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.

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.

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

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

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

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

(2)
\( \hat{H}_0 \) has just one bound state with energy \( \epsilon_0 = -\beta^2 \) and a continuum of states, for \( \epsilon > 0 \). As a result, the Schrödinger equation

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

(3)
can now be studied perturbatively in \( \lambda \), working with a finite \( \beta \) 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 \( \hat{H}(0) \) is used, manifest, at a given order, as inverse powers of \( \beta \), 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 \( \lambda \) one has the eigenvalue equation

\[
\left( -\frac{d^2}{dx^2} - \beta \delta(x) \right) \phi_0(x) = \epsilon_0 \phi_0(x)
\]

(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

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

(5)

with \( \mathcal{D} \equiv \left( -\frac{d^2}{dx^2} - 2\beta \delta(x) + \beta^2 \right) \). To deal with them one needs to consider the Green’s function \( G(x,y) \) defined by

\[
\mathcal{D} G(x,y) = \delta(x-y)
\]

(6)

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

\[
\int \mathcal{S}_n(x)\phi_0(x)dx = 0 ; \ n \geq 1
\]

(7)

which removes the "secular terms" in the expansion. Equation (7) 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

\[
\hat{H} = -i \sigma \cdot \nabla + \sigma_3 m + \lambda W(x)
\]

(8)
and $\psi = (\psi_1 \; \psi_2)$ is a spinor ($\sigma_i$ 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

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

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 (8) have been studied previously, in particular for the case of point-like interactions in one dimension [12] and for graphene and graphite systems, subject to piecewise-constant potentials [13, 14].

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

$$- \psi_1''(x) + \frac{\lambda U'(x) \psi_1'(x)}{E + m + \lambda U(x)} + \left( \frac{\lambda q U'(x)}{E + m + \lambda U(x)} + \lambda (m - E) U(x) \right) \psi_2(x)$$

$$+ \lambda (E + m) V(x) + \lambda^2 U(x) V(x) \right) \psi_1(x)$$

$$= (E^2 - k^2(q)) \psi_1(x),$$

with $k(q) = \sqrt{q^2 + m^2}$. For the special case $U(x) = 0$ 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].

Eq. (11) is now in the appropriate form to be attacked using the approach that we have previously described for the non-relativistic case. We cast this equation in a compact form, formally similar to the nonrelativistic case, as

$$\mathcal{D} \psi_1 = \mathcal{V} \psi_1 ,$$

where $\mathcal{V}(x)$ can be read off the equation (11).

After expressing both the energy and wave function as power series in $\lambda$,

$$E = \sqrt{k^2 - \Delta}, \quad \Delta = \sum_{n=0}^{\infty} \delta_n \lambda^n, \quad \psi_1 = \sum_{n=0}^{\infty} \phi_n \lambda^n$$

and substituting into eq. (12), we obtain an infinite tower of second order differential equations, corresponding to different orders in $\lambda$, which can be solved starting from the lowest order. This situation is completely analogous to the
non-relativistic case, although now $V$ in eq. (12) is an operator and it is non-linear in $\lambda$. The main consequence of this fact is the rapid proliferation of terms contributing at a given perturbative order, as the order is increased.

Applying the method of Gat and Rosenstein to this equation, we have obtained the perturbative expression for the energy of the fundamental mode to fourth order in $\lambda$ for the one-dimensional problem and to second order in $\lambda$ for the two-dimensional model.

Since the solutions for the one-dimensional case can be recovered from the corresponding two-dimensional expressions setting $q = 0$, we first assume $|q| \geq 0$, and report the coefficients of $\Delta$ up to second order

$$
\delta_0 = \beta^2 ,
\delta_1 = -2\beta \mathcal{F}(k) + \mathcal{O}(\beta^2) ,
\delta_2 = \mathcal{F}(k)^2 + \mathcal{O}(\beta) ,
$$

where

$$
\mathcal{F}(k) = \frac{1}{2} \int dx \ ( (m + k) V + (m - k) U ) .
$$

The coefficients $\delta_i$ obtained in the calculation, with $i = 1, 2, \ldots$, are analytic functions of $\beta$, $\delta_i = \sum_{n=0}^{\infty} \delta_i^{(n)} \beta^n$. Although the Green’s functions contain singular contributions at $\beta = 0$, the energy obtained in perturbation theory does not contain infrared divergences for $\beta \to 0^+$, due to exact cancellations, as for the non-relativistic case.

