The Extended Wronskian Determinant Approach and the Iterative Solutions of One-Dimensional Dirac Equation

Ying Xu, Meng Lu

Department of Physics, Fudan University, Shanghai, 200433, P. R. China

Ru-Keng Su

China Center of Advanced Science and Technology (World Laboratory),
P. O. Box 8730, Beijing 100080, P. R. China;
Department of Physics, Fudan University, Shanghai, 200433, P. R. China

Abstract

An approximation method, namely, the Extended Wronskian Determinant Approach, is suggested to study the one-dimensional Dirac equation. An integral equation which can be solved by iterative procedure to find the wave functions is established. We employ this approach to study the one-dimensional Dirac equation with one-well potential, and give the energy levels and wave functions up to the first order iterative approximation. For double-well potential, the energy levels up to the first order approximation are given.

Keywords: Extended Wronskian Determinant Approach, Dirac equation, integral equation, iteration method, double-well potential

PACS numbers: 03.65.Pm, 03.65.Ge, 03.65.Ca
1 Introduction

Since the majority of problems in quantum mechanics lead to very complex equations and cannot be solved exactly, the approximation methods for solving Schrödinger equation are very important for practical use. Recently, Friedberg, Lee and Zhao (FLZ) suggested a new method to decide the wave functions and energy levels of Schrödinger equation by quadrature along a single trajectory [1-3].

Giving a good trial wave function $\Psi$ for one-dimensional (1D) Schrödinger equation with potential $V$,

$$\frac{-1}{2} \frac{d^2 \Phi}{dx^2} + V \Phi = E \Phi$$  \hspace{1cm} (1)

they considered a perturbation equation

$$\frac{-1}{2} \frac{d^2 \Psi}{dx^2} + (V + w) \Psi = (E + \varepsilon) \Psi$$  \hspace{1cm} (2)

where $w$ is the perturbation potential and $\varepsilon$ the energy shift. By means of the Green’s function, they constructed an integral equation and solved it by iterative procedure to find the true ground wave function and the corresponding energy level. The integral equation for wave function $\Psi$ reads

$$\Psi = \Phi - 2 \Phi \int_{x}^{+\infty} \Phi^{-2}(y) dy \int_{y}^{+\infty} \Phi(z)(w - z) \Psi(z) dz$$  \hspace{1cm} (3)

and the corresponding energy is

$$\varepsilon = \frac{\int_{0}^{+\infty} \Phi w \Psi dx}{\int_{0}^{+\infty} \Phi \Psi dx}$$  \hspace{1cm} (4)

Employing a double-well potential [3] and other potentials [4, 5] they gave the ground state energy up to the first order approximation of iterative procedure.

On the other hand, as is well known, the behavior of 1D Schrödinger equation is determined completely by its corresponding Wronskian determinant [6]. Therefore, a Wronskian Determinant Approach (WDA) is suggested by us [7] to study the energy levels and the wave functions of 1D Schrödinger equation. We established an integral equation and employed this equation to study the same problem of double-well potential. A series of expansion of ground state energy up to the second order approximation of iterative procedure is given. We found that the series of energy given by FLZ method and the WDA up to the order of $O(g^{-1})$ where $g$ is the strong coupling constant are the same. This result confirms that the WDA is a successful method to investigate the 1D Schrödinger equation.

The objective of this paper is to extend the WDA to study the 1D Dirac equation. Based on general considerations and an extended Wronskian determinant, we establish an integral equation for Dirac wave function and give the “resonant condition” to determine the energy level. Our approach may be considered as a relativistic generalization.
of the WDA. We will show the formulae of our Extended Wronskian Determinant Approach (EWDA) in next section. In section III, as an example, we will use EWDA to study the 1D Dirac equation with perturbative one-well potential. We will solve the integral equation by iterative procedure up to the first order to find the energy shifts and the wave functions. Since the double-well potential for Schrödinger equation and, in particular, for Dirac equation has wide applications in physics, for example, soliton bag model, instantons and anti-instantons and etc\cite{8-12}, we will address the energy levels and the wave functions for double-well potential in section IV. The last section is a summary.
The Extended Wronskian Determinant Approach

