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Spectroscopy of a Three-Dimensional Isotropic Harmonic Oscillator With a δ -Type Perturbation

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Abstract The self-adjoint Hamiltonian describing a three-dimensional isotropic harmonic oscillator perturbed by an attractive point interaction is rigorously obtained by means of a renormalisation technique. It is shown how the spectrum of the oscillator is modified by such a perturbation. The new bound states can be explicitly obtained by solving a sequence of algebraic nonlinear equations. Numerical results in the computation of the first ones are reported.

1 Introduction

In this paper we investigate the three-dimensional isotropic harmonic oscillator perturbed by a three-dimensional δ -distribution, whose Hamiltonian is formally given by:

$$-\frac{1}{2}\Delta + \frac{1}{2}|x|^2 - \mu\delta = H_0 - \mu\delta.$$

It is worth noting that in the well-known formalism of creation and annihilation operators $a_i \equiv \frac{1}{\sqrt{2}}(x_i + \frac{\partial}{\partial x_i})$ and $a_i^{\dagger} \equiv \frac{1}{\sqrt{2}}(x_i - \frac{\partial}{\partial x_i})$, such a formal Hamiltonian reads:

$$\sum_{i=1}^{3} a_{i}^{\dagger} a_{i} + \frac{3}{2} - \mu \otimes_{i=1}^{3} \delta(\frac{a_{i} + a_{i}^{\dagger}}{\sqrt{2}}),$$

where $a_1^{\dagger}a_1$ is a short notation for $a_1^{\dagger}a_1 \otimes I \otimes I$ and so on (\otimes is the tensor product of operators on Hilbert spaces, [1, VIII.10]).

Since the one-dimensional Hamiltonian studied in [2] was of the type

$$a^{\dagger}a+rac{1}{2}-\mu\delta(rac{a+a^{\dagger}}{\sqrt{2}}),$$

it is clear that the Hamiltonian we are about to study is quite different from the Hamiltonian describing the sum of three one-dimensional δ -perturbed harmonic oscillators.

It turns out that the three-dimensional model is more interesting and more care is required in the limit procedure leading to the self-adjoint operator that gives a rigorous meaning to the formal expression written above.

To be precise, a 'renormalisation' procedure will be required in order to get the proper limit in the sense of resolvents. Such a renormalisation of the coupling constant of the interaction has been used extensively in order to define the correct self-adjoint operator corresponding to a formal expression of the type $-\Delta - \sum_{y \in Y} \mu_y \delta(\cdot - y)$ in three dimensions, as can be seen in [3] and the literature cited therein.

It is clear why we still need such a renormalisation technique also in the case of the harmonic oscillator: the quadratic potential only affects the behaviour of the system at large distances but, in the neighbourhood of the origin the short range interaction prevails and leads to a modification of the bound states of the harmonic oscillator.

The difference between the equation determining the bound states of the perturbed harmonic oscillator in one dimension and its (isotropic) analogue in three dimensions will be pointed out in the specific section.

Since the notation which is going to be used is basically the one used in [2], we refer the reader to that paper as far as the Dirac notation and resolvents are concerned. In addition, throughout this paper we shall identify $L^2(\mathbb{R}^3)$ and $L^2(\mathbb{R}) \otimes L^2(\mathbb{R}) \otimes L^2(\mathbb{R})$. This holds in the sense of isomorphisms and we refer the reader to [1, II.4 and VIII.10] for a description of tensor products of Hilbert spaces and tensor products of operators on Hilbert spaces. In the following l will denote the multi-index (l_1, l_2, l_3) (with $|l|_1 = |l_1| + |l_2| + |l_3|$) and Φ_l the tensor product $\Phi_{l_1} \otimes \Phi_{l_2} \otimes \Phi_{l_3}$. The symbol $\Phi_l^2(0)$ will be a short notation for $\Phi_{l_1}^2(0)\Phi_{l_2}^2(0)\Phi_{l_3}^2(0)$.

