A one dimensional model showing a quantum phase transition based on a singular potential

M.L. Glasser

Department of Physics, Clarkson University, Potsdam, NY 13699-5820

M. Gadella, L.M. Nieto

Departamento de Física Teórica, Atómica y Óptica, Universidad de Valladolid, 47071 Valladolid, Spain

Abstract

We study a one-dimensional singular potential plus three types of regular interactions: constant electric field, harmonic oscillator and infinite square well. We use the Lippman-Schwinger Green function technique in order to search for the bound state energies. In the electric field case the unique bound state coincides with that found in an earlier study as the field is switched off. For non-zero field the ground state is shifted and positive energy "quasibound states" appear. For the harmonic oscillator we find a quantum phase transition of a novel type. This behavior does not occur in the corresponding case of an infinite square well and demonstrates the influence of quantum non-locality.

Key words: Quasibound states, one-dimensional singular point interactions.
PACS: 03.65.-w, 03.65.Db, 03.65.Ge

1. Introduction

Singular potentials of Dirac δ type are frequently used to describe quantum systems, especially as toy models in many textbooks [1] and in some papers on supersymmetry [2]. However, there are a number of recent examples, based on δ interactions, of physical interest. To mention a few: Bose-Einstein condensation in a harmonic trap with a tight and deep “dimple” potential, modeled by a Dirac δ function is studied in [3]. In [4] a nonperturbative study of the entanglement of two directed polymers subjected to repulsive interactions given by a Dirac δ function potential has been carried out. Finally, in a series of three papers [5], light propagation in a one-dimensional realistic dielectric superlattice, modeled by means of a periodic array of Dirac delta functions, is investigated for the cases of transverse electric, transverse magnetic, and omnidirectional polarization modes. Nevertheless, examples of the use of potentials related to the derivative of the Dirac delta function δ′(x) have appeared in the literature only very recently [6], and in a rather abstract context. Indeed, this may be due, in part, to the fact that there has been some controversy on the meaning of the δ′(x) potential [7], since different regularizations produce different reflection and transmission coefficients.

In the present work we examine one-dimensional quantum Hamiltonians with potentials having a regular part V_0(x) and a singular part of the form

\[ W(x) = -a\delta(x) + b\delta'(x), \quad a, b > 0. \]  (1)

Our efforts will concentrate on finding the bound states of these systems using the Green function as the fundamental tool.

Let us consider a one-dimensional quantum system whose dynamical evolution can be governed by two different Hamiltonian operators

\[ H_0 = -\frac{d^2}{dx^2} + V_0(x), \quad H = H_0 + W(x), \]  (2)

the first one will be the regular free Hamiltonian H_0 and the second one the perturbed Hamiltonian H (units have been chosen such that \( \hbar = 2m = 1 \)). Let us assume that H_0 admits a Green function given by \( G_0(x, x', E) \) (the dimension of x and x' is here irrelevant). Then, \( \psi(x) \) represents a bound state of the total Hamiltonian H with energy E if and only if the Lippman-Schwinger bound state equation

\[ \psi(x) = \int G_0(x, x', E)W(x')\psi(x') \, dx'. \]  (3)

is satisfied. In a previous publication [8], this method was used to find the bound states in a one-dimensional system subject to a constant electric field plus a Dirac delta well. In this case, the free Hamiltonian was given by the kinetic term plus the electric field, and the perturbation by the Dirac well. In the present paper, we shall extend this idea to the one-dimensional case in which the free Hamiltonian is a sum of the kinetic term plus either a constant electric field, a harmonic oscillator or an infinite square well. The perturbation is now given by the potential \( W(x) \) introduced in Eq. (1). To be explicit, we shall study...
Hamiltonians of the form $H = H_0 + W(x)$ such that their unperturbed part $H_0$ has one of the following potentials:

$$V_0(x) = -Fx, \quad F > 0,$$

(4)

$$V_0(x) = \frac{k^2}{16} x^2,$$

(5)

$$V_0(x) = \left\{ \begin{array}{ll} 0 & \text{if } |x| < c \\ \infty & \text{if } |x| \geq c \end{array} \right..$$

(6)

We shall see that the presence of the $\delta'(x)$ term has a dramatic effect in the composition of the bound states of $H_0$. In all cases, the presence of the perturbation term $W(x)$ in the potential, may create difficulties in interpretation. These can be overcome by the specification of matching conditions for wave functions at the origin, which is the singular point. This is the approach followed by Kurasov and coworkers [9, 10]; it avoids the controversy on the meaning of the $\delta'(x)$ potential [7] and gives reasonable physical results [6]. These matching conditions show that the wave functions and their derivatives may be discontinuous at the origin. This is opposed to the usual procedure when solving quantum mechanical problems, because the continuity of the wave function is normally taken for granted, a fact that must be discarded here.