For the one-dimensional case ($q = 0$), we have computed the energy corrections up to order four. Terms up to second order are obtained by making $\kappa = m$ in formula (13), while $\delta_3$ and $\delta_4$ are given by

$$
\delta_3 = 2m^3 \mathcal{F}_1 \mathcal{F}_{2,1} + \mathcal{O}(\beta) ,
\delta_4 = m^4 \eta_4 - m^2 \kappa_4 + \mathcal{O}(\beta) ,
$$

where

$$
\eta_4 = (\mathcal{F}_1)^2 \mathcal{F}_{2,2} + 2 \mathcal{F}_1 \mathcal{F}_{3,1} + (\mathcal{F}_{2,1})^2 ,
\kappa_4 = (1/2) \left( \mathcal{F}_1 \mathcal{F}_{3,2} + (\mathcal{F}_1)^3 \right) .
$$

$\mathcal{F}_1, \ldots, \mathcal{F}_{3,2}$ are functionals of $V$ and $U$ given by

$$
\mathcal{F}_1 = \mathcal{F}(m)/m = \int dx V(x) ,
\mathcal{F}_{2,1} = \int \int dx dy V(y) |x - y| V(x) ,
\mathcal{F}_{2,2} = \int \int dx dy V(y) (x - y)^2 V(x) ,
\mathcal{F}_{3,1} = \int \int \int dx dy dz |x - y| |y - z| V(x)V(y)V(z) ,
\mathcal{F}_{3,2} = \int \int \int dx dy dz \frac{|x - y| |x - z|}{(x - y)(x - z)} U(x)V(z)V(y) .
$$
The energy of the bound state in one dimension reads

\[ E^{(1)}(\lambda) = m + \tilde{E}(\lambda) + \lambda^4 \delta E + \mathcal{O}(\lambda^5), \]  

where

\[ \tilde{E} = -\frac{m\lambda^2}{2} F_1^2 - m^2\lambda^3 F_1 F_{2,1} - \frac{m^3\lambda^4}{2} \eta_4 \]  

is the non-relativistic formula previously obtained to fourth order working with the Schrödinger equation and \( \delta E \) is the leading relativistic correction which appears to fourth order

\[ \delta E = \frac{m}{2} \left( \kappa_4 - \frac{1}{4} F_1^4 \right) \]  

Note that, while \( \tilde{E}(\lambda) \) is a functional of \( V \) only, \( \delta E \) is a functional both of \( V \) and \( U \).

In two dimensions, for quasi-bound states of the form \( \psi(x, y) = \exp(iq) \psi(x) \), the energy is given by

\[ E^{(2)}(\lambda) = k - \frac{\lambda^2}{2k} F(k)^2 + \mathcal{O}(\lambda^3). \]  

For the case of a relativistic one-dimensional square well, discussed by Greiner [15] in detail, Eq. (17) reproduces the exact results up to fourth order. As a further test of our perturbation expressions we also consider the simple case in which \( V(x) = -(1 + \gamma)\delta(x), U(x) = -(1 - \gamma)\delta(x) \) and \( q = 0 \). In order to avoid the possible discontinuity of both functions \( \psi_{1,2}(x) \) at \( x = 0 \) we set \( \gamma = 1 \). In this case \( \psi_1(x) \) is continuous at \( x = 0 \) and a straightforward calculation shows that

\[ E^{(1)} = m \left( \frac{1 - \lambda^2}{1 + \lambda^2} \right) = m - 2m\lambda^2 (1 - \lambda^2 + \lambda^4 + \ldots), \]  

and \( \psi(x) = \sqrt{\beta} e^{-\beta|x|} \), with \( \beta = \sqrt{m^2 - E^2} = \frac{2m\lambda}{1 + \lambda^2} \).