2 The resolvent of $H_0 - \mu \delta$ in three-dimensions

As we have anticipated in the introduction, it will not be possible to use the form method (exploited in [2]) in the three-dimensional case.

The reason is basically the divergence of the three-dimensional analogue of the series defining the value of the Green's function at the origin, namely

$$(H_0 + |E|)^{-1}(0,0) = \sum_{l \in \mathbb{N}^3} \frac{\Phi_{2l}^2(0)}{|2l|_1 + \frac{3}{2} + |E|}.$$
(2.1)

The divergence of the series in (2.1) can be easily proved by means of the explicit expression given in [1, Appendix to V.3] and its evaluation using Stirling's formula.

However, $(H_0 + |E|)^{-1}(\cdot, 0)$ and $(H_0 + |E|)^{-1}(0, \cdot)$ are functions in $L^2(\mathbb{R}^3)$. As a matter of fact, we have

$$\|(H_0+|E|)^{-1}(\cdot,0)\|_2^2 = \sum_{l\in\mathbb{N}^3} \frac{\Phi_{2l}^2(0)}{(|2l|_1+\frac{3}{2}+|E|)^2} \le (\sum_{k=0}^\infty \frac{\Phi_{2k}^2(0)}{(2k+\frac{1}{2})^{\frac{2}{3}}})^3 < \infty$$
(2.2)

since $\Phi_{2k}^2(0) \approx k^{-\frac{1}{2}}$. The explicit expression for the Green's function $(H_0 - E)^{-1}(x, y)$ for $Re(\frac{3}{2} - E) > 0$ is given in [4]. In particular, we have $\forall E$ with $Re(\frac{3}{2} - E) > 0$

$$(H_0 - E)^{-1}(x, 0) = \pi^{-\frac{3}{2}} e^{-\frac{|x|^2}{2}} \int_0^1 d\xi \frac{\xi^{\frac{1}{2} - E}}{(1 - \xi^2)^{\frac{3}{2}}} e^{-\frac{|x|^2 \xi^2}{1 - \xi^2}},$$

which shows that $(H_0 - E)^{-1}(\cdot, 0)$ is spherically symmetric. Since the resolvent at any point E with real part greater than $\frac{3}{2}$ can be expressed in terms of the resolvent at the point E = 0 due to the first resolvent identity, it is clear that the spherical symmetry is preserved throughout the resolvent set of H_0 .

This important property will be used in the study of the new energy levels created by the attractive point interaction.

We are now going to follow the procedure that has been used in [3, II.1.1] in order to determine the self-adjoint operator that gives a rigorous meaning to $-\Delta - \mu \delta$.

In our case we introduce a cut-off with respect to the energy eigenvalues and make the coupling constant μ explicitly dependent on the cut-off. We define a finite rank interaction as follows:

$$\delta^{(l)} = P_{|l|_1 \le \tilde{l}} \delta P_{|l|_1 \le \tilde{l}},$$

 $P_{|l|_1 \leq \tilde{l}}$ being the projection onto the finite-dimensional subspace whose basis is given by the restriction of the basis $\{\Phi_{l_1} \otimes \Phi_{l_2} \otimes \Phi_{l_3}\}_{l_1,l_2,l_3=0}^{\infty}$ to the vectors $\Phi_{l_1} \otimes \Phi_{l_2} \otimes \Phi_{l_3}$ with $l_1 + l_2 + l_3 \leq \tilde{l}$.

Because of the energy cut-off, we have now an interaction which is H_0 -small in the sense of forms, that is to say, $\forall E < 0$ and |E| sufficiently large:

$$\|(H_0 - E)^{-\frac{1}{2}} \delta^{(\tilde{l})} (H_0 - E)^{-\frac{1}{2}} \|_{\mathcal{T}_1} = \sum_{|l|_1 \le \tilde{l}} \frac{\Phi_{2l}^2(0)}{|2l|_1 + \frac{3}{2} + |E|} < 1.$$

