Monatsh Math (2009) 157:365–378
DOI 10.1007/s00605-008-0033-7

Polaron with at most one phonon in the weak coupling limit

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Received: 21 December 2007 / Accepted: 6 May 2008 / Published online: 13 August 2008

Abstract We introduce the polaron model with at most one phonon from the H. Fröhlich polaron Hamiltonian by eliminating contributions from more than two phonons. Spectral properties of this 0,1-phonon polaron model are investigated. It is clarified that, in the weak coupling region, the lowest energy and the effective mass obtained from the 0,1-phonon polaron model agree with those of the H. Fröhlich polaron Hamiltonian.

Keywords Polaron · Ground state · Effective mass

Mathematics Subject Classification (2000) 81T10 · 47A10 · 47A75

1 Introduction

Let us consider an electron coupled to the elastic deformations of an ionic crystal. Under approximation proposed by H. Fröhlich [6], the Hamiltonian is formally given by

$$H_{\mathrm{Polaron}} = -\frac{1}{2}\Delta_x + \sqrt{\alpha}\lambda_0 \int_{\mathbb{R}^3} \frac{\mathrm{d}k}{(2\pi)^{3/2}|k|}\left[\mathrm{e}^{\mathrm{i}k\cdot x}a(k) + \mathrm{e}^{-\mathrm{i}k\cdot x}a(k)^*\right] + \int_{\mathbb{R}^3} \mathrm{d}k\, a(k)^* a(k)$$

Communicated by A. Jüngel.

This work was supported by Japan Society for the Promotion of Science (JSPS).

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with $\lambda_0 = (2\sqrt{2}\pi)^{1/2}$. This Hamiltonian is living in the Hilbert space $L^2(\mathbb{R}^3) \otimes \mathfrak{F}$ where $\mathfrak{F}$ is the Fock space over $L^2(\mathbb{R}^3)$ given by $\mathfrak{F} = \oplus_{n=0}^{\infty} L^2(\mathbb{R}^3)^{\otimes_s n}$, $L^2(\mathbb{R}^3)^{\otimes_s n}$ is the n-fold symmetric tensor product of $L^2(\mathbb{R}^3)$ with the convention $L^2(\mathbb{R}^3)^{\otimes_s 0} = \mathbb{C}$. Here Δ_x is the Laplacian on $L^2(\mathbb{R}^3)$ and $a(k), a(k)^*$ are the phonon annihilation and creation operators. Under the natural identification $L^2(\mathbb{R}^3)^{\otimes_s n} = L^2_{\mathrm{sym}}(\mathbb{R}^{3n})$, the symmetric L^2-space over $\mathbb{R}^{3n}$, the annihilation operator is defined by

$$(a(k)\varphi)^{(n)}(k_1, \dots, k_n) = \sqrt{n+1}\varphi^{(n+1)}(k, k_1, \dots, k_n) \ \ a.e.$$

for $\varphi = \oplus_{n=0}^{\infty} \varphi^{(n)} \in \mathfrak{F}$, with $(a(k)\varphi)^{(0)} = 0$. These operators satisfy the so-called canonical commutation relations (CCRs): $[a(k), a(k')^*] = \delta(k-k')$, $[a(k), a(k')] = 0 = [a(k)^*, a(k')^*]$. Since the total momentum of the system is conserved, namely, H_{Polaorn} strongly commutes with $P_{\mathrm{tot}} = -\mathrm{i}\nabla + \int_{\mathbb{R}^3} \mathrm{d}k\, k a(k)^* a(k)$, H_{Polaron} can be decomposed as $H_{\mathrm{Polaron}} = \int_{\mathbb{R}^3}^{\oplus} \mathrm{d}P\, H_{\mathrm{Polaron}}(P)$ with

$$\begin{aligned} H_{\mathrm{Polaron}}(P) = \frac{1}{2}\left(P - \int_{\mathbb{R}^3} \mathrm{d}k\, k a(k)^* a(k)\right)^2 + \sqrt{\alpha}\lambda_0 \int_{\mathbb{R}^3} \frac{\mathrm{d}k}{(2\pi)^{3/2}|k|}[a(k) + a(k)^*] \\ + \int_{\mathbb{R}^3} \mathrm{d}k\, a(k)^* a(k). \end{aligned}$$

