.

Unfortunately our methods do not yield such a strong result.

Theorem 1. Let $\int |\lambda|^2\,(1+\omega^{-1})\, dk < \infty$ and $\lambda \neq 0$ a.s.. If $\int |\lambda|^2\, \omega^{-2}\, dk < \infty$ and if

$$\Sigma - E_0 > \int |\lambda|^2\, \frac{1}{2}\, k^2 \left(\omega + \frac{1}{2}\, k^2\right)^{-1} dk\,, \tag{1.10}$$

then H has a unique ground state.

In the remainder of the paper we give a proof, but before I add some comments.

(i) If $V(x) \to \infty$ as $|x| \to \infty$, then $\Sigma = \infty$ and there is no condition on the coupling strength. But we still cannot allow for the physical case $\omega(k) = |k|$, $\lambda = \alpha\, \hat{\rho}/\sqrt{2\omega}$, $n=3$.

(ii) An instructive simplification is the spin-boson Hamiltonian

$$H_{SB} = -\varepsilon\, \sigma_x \otimes 1 + 1 \otimes H_f + \sigma_z \otimes \int (\lambda(k)\, a^\dagger(k) + \lambda(k)^*\, a(k))\, dk \tag{1.11}$$

with $\omega(k) = |k|$ and σ_x, σ_z the Pauli spin matrices. The corresponding functional integral is a ferromagnetic Ising model over [4]. H_{SB} has a ground state in $^2 \otimes \mathcal{F}$ if and only if the spontaneous magnetization, m^*, of the Ising model vanishes [7]. One has fairly sharp estimates on m^*. E.g. one sufficient condition is $\lim\limits_{t\to\infty}\ t^2 \int |\lambda|^2\, e^{-\omega|t|}\, dk = 0$. On the other hand if we replace $-\sigma_x$ by, say, $-\sigma_x + a\sigma_y$, $a \in$, then in the σ_z representation the kernel $\exp\left[-t\,(-\sigma_x + a\sigma_y)\right]_{\sigma\sigma'}$ is no longer positive for $t>0$, which prevents a functional integral representation at least in the obvious way. The only methods available are then [2,5].

2. Existence

We prove Theorem 1. The strategy is to show that the sequence

$$\psi_T = e^{-TH}\,\psi_0\otimes\Omega/\|e^{-TH}\,\psi_0\otimes\Omega\| \tag{2.1}$$

has a non-zero weak limit as $T\to\infty$. For this purpose we consider

$$\begin{aligned}(\psi_T, e^{-\tau H_e}\otimes P_\Omega\,\psi_T) = [(\psi_0\otimes\Omega, e^{-TH}\,e^{-\tau H_e}\otimes P_\Omega\,e^{-TH}\,\psi_0\otimes\Omega)/\\ (\psi_0\otimes\Omega, e^{-(2T+\tau)H}\,\psi_0\otimes\Omega)]\,[(\psi_0\otimes\Omega, e^{-(2T+\tau)H}\,\psi_0\otimes\Omega)/\\ (\psi_0\otimes\Omega, e^{-2TH}\,\psi_0\otimes\Omega)]\end{aligned} \tag{2.2}$$

with $\tau>0$ and P_Ω the projection onto the Fock vacuum. Let E_m be the infimum of the spectrum of H.

Lemma 2. We have

$$\lim_{T\to\infty}\,(\psi_0\otimes\Omega, e^{-(2T+\tau)H}\,\psi_0\otimes\Omega)/(\psi_0\otimes\Omega, e^{-2TH}\,\psi_0\otimes\Omega) = e^{-\tau E_m}\,. \tag{2.3}$$

Proof. Let μ be the spectral measure for $\psi_0\otimes\Omega$. We claim that inf supp $\mu = E_m$. If so, (2.3) follows from the spectral theorem.

Let $W(f) = \exp\left[\int (f(k)\,a^\dagger(k) - f(k)^*\,a(k))\,dk\right]$ be the Weyl operator with test function $f\in L^2$. For bounded functions g we have

$$\begin{aligned}&(g\,\psi_0\otimes W(f)\,\Omega, e^{-TH}\,g\,\psi_0\otimes W(f)\,\Omega)\\ &= {}_{[0,T]}\Bigg(\psi_0(x_0)\,\psi_0(x_t)\,\exp\left[-\int_0^T dt\,V(x_t) - S_{[0,T]}\right]\,g(x_0)\,g(x_t) \qquad (2.4)\\ &\exp\left[-\frac{1}{2}\int |f|^2 dk + \frac{i}{2}\int_0^T dt\int (f^*\lambda e^{ikx_t}e^{-\omega t} + f\lambda^* e^{-ikx_t}e^{-\omega(T-t)})dk\right]\Bigg)\,.\end{aligned}$$

Let $\kappa =$ inf supp μ. By the spectral theorem

$$\lim_{T\to\infty}\,-\frac{1}{T}\,\log\,(\psi_0\otimes\Omega, e^{-TH}\,\psi_0\otimes\Omega) = \kappa\,. \tag{2.5}$$

By (2.4) the ratio $(g\,\psi_0 \otimes W(f)\,\Omega, e^{-TH}\, g\,\psi_0 \otimes W(f)\,\Omega)/(\psi_0 \otimes \Omega, e^{-TH}\,\psi_0 \otimes \Omega)$ is bounded uniformly in T. Thus also

$$\lim_{T\to\infty} -\frac{1}{T}\,\log\,(g\,\psi_0 \otimes W(f)\,\Omega, e^{-TH}\, g\,\psi_0 \otimes W(f)\,\Omega) = \kappa\,. \tag{2.6}$$