The 1D Dirac equation reads

\[
\left( \hat{\alpha} \hat{p} + \hat{\beta} m \right) \psi(y) = (E - V) \psi(y) \tag{5}
\]

where \( \psi = \begin{pmatrix} u \\ v \end{pmatrix} \) is a 2-component spinor. Choose \( \hat{\alpha} = \hat{\sigma}_2, \hat{\beta} = \hat{\sigma}_3 \) and define

\[
\hat{A} \equiv \begin{pmatrix} 0 & m + E - V \\ m - E + V & 0 \end{pmatrix} \tag{6}
\]

then Eq. (5) could be rewritten as

\[
\psi'(y) - \hat{A} \psi(y) = 0 \tag{7}
\]

Eq. (7) is called the homogeneous equation in our approach. We need its specific solution as a zeroth order approximation to construct the solution of the perturbation equation. Assume a perturbative potential \( w \) is added to Eq. (5)

\[
\mathcal{V} = V + w \tag{8}
\]

and the eigenenergy is shifted to

\[
\mathcal{E} = E + \varepsilon \tag{9}
\]

We get the perturbation equation

\[
\psi'(y) - \hat{A} \psi = (\varepsilon - w) \hat{f} \psi \tag{10}
\]

where

\[
\hat{f} \equiv \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{11}
\]

Eq. (10) is called an inhomogeneous equation and the inhomogeneous term is \((\varepsilon - w) \hat{f} \psi\) in our approach.

As is well known, in ordinary differential equation theory, with a specific solution of a homogeneous differential equation given, we can try to find another linearly independent solution of this equation and the general solutions of the corresponding inhomogeneous differential equation through Wronskian determinant calculation. This procedure can also be employed to discuss the solution of 1D Dirac equation.

Suppose \( \psi_1 = \begin{pmatrix} u_1 \\ v_1 \end{pmatrix} \) is a specific solution of Eq. (7). It is a normalized bound state and satisfies the boundary condition

\[
\lim_{y \to \pm \infty} \psi_1 = 0.
\]

Now we construct another solution \( \psi_2 = \begin{pmatrix} u_2 \\ v_2 \end{pmatrix} \) which is a linearly independent solution with \( \psi_1 \) by using the extended Wronskian determinant approach. Obviously we have

\[
(v_2 - u_2) \psi_1' - (v_1 - u_1) \psi_2' = (v_2 - u_2) \hat{A} \psi_1 - (v_1 - u_1) \hat{A} \psi_2 \tag{12}
\]
A straightforward calculation can show the right hand side of Eq. (12) be zero, we get

\[(u_1v_2 - u_2v_1)' = 0\]  (13)

Define a matrix \(\hat{U}\) as

\[\hat{U} \equiv \begin{pmatrix} u_1 & u_1 \\ v_1 & v_2 \end{pmatrix}\]  (14)

We find

\[\det \hat{U} = C (\text{Const.})\]  (15)

Here \(\det \hat{U}\) is called an extended Wronskian determinant. The constant \(C\) is nonzero because \(\psi_1\) and \(\psi_2\) are linearly independent. Since \(\psi_1\) satisfies the boundary condition

\[\lim_{y \to \pm \infty} \psi_1 = 0,\]

we get that \(\psi_2\) must be divergent when \(y \to \pm \infty\) because of Eq. (15). Eqs. (15) and (7) yield

\[u_1v_2 - \frac{1}{m - E + V}v_2v_1 = C\]  (16)

Assume \(v_2(y)\) has the form \(v_2(y) = h(y)v_1(y)\) where \(h(y)\) is an unknown function which can be solved from Eqs. (16) and (7), we find

\[h(y) = -C \int dy \frac{m - E + V}{v_1^2}\]  (17)

and

\[v_2 = -Cv_1 \int dy \frac{m - E + V}{v_1^2}\]  (18)

Similar procedure can be used to construct \(u_2\), we finally obtain

\[\psi_2 = \begin{pmatrix} u_2 \\ v_2 \end{pmatrix} = -C \left( \begin{pmatrix} u_1 \\ v_1 \end{pmatrix} \int dy \frac{m - E + V}{v_1^2} \right)\]  (19)

\(\psi_2\) does not satisfy the boundary condition of \(\psi_1\), because of the uniqueness theorem.