Then, the resolvent of $H_0 - \mu(\tilde{l})\delta^{(\tilde{l})}$ is given by the operator-valued function meromorphic for $E \in \mathcal{C} \setminus \mathbb{R}_+$:

$$[\dot{H_0} - \mu(\tilde{l})\delta^{(\tilde{l})} - E]^{-1} = (H_0 - E)^{-1} + \frac{C(H_0^{(l)}; E)}{\frac{1}{\mu(\tilde{l})} - (H_0^{(\tilde{l})} - E)^{-1}(0, 0)}$$
(2.3)

where

$$C(H; E) \equiv |(H - \bar{E})^{-1}(\cdot, 0)\rangle \langle (H - E)^{-1}(0, \cdot)|$$

and

$$H_0^{(\bar{l})} = P_{|l|_1 \le \bar{l}} H_0 P_{|l|_1 \le \bar{l}}.$$

The only simple pole on the negative semiaxis $E \leq 0$ is determined by the equation:

$$\frac{1}{\mu(\tilde{l})} = (H_0^{(\tilde{l})} - E)^{-1}(0,0).$$

The operator in (2.3) belongs to $\mathcal{T}_{3+\epsilon}$ since the second summand is a finite rank operator and $(H_0 - E)^{-1} \in \mathcal{T}_{3+\epsilon}$ for any $E \in \rho(H_0)$. The latter statement can be proved as follows.

For any $E \leq 0$ the eigenvalues of $(H_0 - E)^{-1} = (H_0 + |E|)^{-1}$ are given by

$$\{(l_1+l_2+l_3+\frac{3}{2}+|E|)^{-1}\}_{l_1,l_2,l_3=0}^{\infty}$$

and such a sequence is bounded from above by

$$\prod_{i=1}^{3} (l_i + \frac{1}{2})^{-\frac{1}{3}} \in l^{3+\epsilon}(\mathbb{I} \mathbb{N}^3).$$

Thus, for any $E \leq 0$, $(H_0 - E)^{-1} \in \mathcal{T}_{3+\epsilon}$. Then, by using the first resolvent identity, for any $E' \in \rho(H_0)$ and any $E \leq 0$:

$$(H_0 - E')^{-1} = (H_0 - E)^{-1} + (E' - E)(H_0 - E')^{-1}(H_0 - E)^{-1} \in \mathcal{T}_{3+\epsilon}$$

since the second summand belongs to $\mathcal{T}_{3+\epsilon}$ being the product of a $\mathcal{T}_{3+\epsilon}$ operator and a bounded one.

If we choose

$$\frac{1}{\mu(\tilde{l})} = \sum_{|l|_1 \le \tilde{l}} \frac{\Phi_{2l}^2(0)}{|2l|_1 + \frac{3}{2}} + \alpha = H_0^{(\tilde{l})^{-1}}(0,0) + \alpha$$

with $\alpha \in I\!\!R$, then for any $E \leq 0$

$$(\| \|_{1}) - \lim_{\tilde{l} \to \infty} (H_{\alpha}^{(l)} - E)^{-1} = (\| \|_{1}) - \lim_{\tilde{l} \to \infty} [H_{0} - \mu(\tilde{l})\delta^{(l)} - E]^{-1} = R_{\alpha}(E)$$

$$= (H_{0} - E)^{-1} + \frac{C(H_{0}; E)}{\alpha - E \sum_{l \in \mathbb{N}^{3}} \frac{\Phi_{2l}^{2}(0)}{(|2l|_{1} + \frac{3}{2})(|2l|_{1} + \frac{3}{2} - E)}}$$
(2.4)

The proof is obtained taking account that the numerator of the second summand on the r.h.s. of (2.3) converges to $C(H_0; E)$ in the trace class norm as a consequence of (2.2) while the denominator converges to the one of the second summand on the r.h.s. of (2.4) as a consequence of our definition of $\mu^{(\tilde{l})}$. It is not difficult to check that $R_{\alpha}(E)$ ($\alpha > 0$) is well defined $\forall E \in \mathbb{C} \setminus \mathbb{R}_+$ and satisfies the resolvent identity in the region. Furthermore, it is obviously injective since there is no $f \in L^2(\mathbb{R}^3)$ satisfying

$$(H_0 - E)^{-1}f = -\frac{C(H_0; E)f}{\alpha - E\sum_{l \in \mathbb{N}^3} \frac{\Phi_{2l}^2(0)}{(|2l|_1 + \frac{3}{2})(|2l|_1 + \frac{3}{2} - E)}}$$

for any $E \in \mathcal{C} \setminus \mathbb{R}_+$.