$H_{\mathrm{Polaron}}(P)$ is understood as the polaron Hamiltonian with a fixed total momentum P and it is living in $\mathfrak{F}$. Mathematically rigorous study of this model has been done by some authors [3,7,8,16] succesfully. As we saw in the above, the operator $H_{\mathrm{Polaron}}(P)$ contains the field operators $a(k)$ and $a(k)^*$, and these objects make our analysis difficult. In particular if α is not so small, namely non-perturbative case, we seriously take the effects coming from many phonons into consideration in order to investigate the property of the lowest energy. On the other hand, if α is small or weak coupling region, only few phonons would affect the phenomena and, as Spohn and Minlos did in [12], we could ignore the effects from multi-phonon. Now our approximated Hamiltonian is given by

$$H(P) = E H_{\mathrm{Polaron}}(P) E,$$

where E is the orthogonal projection onto 0,1-phonon subspace $\mathbb{C} \oplus L^2(\mathbb{R}^3) \subset \mathfrak{F}$. Formally $H(P)$ can be written as

$$H(P) = \begin{pmatrix} \frac{1}{2}P^2 & \lambda \left\langle \frac{1}{|k|} \right| \\ \lambda \left| \frac{1}{|k|} \right\rangle & \frac{1}{2}(P-k)^2 + 1 \end{pmatrix} \tag{1}$$

acting in the 0,1-phonon subspace $\mathbb{C} \oplus L^2(\mathbb{R}^3)$ with $\lambda = \sqrt{\alpha}(2\pi)^{-3/2}(2\sqrt{2}\pi)^{1/2}$, and it is a model of Friedrichs' type [5]. Here $\langle \frac{1}{|k|}|$ is a linear operator from $L^2(\mathbb{R}^3)$ to $\mathbb{C}$, defined by $\langle \frac{1}{|k|} | f \rangle = \int_{\mathbb{R}^3} \mathrm{d}k \, \frac{f(k)}{|k|}$ for a suitable f in $L^2(\mathbb{R}^3)$ and $| \frac{1}{|k|} \rangle$ is its adjoint (we refer [9] for recent developments of the Friedrichs model). Our aim of this paper is to investigate the spectral property of $H(P)$ and clarify a connection between the known results for $H_{\text{Polaron}}(P)$ and obtained results for $H(P)$ which could justify our 0,1-phonon approximation in the weak coupling limit.

It is obvious that the structure of $H(P)$ is much simpler than $H_{\text{Polaron}}(P)$. Indeed the approximated Hamiltonian $H(P)$ is solvable as we will see in the latter sections. It is worthy to emphasize that $H(P)$ is slightly singular because $1/|k|$ is not in $L^2(\mathbb{R}^3)$ which means the off-diagonal interaction term is unbounded. This point is one of differences between $H(P)$ and the Friedrichs model, cf.[2]. Thus we have to pay extra attentions for our analysis of $H(P)$. Also we should remark that this model is very instructive because (I) we could be away from the rigorous treatments of the second quantization which are complicated for beginners, (II) mathematical tools we need are elementary although obtained results well explain the behaviors of the polaron, especially in the weak coupling region (to describe the polaron in the strong coupling regime, our model (1) is powerless, and readers should consult [1,10,11,15] about this direction).

This paper is organized as follow. In Sect. 2, we give a precise definition of the Hamiltonian (1) and state main results, that is, existence and nonexistence of ground states and properties of spectrum, the lowest energy and the effective mass. Sections 3, 4 and 5 are devoted to the proof of the main results.

2 Main results

We denote the inner product and the norm of a Hilbert space $\mathfrak{h}$ by $\langle . , . \rangle_{\mathfrak{h}}$ and $\| \cdot \|_{\mathfrak{h}}$ respectively. If there is no danger of confusion, then we omit the subscript $\mathfrak{h}$ in $\langle . , . \rangle_{\mathfrak{h}}$ and $\| \cdot \|_{\mathfrak{h}}$. For a linear operator a on a Hilbert space, we denote its domain by $\mathrm{dom}(a)$. For a self-adjoint operator b on a Hilbert space, we denote its spectrum (resp. essential spectrum) by $\mathrm{spec}(b)$ (resp. $\mathrm{ess.\,spec}(b)$).

First of all, we have to clarify the exact meaning of the Hamiltonian

$$H(P) = \begin{pmatrix} \frac{1}{2}P^2 & \lambda \left\langle \frac{1}{|k|} \right| \\ \lambda \left| \frac{1}{|k|} \right\rangle & \frac{1}{2}(P-k)^2 + 1 \end{pmatrix}$$

with $\lambda = \sqrt{\alpha}(2\pi)^{-3/2}(2\sqrt{2}\pi)^{1/2}$. As we pointed out in the introduction, problem is coming from the fact that the function $1/|k|$ is not in $L^2(\mathbb{R}^3)$ which means the interaction term

$$H_{\mathrm{I}} = \begin{pmatrix} 0 & \lambda \left\langle \frac{1}{|k|} \right| \\ \lambda \left| \frac{1}{|k|} \right\rangle & 0 \end{pmatrix}$$

is not bounded. However the following lemma tells us that this singularity would not be so serious.

Lemma 2.1 *Let*

$$H_0(P) = \begin{pmatrix} \frac{1}{2}P^2 & 0 \\ 0 & \frac{1}{2}(P-k)^2 + 1 \end{pmatrix}.$$

For any $\varepsilon > 0$*, there exists a* $C_{\varepsilon,P} > 0$ *such that*

$$|\langle \varphi, H_{\mathrm{I}}\varphi\rangle| \le \varepsilon \langle \varphi, H_0(P)\varphi\rangle + C_{\varepsilon,P}\|\varphi\|^2$$

for all $\varphi = \varphi_0 \oplus \varphi_1 \in \mathbb{C} \oplus \mathrm{dom}(|k|)$.

