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On the spectrum of the harmonic oscillator with a δ-type perturbation. II

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Abstract. In this paper we study the spectrum of the Hamiltonian H of a one-dimensional harmonic oscillator perturbed by an attractive point interaction. The point interaction is assumed of the form $-\alpha\delta(x - x_0)$ ($\alpha > 0$ and $x_0 \neq 0$) so that it can act away from the equilibrium position of the oscillator. If the parameters α and x_0 are known, all the eigenvalues of H can be computed with high accuracy. On the other hand, recovering these two parameters from the knowledge of the first two eigenvalues of H turns out to be an extremely unstable problem.

1 Introduction

In this brief note we extend the results of [1] to the case in which the δ-interaction is located at a point x_0 which is not the equilibrium position of the harmonic oscillator.

Such a situation is of interest in quantum chemistry since it can be regarded as a simplified model for the interaction of a diatomic molecule with a neutral atom when the centre of the point interaction lies along the vibrational direction. A similar model (in 3D) is studied in [2] in the limit $|x_0| \to \infty$. The point interaction is given there by the so-called Fermi pseudopotential (see [3] pp.46-48) located at a point which might not be the origin. Of course, the harmonic potential in quantum chemistry is an approximation of the more realistic Morse potential (see [4] pp.451-454).

Following the strategy used in [1], we shall determine the ground state and the first excited state by means of the equations determining the poles of the resolvent of the self-adjoint operator

$$H = H_0 - \|v\|_1 \delta(x - x_0)$$

where

$$H_0 = \frac{1}{2}(-\frac{d^2}{dx^2} + x^2).$$

As usual, here $\|v\|_1$ is the L^1 norm of v i.e. $\int_{\mathbb{R}} |v(x)| dx$.

We shall see that the main difference between the spectrum of this Hamiltonian and the spectrum of $H_0 - \|v\|_1 \delta$ (considered in [1]) is that, due to the removal of the symmetry, the odd-labelled eigenvalues are also affected by the perturbation.

We shall also see that, if x_0 coincides with a zero of an eigenfunction of the unperturbed harmonic oscillator, then the eigenvalue corresponding to that particular eigenfunction will not be affected.

2 The resolvent of H

In this section we simply restate theorem 2.2 of [1] for the more general case being considered, i.e. the centre of the attractive δ-interaction is not the origin, but a point x_0 on the real axis.

Following [1], in order to determine the resolvent of H, it is convenient to use the limit procedure known as *convergence in the norm resolvent sense.* Therefore, after introducing the self-adjoint Hamiltonians ($\epsilon \in \mathbb{R}_+$)

$$H_\epsilon = H_0 - v_\epsilon$$

(where $v_\epsilon(x - x_0) = \frac{1}{\epsilon} v(\frac{x - x_0}{\epsilon})$, $v \geq 0$ and $v \in L^1(\mathbb{R})$) we can get the resolvent of H as the limit when $\epsilon \to 0_+$ of the resolvent of H_ϵ in the norm topology by following the steps in section 2 of [1]. The result can be summarised in the following theorem whose proof is omitted since it is practically identical to that of theorem 2.2 in [1].

Theorem 2.1. *Let $\{H_\epsilon\}_{\epsilon \in (0,1]}$, H be the self-adjoint operators defined above. Then, $H_\epsilon \to H$ as $\epsilon \to 0_+$ in the norm resolvent sense and*

$$(H - E)^{-1} = (H_0 - E)^{-1} + \frac{|(H_0 - E)^{-1}(\cdot, x_0)\rangle\langle(H_0 - E)^{-1}(x_0, \cdot)|}{\frac{1}{\|v\|_1} - (H_0 - E)^{-1}(x_0, x_0)} \tag{2.1}$$

with $(H_0 - E)^{-1}(x, y) = \sum_{l=0}^{\infty} \frac{\Phi_l(x)\Phi_l(y)}{(l + \frac{1}{2} - E)}$, $\{\Phi_l\}_{l=0}^{\infty}$ being the eigenfunctions of the harmonic oscillator.

Having determined explicitly the resolvent of H, we can now find the eigenvalues by studying the poles of $(H - E)^{-1}$. This will be the main subject of the next section.