Therefore, we must simply invoke the argument in [3, II.1.1] above the statement of theorem 1.1 to get that

$$R_{\alpha}(E) = (H_{\alpha} - E)^{-1}$$

that is to say, the limit $R_{\alpha}(E)$ is the resolvent of a densely defined self-adjoint operator H_{α} for any $\alpha > 0$.

If $\alpha \leq 0$, it is possible to have a singularity in the second term of the expression defining $R_{\alpha}(E)$ as an operator-valued function of E. As we shall see more in detail in the next section regarding the spectral analysis of H_{α} , if $\alpha \leq 0$ the denominator has only a simple zero in the whole of $\mathcal{C} \setminus \mathbb{R}_+$ along the negative semiaxis $E \leq 0$. Therefore, also for $\alpha \leq 0$, $R_{\alpha}(E)$ defines the resolvent of a densely defined self-adjoint operator H_{α} .

Let us summarise the result we have just obtained in a theorem.

Theorem 2.2. Let $\{H_{\alpha}^{(\tilde{l})}\}_{\tilde{l}=1}^{\infty}$ be the sequence of self-adjoint operators defined above. Then $H_{\alpha}^{(\tilde{l})} \to H_{\alpha}$ in the norm resolvent sense [1, VIII.7] and

$$(H_{\alpha} - E)^{-1} = (H_0 - E)^{-1} + \frac{C(H_0; E)}{\alpha - E \sum_{l \in \mathbb{N}^3} \frac{\Phi_{2l}^2(0)}{(|2l|_1 + \frac{3}{2})(|2l|_1 + \frac{3}{2} - E)}}.$$
 (2.5)

3 The bound state equation

The bound states of the perturbed three-dimensional oscillator are the poles of the resolvent of its Hamiltonian H_{α} .

As we have already seen in the one-dimensional situation, states belonging to energy levels of the type $|l|_1 + \frac{3}{2} = (2k+1) + \frac{3}{2}$ are not affected by the perturbation since $(H_0 - E)^{-1}(\cdot, 0)$ is obviously orthogonal to their eigenfunctions.

There is instead a major difference between the two models in the behaviour of the even levels, i.e. eigenenergies of the type $|l|_1 + \frac{3}{2} = 2k + \frac{3}{2}$, due to the $\frac{1}{2}(|l|_1 + 1)(|l|_1 + 2)$ -degeneracy of the eigenvalues of the spectrum of the 3-dimensional isotropic harmonic oscillator.

For the sake of simplicity, let us see this for the first excited even level, namely $E_2 = \frac{7}{2}$. As we have seen in [2], the corresponding one-dimensional level $E_2 = \frac{5}{2}$ is lowered by the attractive perturbation considered therein.

In three dimensions instead, three of the six states belonging to the level E_2 , precisely the states (1,1,0), (1,0,1) and (0,1,1), are obviously not affected by the perturbation. Let us consider what happens in the three-dimensional subspace spanned by (2,0,0), (0,2,0)and (0,0,2).

Following [5, Problem 65], after performing a unitary transformation (into the usual spherical coordinates r, θ, ϕ), we get a new orthogonal basis for this subspace given by the functions $\psi_{2,0,0}, \psi_{2,2,-2}, \psi_{2,2,2}$ with

$$\psi_{n,l,m} = \text{const} \cdot r^l e^{-\frac{r^2}{2}} Y_{l,m}(\theta,\phi) F(-\frac{n-l}{2},l+\frac{3}{2},r^2)$$

where $Y_{l,m}$ are the normalised spherical harmonics and F is the confluent hypergeometric function. As is well known, $Y_{0,0} = \frac{1}{4\pi}$. Hence, the only spherically symmetric vector in the new basis is $\psi_{2,0,0}$. As a consequence, the operator $C(H_0; E)$ reduced to the subspace with $E_2 = 2 + \frac{3}{2}$ is a rank-one operator with kernel given by $\{\psi_{2,0,0}\}^{\perp}$. Therefore, the new eigenvalue created by the perturbation in the interval $(\frac{3}{2}, \frac{7}{2})$ is a simple eigenvalue.