Proof For $\varphi = \varphi_0 \oplus \varphi_1 \in \mathbb{C} \oplus \mathrm{dom}(|k|)$, one has

$$\langle \varphi, H_{\mathrm{I}}\varphi\rangle = 2\Re \varphi_0 \langle \varphi_1, \varrho\rangle$$

with $\varrho(k) = \lambda/|k|$. Note that, with $\beta_P(k)^2 = \frac{1}{2}(P-k)^2 + 1$,

$$\begin{aligned} |\langle \varphi_1, \varrho\rangle| &= \left| \lambda \int_{\mathbb{R}^3} \frac{\mathrm{d}k}{|k|\beta_P(k)^{1/2}} \beta_P(k)^{1/2}\varphi_1^*(k)\right| \le \left[\lambda^2 \int_{\mathbb{R}^3} \frac{\mathrm{d}k}{k^2\beta_P(k)}\right]^{1/2} \|\beta_P^{1/2}\varphi_1\| \\ &=: C_P \|\beta_P^{1/2}\varphi_1\| \end{aligned}$$

which implies, for arbitrary $\varepsilon > 0$,

$$\begin{aligned} |\langle \varphi, H_{\mathrm{I}}\varphi\rangle| &\le 2|\varphi_0| C_P \|\beta_P^{1/2}\varphi_1\| \le \varepsilon \|\beta_P^{1/2}\varphi_1\|^2 + 2\varepsilon^{-1}C_P^2|\varphi_0|^2 \\ &< \varepsilon \|H_0(P)\varphi\|^2 + C_{P,\varepsilon}\|\varphi\|^2 \end{aligned}$$

with $C_{P,\varepsilon} = 2\varepsilon^{-1}C_P^2$. □

Now we can give a precise definition of $H(P)$.

Definition 2.2 By the KLMN theorem, one can define a self-adjoint operator $H(P) = H_0(P) + H_{\mathrm{I}}$ as a form sum with the form domain $\mathbb{C} \oplus \mathrm{dom}(|k|)$.

Theorem 2.3 *(Essential spectrum) We have*

$$\text{ess.spec}(H(P)) = [1, \infty).$$

Theorem 2.4 (i) *(Existence of a unique ground state) Let* P_{c} *be the unique positive solution of the equation*

$$\frac{1}{2}P_{\mathrm{c}}^2 - 1 - \frac{\pi\alpha}{\sqrt{2}}\frac{1}{P_{\mathrm{c}}} = 0.$$

Clearly $P_{\mathrm{c}} > \sqrt{2}$ *for all* $\alpha > 0$. *Then, for* $P \in \mathbb{R}^3$ *with* $|P| < P_{\mathrm{c}}$, $H(P)$ *has a unique ground state* φ_P *given by*

$$\varphi_P = \frac{1}{\sqrt{1 + \frac{\alpha}{\sqrt{1-E(P)}(P^2+2-2E(P))}}} \begin{pmatrix} 1 \\ -\frac{\lambda}{|k|} \frac{1}{\frac{1}{2}(P-k)^2+1-E(P)} \end{pmatrix}, \tag{2}$$

where $E(P) := \inf \operatorname{spec}(H(P)) < \min\{\frac{1}{2}P^2, 1\}$. *Moreover*

$$\operatorname{spec}(H(P)) = \{E(P)\} \cup [1, \infty)\,.$$

(ii) *(Nonexistence of a ground state) For* $|P| \geq P_{\mathrm{c}}$, $H(P)$ *has no ground state and*

$$\operatorname{spec}(H(P)) = [1, \infty).$$

By the concrete expression (2), one can immediately obtain the following corollary.

Corollary 2.5 *(Properties of ground states) Let* l *be the angular momentum operator defined by* $l = 0 \oplus k \times (-\mathrm{i}\nabla_k)$.

(i) *For* $P = 0$, $\mathrm{e}^{\mathrm{i}\phi\omega\cdot l}\varphi_0 = \varphi_0$ *for all* $\phi \in \mathbb{R}$ *and* $\omega \in \mathbb{S}^2$.
(ii) *For* $P \neq 0$ *with* $|P| < P_{\mathrm{c}}$, *set* $\omega_P = P/|P|$. *Then* $\mathrm{e}^{\mathrm{i}\phi\omega_P\cdot l}\varphi_P = \varphi_P$ *for all* $\phi \in \mathbb{R}$.
(iii) φ_P *weakly converges to* 0 *as* $|P| \uparrow P_{\mathrm{c}}$.