3 The bound state equation

The eigenvalues of the operator H are given by the poles of its resolvent. Similarly to what has been seen in [1], it is not difficult ot check that, because of a cancellation, $(\Phi_{2k}, (H-E)^{-1}\Phi_{2k})$ no longer diverges at $E = 2k+\frac{1}{2}, \forall k = 0, 1, 2, \ldots$. Therefore, the even-labelled eigenvalues of the unperturbed Hamiltonian H_0 are no longer poles of the resolvent of H and, consequently, eigenvalues of H itself. However, due to the lack of symmetry of $(H_0 - E)^{-1}(x_0, \cdot)$, differently from the situation described in [1], the rank-one operator on the r.h.s. of (2.1) no longer vanishes on the subspace of antisymmetric functions. Also in the case of the antisymmetric eigenfunctions of H_0, i.e. Φ_{2k+1}, it is not difficult to check that $(\Phi_{2k+1}, (H-E)^{-1}\Phi_{2k+1})$ does not diverge at $E = 2k + \frac{3}{2}, \forall k = 0, 1, 2, \ldots$. Therefore, in this case the δ-perturbation modifies also the odd-labelled eigenvalues.

Thus, the spectrum of H is given by the solutions of the following equation:

$$\frac{1}{\|v\|_1} = (H_0 - E)^{-1}(x_0, x_0) = \sum_{l=0}^{\infty} \frac{\Phi_l^2(x_0)}{l + \frac{1}{2} - E}. \tag{3.1}$$

It is worth noting that, since Φ_l^2 is symmetric for all integers l, we have the same bound state equation in both cases $x_0 > 0$ and $x_0 < 0$.

In [1] we computed $(H_0 - E)^{-1}(0, 0), \forall E < \frac{1}{2}$ by using the relationship between the resolvent and the semigroup of H_0. After writing [1] we encountered the explicit formula for the Green's function of H_0 in the literature on the harmonic oscillator (see [5]). In the particular case $x = y = x_0$ and $E < \frac{1}{2}$, we have:

$$(H_0 - E)^{-1}(x_0, x_0) = \pi^{-\frac{1}{2}} e^{-x_0^2} \int_0^1 \frac{\xi^{-(E+\frac{1}{2})}}{(1-\xi^2)^{\frac{1}{2}}} e^{2x_0^2 \xi \frac{1}{1+\xi}} d\xi. \tag{3.2}$$

By setting $E = \frac{1}{2} - \epsilon$, the r.h.s. in (3.2) can be written as follows

$$\pi^{-\frac{1}{2}} e^{-x_0^2} \int_0^1 \frac{\xi^{-1+\epsilon}}{(1-\xi^2)^{\frac{1}{2}}} e^{2x_0^2 \xi \frac{1}{1+\xi}} d\xi = \pi^{-\frac{1}{2}} \int_0^1 \frac{\xi^{-1+\epsilon}}{(1-\xi^2)^{\frac{1}{2}}} e^{-x_0^2 \frac{1-\xi}{1+\xi}} d\xi.$$

Using a well-known calculus theorem, the latter integral becomes

$$\pi^{-\frac{1}{2}} e^{-x_0^2(1-\tilde{\xi})(1+\tilde{\xi})^{-1}} \int_0^1 \frac{\xi^{-1+\epsilon}}{(1-\xi^2)^{\frac{1}{2}}} d\xi = e^{-x_0^2(1-\tilde{\xi})(1+\tilde{\xi})^{-1}} (H_0 - \frac{1}{2} + \epsilon)^{-1}(0, 0)$$

for some $\tilde{\xi} \in (0, 1)$.

Therefore, we have the chain of inequalities:

$$\begin{aligned} e^{-x_0^2}(H_0 - \frac{1}{2} + \epsilon)^{-1}(0,0) &< e^{-x_0^2(1-\tilde{\xi})(1+\tilde{\xi})^{-1}} (H_0 - \frac{1}{2} + \epsilon)^{-1}(0,0) \\ &= (H_0 - \frac{1}{2} + \epsilon)^{-1}(x_0, x_0) \\ &< (H_0 - \frac{1}{2} + \epsilon)^{-1}(0,0). \end{aligned}$$

It follows that the solution $E_0(x_0) = \frac{1}{2} - \epsilon_0(x_0)$ of (3.1) is inside the interval $(\frac{1}{2} - \epsilon_0^-(0), \frac{1}{2} - \epsilon_0^+(0))$, where $\epsilon_0^-(0)$ solves the equation (in ϵ)

$$\frac{1}{\|v\|_1} = (H_0 - \frac{1}{2} + \epsilon)^{-1}(0,0)$$

and $\epsilon_0^+(0)$ solves

$$\frac{1}{\|v\|_1} e^{x_0^2} = (H_0 - \frac{1}{2} + \epsilon)^{-1}(0,0).$$

Thus, the ground state of the Hamiltonian with the attractive interaction centred at the origin, is the lowest ground state amongst the ground states of the Hamiltonians $H_0 - \|v\|_1 \delta(x - x_0)$.