The presence of $\delta(x)$ and $\delta'(x)$ together in the potential implies that the Schrödinger equation necessarily be a distributional equation. In addition as the wave functions are discontinuous at the origin, we have to define the product of a discontinuous function $\psi(x)$ times $\delta(x)$ and $\delta'(x)$. This can be done as follows [6]:

$$\psi(x)\delta(x) = \frac{\psi(0+) + \psi(0-)}{2}\delta(x),$$

(7)

$$\psi(x)\delta'(x) = \frac{\psi(0+) + \psi(0-)}{2}\delta'(x),$$

where $\psi(0+)$ and $\psi(0-)$ are the right and left limits of $\psi(x)$ at the origin (here, $\psi(x)$ is either $\psi(x)$ or its derivative). The two equations [7] are essential in the present study.

The next section consists of three parts. First of all, starting from the explicit form of (3) with $W(x) = -a\delta(x) + b\delta'(x)$, we obtain a determinant whose root give the energy values for the bound state of the total Hamiltonian $H = H_0 + W(x)$. Then, in the following three subsections we search for bound states for the total Hamiltonian, where $H_0$ is given by (4) (constant electric field), (5) (harmonic oscillator) and (6) (infinite square well) respectively. The most striking result appears in the case (5). For values of the parameter $b^2$ above a threshold, the harmonic oscillator loses its bound states which become resonances grouped in complex conjugate pairs. If $b^2$ takes values below the threshold, there is an infinite number of bound states. In the case (6), there exists the possibility for a unique bound state with negative energy in a narrow range of values of $b$. This negative value has no lower bound. The results are summarized in the Concluding Remarks.

2. The search for bound states

We can apply formula (3) to all the three cases considered above, because for them we explicitly know the Green function $G_0(x, x', E)$ of the corresponding $H_0$. In this case, (3) has the form

$$\psi(x) = \int G_0(x, x', E)[-a\delta(x') + b\delta'(x')] \psi(x') dx',$$

(8)

In all other cases, we shall use the Green function $G_{free}(x, x', E)$ for the Hamiltonian of a free particle, and then apply (3) with $W(x)$ as the total potential.

From now on we shall use the following notation for simplicity

$$G_{ij}(x, x') := \frac{\partial^i j}{\partial x^i \partial x'^j} G_0(x, x', E), \quad i, j = 0, 1.$$

(9)

Then, from (3) we readily obtain

$$2\psi(x) = -aG_0(x, 0)[\psi(0+) + \psi(0-)]$$

$$-b[\psi(0+) + G_0(0, 0)\psi'(0) + G_0(0, 0)\psi'(0-)] + G_0(0, 0)\psi(0-) + G(x, 0)\psi'(0-)].$$

(10)

Next, we introduce the following notation to simplify our expressions:

$$A := G_0(0+, 0) = G_0(0-, 0),$$

(11)

$$B := G_0^{01}(0+, 0) = G_0^{01}(0-, 0),$$

(12)

$$C := G_0^{10}(0-, 0) = G_0^{10}(0+, 0),$$

(13)

$$D := G_0^{11}(0+, 0) = G_0^{11}(0-, 0),$$

(14)

where the signs plus and minus after a 0 denote right and left limits, respectively. Identities such as $G_0(0+, 0) = G_0(0-, 0)$ are intrinsic properties of the Green functions considered in this paper.