Remark 2.6 Corollary 2.5 (i) means that the polaron at rest is distributed as a rotationally symmetric form. On the other hand, (ii) suggests that the polaron in motion with a momentum $P(\neq 0)$ maintains the rotational symmetry along to its motion only. The property (iii) tells us that the ground state in motion melts into an unstable state as $|P| \uparrow P_{\mathrm{c}}$.

Theorem 2.7 *(Properties of* $E(P)$*) We have the following.*

(i) $E(P_1) = E(P_2)$ *if* $|P_1| = |P_2|$.
(ii) *For* P *with* $|P| < P_{\mathrm{c}}$, $E(P)$ *is given by the unique solution of the following equation:*

$$\frac{1}{2}P^2 - E(P) = \frac{\sqrt{2}\alpha}{|P|} \arcsin\sqrt{\frac{P^2}{P^2+2-2E(P)}}.$$

Moreover $-\alpha \leq E(P) < \min\{\frac{1}{2}P^2, 1\}$ *for* P *with* $|P| < P_{\mathrm{c}}$.

(iii) *For* P *with* $0 < |P| < P_{\mathrm{c}}$, *we have* $\dfrac{\partial}{\partial |P|}E(P) > 0$.
(iv) $\left.\dfrac{\partial}{\partial |P|}E(P)\right|_{P=0} = 0.$

Theorem 2.8 *(Effective mass) One has*

$$\frac{1}{m_{\text{eff}}} := \frac{\partial^2}{\partial |P|^2} E(P)\bigg|_{P=0} = \frac{(1-E(0))^{3/2} + \frac{1}{3}\alpha - 2\alpha E(0)}{(1-E(0))^{3/2} + \frac{1}{2}\alpha}. \tag{3}$$

Especially the right hand side of (3) *is strictly positive whenever* $\alpha > 0$. *Moreover if* $E(0) > -\frac{1}{12}$, *then*

$$1 < m_{\text{eff}} \tag{4}$$

holds.

Remark 2.9 m_{eff} is called the *effective mass* of the polaron. The origin of this naming is coming from the following formula:

$$E(P) - E(0) = \frac{P^2}{2m_{\text{eff}}} + \mathcal{O}(|P|^3).$$

Namely m_{eff} behaves as a mass of the polaron. The strict inequality (4) means that the mass of electron in an ionic crystal becomes to be heavier because the electron is dressed with the phonon cloud, or the lattice distortion field. In the weak coupling limit mentioned below, we will see that this strict inequality actually holds.

Taking the weak coupling limit $\alpha \to 0$, one can rediscover the following well-known results [4].

Corollary 2.10 *(Weak coulping limit) For sufficiently small* α, *we have the following.*

(i)

$$E(P) = \frac{1}{2}P^2 - \alpha \frac{\sqrt{2}}{|P|} \arcsin \frac{|P|}{\sqrt{2}} + \mathcal{O}(\alpha^2).$$

In particular,

$$E(0) = -\alpha + \mathcal{O}(\alpha^2).$$

(ii)

$$m_{\text{eff}} = 1 + \frac{1}{6}\alpha + \mathcal{O}(\alpha^2).$$

3 Proof of Theorem 2.3

Let us define a Hamiltonian with an ultraviolet cutoff κ by

$$H_\kappa(P) = \begin{pmatrix} \frac{1}{2}P^2 & \lambda \left\langle \frac{1}{|k|}\chi_\kappa(k) \right| \\ \lambda \left| \frac{1}{|k|}\chi_\kappa(k) \right\rangle & \frac{1}{2}(P-k)^2 + 1 \end{pmatrix},$$

where $\chi_\kappa(k) = 1$ if $|k| < \kappa$, $\chi_\kappa(k) = 0$ otherwise. Since $\chi_\kappa(k)/|k| \in L^2(\mathbb{R}^3)$, $H_\kappa(P)$ is self-adjoint on $\mathbb{C} \oplus \mathrm{dom}(k^2)$ for all $\kappa < \infty$. Moreover, since the interaction term is rank 2 perturbation, one has

$$\text{ess.spec}(H_\kappa(P)) = [1, \infty). \tag{5}$$

Lemma 3.1 *Let $H_{\mathrm{I},\kappa}$ be the off-diagonal interaction term in $H_\kappa(P)$. Then one has*

$$|\langle \varphi, (H_{\mathrm{I}} - H_{\mathrm{I},\kappa})\varphi \rangle| \le \lambda D_P(\kappa) \left(\| H_0(P)^{1/2} \varphi \|^2 + \|\varphi\|^2 \right)$$

for all $\varphi \in \mathbb{C} \oplus \mathrm{dom}(|k|)$, where

$$D_P(\kappa)^2 = \int\limits_{|k|>\kappa} \frac{\mathrm{d}k}{k^2 \beta_P(k)}.$$

Proof For every $\varphi \in \mathbb{C} \oplus \mathrm{dom}(|k|)$, one can check that

$$\begin{aligned} |\langle \varphi, (H_{\mathrm{I}} - H_{\mathrm{I},\kappa})\varphi \rangle| &\le 2\lambda D_P(\kappa) \|\beta_P^{1/2}\varphi_1\| |\varphi_0| \le \lambda D_P(\kappa) \left(\|\beta_P^{1/2}\varphi_1\|^2 + |\varphi_0|^2 \right) \\ &\le \lambda D_P(\kappa) (\|H_0(P)^{1/2}\varphi\|^2 + \|\varphi\|^2). \end{aligned}$$