In order to perform numerical computations, we rewrite the ground state equation in the more suitable form (obtained by means of the two changes of variable: $\xi = \cosh t$ and $e^{-\epsilon t} = x$)

$$\frac{\pi^{\frac{1}{2}}}{\|v\|_1} = \frac{e^{-x_0^2}}{\epsilon} \int_0^1 \left(\frac{2}{1 + x^{\frac{2}{\epsilon}}}\right)^{\epsilon} e^{4x_0^2 x^{\frac{1}{\epsilon}} (1 + x^{\frac{1}{\epsilon}})^{-2}} dx. \tag{3.3}$$

We now turn our attention to the first excited state ($l = 1$). As stated at the beginning of this section, differently from the case in which the δ is centred at the origin, its eigenenergy is modified by the δ_{x_0}-perturbation.

Since the integral expression of the Green's function of H_0 given in [6] is only valid for $E < \frac{1}{2}$, it is clear that we shall have to use a trick similar to that used in [1] to determine an integral formula for $(H_0 - E)^{-1}(0,0)$ in the left neighbourhood of the second even-labelled eigenvalue of H_0, namely $E_2 = \frac{5}{2}$.

Therefore, we start by writing:

$$(H_0 - E)^{-1}(x_0, x_0) = \sum_{l=1}^{\infty} \frac{\Phi_l^2(x_0)}{l + \frac{1}{2} - E} - \frac{\Phi_0^2(x_0)}{E - \frac{1}{2}}$$

for any $E \in (\frac{1}{2}, \frac{3}{2})$. After setting $E = \frac{3}{2} - \epsilon$, the r.h.s. becomes:

$$\sum_{l=1}^{\infty} \frac{\Phi_l^2(x_0)}{l + \epsilon - 1} - \frac{\Phi_0^2(x_0)}{1 - \epsilon}.$$

The trick is once again to find an integral formula for the series starting at $l = 1$, which holds also in the left neighbourhood of $E_1 = \frac{3}{2}$. Hence,

$$\sum_{l=1}^{\infty} \frac{\Phi_l^2(x_0)}{l + \epsilon - 1} = \sum_{l=0}^{\infty} \frac{\Phi_l^2(x_0)}{l + \epsilon - 1} - \frac{\Phi_0^2(x_0)}{\epsilon - 1}.$$

For $\epsilon > 1$ (corresponding to $E < \frac{1}{2}$), the r.h.s. is equal to:

$$\begin{aligned} &\pi^{-\frac{1}{2}} \int_0^1 \frac{\xi^{-2+\epsilon}}{(1-\xi^2)^{\frac{1}{2}}} e^{-x_0^2 \frac{1-\xi}{1+\xi}} d\xi - \pi^{-\frac{1}{2}} \frac{e^{-x_0^2}}{\epsilon - 1} \\ &= \pi^{-\frac{1}{2}} \left[\int_0^1 \frac{\xi^{-2+\epsilon}}{(1-\xi^2)^{\frac{1}{2}}} e^{-x_0^2 \frac{1-\xi}{1+\xi}} d\xi - e^{-x_0^2} \int_0^1 \xi^{-2+\epsilon} d\xi \right] \\ &= \pi^{-\frac{1}{2}} e^{-x_0^2} \int_0^1 \frac{\xi^{-1+\epsilon}}{(1-\xi^2)^{\frac{1}{2}}} \frac{e^{\frac{2\xi x_0^2}{1+\xi}} - (1-\xi^2)^{\frac{1}{2}}}{\xi} d\xi. \end{aligned} \tag{3.4}$$

It is immediate to notice that the integral on the r.h.s. of (3.4) is well defined now for any $\epsilon > 0$, since $\frac{\xi^{-1+\epsilon}}{(1-\xi^2)^{\frac{1}{2}}} \in L^1[0,1]$ and the other fraction in the integrand is bounded.

Hence, the equation determining the first excited state eigenenergy is:

$$\frac{\pi^{\frac{1}{2}}}{\|v\|_1} = e^{-x_0^2} \left[\int_0^1 \frac{\xi^{-1+\epsilon}}{(1-\xi^2)^{\frac{1}{2}}} \frac{e^{\frac{2\xi x_0^2}{1+\xi}} - (1-\xi^2)^{\frac{1}{2}}}{\xi} d\xi - \frac{1}{1-\epsilon} \right] \tag{3.5}$$

with $\epsilon = \frac{3}{2} - E$ and $E \in (\frac{1}{2}, \frac{3}{2})$.

