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Weakly (and not so weakly) bound states of a relativistic particle in one dimension

Paolo Amore [a,*], Francisco M. Fernández [b], Enrique Jiménez [c]

[a] Facultad de Ciencias, CUICBAS, Universidad de Colima, Bernal Díaz del Castillo 340, Colima, Colima, Mexico
[b] INIFTA, Division Quimica Teorica, Blvd. 113 S/N, Sucursal 4, Casilla de Correo 16, 1900 La Plata, Argentina
[c] Facultad de Ciencias and Dual CP Institute of High Energy Physics, Universidad de Colima, Bernal Díaz del Castillo 340, Colima, Colima, Mexico

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ABSTRACT

We present the first exact calculation of the energy of the bound state of a one dimensional Dirac massive particle in weak short-range arbitrary potentials, using perturbation theory to fourth order (the analogous result for two dimensional systems with confinement along one direction and arbitrary mass is also calculated to second order). We show that the non-perturbative extension obtained using Padé approximants can provide remarkably good approximations even for deep wells, in certain range of physical parameters. As an example, we discuss the case of two gaussian wells, comparing numerical and analytical results, predicted by our formulas.

1. Introduction

Almost 90 years have passed since Dirac established his famous equation, successfully combining Quantum Mechanics and Special Relativity, the two physical theories that completely changed our understanding of Nature at the beginning of the previous century. The importance of the Dirac equation can hardly be overstated: it predicts the existence of antimatter (discovered by Anderson in 1932), it explains the spin of the electron, recovering Pauli's theory in the low energy limit, and it also describes correctly the observed spectrum of the hydrogen atom, all at once. Another consequence of the Dirac equation, the *Zitterbewegung* (*trembling motion*) of the electron, has not been experimentally observed, although recently it has been simulated on physical systems composed of atoms which mimic the behavior of a free relativistic particle [1,2]. In recent years, the Dirac equation has also been used to describe the low energy spectrum of graphene, with either massless [3] or massive [4] excitations.

It is interesting to observe that even from the point of view of the theory, there are consequences of the Dirac equation that still need to be explored; our attention in the present paper is devoted to the study of the behavior of weakly bound relativistic states in one and two dimensional systems. The non-relativistic counterpart of this problem, has been settled long time ago in a seminal paper by Simon [5], where the conditions for the existence of this bound state have been given and the analyticity (non-analyticity) of the energy in one (two) dimension has been established.

For the relativistic case, the conditions under which a Dirac particle is trapped in a one-dimensional potential have been identified in ref. [6]; more recently Cuenin and Siegel [7] have studied the weakly coupling eigenvalue asymptotics for the bound state of the one dimensional Dirac operator, perturbed by a matrix-valued and non-symmetric potential.

For the case of a non-relativistic particle in a one dimensional short-range potential, a formula for the energy of the bound state has been derived up to sixth order: Simon [5] reports an unpublished result obtained by Abarbanel, Callan and Goldberger [8], which is exact to third order in the parameter controlling the strength of the potential, whereas higher order corrections (up to order six) have been derived later [11,10,9] using different techniques. Interestingly, a similar analysis for the relativistic case is still lacking and this constitutes the main goal of the present paper.

The approach that we will follow in this paper has been originally proposed by Gat and Rosenstein [10], and applied to the non-relativistic version of the present problem (to third order in the perturbation parameter) and to a $(1+1)$ dimensional QFT; in a recent work by two of the present authors, ref. [9], the method has been applied to calculate the energy of the bound state of an arbitrary shallow short range potential to sixth order.

* Corresponding author.
E-mail addresses: paolo.amore@gmail.com (P. Amore), fernande@quimica.unlp.edu.ar (F.M. Fernández), ejimenezr@ucol.mx (E. Jiménez).

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2. The method

We will first briefly describe how the method works for the non-relativistic problem and then discuss how it can be extended to its relativistic counterpart.

Let $\hat{H}$ be the hamiltonian of the problem

$$\hat{H}(\lambda) = -\frac{d^2}{dx^2} + \lambda V(x) \tag{1}$$

where $V(x) < 0$ for $x \in (-\infty, \infty)$ and $\lim_{|x|\to\infty} V(x) = 0$. Here $\lambda > 0$ is a parameter that controls the strength of the potential well. As noticed in [10], one cannot use $\hat{H}(0)$ as the unperturbed hamiltonian, since, for $\lambda > 0$ the spectrum of $\hat{H}$ contains (at least) one bound state, whereas the spectrum of $\hat{H}(0)$ is continuous.

Instead we use as unperturbed Hamiltonian the operator

$$\hat{H}_0 \equiv -\frac{d^2}{dx^2} - 2\beta\delta(x) \quad , \quad \beta > 0 \quad . \tag{2}$$

$\hat{H}_0$ has just one bound state with energy $\epsilon_0 = -\beta^2$ and a continuum of states, for $\epsilon > 0$ (the reader may refer to ref. [12] for a discussion of the one center δ interaction in one dimension). As a result, the Schrödinger equation

$$\left[\hat{H}_0 + \lambda V(x)\right]\psi(x) = E\psi(x) \tag{3}$$

can now be studied perturbatively in λ, working with a finite β and assuming $E = \sum_{n=0}^{\infty}\lambda^n\epsilon_n$ and $\psi(x) = \sum_{n=0}^{\infty}\lambda^n\phi_n(x)$. The infrared divergencies, which would spoil the perturbative expansion when $H(0)$ is used, manifest, at a given order, as inverse powers of β, and cancel out exactly, rendering each order perfectly finite.