This completes the proof. □

Corollary 3.2 *$H_\kappa(P)$ converges to $H(P)$ in the norm resolvent sense as $\kappa \to \infty$.*

Proof This is a direct consequence of the above lemma and [14, Theorem VIII. 25]. □

Proof of Theorem 2.3 By Lemma 3.1, it follows that

$$H(P) \le H_\kappa(P) + \lambda D_P(\kappa)(H_0(P) + \mathbb{1}). \tag{6}$$

On the other hand, there exists a C such that $\langle \varphi, H_0(P)\varphi \rangle \le C(\langle \varphi, H(P)\varphi \rangle + \|\varphi\|^2)$ by Lemma 2.1. Combining this with (6), one arrives at

$$H(P) \le H_\kappa(P) + C' D_P(\kappa)(H(P) + \mathbb{1}),$$

where C' is a some positive constant independent of κ. Choosing κ sufficiently large as $C' D_P(\kappa) < 1$, we obtain

$$(1 - C' D_P(\kappa)) H(P) \le H_\kappa(P).$$

By changing the role of $H(P)$ and $H_\kappa(P)$ in the above arguments, we also obtain

$$(1 - C' D(\kappa)) H_\kappa(P) \le H(P).$$

Applying the min-max principle, one has

$$(1 - C'D_P(\kappa)) \inf \mathrm{ess.\,spec}(H(P) \le \inf \mathrm{ess.\,spec}(H_\kappa(P))$$

and

$$(1 - C'D_P(\kappa)) \inf \mathrm{ess.\,spec}(H_\kappa(P) \le \inf \mathrm{ess.\,spec}(H(P)).$$

Taking the limit $\kappa \to \infty$, we can conclude that

$$\inf \mathrm{ess.\,spec}(H(P)) = \lim_{\kappa\to\infty} \inf \mathrm{ess.\,spec}(H_\kappa(P)) = 1.$$

This is the desired assertion. □

4 Proof of Theorem 2.4

Let

$$\eta(P, z) = \frac{1}{2}P^2 - z - \lambda^2 \int_{\mathbb{R}^3} \frac{\mathrm{d}k}{k^2} \frac{1}{\frac{1}{2}(P-k)^2 + 1 - z}$$

for $z \in \mathbb{C}\backslash[1, \infty)$ if $P \ne 0$ and $z \in \mathbb{C}\backslash(1, \infty)$ if $P = 0$. The reason why η is important is explained by the following.

Lemma 4.1 *For $\varphi = \varphi_0 \oplus \varphi_1 \in \mathbb{C} \oplus L^2(\mathbb{R}^3)$ and $z \in \mathbb{C}\backslash[1, \infty)$, one has*

$$(H(P) - z)^{-1}\varphi = F_0[\varphi] \oplus F_1[\varphi]$$

with

$$F_0[\varphi] = \eta(P, z)^{-1} \left(\varphi_0 - \lambda \int_{\mathbb{R}^3} \frac{\mathrm{d}k}{|k|} \frac{1}{\frac{1}{2}(P-k)^2 + 1 - z} \right),$$

$$F_1[\varphi](k) = \frac{\varphi_1(k)}{\frac{1}{2}(P-k)^2 + 1 - z} - \frac{\lambda F_0[\varphi]}{|k|[\frac{1}{2}(P-k)^2 + 1 - z]}.$$

Proof First one can see the corresponding formula for $H_\kappa(P)$. Then taking the limit $\kappa \to \infty$, one obtains the assertion in the lemma by applying Corollary 3.2 (readers who are not familiar with a model of Friedrichs' type should check that $(H(P) - z)F_0[\varphi] \oplus F_1[\varphi] = \varphi$ actually holds). □

The above lemma tells us that the behavior of the ground states is reduced to that of $\eta(P, z)$. Therefore we will concentrate our attention to the analysis of η.

Lemma 4.2 *We have the following.*

(i) $\eta(P, E) = \dfrac{1}{2}P^2 - E - \dfrac{\sqrt{2}\alpha}{|P|} \arcsin\sqrt{\dfrac{P^2}{P^2 + 2 - 2E}}$ *for* $(P, E) \in \mathbb{R}^3\backslash\{0\} \times (-\infty, 1]$.

(ii) $\eta(0, E) = -E - \dfrac{\alpha}{\sqrt{1-E}}$ *for* $E < 1$.

