Solution of one-dimensional Dirac equation via Poincaré map

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Abstract – We solve the general one-dimensional Dirac equation using a “Poincaré map” approach which avoids any approximation to the spacial derivatives and reduces the problem to a simple recursive relation which is very practical from the numerical implementation point of view. To test the efficiency and rapid convergence of this approach we apply it to a vector coupling Woods-Saxon potential, which is exactly solvable. Comparison with available analytical results is impressive and hence validates the accuracy and efficiency of this method.

The Dirac equation describes a relativistic particle of spin one-half at high velocities (below the threshold of pair production) [1]. It describes the state of electrons in a way consistent with special relativity, requiring that electrons have spin 1/2, and predicting the existence of an antiparticle partner to the electron (the positron). The physics and mathematics of the Dirac equation is very rich, it is a first-order matrix linear differential equation whose solution is a 4-component wave function (a spinor). Nevertheless, it was hard to find nontrivial exact solutions of this equation. Until 1989, there was only one nontrivial exact solution of the Dirac equation for the very important Coulomb problem. By convention, a nontrivial exact solution of the Dirac equation is a solution that, in the nonrelativistic limit, reproduces a known solution of Schrödinger equation with that specific potential and hence carries the same relativistic potential name.

In this regard, Moshinsky and Szczepaniak [2] in 1989 were able to formulate and solve the relativistic oscillator problem (Dirac-Oscillator). During the last decade, Alhaidari has introduced an effective approach to the solution of the Dirac equation for spherically symmetric potentials [3–7]. His method was initiated by the observation that different potentials can be grouped into classes; for example, the nonrelativistic Coulomb, oscillator and S-wave Morse problems constitute one such class.

Therefore, the solution of two problems in one class implies solution for the remaining one. By this method, the S-wave Dirac-Morse problem was formulated and solved [3].

Using the above-mentioned method, other potentials were treated; among these are Dirac-Scarf, Dirac-Rosen-Morse I & II, Dirac-Poschl-Teller, Dirac-Eckart [4], Dirac-Hulthen, and Dirac-Woods-Saxon potentials [8] as well as other potentials [9,10]. On the other hand, alternative methods such as quasi-exactly solvable problems at rest mass energies with power-law relativistic potentials were investigated following the same procedure [5]. Orthogonal polynomials were also used to find series solutions of Dirac equation for scattering and bound states [6]. In this work we will be interested in solving the one-dimensional (1D) Dirac equation in general using a Poincaré map which enables us to treat exactly the spacial derivative operator while the only approximation is made upon discretizing the scattering potential. The approach is very efficient and converges rapidly. To exhibit the efficiency of our method we use it to solve the vector coupling Woods-Saxon potential and compare our results for the transmission coefficient with the analytic one. The accuracy and easy implementation of our method are impressive and suggest its suitability in dealing with 1D Dirac equation for an arbitrary potential.

We consider a one-dimensional Dirac equation for a particle of mass \( m \), subject to a vector potential coupling...
by the Dirac Hamiltonian
\[ H = p_x \sigma_x + m \sigma_z + V(x) \]
with \( \sigma_x \) and \( \sigma_z \) being the Pauli matrices. The stationary eigenvalue equation can be written explicitly in the following form:
\[ \begin{pmatrix} m + V(x) - \varepsilon & -i \frac{d}{dx} \\ -i \frac{d}{dx} & -m + V(x) - \varepsilon \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = 0, \tag{2} \]
where \( \psi(x) = (\psi_1 \ \psi_2)^t \) is the eigenspinor made of two components. Generally speaking for an arbitrary potential \( V(x) \), this equation is difficult to solve analytically except for a very limited number of solvable potentials as classified by supersymmetric quantum mechanics [11].

Using this approach we are going to show that the above 1D Dirac equation can be replaced by a Poincaré map associated with the above wave equation. This approach will enable us to solve the Dirac equation and generate the spinor wave function iteratively, a method very suitable for numerical implementations. In addition, we will be able to use the transfer matrix approach to compute the transmission coefficient.