Note that \( 0 < \beta \leq \beta(\lambda = 1) = m \). Present perturbation theory yields the first three terms of the series exactly.

In the perturbative region, \( 0 < \lambda \ll 1 \), the relativistic correction \( \delta E \) provides in general a tiny correction to the corresponding non-relativistic expression, \( \tilde{E} \), implying that the weakly bound electron is essentially non-relativistic. This hierarchy can however be modified already at moderate values of \( \lambda \). In this case, the energy of the bound state cannot lower indefinitely as the well becomes deeper and deeper, as in the non–relativistic case, since it is trapped between two continua, the continuum of positive energy states, for \( E \geq m \), and the continuum of negative energy states, for \( E \leq -m \). This behavior can be captured using a diagonal Pade approximant, which tends to a constant for \( \lambda \to \infty \):

\[ E^{(1)}_{\text{Pade}} = m + \frac{m^2\lambda^2 F_1^4}{-2mF_1^2 + 4m^2\lambda F_1 F_{2,1} + 2\lambda^2 (-2\delta E + m^3 (\eta_4 - 4F_{2,1}^2))}. \]
This formula provides a completely analytical expression for the energy of the relativistic bound state which can be used for larger values of \( \lambda \); the non-relativistic case can either be obtained setting \( \delta E \to 0 \) in this expression, or using the simpler [2, 1] Padé approximant, which is linear as \( \lambda \to \infty \):

\[
E_{\text{Pade--nr}}^{(1)} = -\frac{m \lambda^2 F_3^3}{4m \lambda F_{2,1}^2 - 2F_1}
\]  

(23)

One way to assess the region of applicability of Eq. (22) is by identifying the region in parameter space where

\[
\delta E > \frac{m^3}{2} \left( \eta_4 - 3F_{2,1}^2 \right)
\]  

(24)

is fulfilled. When this condition is met, the denominator of \( E_{\text{Pade}}^{(1)} \) has no real pole and consequently the resummation is more accurate.

As an example, we consider the gaussian wells \( V(x) = -(1 + \gamma)e^{-\alpha x^2} \) and \( U(x) = -(1 - \gamma)e^{-\alpha x^2} \), where \(-1 \leq \gamma \leq 1\) is a parameter which controls the depths of \( V(x) \) and \( U(x) \).

In this case the inequality (24) reads

\[
\pi \alpha (\gamma + 5) > 8 \left( -6 + 3\sqrt{3} + 2\pi \right) (\gamma + 1)m^2
\]  

(25)

The region in parameter space where the inequality is fulfilled is displayed in Fig. 1 for three values of \( \alpha \). Notably the Padé has always real poles when \( \delta E \) is set to zero.

Figure 1: Parameter space for the inequality (25) for three different values of \( \alpha \). (color online)

In Fig. 2 we plot the quantity \( m - E \) for the case \( m = 0.1 \) and \( \alpha = 1 \), as a function of \( \lambda \), for \( \gamma = 1 \) (the plot for \( \gamma = 0 \), not reported here is quite

\textsuperscript{1}Note that the case \(|\gamma| > 1\) can be reduced to the present case by means of a redefinition of \( \lambda \).
similar). The blue points represent the numerical values obtained applying the shooting method directly to Eq. (11); the red points are obtained solving the corresponding non-relativistic Schrödinger equation. These values are compared with the relativistic Padé of Eq. (22) (solid line), the non-relativistic [2, 2] Padé obtained setting $\delta E = 0$ (dashed line) and the non–relativistic Padé of Eq. (23) (dot-dashed line). The horizontal lines correspond to the limit values $m(1 + \gamma)$.

While $\delta E$ provides a tiny contribution at small $\lambda$, it plays an essential role at larger values of $\lambda$.