It is not difficult to extend the argument to higher levels.

Thus, the important difference between the one-dimensional case and the threedimensional one is that in the latter the even excited states are still in the spectrum of the perturbed Hamiltonian, even though their degeneracy is lowered by the emergence of an adjacent new simple eigenvalue.

Hence, the new bound states are the roots of the following equation for $E \in \rho(H_0)$:

$$\alpha = E \sum_{l \in \mathbb{N}^3} \frac{\Phi_{2l}^2(0)}{(|2l|_1 + \frac{3}{2})(|2l|_1 + \frac{3}{2} - E)} = \lim_{\tilde{l} \to \infty} ((H_0^{(\tilde{l})} - E)^{-1}(0, 0) - H_0^{(\tilde{l})^{-1}}(0, 0)). \quad (3.1)$$

In order to determine the new ground state, we can rewrite the series on the r.h.s. of (3.1) as an integral.

In fact, for any $E < \frac{3}{2}$ we have:

$$\begin{split} (H_0^{(\tilde{l})} - E)^{-1}(0,0) - H_0^{(\tilde{l})^{-1}}(0,0) &= \sum_{|l|_1 \le \tilde{l}} \frac{\Phi_{2l}^2(0)}{|2l|_1 + \frac{3}{2} - E} - \sum_{|l|_1 \le \tilde{l}} \frac{\Phi_{2l}^2(0)}{|2l|_1 + \frac{3}{2}} \\ &= \sum_{|l|_1 \le \tilde{l}} \Phi_{2l}^2(0) \int_0^\infty (e^{-(|2l|_1 + \frac{3}{2} - E)t} - e^{-(|2l|_1 + \frac{3}{2})t}) dt \\ &= \int_0^\infty \sum_{|l|_1 \le \tilde{l}} \Phi_{2l}^2(0) e^{-(|2l|_1 + \frac{3}{2})t} (e^{Et} - 1). \end{split}$$

We take the limit of the latter as $\tilde{l} \to \infty$: thanks to the monotone convergence Lebesgue theorem we are allowed to perform the limit under the integral so that the finite summation

becomes a series, convergent for t > 0. By using the same technique as in [2] sect.3 we obtain

$$\lim_{\tilde{l}\to\infty} \left((H_0^{(\tilde{l})} - E)^{-1}(0,0) - H_0^{(\tilde{l})^{-1}}(0,0) \right) = \int_0^\infty \left(\sum_{k=0}^\infty \Phi_{2k}^2(0) e^{-(2k+\frac{1}{2})t} \right)^3 (e^{Et} - 1) dt$$

$$= \frac{1}{\sqrt{\pi^3}} \int_0^\infty \frac{e^{\frac{3}{2}t}}{(e^{2t} - 1)^{\frac{3}{2}}} (e^{Et} - 1) dt.$$
(3.2)

The integral in (3.2) shows again clearly why we need the renormalisation procedure: the denominator goes to zero like $t^{\frac{3}{2}}$ as $t \to 0$, which implies that without the numerator we should have a non-integrable singularity, differently from the one-dimensional situation, as can be seen by looking at the integral on the r.h.s of (3.3) in [2].

Therefore, for any $E < \frac{3}{2}$, (3.1) can be rewritten as

$$\alpha = \frac{1}{\sqrt{\pi^3}} \int_0^\infty \frac{e^{\frac{3}{2}t}}{(e^{2t} - 1)^{\frac{3}{2}}} (e^{Et} - 1) dt.$$
(3.3)

It is immediate to notice that if $\alpha = 0$, then the solution of (3.3) is E = 0.