If we take right and left limits at the origin in (10), we obtain respectively.

$$\left[ 1 + \frac{a}{2} A + \frac{b}{2} B \right] \psi(0+) + \left[ \frac{a}{2} A + \frac{b}{2} B \right] \psi(0-)$$

$$+ \frac{b}{2} A\psi'(0+) + \frac{b}{2} A\psi'(0-) = 0,$$

(15)

$$\left[ \frac{a}{2} C + \frac{b}{2} D \right] \psi(0+) + \left[ 1 + \frac{a}{2} A + \frac{b}{2} C \right] \psi(0-)$$

$$+ \frac{b}{2} A\psi'(0+) + \frac{b}{2} A\psi'(0-) = 0.$$
Taken together, the four linear equations (15)–(18) give a 4 × 4 system which has a non-trivial solution if and only if
\[
\det \begin{pmatrix}
1 + \frac{\pi}{2} A + \frac{\pi}{2} B & \frac{\pi}{2} A + \frac{\pi}{2} B & \frac{\pi}{2} A & \frac{\pi}{2} A \\
\frac{\pi}{2} A + \frac{\pi}{2} C & 1 + \frac{\pi}{2} A + \frac{\pi}{2} C & \frac{\pi}{2} A & \frac{\pi}{2} A \\
\frac{\pi}{2} C + \frac{\pi}{2} D & \frac{\pi}{2} C + \frac{\pi}{2} D & 1 + \frac{\pi}{2} C & \frac{\pi}{2} C \\
\frac{\pi}{2} B + \frac{\pi}{2} D & \frac{\pi}{2} B + \frac{\pi}{2} D & \frac{\pi}{2} B & 1 + \frac{\pi}{2} B
\end{pmatrix} = 0.
\]
This determinant can be simplified by subtracting the third column from the last, adding the fourth row to the third and then subtracting the second row from the first. Then, by subtracting the second column from the first one obtains,
\[
\det \begin{pmatrix}
2 & -1 - \frac{\pi}{2} (B - C) & 0 \\
-1 & 1 + \frac{\pi}{2} A + \frac{\pi}{2} C & \frac{\pi}{2} A \\
0 & \frac{\pi}{2} (B + C) + bD & 1 + \frac{\pi}{2} (B + C)
\end{pmatrix} = 0. \quad (19)
\]
Equation (19) will give us the values of the energy for the bound states in three cases under consideration, which we analyze separately below.

2.1. Constant electric field

In this case, \( V_0 \) is given by (4). The appropriate Green function \( G_0(x, x', E) := G_0(x, x') \), given in [8], is
\[
G_0(x, x') = -\frac{\pi}{F^{1/3}} \text{Ai} \left( \frac{x_c - E/F}{F^{-1/3}} \right) \text{Bi} \left( \frac{x_c - E/F}{F^{-1/3}} \right). \quad (20)
\]
Since \( E \) is fixed, the notation \( G_0(x, x') \) will be used where no confusion is possible (see (9)). In (20), Ai(\( x \)) and Bi(\( x \)) are the Airy functions of first and second kind, respectively, and \( x_s \) and \( x_c \) are the maximum and minimum of \( x \) and \( x' \) respectively. As we already pointed out in (11), this Green function is continuous at the origin with respect both arguments, so that, if we denote \( z = -E/F^{1/3} \),
\[
A = G_0(0+, 0) = G_0(0-, 0) = -\frac{\pi}{F^{1/3}} \text{Ai}(z) \text{Bi}'(z). \quad (21)
\]
At the origin, partial derivatives with respect to the arguments \( x \) and \( x' \) have jumps and fulfill the identities given in (12)–(14). Then, we have
\[
B = -\pi \text{Ai}(z) \text{Bi}'(z), \quad (22)
\]
\[
C = -\pi \text{Ai}'(z) \text{Bi}(z), \quad (23)
\]
\[
D = -\pi F^{1/3} \text{Ai}'(z) \text{Bi}'(z). \quad (24)
\]
By inserting these values into (19), we obtain a transcendental equation that gives the energy values for the total Hamiltonian (2) \( H = H_0 + W(x) \), with \( V_0(x) \) as in (4). A plot of the bound states resulting from the transcendental equation (19), which involves Airy functions, is shown in Figure 1 for different values of \( a \) and \( b \).