We consider our one-dimensional system where the particle is moving under the action of a scattering potential \( V(x) \) bound to a region of size \( L \) of our system. So our space can be decomposed into three major regions: two extremes free-like regions where the potential is almost zero and an intermediate region where the potential is \( V(x) \). Now we proceed in subdividing the potential interval \( L \) into \( N+1 \) equal regions, in every region we approximate the potential by a constant local value \( V_n = V(x_n) \), where \( x_n = nh \) and \( h = \frac{L}{N+1} \), with \( N \) the maximum value of \( n \), see fig. 1. Hence, the Hamiltonian in each region \( n \), defined by \( h(n-1) < x < nh \), is given by
\[ H_n = p_x \sigma_x + m \sigma_z + V_n. \tag{3} \]

Actually we can even generalize this approach to treat spatially dependent masses in which case \( m_n = m(x_n) \) in the above equation, however from now on we limit ourselves to a uniform mass distribution. In each spacial region we have a 1D Dirac fermion subject to a constant potential, hence the solution is easily generated. The complete solution for (3) satisfying the eigenequation with spinor \( \psi_n(x) = (\psi_n^1 \psi_n^2)^t \) in the \( n \)-th space region where the potential is approximated by its local value \( V_n \) will depend on the energy range and can be written as
\[
\psi_n(x) = A_n \begin{pmatrix} i \alpha_n \1 \1 \end{pmatrix} e^{ip_n x} + B_n \begin{pmatrix} -i \alpha_n \1 \1 \end{pmatrix} e^{-ip_n x}, \quad \varepsilon \leq V_n - m, \tag{4}\]
\[
\psi_n(x) = A_n \begin{pmatrix} \alpha_n \1 \1 \end{pmatrix} e^{ip_n x} + B_n \begin{pmatrix} -\alpha_n \1 \1 \end{pmatrix} e^{-ip_n x}, \quad V_n - m \leq \varepsilon \leq V_n, \tag{5}\]
\[
\psi_n(x) = A_n \begin{pmatrix} 1 \alpha_n \1 \1 \end{pmatrix} e^{ip_n x} + B_n \begin{pmatrix} 1 -\alpha_n \1 \1 \end{pmatrix} e^{-ip_n x}, \quad V_n \leq \varepsilon \leq V_n + m, \tag{6}\]
\[
\psi_n(x) = A_n \begin{pmatrix} 1 i \alpha_n \1 \1 \end{pmatrix} e^{ip_n x} + B_n \begin{pmatrix} 1 -i \alpha_n \1 \1 \end{pmatrix} e^{-ip_n x}, \quad \varepsilon \geq V_n + m, \tag{7}\]
where we have set
\[
\alpha_n = \sqrt{\left| \varepsilon - V_n - m \right| \left| \varepsilon - V_n + m \right|}, \quad \tag{8}\]
\[
p_n = \sqrt{\left| (m + V_n - \varepsilon) (m - V_n + \varepsilon) \right|}. \]

The coefficients \( A_n \) and \( B_n \) are two normalization constants. The above solutions can be written in a compact matrix form, such as
\[
\psi_n(x) = M_n^\star(x) \begin{pmatrix} A_n \\ B_n \end{pmatrix}, \tag{9}\]
where the matrix \( M_n^\star(x) \) is given by see eq. (10) above

\[
M_n^\star(x) = \begin{pmatrix} \left(1 + \frac{1}{2} \frac{x}{\alpha_n} \right) e^{1/2 \frac{x}{\alpha_n}} & \left(-1 + \frac{1}{2} \frac{x}{\alpha_n} \right) e^{-1/2 \frac{x}{\alpha_n}} \\ \left(-1 + \frac{1}{2} \frac{x}{\alpha_n} \right) e^{1/2 \frac{x}{\alpha_n}} & \left(1 + \frac{1}{2} \frac{x}{\alpha_n} \right) e^{-1/2 \frac{x}{\alpha_n}} \end{pmatrix} \tag{10}\]
continuity of the spinor wave function at the junction

and

where the explicit matrix elements of $c$ of wave propagating from right to left, this amounts to

for a positive and negative

Just outside the potential region on the right-hand side in the $(N+2)$-th region the spinor wave is given by