Therefore, the perturbed harmonic oscillator with Hamiltonian defined by means of (2.3) for $\alpha = 0$ has ground state energy equal to 0.

4 Computation of the first eigenvalues of H_{α}

We set $b_k = \Phi_{2k}^2(0)e^{-(2k+\frac{1}{2})t}$ for the sake of reducing the notation. In this section we will make use of the following explicit expressions: $b_0 = \frac{1}{\sqrt{\pi}}e^{-\frac{t}{2}}$, $b_1 = \frac{1}{2\sqrt{\pi}}e^{-\frac{5}{2}t}$ and $b_2 = \frac{3}{8\sqrt{\pi}}e^{-\frac{9}{2}t}$.

Ground state. To study the ground state of the perturbed system we set $E = \frac{3}{2} - \epsilon$, in analogy with [2]. If we set $x = e^{-t\epsilon}$ the integral in (3.3) takes the form $\frac{1}{\epsilon}I_{\epsilon}^{(0)}$ where

$$I_{\epsilon}^{(0)} = \int_{0}^{1} \frac{1 - x^{\frac{1}{\epsilon}(\frac{3}{2} - \epsilon)}}{(1 - x^{\frac{2}{\epsilon}})^{\frac{3}{2}}} dx.$$
(4.1)

 $I_{\epsilon}^{(0)}$ exists for any $\epsilon \in (0, \frac{3}{2})$ and its value is uniformly bounded, so that (4.1) is very convenient for computing: in figure 1 we plot α vs E in $(-\frac{1}{2}, \frac{3}{2})$. The ground state can be computed with very high precision once α is given.

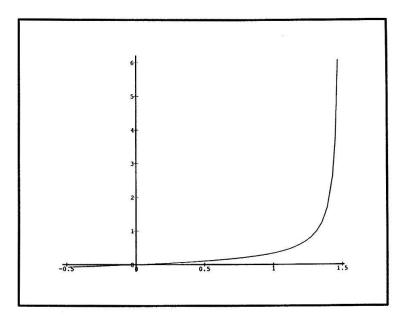


Figure 1. The parameter α as a function of E in $\left(-\frac{1}{2}, \frac{3}{2}\right)$.

First even level. As we have anticipated in the previous section, the first even level of the unperturbed oscillator $E_2 = \frac{7}{2}$ gives rise to two levels because of the perturbation. Since the states (1,1,0), (1,0,1) and (0,1,1) are orthogonal to $(H_0 - E)^{-1}(0,\cdot)$, they are not affected by the perturbation and consequently $\frac{7}{2}$ is still in the spectrum even though its degeneracy is lower.

In order to study the energy levels created by the states (2,0,0), (0,2,0) and (0,0,2), we set $E = \frac{7}{2} - \epsilon$ ($\epsilon \in (0,2)$) and rewrite the difference on the l.h.s. of (3.2) as

$$\frac{2(\frac{7}{2}-\epsilon)}{3\sqrt{\pi^3}}\frac{1}{\epsilon-2} + \int_0^\infty \sum_{l\neq(0,0,0)} b_{l_1}b_{l_2}b_{l_3}(e^{(\frac{7}{2}-\epsilon)t}-1)dt.$$

If we suitably handle the first terms of the multiple series, we obtain

$$\frac{2(\frac{7}{2}-\epsilon)}{3\sqrt{\pi^3}}\frac{1}{\epsilon-2} + \int_0^\infty \sum_{k=1}^\infty b_k (b_0^2 + b_0 \sum_{k=0}^\infty b_k + (\sum_{k=0}^\infty b_k)^2) (e^{(\frac{7}{2}-\epsilon)t} - 1)dt.$$
(4.2)