Proof (i) We first note the Feynman's formula:

$$\frac{1}{ab} = \int_0^1 \mathrm{d}x \, \frac{1}{[ax + b(1-x)]^2}, \quad a > 0, b > 0. \tag{7}$$

For $E \leq 1$, by applying (7), one has

$$\begin{aligned}
&\int_{\mathbb{R}^3} \frac{\mathrm{d}k}{k^2} \frac{1}{\frac{1}{2}(P-k)^2 + 1 - E} \\
&= 2\int_0^1 \mathrm{d}x \int_{\mathbb{R}^3} \mathrm{d}k \, \frac{1}{\left[\{(P-k)^2 + 2 - 2E\}x + k^2(1-x)\right]^2} \\
&= 2\int_0^1 \mathrm{d}x \int_{\mathbb{R}^3} \mathrm{d}k \, \frac{1}{\left[(k - xP)^2 - x^2P^2 + (P^2 + 2 - 2E)x\right]^2}.
\end{aligned} \tag{8}$$

Here we remark the following elementary facts:

(a) $\displaystyle\int_{\mathbb{R}^3} \mathrm{d}k \, \frac{1}{(k^2 + a)^2} = \frac{\pi^2}{\sqrt{a}}, \quad a > 0,$

(b) $\displaystyle\int \frac{\mathrm{d}x}{\sqrt{-ax^2 + bx}} = -\frac{1}{\sqrt{a}} \arcsin\left(1 - \frac{2a}{b}x\right), \quad a, b > 0.$

By noting the fact $-x^2P^2 + (P^2 + 2 - 2E)x \geq 0$ for all $x \in [0, 1]$, one can see that

$$\text{RHS of (8)} = 2\int_0^1 \mathrm{d}x \frac{\pi^2}{\sqrt{(P^2+2-2E)x - P^2x^2}} \quad \text{(by (a))}$$

$$= -\frac{2\pi^2}{|P|}\left\{\underbrace{\arcsin\left(1-\frac{2P^2}{P^2+2-2E}\right)-\frac{\pi}{2}}_{=:-A}\right\} \quad \text{(by (b))}.$$

By the definition of A, one has $\arcsin\left(1-\frac{2P^2}{P^2+2-2E}\right) = -A+\frac{\pi}{2}$. Therefore

$$1-\frac{2P^2}{P^2+2-2E} = \cos A = 1-2\sin^2\frac{A}{2},$$

that is,

$$\sin\frac{A}{2} = \sqrt{\frac{P^2}{P^2+2-2E}},$$

equivalently $A = 2\arcsin\sqrt{\frac{P^2}{P^2+2-2E}}$. Summarizing these results, one arrives at

$$\int_{\mathbb{R}^3} \frac{\mathrm{d}k}{k^2}\frac{1}{\frac{1}{2}(P-k)^2+1-E} = \frac{4\pi^2}{|P|}\arcsin\sqrt{\frac{P^2}{P^2+2-2E}}.$$

Now we can conclude (i). Similarly one can show (ii). □

Corollary 4.3 (i) *For* $(P,E)\in\mathbb{R}^3\backslash\{0\}\times(-\infty,1]$, *one has*

$$\frac{\partial}{\partial|P|}\eta(P,E) = |P| + \frac{\sqrt{2}\alpha}{P^2}\arcsin\sqrt{\frac{P^2}{P^2+2-2E}} - \frac{\sqrt{2}\alpha}{|P|}\frac{\sqrt{2-2E}}{P^2+2-2E}.$$

In particular $\frac{\partial}{\partial|P|}\eta(P,E) > 0$ *for* $(P,E)\in\mathbb{R}^3\backslash\{0\}\times(-\infty,1]$.

(ii) *For* $(P,E)\in\mathbb{R}^3\times(-\infty,1)$, *one has*

$$\frac{\partial}{\partial|P|}\eta(P,E) = -1 - \frac{\sqrt{2}\alpha}{\sqrt{2-2E}(P^2+2-2E)}.$$

In particular $\frac{\partial}{\partial E}\eta(P,E) < 0$ *for* $(P,E)\in\mathbb{R}^3\times(-\infty,1)$.

Lemma 4.4 *Let $E_0(P) = \min\{\frac{1}{2}P^2, 1\}$. Then $\eta(P, E_0(P)) = 0$ if and only if $|P| = P_c (> \sqrt{2})$, where P_c is the unique positive solution of the following equation*

$$\frac{1}{2}P_c^2 - 1 - \frac{\pi\alpha}{\sqrt{2}}\frac{1}{P_c} = 0.$$

Moreover $\eta(P, E_0(P)) < 0$ if $|P| < P_c$ and $\eta(P, E_0(P)) > 0$ if $|P| > P_c$.