If we take \( b = 0 \) in the perturbation part of the potential \( W(x) \) given by (1), then Eq. (15) reduces to \( 1 + aA = 0 \), which is the problem treated in [8]. On taking the limit \( F \to 0 \) we find that the energy is \( E = -a^2/4 \) as expected. In the case of low field strength, where \( F \) is small, the properties of Airy functions yield,
\[
A = -\frac{1}{2F^{1/3} \sqrt{F}} \quad B = -C = -\frac{1}{2} \quad D = \frac{F^{1/3} \sqrt{F}}{2}. \quad (25)
\]
For \( b \neq 0 \), (19) simplifies to \( aA = b^2 AD - 1 \). Using (25) and taking into account the definition of \( z \), we obtain the value of the energy of the bound state in the limit \( F \to 0 \), which is
\[
E = \frac{-4a^2}{(4 + b^2)^2}, \quad (26)
\]
in agreement with (6) (remember that throughout the present work we have chosen \( m = 1/2 \)).

A striking result found in [8] is the existence of positive energy solutions to the bound state equation for the \( \delta \) well, which correspond to “quasibound” levels embedded in the continuum of scattering states. To check whether these are seriously affected by the presence of the \( \delta' \) potential we examined the evolution of the spectrum, numerically for the case \( a = b = 1 \) and \( m = 1/2 \), as \( F \) increases. The findings, shown in Figure 2, suggest that the quasibound state spectrum is similar to that found in [8]. In particular, the ionization field \( F_c \) is 0.076 [8] is decreased by about 10% to 0.062 due to the influence of \( b \neq 0 \).

2.2. The Harmonic Oscillator

The next Hamiltonian to be considered is the one coming from the potential in Eq. (5):
\[
H = -\frac{\partial^2}{\partial x^2} - a\delta(x) + b\delta'(x) + \frac{k^2 x^2}{16}, \quad (27)
\]
where the total potential is a sum of a harmonic oscillator well, where the form of the coupling constant has been chosen for
convenience, and the singular potential at the origin. By setting $k = 0$, i.e., dropping the oscillator term in the potential, we can verify that our method gives the same value as obtained in [6]. It is well known that the Green function for the free particle is given by (2m = $\hbar = 1$)

$$G_0(x, x', E) = \frac{\exp[i \sqrt{E} |x - x'|]}{2i \sqrt{E}}, \quad E > 0. \quad (28)$$

If we use (28) in (11)–(14) with $a \neq 0 \neq b, k = 0$, we obtain

$$A = \frac{1}{2i \sqrt{E}}, \quad B = -C = \frac{1}{2}, \quad D = -\frac{i}{2} \sqrt{E}. \quad (29)$$

Then, by using (29) in (19), we get the equation:

$$1 + \frac{1}{2i \sqrt{E}} + \frac{b^2}{4} = 0. \quad (30)$$

Eq. (30) makes sense if and only if $E$ takes negative values. Indeed, this is what happens and we find again the result given in Eq. (20), which coincides with the one given in [6].

Now let us assume that the three coefficients in (27) are different from zero. In this case, one has to calculate the Green function corresponding to $V_0$ in (5) which has been obtained in [11] and gives

$$A = \frac{1}{2 \sqrt{k}} \frac{\Gamma(\frac{1}{4} - \frac{E}{2k})}{\Gamma(\frac{1}{4} - \frac{E}{2k})}, \quad B = C = 0, \quad D = -kA. \quad (31)$$

Accordingly, (19) becomes:

$$\frac{b^2}{2} \frac{\Gamma^2(\frac{1}{4} - \frac{E}{2k})}{\Gamma^2(\frac{1}{4} - \frac{E}{2k})} + \frac{a}{\sqrt{k}} \frac{\Gamma(\frac{1}{4} - \frac{E}{2k})}{\Gamma(\frac{1}{4} - \frac{E}{2k})} + 2 = 0. \quad (32)$$

Note that (32) is strictly positive for $k > 0$ and $E < 0$ (since $\Gamma(x) > 0$ whenever $x > 0$). This shows that the action of the potential given in (5) removes the negative energy bound state that appeared with the singular potential and $a > 0$.