Now we are in a position to find the solution \(\psi = \begin{pmatrix} u \\ v \end{pmatrix}\) of the corresponding inhomogeneous perturbation equation (10). Suppose \(\psi\) has the form

\[\psi = \begin{pmatrix} u \\ v \end{pmatrix} = \hat{U}(y)g(y)\]  (20)

where \(g(y)\) is a column matrix. Substituting Eqs. (20) and (14) into Eq. (10) we obtain

\[g' = (\varepsilon - w)\hat{U}^{-1}\hat{f}\hat{U}g \equiv \hat{B}g\]  (21)

where \(\hat{U}^{-1}\) is the inverse matrix of \(\hat{U}\). A simple calculation can show that

\[\hat{B}(\varepsilon - w, y) \equiv (\varepsilon - w)\hat{U}^{-1}\hat{f}\hat{U} = \frac{1}{C}(\varepsilon - w)\begin{pmatrix} u_1u_2 + v_1v_2 & u_2^2 + v_2^2 \\ -(u_1^2 + v_1^2) & -(u_1u_2 + v_1v_2) \end{pmatrix}\]  (22)
and the wave function
\[ \psi = \hat{U} \int dy \hat{B} g = \hat{U} \int dy (\varepsilon - w) \hat{U}^{-1} \hat{f} \psi \]  \hspace{1cm} (23)

or, explicitly,
\[ \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} u_1 & u_2 \\ v_1 & v_2 \end{pmatrix} \int dy \frac{1}{C} (\varepsilon - w) \begin{pmatrix} v_2 & -u_2 \\ -v_1 & u_1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} \]  \hspace{1cm} (24)

Eq. (24) is an integral equation and can be solved by iterative procedure step by step. It can be proven that the choice of the constant \( C \) does not affect on our result remarkably.

For simplicity, we choose \( C = 1 \) in the following calculations. The integration bound of Eq. (24) is determined by the boundary condition and the normalized condition. Based on Eq. (21), we obtain an iterative sequence of \( g \) as
\[ \begin{cases} g^{(0)} (\varepsilon - w, y) = g (\varepsilon - w, a) \\ g^{(1)} (\varepsilon - w, y) = g (\varepsilon - w, a) + \int_a^y dy' \hat{B} (\varepsilon - w, y') g^{(0)} (\varepsilon - w, y') \\ \vdots \\ g^{(n)} (\varepsilon - w, y) = g (\varepsilon - w, a) + \int_a^y dy' \hat{B} (\varepsilon - w, y') g^{(n-1)} (\varepsilon - w, y') \end{cases} \]  \hspace{1cm} (25)

The corresponding formal solution of wave function \( \psi \) is given by Eq. (20).

Now we turn to discuss the energy shift \( \varepsilon \). We get
\[ \varepsilon = \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} u_1 g_1 + u_2 g_2 \\ v_1 g_1 + v_2 g_2 \end{pmatrix} \]  \hspace{1cm} (26)

from Eq. (20), where \( g = \begin{pmatrix} g_1 \\ g_2 \end{pmatrix} \). Noting that the boundary conditions for \( \psi_1 \) and \( \psi_2 \) are
\[ \lim_{y \to \pm \infty} \psi_1 = \lim_{y \to \pm \infty} \begin{pmatrix} u_1 \\ v_1 \end{pmatrix} = 0 \]
and
\[ \lim_{y \to \pm \infty} \psi_2 = \lim_{y \to \pm \infty} \begin{pmatrix} u_2 \\ v_2 \end{pmatrix} = \infty \]
respectively, we have
\[ \lim_{y \to \pm \infty} g_2 = 0 \]  \hspace{1cm} (27)