Using the above notation we can easily define the transmission amplitude as

Hence to evaluate the transmission amplitude all we need is to find $A_{N+2}$ using the above recursive scheme. Our strategy now is to express $A_{N+2}$ in terms of the two end points spinors $\psi_{N+1} = \psi_{N+1}(x_{N+1})$ and $\psi_{N+2} = \psi_{N+2}(x_{N+2})$. This can be easily done using our previous relations and leads to the form

Summing up, we iterate the Poincaré map (13) to obtain the end point spinors, $\psi_{N+1}$ and $\psi_{N+2}$, in terms of the transmitted spinor $\psi_0$. These spinors will then be injected in eqs. (20) and (19) to determine the transmission amplitude.

To test the validity of our previous approach we will now implement it for a test potential, the Woods-Saxon potential which has an exact analytical solution [13,14]. This potential is defined by [14]

where $V_0$ is real and positive for a barrier or negative for a well, $a$ and $L$ are real and positive. $\theta(x)$ is the Heaviside step function. The analytical solutions provided in ref. [14] is used to evaluate the exact transmission coefficient for the potential (21) from the asymptotic behavior of the wave functions. This analysis leads to

$$T = 1 - \frac{B}{A} \left| \frac{E + k}{E - k} \right|^2,$$
where $A$ and $B$ are given by

$$A = D_1 \frac{\Gamma(1 - 2\mu)\Gamma(-2\nu)}{\Gamma(-\mu - \nu - \lambda)\Gamma(1 - \mu - \nu + \lambda)} e^{-i\pi\mu} + D_2 \frac{\Gamma(1 + 2\mu)\Gamma(-2\nu)}{\Gamma(\mu - \nu - \lambda)\Gamma(1 + \mu - \nu + \lambda)} e^{i\pi\mu},$$

$$B = D_1 \frac{\Gamma(1 - 2\mu)\Gamma(2\nu)}{\Gamma(-\mu + \nu - \lambda)\Gamma(1 - \mu + \nu + \lambda)} e^{-i\pi\mu} + D_2 \frac{\Gamma(1 + 2\mu)\Gamma(2\nu)}{\Gamma(\mu + \nu - \lambda)\Gamma(1 + \mu + \nu + \lambda)} e^{i\pi\mu},$$

with the ratio

$$\frac{D_2}{D_1} = \frac{\Gamma(2\mu)\Gamma(1 - \mu - \nu + \lambda)\Gamma(-\mu - \nu + \lambda)}{\Gamma(-2\mu)\Gamma(1 + \mu - \nu - \lambda)\Gamma(\mu - \nu + \lambda)} e^{-2i\pi\mu} e^{4aL\mu},$$

and the abbreviations $\mu = \frac{\alpha p}{c}$, $\nu = \frac{V_0 a}{c}$, $\lambda = \frac{V_0}{a}$, $p^2 = (E - V_0)^2 - m^2$, $k^2 = E^2 - m^2$ have been used.

For scattering states, of interest to us, $|E| > m$ ensures that $k$ is real while the momentum $p$ is real for $m < E < V_0 - m$ (the Klein range) and $E > V_0 + m$, it is imaginary for $V_0 - m < E < V_0 + m$. The potential strength $V_0$ is real and positive in our computations. In fig. 3 we show the shape of the Woods-Saxon potential for the parameters $L = 10$, $a = 5$ and $V_0 = 1.2$, the vertical lines represent the discretization of this potential. We shifted the potential to the right by an amount $L$ for convenience, such a translation does not affect the physics of the problem.