Concerning the oscillator bound states, note that the first term on the left hand side of (32) is always positive. The second term could be either positive or negative, but for large values of $k$ one expects that eventually this term will be smaller than 2. In this case, the left hand side of (32) is positive and, therefore, no solutions for $E$ exist; i.e. no bound states exist for (27). To show when this happens, let us write (32) as

$$b^2 \alpha^2 + 2 \frac{a}{\sqrt{k}} \alpha + 4 = 0, \quad \text{where} \quad \alpha := \frac{\Gamma(\frac{1}{4} - \frac{E}{2k})}{\Gamma(\frac{1}{4} - \frac{E}{2k})}. \quad (33)$$

The discriminant of (33) is $\sqrt{(a^2/k) - 4b^2}$; if it is negative, equation (33) has no real root $\alpha$ and therefore, no solutions $E$ exist when

$$b^2 > a^2/(4k). \quad (34)$$

Hence, there are no solutions $E$ for Eq. (32) for values of $b$ above $a/(2 \sqrt{k})$ (or below $-a/(2 \sqrt{k}$), since this equation is symmetric with respect to a change of sign in $b$), and thus there are no bound states! This is a very striking result, that can be appreciated in Figure 3: the action of the singular potential $W(x) = -a\delta(x) + b\delta'(x)$ erases all bound states of the harmonic oscillator well provided that the absolute value of $b$ is bigger than a critical value. This effect is produced solely by the presence of the $\delta'(x)$ interaction with sufficient intensity. For values of $b$ in the interval $(-a/(2 \sqrt{k}), a/(2 \sqrt{k}))$, including $b = 0$, equation (31) has an infinite number of solutions grouped in pairs (due to the double sign in the solution $\alpha$ in (33), see (35)). This is illustrated in Figures 3 and 4.
For values of $b$ in the range given by Eq. (34), equation (32) has complex solutions. Solving for $c$, we obtain

$$\alpha = \frac{\Gamma \left( \frac{1}{4} - \frac{E}{E} \right)}{\Gamma \left( \frac{1}{4} - \frac{E}{E} \right)} = \frac{1}{b^2} \left( -\frac{a}{\sqrt{k} \pm \sqrt{\frac{a^2}{k} - 4b^2}} \right).$$  \tag{35}$$

This gives for $b$, satisfying Eq. (34), complex solutions of (32) for $E$ grouped in pairs. Since the gamma function has the property $\Gamma(z^*) = [\Gamma(z)]^*$, where the star denotes complex conjugation, these pairs are complex conjugates, so that if $E_R + i\gamma$ is a solution of (35), then $E_R - i\gamma$ is also a solution. These solutions can be considered to be resonances. Unlike the case $b = 0$, treated in [5], both the even and odd oscillator states are affected by the perturbation.

### 2.3. The infinite square well

The last case under our study is the Hamiltonian $H = H_0 + W(x)$, where $V_0$ is given by Eq. (6). The corresponding Green function has already been calculated in [12] and gives for $A, B, C$ and $D$ in Eqs. (11)–(14) the following values

$$A = \frac{\tan(e \sqrt{E})}{2\pi \sqrt{E}}, \quad B = C = 0, \quad D = \frac{\sqrt{E}}{2\tan(e \sqrt{E})},$$  \tag{36}$$

$2c$ being the well width of the potential Eq. (6). If we insert these values into Eq. (19), we obtain the transcendental equation

$$\frac{\tan(e \sqrt{E})}{\sqrt{E}} = \frac{b^2 - 4\pi}{2a},$$  \tag{37}$$

which has an infinite number of solutions. Note that if $a = 0$ this equation is meaningless.

In order to search for solutions of (37), let us choose $c = 1$, fix some value of $a$, and then plot the resulting function of $b$ in terms of the energy. This is done in Figure 5, and we can see that for each value of $b$ (37) has an infinite number of positive solutions, each giving the energy of a bound state. However, for values of $b$ in the interval $[2\sqrt{\pi}, \sqrt{2 + 4\pi}]$ there exists an additional negative solution for $E$. This energy is zero for $b = \sqrt{2 + 4\pi}$, but goes to $-\infty$ as $b$ approaches to $2\sqrt{\pi}$ from above.

In Figure 6 we display the bound state spectrum as a function of $a$ for $b = 1, 5, 10$. The vertical line $E = \pi^2$ comes from the numerical algorithm and is spurious.

### 3. Concluding remarks

To summarize this work, the Lippman-Schwinger Green function technique has been used to study the energy of possible bound states for a quantum Hamiltonian of the form $H = -\frac{d^2}{dx^2} + V_0(x) - a\delta(x) + b\delta'(x)$. Three particular cases have been studied.
(i) $V_0(x) = -Fx$ with $F$ constant. The case $b = 0$ was studied previously. In the limit $F \to 0$, we obtain one negative eigenvalue which coincides with the value found in [6] that uses a quite different technique.