According to Eqs. (21) and (22) we find
\[ g_2 (\varepsilon - w, y) = g_2 (\varepsilon - w, a) + \frac{1}{C} \int_a^y dy (\varepsilon - w) [- (u_1^2 + v_1^2) g_1 - (u_1 u_2 + v_1 v_2) g_2] \]  \hspace{1cm} (28)

By means of Eq. (27), we get
\[ \int_{-\infty}^{+\infty} dy (\varepsilon - w) \left[ (u_1^2 + v_1^2) g_1 + (u_1 u_2 + v_1 v_2) g_2 \right] = 0 \]  \hspace{1cm} (29)
Eq. (29) is called the “resonant condition”. The energy shift reads

\[
\varepsilon = \frac{\int_{-\infty}^{+\infty} dy \left[ \left( u_1^2 + v_1^2 \right) g_1 + \left( u_1 u_2 + v_1 v_2 \right) g_2 \right]}{\int_{-\infty}^{+\infty} dy \left[ p_1^2 \right] g_1 + \left( u_1 u_2 + v_1 v_2 \right) g_2}
\]  

(30)

Eqs. (24), (25), (30) as well as the normalization condition of \( \psi \) are the basic formulae in EWDA. The zeroth order wave function can be taken as \( \psi^{(0)} = \psi_1 \) when \( w \) is a perturbation potential. Starting from \( \psi^{(0)} \), we can find the wave function and the energy level up to any order which we need in principle by iterative procedure.
3 One-Well Potential

3.1 Square-Well Potential

As an application and example, now we study how to find the bound state wave functions and the energy levels of 1D Dirac equation with one well-potential. As a homogeneous equation, we study the square-well potential first.

The 1D Dirac equation with square-well potential

\[ V(y) = -V_0 \theta \left( y + \frac{a}{2} \right) \theta \left( -y + \frac{a}{2} \right) \]  \hspace{1cm} (31)

where \( \theta (y) \) is the step function

\[ \theta(y) = \begin{cases} 1 & (y > 0) \\ 0 & (y < 0) \end{cases} \]  \hspace{1cm} (32)

(Fig. 1) can be solved exactly [13]. The bound state solution \( \psi_1 \) is

\[ \psi_1 = \begin{pmatrix} u_1 \\ v_1 \end{pmatrix} = \left( \frac{1}{m-E} \right) u_A e^{\kappa y} \theta \left( -y - \frac{a}{2} \right) \]

\[ + \left[ \left( \frac{\cos py}{p} \right) u_B + \left( \frac{\sin py}{p} \right) \sin py \right] \theta \left( y + \frac{a}{2} \right) \theta \left( -y + \frac{a}{2} \right) \]

\[ + \left( \frac{1}{m-E} \right) u_D e^{-\kappa y} \theta \left( y - \frac{a}{2} \right) \]  \hspace{1cm} (33)

in which

\[ \kappa = \sqrt{m^2 - E^2} \]  \hspace{1cm} (34)

\[ p = \sqrt{(E + V_0)^2 - m^2} \]  \hspace{1cm} (35)

The coefficients \( u_A, u_B, u_C \) and \( u_D \) in one case are given by

\[ u_A = u_D = u_B e^{\frac{\kappa a}{2}} \cos \frac{1}{2} pa \]  \hspace{1cm} (36)

\[ u_B = \left[ \frac{m}{m+E} \frac{1}{\kappa} (1 + \cos pa) + \frac{E + V_0}{E + V_0 + m} a + \frac{m}{E + V_0 + m} \frac{1}{p} \sin pa \right]^{-\frac{1}{2}} \]  \hspace{1cm} (37)

\[ u_C = 0 \]  \hspace{1cm} (38)