Proof For P with $|P| < \sqrt{2}$, one has

$$\eta(P, E_0(P)) = \eta(P, \tfrac{1}{2}P^2) = -\frac{\sqrt{2}\alpha}{|P|}\arcsin\frac{|P|}{\sqrt{2}} < 0.$$

On the other hand, for P with $|P| \geq \sqrt{2}$, we have

$$\eta(P, E_0(P)) = \eta(P, 1) = \frac{1}{2}P^2 - 1 - \frac{\pi\alpha}{\sqrt{2}|P|}.$$

Clearly $\eta(P, 1)$ is strictly increasing in $|P|$ and hence $\eta(P, 1) = 0$ if and only if $|P| = P_c$. Remainder assertions are trivial. □

Proposition 4.5 (i) *For P with $|P| < P_c$, the equation $\eta(P, E) = 0$ has a unique solution $E(P)$ such that*

(i-a) $0 < -E(0) \leq \alpha$,

(i-b) $0 < E_0(P) - E(P) < \dfrac{\pi\alpha}{\sqrt{2}|P|} - \dfrac{1}{2}P^2 + E_0(P)$ *for* $P \neq 0$.

(ii) *For P with $|P| \geq P_c$, the equation $\eta(P, E) = 0$ has no solution in $(P, E) \in \{P \in \mathbb{R}^3 \,|\, |P| \geq P_c\} \times (-\infty, 1)$.*

Proof (i) For P with $|P| < P_c$, $\eta(P, E_0(P)) < 0$ holds by Lemma 4.4. Moreover $\eta(P, E)$ is strictly increasing in E by Corollary 4.3. Thus there exists a unique $E(P)$ such that $\eta(P, E(P)) = 0$ with $E(P) < E_0(P)$. More precisely

$$\frac{1}{2}P^2 - E(P) = \frac{\sqrt{2}\alpha}{|P|}\arcsin\sqrt{\frac{P^2}{P^2 + 2 - 2E(P)}}. \tag{9}$$

Let us write $E(P) = E_0(P) - \Delta(P)$.

(i-a) $P = 0$: In this case, $E(0) = -\Delta(0)$ and (9) becomes

$$\Delta(0) = \frac{\alpha}{\sqrt{1 + \Delta(0)}}.$$

Thus the solution must statisfy $0 < \Delta(0) < \alpha$.

(i-b 1) $0 < |P| < \sqrt{2}$: In this case, (9) becomes

$$\Delta(P) = \frac{\sqrt{2}\alpha}{|P|}\arcsin\sqrt{\frac{P^2}{2 + 2\Delta(P)}}.$$

Equivalently

$$\sin \frac{|P|}{\sqrt{2}\alpha}\Delta(P) = \sqrt{\frac{P^2}{2+2\Delta(P)}}$$

with $\frac{|P|}{\sqrt{2}\alpha} \le \frac{\pi}{2}$. Hence $\Delta(P)$ satisfies $0 < \Delta(P) < \frac{\pi\alpha}{\sqrt{2}|P|}$.

(i-b 2) $\sqrt{2} \le |P| < P_{\rm c}$: We have

$$\frac{1}{2}P^2 - 1 + \Delta(P) = \frac{\sqrt{2}\alpha}{|P|}\arcsin\sqrt{\frac{P^2}{P^2+2\Delta(P)}}$$

or

$$\sin \frac{|P|}{\sqrt{2}\alpha}\left(\frac{1}{2}P^2 - 1 + \Delta(P)\right) = \frac{|P|}{\sqrt{P^2+2\Delta(P)}}$$

with $\frac{|P|}{\sqrt{2}\alpha}\left(\frac{1}{2}P^2 - 1 + \Delta(P)\right) \le \frac{\pi}{2}$. Thus we obtain

$$0 < \Delta(P) < \frac{\pi\alpha}{\sqrt{2}|P|} - \frac{1}{2}P^2 + 1.$$

Summarizing (i-b 1) and (i-b 2), one arrives at

$$0 < E_0(P) - E(P) < \frac{\pi\alpha}{\sqrt{2}|P|} - \frac{1}{2}P^2 + E_0(P).$$

(ii) This immediately follows from Corollary 4.3 (ii) and Lemma 4.4. □

Proof of Theorem 2.4 By Lemma 4.4 and Proposition 4.5, $\mathbb{C}\backslash[1,\infty) \ni z \to (H(P)-z)^{-1}$ is meromorphic with a simple pole at $z = E(P)$ if $|P| < P_{\rm c}$, and is holomorphic if $|P| \ge P_{\rm c}$, where $E(P)$ is given by Proposition 4.5. Thus $H(P)$ has a unique ground state with the corresponding eigenvalue $E(P)$ and $\mathrm{spec}(H(P)) = \{E(P)\} \cup [1,\infty)$. For $|P| \ge P_{\rm c}$, $H(P)$ has no ground state with $\mathrm{spec}(H(P)) = [1,\infty)$. The concrete expression (2) of the unique ground state is proven by Proposition 4.6 below. □

Proposition 4.6 *For P with $|P| < P_{\rm c}$, the unique ground state φ_P for $H(P)$ is given by* (2).