Higher eigenenergies can be determined by means of equations like (3.5) obtained by using 'renormalisation tricks'. The integral formulae, however, are bound to become increasingly more complicated.

We proceed in the same way as in the ground state equation and transform the integral on the r.h.s. of (3.5). The latter becomes:

$$\begin{aligned} \frac{\pi^{\frac{1}{2}}}{\|v\|_1} = \frac{e^{-x_0^2}}{\epsilon} \int_0^1 \left(\frac{2}{1 + x^{\frac{2}{\epsilon}}} \right)^{\epsilon} \Big[x^{-\frac{1}{\epsilon}} \big(e^{4x_0^2 x^{\frac{1}{\epsilon}} (1+x^{\frac{1}{\epsilon}})^{-2}} - 1 \big) \\ + x^{\frac{1}{\epsilon}} \big(e^{4x_0^2 x^{\frac{1}{\epsilon}} (1+x^{\frac{1}{\epsilon}})^{-2}} + 1 \big) \Big] dx - \frac{e^{-x_0^2}}{1-\epsilon}. \end{aligned} \tag{3.6}$$

Before ending this section, we want to single out a special situation, i.e. the case in which x_0 coincides with a zero of an eigenfunction of H_0 but $x_0 \neq 0$ (if $x_0 = 0$, all the antisymmetric eigenfunctions vanish at 0 and we are exactly in the situation fully described in [1]). Let us assume that $x_0 = \tilde{x}_{\bar{l}}$, where $\tilde{x}_{\bar{l}}$ is such that $\Phi_{\bar{l}}(\tilde{x}_{\bar{l}}) = 0$.

Thus, the series expressing $(H_0 - E)^{-1}(\tilde{x}_{\bar{l}}, \cdot)$ is equal to

$$\sum_{l \neq \bar{l}} \frac{\Phi_l(\tilde{x}_{\bar{l}}) \langle \Phi_l |}{l + \frac{1}{2} - E}.$$

Hence,

$$((H_0 - E)^{-1}(\tilde{x}_{\bar{l}}, \cdot), \Phi_{\bar{l}}) = 0$$

which implies that the energy of the $\tilde{l}$-th level is not modified by the $\delta_{\bar{x}_{\tilde{l}}}$-perturbation. For example, if $x_0 = \pm\frac{1}{\sqrt{2}}$, then the eigenenergy $E_2 = \frac{5}{2}$ will not be affected by the δ-perturbation centred at x_0.

4 Identifying the potential from measured values of the energy

We can change the point of view of section 3 and regard the derivation of (3.3) and (3.6) as part of the solution of an inverse problem for the one-dimensional Schrödinger equation.

In the present case, the form of the potential is *a priori* known to be $\frac{x^2}{2} - \alpha\delta(x \mp \sqrt{\beta})$ where $\alpha = \|v\|_1$ and $\beta = x_0^2$, so that the inverse problem reduces to determining the location of two real parameters only. In fact, suppose that $E_0 = \frac{1}{2} - \epsilon_0$ and $E_1 = \frac{3}{2} - \epsilon_1$ are given. By equating the r.h.s. of (3.3) and (3.6) we get the following non linear equation in β

$$\begin{aligned}\phi_{\epsilon_0,\epsilon_1}(\beta) \equiv e^{-\beta}\Big\{\frac{1}{\epsilon_0}\int_0^1\Big(\frac{2}{1+x^{\frac{2}{\epsilon_0}}}\Big)^{\epsilon_0} e^{4\beta x^{\frac{1}{\epsilon_0}}(1+x^{\frac{1}{\epsilon_0}})^{-2}}dx \\ -\frac{1}{\epsilon_1}\int_0^1\Big(\frac{2}{1+x^{\frac{2}{\epsilon_1}}}\Big)^{\epsilon_1}\big[x^{-\frac{1}{\epsilon_1}}(e^{4\beta x^{\frac{1}{\epsilon_1}}(1+x^{\frac{1}{\epsilon_1}})^{-2}}-1) \\ +x^{\frac{1}{\epsilon_1}}(e^{4\beta x^{\frac{1}{\epsilon_1}}(1+x^{\frac{1}{\epsilon_1}})^{-2}}+1)\big]dx + \frac{1}{1-\epsilon_1}\Big\} = 0.\end{aligned}$$

Once β has been computed, we get α by a simple substitution in (3.3). Computations confirm the prediction that the solution of such an inverse problem is quite unpractical unless the data are available with extremely large precision. This is due to the severe instability of β and α with respect to the error possibly affecting ϵ_0 and ϵ_1.