Furthermore, if we observe that

$$\sum_{k=1}^{\infty} b_k = \frac{1}{\sqrt{\pi}} \left(\frac{e^{\frac{1}{2}t}}{(e^{2t} - 1)^{\frac{1}{2}}} - e^{-\frac{t}{2}} \right)$$

and substitute in (4.2), we get

$$\begin{aligned} \alpha &= \frac{1}{\sqrt{\pi^3}} \frac{2(\frac{7}{2} - \epsilon)}{3} \frac{1}{\epsilon - 2} \\ &+ \frac{1}{\sqrt{\pi^3}} \int_0^\infty \frac{e^{\frac{t}{2}} (1 - (1 - e^{-2t})^{\frac{1}{2}})}{(e^{2t} - 1)^{\frac{3}{2}}} (e^t + (e^{2t} - 1)^{\frac{1}{2}} + e^{-t}(e^{2t} - 1))(e^{(\frac{7}{2} - \epsilon)t} - 1)dt. \end{aligned}$$

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The integral on the r.h.s. is convergent in the range of ϵ and can be transformed into $\frac{1}{\epsilon}I_{\epsilon}^{(1)}$ where

$$I_{\epsilon}^{(1)} = \int_{0}^{1} \frac{1 - x^{\frac{1}{\epsilon}(\frac{1}{2} - \epsilon)}}{(1 - x^{\frac{2}{\epsilon}})^{\frac{3}{2}}} \frac{1}{1 + (1 - x^{\frac{2}{\epsilon}})^{\frac{1}{2}}} (1 + (1 - x^{\frac{2}{\epsilon}})^{\frac{1}{2}} + (1 - x^{\frac{2}{\epsilon}})) dx$$

is uniformly bounded for $\epsilon \in (0,2)$ and very convenient for computation. Hence we have

$$\alpha = \frac{1}{\sqrt{\pi^3}} \frac{2(\frac{7}{2} - \epsilon)}{3} \frac{1}{\epsilon - 2} + \frac{1}{\sqrt{\pi^3}} \frac{I_{\epsilon}^{(1)}}{\epsilon}.$$
(4.3)

In figure 2 we plot α vs E for $E \in (\frac{3}{2}, \frac{7}{2})$.

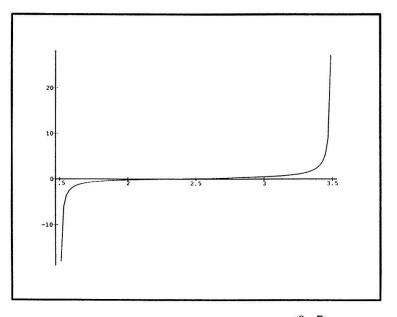


Figure 2. The parameter α as a function of E in $(\frac{3}{2}, \frac{7}{2})$.

Second even level. For the second even level we obtain the following equation

$$\frac{2(\frac{11}{2}-\epsilon)}{3\sqrt{\pi^3}}\frac{1}{\epsilon-4} + \frac{3(\frac{11}{2}-\epsilon)}{7\sqrt{\pi^3}}\frac{1}{\epsilon-2} + \sum_{|l|\geq 2} (\frac{\Phi_{2l}^2(0)}{|2l|_1 + \frac{3}{2} - E} - \frac{\Phi_{2l}^2(0)}{|2l|_1 + \frac{3}{2}}).$$

The same method used to derive the equation for the first even level leads us to the equation

$$\begin{split} \sum_{|l|\geq 2} (\frac{\Phi_{2l}^2(0)}{|2l|_1 + \frac{3}{2} - E} - \frac{\Phi_{2l}^2(0)}{|2l|_1 + \frac{3}{2}}) &= \int_0^\infty (e^{Et} - 1) \left(3b_0^2 \sum_{k=2}^\infty b_k + 3b_0 (\sum_{k=1}^\infty b_k)^2 + (\sum_{k=1}^\infty b_k)^3 \right) dt \\ &= \frac{1}{\sqrt{\pi^3}} \int_0^\infty 3e^{-\frac{3}{2}t} \left(\frac{1 - (1 - e^{-2t})^{\frac{1}{2}}}{(1 - e^{-2t})^{\frac{1}{2}}} - \frac{e^{-2t}}{2} + \frac{(1 - (1 - e^{-2t})^{\frac{1}{2}})^2}{(1 - e^{-2t})} + \frac{1}{3} \frac{(1 - (1 - e^{-2t})^{\frac{1}{2}})^3}{(1 - e^{-2t})^{\frac{3}{2}}} \right) (e^{(\frac{11}{2} - \epsilon)t} - 1) dt. \end{split}$$