Proof Let $Q_{\rm GS}$ be the orthogonal projection onto the one dimensional subspace spanned by the ground state φ_P. Then one has

$$Q_{\rm GS} = \text{s-}\lim_{E \to E(P)} (E(P) - E)(H(P) - E)^{-1},$$

where s-lim means the strong limit. Since $Q_{\rm GS}(1 \oplus 0) \neq 0$, we have

$$\begin{aligned}\varphi_P &= \|Q_{\mathrm{GS}}(1\oplus 0)\|^{-1} Q_{\mathrm{GS}}(1\oplus 0)\\ &= \left(-\frac{\partial}{\partial E}\eta(P,E)\Big|_{E=E(P)}\right)^{-1/2}\left(\begin{array}{c}1\\ -\frac{\lambda}{|k|}\frac{1}{\frac{1}{2}(P-k)^2+1-E(P)}\end{array}\right).\end{aligned}$$

A concrete calculation yields (2). □

5 Proof of Theorems 2.7 and 2.8

Proposition 5.1 *One has the following.*

(i) $\frac{\partial}{\partial|P|}E(P) \geq 0$ *for P with $|P| < P_{\mathrm{c}}$. The equality holds only if $P = 0$.*

(ii) $\frac{\partial^2}{\partial|P|^2}E(P)\Big|_{P=0} = \frac{(1-E(0))^{3/2}+\frac{1}{3}\alpha-2\alpha E(0)}{(1-E(0))^{3/2}+\frac{1}{2}\alpha}$.

Proof (i) This is a direct consequence of Corollary 4.3 (i) (notice that

$$\arcsin\sqrt{\frac{P^2}{P^2+2-2E}} - |P|\frac{\sqrt{2-2E}}{P^2+2-2E} \geq 0$$

with $\frac{P^2}{P^2+2-2E} \leq 1$).

(ii) By (i) and the implicite function theorem, one obtains

$$\frac{\partial^2}{\partial|P|^2}E(P)\Big|_{P=0} = -\frac{\frac{\partial^2}{\partial|P|^2}\eta(P,E)\Big|_{P=0,E=E(0)}}{\frac{\partial}{\partial E}\eta(P,E)\Big|_{P=0,E=E(0)}}.$$

Finally we remark that

$$\begin{aligned}\frac{\partial^2}{\partial|P|^2}\eta(P,E) = 1 &- \frac{2\sqrt{2}\alpha}{|P|^3}\arcsin\sqrt{\frac{P^2}{P^2+2-2E}} + \frac{2\sqrt{2}\alpha}{P^2}\frac{\sqrt{2-2E}}{P^2+2-2E}\\ &+2\sqrt{2}\alpha\frac{\sqrt{2-2E}}{P^2+2-2E}\end{aligned}$$

which implies

$$\frac{\partial^2}{\partial|P|^2}\eta(P,E)\Big|_{P=0} = 1 - \frac{\alpha}{6}(1-E)^{-3/2} + 2\alpha(1-E)^{-1/2}.$$

□

Proof of Theorem 2.7 (i) Note that, for all $\phi \in \mathbb{R}$ and $\omega \in \mathbb{S}^2 := \{P \in \mathbb{R}^3 \mid |P| = 1\}$,

$$\mathrm{e}^{\mathrm{i}\phi\omega\cdot l} H(P) \mathrm{e}^{-\mathrm{i}\phi\omega\cdot l} = H(g(\phi, \omega)^{-1} P), \tag{10}$$

where $g(\phi, \omega) \in SO(3)$ is the rotation around ω with angle ϕ (Proof: For each finite κ, one can check that

$$\mathrm{e}^{\mathrm{i}\phi\omega\cdot l} H_\kappa(P) \mathrm{e}^{-\mathrm{i}\phi\omega\cdot l} = H_\kappa(g(\phi, \omega)^{-1} P), \tag{11}$$

that is, $\mathrm{e}^{\mathrm{i}\phi\omega\cdot l}\mathrm{e}^{\mathrm{i}tH_\kappa(P)}\mathrm{e}^{-\mathrm{i}\phi\omega\cdot l} = \mathrm{e}^{\mathrm{i}tH_\kappa(g(\phi,\omega)^{-1}P)}$. By applying Corollary 3.2, $\mathrm{e}^{\mathrm{i}\phi\omega\cdot l}\mathrm{e}^{\mathrm{i}tH(P)}\mathrm{e}^{-\mathrm{i}\phi\omega\cdot l} = \mathrm{e}^{\mathrm{i}tH(g(\phi,\omega)^{-1}P)}$ holds). The assertion (i) is a direct consequence of (10).

(ii) As we saw, the ground state energy inf spec$(H(P))$ is given by a unique simple zero $E(P)$ of $\eta(P, E)$ for $|P| < P_\mathrm{c}$. Hence Lemma 4.4 and Proposition 4.5 give the desired results.

(iii) and (iv) are proven in Proposition 5.1 (i). □

Proof of Theorem 2.8 This is an immediate consequence of Proposition 5.1 (ii). □

Acknowledgments The author thanks M. Hirokawa and A. Arai for useful discussions.

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