The normalized upper and lower components of the Dirac spinor, $\psi_{1,2}(x)$, are plotted in Fig. 3, for the case $m = 0.1$, $\alpha = 1$, $\gamma = 0$ and $\lambda = 1$. The corresponding probability density $\rho(x)$ is also displayed. $\psi_1(x)$ is obtained numerically using the shooting method. By inspection of the Eq. (11) we see that the coefficient of $\psi'_1(x)$ is singular when $E + m + \lambda U(x) = 0$: this forces the first derivative of the wavefunction to vanish at the singularity, represented by a vertical line in the plot. Out of this region the wave function decays exponentially as $\psi_1(x) \propto e^{-\sqrt{m^2 - E^2}x}$. The dashed line is a fit of the numerical results, within the interval $5 \leq x \leq 50$ and it corresponds to $\psi_1^{(fit)}(x) = 0.5929 \cdot e^{-0.0931 \cdot x}$. Note that $\Gamma^{(fit)} = 0.0931$ is in perfect agreement with the expected expression $\Gamma = \sqrt{m^2 - E^2}$.

This remarkable agreement can be appreciated from Fig. 4, where the constant $\Gamma$ is extracted from the fit of the numerical results of the wave function $\psi_1(x)$, at different values of $\lambda$ (the dots in the plot), and contrasted with the explicit expressions obtained using the Padé approximant of Eq. (22). While, in the non-relativistic case, the wave function decays more and more strongly as $\lambda \rightarrow \infty$, in the relativistic case the energy of the bound state obeys the inequality $-m < E < m$, and therefore $0 < \Gamma \leq m$. The particular behavior of the analytic formula for $\Gamma$ when $\gamma = 0$, which breaks down at $\lambda \approx 10$, is easily explained by the fact that the Padé slightly underestimates the limiting energy for $\lambda > 10$, and as a result $\sqrt{m^2 - E^2}$ becomes imaginary.

Conclusions. We have calculated for the first time the energy of a relativistic bound state in a shallow short range potential in one dimension to fourth order in perturbation theory, proving that the first genuinely relativistic correction appears only at order four. We have confirmed this generally tiny contribution in a number of cases where it was possible to contrast our results with exact results available in the literature and with precise numerical calculations, carried out for the case of a pair of gaussian potentials.

We have also shown that it is possible to extend the perturbative analysis to the study of deep wells, by using a Padé approximant which captures the asymptotic behavior of the energy for $\lambda \rightarrow \infty$. The simple analytical formula that we have obtained has been tested for the (not exactly solvable) case of gaussian well, finding that the analytical approximation is in excellent agreement with the numerical results.
Figure 2: Energy of the relativistic and non-relativistic bound states (blue and red dots respectively) compared with the relativistic and non-relativistic Padé approximants (solid, dashed and dot-dashed lines respectively). Here \( m = 0.1, \alpha = 1 \) and \( \gamma = 1 \). The horizontal lines are the limit values \( m - E = m(1 + \gamma) \).

(color online)

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Figure 3: Normalized upper and lower components $\psi_{1,2}(x)$ and probability density of the Dirac spinor for $m = 0.1$, $\alpha = 1$, $\gamma = 0$ and $\lambda = 1$, obtained using the shooting method. The vertical line is the location of the singularity $E + m + \lambda U(x)$, where $\psi'_1(x) = 0$. The dashed line is the fit of the numerical results between $x = 5$ and $x = 50$, $\psi_{1}^{(fit)}(x) = 0.5929 \cdot e^{-0.0931 \cdot x}$. (color online)

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Figure 4: Constant $\Gamma$ of the exponential decay of the wave function. The dots (blue and green) are the values of $\Gamma$ obtained from the fit of the numerical wave function at different values of $\lambda$ at $\gamma = 1$ and $\gamma = 0$ respectively. The solid and dashed lines are the explicit expressions obtained using the Padé of Eq. (22). (color online)