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If $\epsilon \in (0,2)$ the improper integral is convergent and can be computed by means of the usual change $x = e^{-\epsilon t}$. In fact, the integral is transformed into $\frac{1}{\epsilon}I_{\epsilon}^{(2)}$ where

$$\begin{split} I_{\epsilon}^{(2)} &= 3 \int_{0}^{1} \frac{1 - x^{\frac{1}{\epsilon}(\frac{11}{2} - \epsilon)}}{(1 - x^{\frac{2}{\epsilon}})^{\frac{3}{2}}} \Big(\frac{1 - x^{\frac{2}{\epsilon}}}{2} \frac{1}{1 + (1 - x^{\frac{2}{\epsilon}})^{\frac{1}{2}}} \Big(1 + \frac{1}{1 + (1 - x^{\frac{2}{\epsilon}})^{\frac{1}{2}}} \Big) \\ &+ \frac{(1 - x^{\frac{2}{\epsilon}})^{\frac{1}{2}}}{(1 + (1 - x^{\frac{2}{\epsilon}})^{\frac{1}{2}})^{2}} + \frac{1}{3} \frac{x^{\frac{2}{\epsilon}}}{(1 + (1 - x^{\frac{2}{\epsilon}})^{\frac{1}{2}})^{3}} \Big) dx. \end{split}$$

Hence, the equation which allows us to compute with high accuracy the third eigenvalue is

$$\alpha = \frac{2(\frac{11}{2} - \epsilon)}{3\sqrt{\pi^3}} \frac{1}{\epsilon - 4} + \frac{1}{\sqrt{\pi^3}} \frac{3(\frac{11}{2} - \epsilon)}{7} \frac{1}{\epsilon - 2} + \frac{1}{\sqrt{\pi^3}} \frac{I_{\epsilon}^{(2)}}{\epsilon}.$$
 (4.4)

In figure 3 we plot α when $E \in (\frac{7}{2}, \frac{11}{2})$.

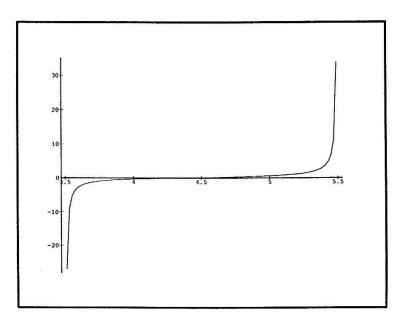


Figure 3. The parameter α as a function of E in $(\frac{7}{2}, \frac{11}{2})$.

Observe that, in analogy with the one-dimensional problem, α is related to ϵ by a formula like

$$\frac{c_1}{\epsilon - 2} + \frac{c_2}{\epsilon} + c_3$$

at any energy level.

Remark. $I_{\epsilon}^{(1)}$ and $I_{\epsilon}^{(2)}$ require some care when they are regarded from a numerical point of view: although they involve the computation of a family of *proper* integrals (uniformly bounded in ϵ), we get meaningless results if terms like $\frac{1-(1-x_{\epsilon}^2)^{\frac{1}{2}}}{x_{\epsilon}^2}$ (obtained during their derivation) are not transformed into $\frac{1}{1+(1-x_{\epsilon}^2)^{\frac{1}{2}}}$ in such a way to avoid subtractions between almost equal numbers which are very dangerous operations in floating-point arithmetics. Ackowledgements We would like to thank Prof. M. Klaus for pointing out Ref.4 and for many useful suggestions. S.F. gratefully acknowledges the constant encouragement and the financial support given to him by the Centre for Transport Theory and Mathematical Physics and Prof. Zweifel in particular. The computations were performed at the Computer Centre of the CNR-IAGA.

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