Contrary to the approach followed in [10,9], where the standard Rayleigh–Schrödinger approach involving matrix elements was applied, here we obtain a perturbative solution of the Schrödinger equation in terms of the appropriate Green's functions.

To lowest order in λ one has the eigenvalue equation

$$\left(-\frac{d^2}{dx^2} - 2\beta\,\delta(x)\right)\phi_0(x) = \epsilon_0\phi_0(x) \tag{4}$$

In this case the eigenvalue and eigenfunction are $\epsilon_0 = -\beta^2$ and $\phi_0(x) = \sqrt{\beta}e^{-\beta|x|}$ respectively.

To higher orders one obtains the equations

$$\mathcal{D}\phi_n(x) = -V(x)\phi_{n-1}(x) + \sum_{k=1}^{n}\epsilon_k\phi_{n-k}(x) \equiv \mathcal{S}_n(x) \tag{5}$$

where

$$\mathcal{D} \equiv \left(-\frac{d^2}{dx^2} - 2\beta\delta(x) + \beta^2\right) \tag{6}$$

To deal with them one needs to consider the Green's function $G(x, y)$ defined by

$$\mathcal{D}G(x, y) = \delta(x - y) \tag{7}$$

and write the solution of order n as $\phi_n(x) = \int G(x, y)\mathcal{S}_n(y)dy$. The exact form of this and higher orders Green's functions can be found in ref. [9]. This equation needs to be complemented by the condition

$$\int \mathcal{S}_n(x)\phi_0(x)dx = 0\ ;\ n \geq 1\ , \tag{8}$$

which removes the "secular terms" in the expansion. Equation (8) only gives the energy and the wave function at a given order.

This approach has the advantage of avoiding the appearance of infinite series and it allows one to consider more general eigenvalue equations, as in the case of a relativistic particle.

Let us now discuss the case of a relativistic particle in one or two dimensions, obeying the Dirac equation $\hat{H}\psi = E(\lambda)\psi$, where

$$\hat{H} = -i\,\sigma\cdot\nabla + \sigma_3 m + \lambda W(x) \tag{9}$$

and $\psi = (\psi_1\ \psi_2)$ is a spinor (σ_i are the usual Pauli matrices).

Here $\sigma\cdot\nabla = \sigma_1\partial_x$ for the one dimensional case and $\sigma\cdot\nabla = \sigma_1\partial_x + \sigma_2\partial_y$ for the two-dimensional one.

The potential, which depends only on x, is given by

$$W(x) = \frac{1}{2}\left[\sigma_3\,(V(x) + U(x)) + \mathbf{1}\,(V(x) - U(x))\right]\ ,$$

where $(V(x) + U(x))/2$ and $(V(x) - U(x))/2$ are a vector and a scalar potential respectively.

Equations of the form of (9) have been studied previously, in particular for the case of point-like interactions in one dimension [13] and for graphene and graphite systems, subject to piecewise-constant potentials [14,15].

We can work in one or two dimensions in an unified framework by using the ansatz $\exp[iqy]\psi(x)$ (the one dimensional case is recovered for $q = 0$) and write explicitly the Dirac equation in terms of its components

$$\begin{aligned}(-E + m + \lambda V)\psi_1 - i\,(q + \partial_x)\,\psi_2 &= 0\\ -(E + m + \lambda U)\psi_2 + i\,(q - \partial_x)\,\psi_1 &= 0\end{aligned} \tag{10}$$

Using the second equation we can express ψ_2 in terms of ψ_1 and then use it inside the first equation to obtain a second order differential equation for ψ_1 alone:

$$\begin{aligned}&-\psi_1''(x) + \frac{\lambda U'(x)\psi_1'(x)}{E + m + \lambda U(x)} + \mathcal{V}(x)\psi_1(x)\\ &\quad = \left(E^2 - k^2(q)\right)\psi_1(x)\end{aligned} \tag{11}$$

with

$$\mathcal{V}(x) \equiv \left(\lambda(m - E)U(x) + \lambda(E + m)V(x) + \lambda^2U(x)V(x)\right) \tag{12}$$

and $k(q) \equiv \sqrt{q^2 + m^2}$.

When $U(x) = 0$ this equation takes a simpler form of a Schrödinger-like equation, with an energy dependent potential, as already pointed out by Coutinho and Nogami [6]. For the special case $E + m + \lambda U(x_0) = 0$ for some $x_0 \in \mathbb{R}$, in which the denominator in the second term of eq. (11) vanishes, the eigenfunction needs to obey the additional boundary condition $\psi_1'(x_0) = 0$ (see the discussion in Fig. 3).

Eq. (11) is now in the appropriate form to be attacked using the approach that we have previously described for the non-relativistic case, introducing an attractive delta potential of strength β, that allows to separate a single bound state from the continuum. This amounts to substituting $-\frac{d^2}{dx^2} \to -\frac{d^2}{dx^2} - 2\beta\delta(x) = \mathcal{D} - \beta^2$, previously defined, and then casting equation (11), in a compact form, formally similar to the nonrelativistic case, as

$$\left(\mathcal{D} - \beta^2\right)\psi_1 = \tilde{\mathcal{V}}\,\psi_1\ , \tag{13}$$

where

$$\tilde{\mathcal{V}}(x) \equiv -\frac{\lambda U'(x)}{E + m + \lambda U(x)}\frac{d}{dx} + \left(E^2 - k^2(q) - \mathcal{V}(x)\right) \tag{14}$$

is an operator defined on the real line (with the possible exception of x_0 for which the denominator $E + m + \lambda U(x)$ vanishes).