The lsp $\{g\,\psi_0 \otimes W(f)\,\Omega \mid g \text{ bounded}, f \in L^2\}$ is dense in $\mathcal{H}$ and each vector has a spectral measure with infimum κ. This is possible only if $\kappa = E_m$. ∎

We write the first factor in (2.4) as

$$
\begin{aligned}
{}_{[0,2T+\tau]}\Big(\exp\Big[-\int_0^{2T+\tau} V(x_t)\,dt - S_{[0,T]} - S_{[T+\tau,2T+\tau]} + \\
S_{[0,2T+\tau]} - S_{[0,2T+\tau]}\Big]\psi_0(x_0)\,\psi_0(x_{2T+\tau})\Big)\Big/ \\
{}_{[0,2T+\tau]}\left(\exp\left[-\int_0^{2T+\tau} V(x_t)\,dt - S_{[0,2T+\tau]}\right]\psi_0(x_0)\,\psi_0(x_{2T+\tau})\right)\,.
\end{aligned}
\tag{2.7}$$

Using $|\cos kx| \le 1$ we obtain the pathwise bound

$$
\begin{aligned}
S_{[0,T]} + S_{[T+\tau,2T+\tau]} - S_{[0,2T+\tau]} \le \\
\frac{1}{2}\int |\lambda|^2 \left(\left(2\int_{-\infty}^0\int_\tau^\infty + 4\int_0^\tau\int_\tau^\infty + \int_0^\tau\int_0^\tau\right) e^{-\omega|t-s|}\,dt\,ds\right) dk \le \\
\int |\lambda|^2\,(\tau\omega^{-1} + \omega^{-2}\,(3 - 2e^{-\tau\omega})\,dk = \ell(\tau)\,.
\end{aligned}
\tag{2.8}$$

Let $E(d\lambda)$ be the spectral resolution of H_e. By assumption for sufficiently small δ the spectral projection $E([E_0, \Sigma-\delta])$ is finite dimensional. (If $\Sigma = \infty$, we take $\Sigma - \delta < \infty$.) From the argument above and by Lemma 1 we conclude

$$
\begin{aligned}
\liminf_{T\to\infty}\left(\int_{E_0}^{\Sigma-\delta} e^{-\lambda\tau}\,(\psi_T, E(d\lambda)\otimes P_\Omega\,\psi_T) + \right. \\
\left.\int_{\Sigma-\delta}^\infty e^{-\lambda\tau}\,(\psi_T, E(d\lambda)\otimes P_\Omega\,\psi_T)\right) \ge e^{-\tau E_m}\,e^{-\ell(\tau)}\,.
\end{aligned}
\tag{2.9}$$

The second term on the left hand side is bounded by $e^{-\tau(\Sigma-\delta)}$. Finally we optimize with respect to τ with the result

Lemma 3. If $\int |\lambda|^2\, \omega^{-2}\, dk < \infty$ and if $\int |\lambda|^2\, \omega^{-1}\, dk < \Sigma - E_m$, then for sufficiently small $\delta > 0$

$$\liminf_{T\to\infty}\, (\psi_T, E([E_0, \Sigma - \delta]) \otimes P_\Omega\, \psi_T) > 0\,. \tag{2.10}$$

We still have to convert the condition in Lemma 3 to a condition on $\Sigma - E_0$. This can be achieved through a variational bound on E_m.

Lemma 4. We have the bound

$$E_m \le E_0 - \int |\lambda|^2 \left(\omega + \frac{1}{2}\, k^2\right)^{-1} dk\,. \tag{2.11}$$

Proof. Let $P = \int dk\, k\; a^\dagger(k)\, a(k)$ be the total momentum of the field. We choose as trial function $\psi_f = \psi_0(x)\, e^{ixP}\, W(f)\, \Omega$ with f yet to be determined. Then

$$E_m \le (\psi_f, H\, \psi_f) = E_0 + \frac{1}{2}\left(\int k |f|^2\, dk\right)^2 + \int \left(\omega + \frac{1}{2}\, k^2\right) |f|^2\, dk + \int (\lambda f^* + \lambda^* f)\, dk\,. \tag{2.12}$$

The minimizing $f = \lambda\left(\omega + \frac{1}{2}\, k^2\right)^{-1}$ yields the bound (2.11). ∎

Lemma 3 and Lemma 4 imply the existence of a ground state provided

$$\Sigma - E_0 \ge \int |\lambda|^2\, \omega^{-1}\, dk - \int |\lambda|^2 \left(\omega + \frac{1}{2}\, k^2\right)^{-1} \tag{2.13}$$

as claimed in Theorem 1.

Acknowledgement. I thank V. Bach for illuminating discussions.

References

[1] M. Reed and B. Simon, Methods of Modern Mathematical Physics : Analysis of Operators, Vol. 4. Academic Press, 1978.

[2] V. Bach, J. Fröhlich and I. Sigal, Quantum electrodynamics of confined non-relativistic particles. Preprint, 1996.

[3] H. Spohn, The effective mass of the polaron – a functional integral approach, *Annals of Physics* **175**, 278-318 (1987).

[4] H. Spohn, Ground state(s) of the spin-boson Hamiltonian, *Comm. Math. Phys.* **123**, 277-304 (1988).

[5] A. Arai and M. Hirokawa, On the existence and uniqueness of ground states of a generalized spin-boson model. Preprint, 1996.

[6] E. Nelson, Schrödinger particles interacting with a quantized scalar field. Theory and Applications of Analysis in Function Space, ed. by W.T. Martin and I. Segal. MIT Press, Cambridge, Mass., 1964.

[7] H. Spohn, unpublished note, 1991.