Using the above-mentioned numerical procedure (Poincaré map) we evaluate the transmission coefficient associated with the potential characterized by the above-mentioned parameters $(L, a, V_0)$ and a mass $m = 0.4$ in our atomic units. Moreover, using the same parameters as in the literature [13], we have plotted the transmission coefficient in the Klein zone for a constant mass $m$. As shown in fig. 4 the solid lines correspond to the exact transmission [13], and the dashed lines are generated by our Poincaré iterative map. We notice from this figure, as expected, that as $N$ increases, the dotted-line curve converges to the exact solid-line curve. We see a satisfactory agreement between our fast-converging numerical approach and the analytical results [13,14]. In fig. 5 we show the transmission coefficient as a function of the potential strength $V_0$ for two values of the iteration parameter $N$. The agreement between our numerical approach and the analytical results is impressive. Thus we expect that we can apply our iterative approach to very general potentials, which do not lend themselves to analytical solutions. In summary, we believe that the Poincaré map exposed in this work is very simple and enables us to solve the 1D Dirac equation for any arbitrary short-range potential with high accuracy and simple computational means. This approach can be easily extended to handle the two-dimensional Dirac equation, which plays an important role in describing the recently discovered graphene system [15].
Fig. 5: (Colour on-line) The transmission coefficient as a function of $V_0$ for two different iterations, (a) $N = 400$ and (b) $N = 1000$.

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REFERENCES

[1] Greiner W., Relativistic Quantum Mechanics: Wave Equations (Springer, Berlin) 1994; Bjorken J. D. and Drell S. D., Relativistic Quantum Mechanics (McGraw-Hill, New York) 1964; Greiner W., Miller B. and Rafeelski J., Quantum Electrodynamics of Strong Fields (Springer, Berlin) 1985.

[2] Moshinsky M. and Szczepaniak A., J. Phys. A, 22 (1989) L817.

[3] Alhaidari A. D., Phys. Rev. Lett., 87 (2002) 210405; 88 (2002) 189901.

[4] Alhaidari A. D., J. Phys. A, 34 (2001) 9827; 35 (2002) 9207.

[5] Alhaidari A. D., Int. J. Mod. Phys. A, 17 (2002) 4551.

[6] Alhaidari A. D., Phys. Rev. A, 65 (2002) 042109; 66 (2002) 019902.

[7] Alhaidari A. D., Int. J. Mod. Phys. A, 18 (2003) 4955.

[8] Guo J.-Y., Fang X. Z. and Xu F.-X., Phys. Rev. A, 66 (2002) 062105; Guo J.-Y., Meng J. and Xu F.-X., Chin. Phys. Lett., 20 (2003) 602.

[9] Alhaidari A. D., Ann. Phys. (N.Y.), 312 (2004) 144; Phys. Lett. A, 326 (2004) 58; J. Phys. A, 37 (2004) 11229.

[10] Alhaidari A. D., Phys. Lett. A, 322 (2004) 72.

[11] Cooper F., Khare A. and Sukhatme Uday, Supersymmetry in Quantum Mechanics (World Scientific Publishing Co.) 2001.

[12] Bellisard J., Formoso A., Lima R. and Testard D., Phys. Rev. B, 26 (1982) 3024; Dominguez-Adamé F., Marcia E. and Sanchez A., Phys. Rev. B, 48 (1993) 6054; Diez E., Sanchez A. and Dominguez-Adamé F., Phys. Rev. B, 50 (1994) 14359.

[13] Panella O., Biondini S. and Arda A., J. Phys. A: Math. Theor., 43 (2010) 325302.

[14] Kennedy P., J. Phys. A: Math. Gen., 35 (2002) 689.

[15] Geim A. K. and Novoselov K. S., Nat. Mater., 6 (2007) 183.