Let β be regarded as a real positive function defined for $(\epsilon_0, \epsilon_1) \in (0, \infty) \times (0, 1)$. In figure 1 we show the graph of $\beta(\epsilon_0, \epsilon_1)$ in the domain $(0, 2) \times (0, 1)$. Observe the bad behaviour of β in the physically more interesting range in which $\beta > 1$. The level lines plotted on the surface correspond to $\beta = \frac{1}{2}$ and $\beta = 1$.

When β goes to zero, the potential should tend to the one analysed in [1]. Since from the point of view of this article values of β close to zero are unphysical, we disregard here an accurate analysis of such a limit procedure.

In figure 2 we plot α as a function of ϵ_0 when $\beta = x_0^2 = 5$.

Finally, we observe that it is not possible to distinguish between the two cases $x_0 = \pm\sqrt{\beta}$ from energy measurements only.

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Figure 1

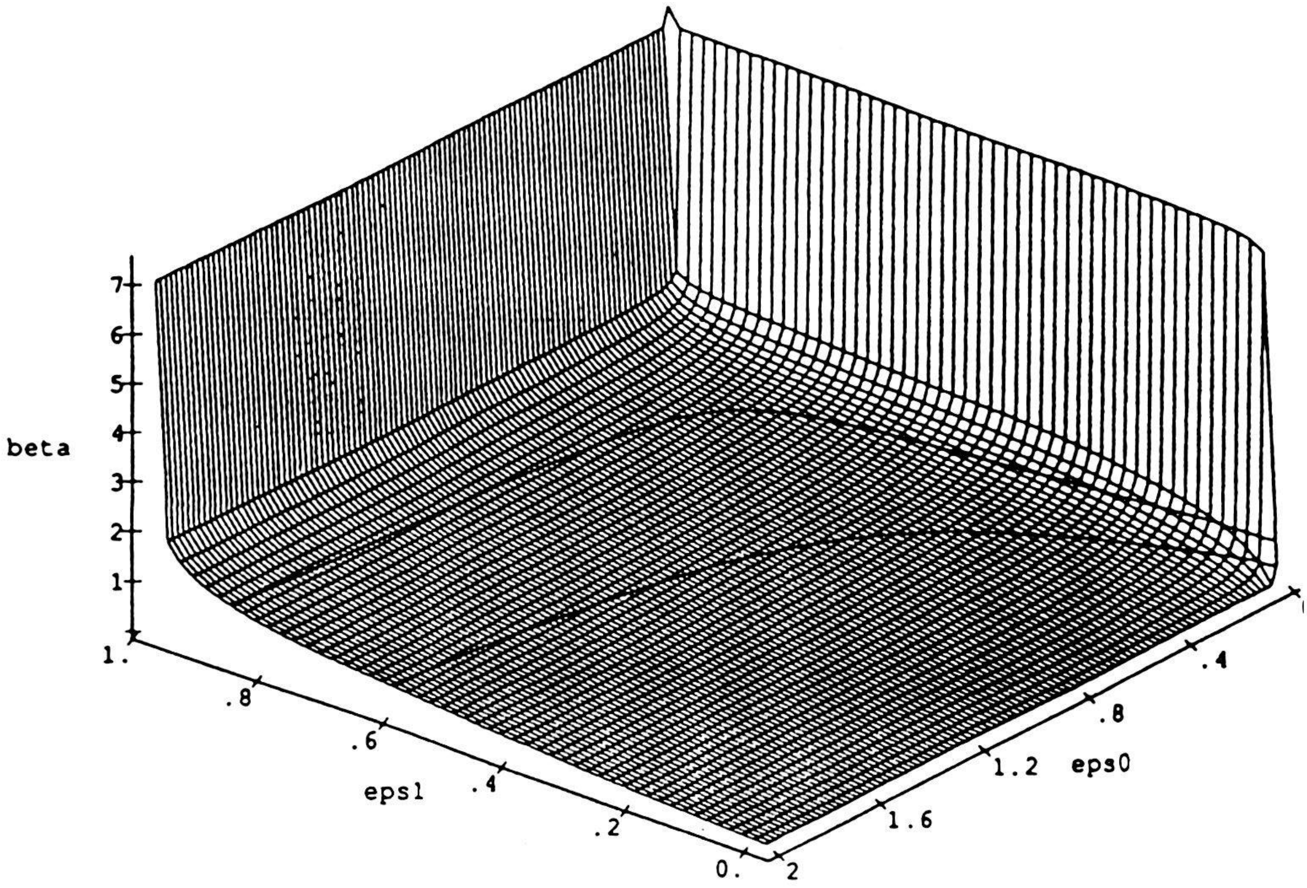

Figure 2