(ii) $V_0(x) = k^2 x^2 / 16$. In this case, there can be no state with negative energy. But the most striking result is the existence of a quantum phase transition [13] characterized by a threshold for the absolute value of $b$ (that also depends on $a$ and $k$). Below this threshold, there is an infinite number of bound states which group into pairs. Above this threshold, the infinite ladder of harmonic oscillator states evaporates and is replaced by an infinite number of resonances, which group in complex conjugate pairs.

(iii) If $V_0(x)$ is an infinite square well potential, the singular interaction $W(x)$ does not eliminate the bound states of the free Hamiltonian $H_0 = -d^2/dx^2 + V_0(x)$, which are merely shifted. For values of $b$ in a narrow interval, there exists a unique negative energy bound state whose absolute value can be arbitrarily large.

The difference in behavior between the square well and the harmonic well cases can only be due to the influence of boundary conditions, “soft” in the harmonic case and impenetrable in the square well, in a region where the singular potential is zero. This provides a striking demonstration of non-locality.

Some other examples of more realistic potentials $V_0(x)$ should be studied to obtain more conclusions about the emergence of the quantum phase transitions mentioned above. To analyze this phenomenon in two and three dimensions is also a very attractive project, that is presently in progress.

Acknowledgements

Partial financial support is acknowledged to the Spanish Junta de Castilla y León (Project GR224) and the Ministry of Education and Science (Project MTM2009-10751).

References

[1] S. Flügge, Practical Quantum Mechanics, Springer-Verlag, New York, 1974; C. Cohen–Tannoudji, B. Diu y F. Laloe, Quantum Mechanics, John Wiley, New York, 1977.
[2] J.I. Díaz, J. Negro, L.M. Nieto, and O. Rosas-Ortiz, J. Phys. A: Math. Gen. 32 (1999) 8447; J. Negro, L.M. Nieto, and O. Rosas-Ortiz, in Foundations of Quantum Physics, R. Blanco et al (Eds.), p 259, CIEMAT/RSEF, Madrid, 2002.
[3] H. Uncu, D. Tarhan, E. Demiralp, and O. E. Mustecaplıoğlu, Phys. Rev. A 76 (2007) 013618.
[4] F. Ferrari, V. G. Rostiashvili, and T. A. Vilgis, Phys. Rev. E 71 (2005) 061802.
[5] I. Alvarado-Rodríguez, P. Halevi, and J. J. Sánchez-Mondragón, Phys. Rev. E 59 (1999) 3624; J. R. Zurita-Sánchez and P. Halevi, Phys. Rev. E 61 (2000) 5802; Ming-Chieh Lin and Ruei-Fu Jao, Phys. Rev. E 74 (2006) 046613.
[6] M. Gadella, J. Negro, L.M. Nieto, Phys. Lett. A 373 (2009) 1310.
[7] P. Seba, Rep. Math. Phys. 24 (1986) 111; F.M. Toyama, Y. Nogami, J. Phys. A: Math. Theor. 40 (2007) F685; F.A.B. Coutinho, Y. Nogami, J. Fernando Pérez, J. Phys. A: Math. Gen. 30 (1997) 3937; P.L. Christiansen, H.C. Arnbak, A.V. Zolotaryuk, V.N. Ermakov, Y.B. Gaididei, J. Phys. A: Math. Gen. 36 (2003) 7589.
[8] M.L. Glasser, W. Jaskólski, F. García-Moliner, V.R. Velasco, Phys. Rev. B 42 (1990) 7630.
[9] P. Kurasov, J. Math. Anal. Appl. 201 (1996) 297; S. Albeverio, L. Dabrowski, P. Kurasov, Lett. Math. Phys. 45 (1998) 33.
[10] S. Albeverio, P. Kurasov, Singular perturbations of differential operators. Solvable Schrödinger type operators, London Mathematical Society Lecture Notes 271, Cambridge UP, Cambridge, 2000.
[11] M.L. Glasser, F. García-Moliner, V.R. Velasco, J. Appl. Phys. 68 (1990) 4319.
[12] M.L. Glasser, Am. J. Phys. 47 (1979) 738.
[13] S. Sachdev, Quantum Phase Transitions, Cambridge UP, London, 1999.