and the energy spectrum satisfies

\[ \cot \frac{1}{2} pa = -\left[ \frac{(m+E)(E+V_0-m)}{(m-E)(E+V_0+m)} \right]^\frac{1}{2} \]  \hspace{1cm} (39)
The upper component \( u_1 \) and the lower component \( v_1 \) of this solution \( \psi_{1,I} \) are even symmetric and odd symmetric respectively. In another case, the coefficients of the alternative solution \( \psi_{1,II} \) in which the symmetry exchanges are given by

\[
\begin{align*}
  u_A &= -u_D = -u_C e^{\frac{1}{2} \kappa a} \sin \frac{1}{2} pa \\
  u_B &= 0 \\
  u_C &= \left[ \frac{m}{m + E} \frac{1}{\kappa} (1 - \cos pa) + \frac{E + V_0}{E + V_0 + m} a - \frac{m}{E + V_0 + m} \frac{1}{p} \sin pa \right]^{-\frac{1}{2}} \tag{41}
\end{align*}
\]

and the energy spectrum satisfies

\[
\tan \frac{1}{2} pa = \left[ \frac{(m + E)(E + V_0 - m)}{(m - E)(E + V_0 + m)} \right]^\frac{1}{2}. \tag{42}
\]

Another linearly independent solution \( \psi_2 \) can be obtained by using Eq. (19). The result reads

\[
\psi_2 = \begin{pmatrix} u_2 \\ v_2 \end{pmatrix} = \frac{1}{2} \left( \begin{pmatrix} \frac{m + E}{\kappa} \\ -1 \end{pmatrix} \right) \frac{1}{u_A} e^{-\kappa \theta} (-y - \frac{a}{2}) \\
+ \left[ \begin{pmatrix} \frac{m + E + V_0}{p} \sin py \\ \frac{m + E + V_0}{p} \cos py \end{pmatrix} \right] \frac{1}{u_B} + \left[ \begin{pmatrix} -\frac{m + E + V_0}{p} \cos py \\ \frac{m + E + V_0}{p} \sin py \end{pmatrix} \right] \frac{1}{u_C} \theta (-y + \frac{a}{2}) \theta \left( y + \frac{a}{2} \right) \\
+ \frac{1}{2} \left( \begin{pmatrix} \frac{m + E}{\kappa} \\ 1 \end{pmatrix} \right) \frac{1}{u_D} e^{\kappa \theta} \left( y - \frac{a}{2} \right) \tag{43}
\]

where \( u_A, u_B, u_C \) and \( u_D \) are given by Eqs. (38-40) for \( \psi_{1,I} \) and Eqs. (42-44) for \( \psi_{1,II} \) respectively.

### 3.2 Perturbation of the Square Well Potential

Now we go to discuss the inhomogeneous equation (10). The one-well potential is given by

\[
V = -V_0 \left[ 1 - \left( \frac{2y}{a} \right)^2 \right] \theta \left( y + \frac{a}{2} \right) \theta \left( -y + \frac{a}{2} \right) \tag{45}
\]

(Fig. 2) and the perturbation potential reads

\[
w(y) = \frac{4V_0}{a^2} y^2 \theta \left( y + \frac{a}{2} \right) \theta \left( -y + \frac{a}{2} \right) \tag{46}
\]

We calculate the first order energy shift \( \varepsilon^{(1)} \). Using \( \psi_1 \) as the zeroth order non-perturbation wave function \( \psi^{(0)} \), then \( g^{(0)} = \binom{1}{0} \) from Eq. (20). Substituting Eq. (38)
and \(g^{(0)}\) into Eq. (40), we obtain

\[
\varepsilon^{(1)}_I = \frac{4V_0}{a^2} \left[ \frac{E + V_0}{E + V_0 + m} \frac{1}{12} a^3 + m \left( \frac{a^2}{4p} \sin pa + \frac{a}{2p^2} \cos pa - \frac{1}{2p^3} \sin pa \right) \right]
\]

\[
\frac{m}{E + m \kappa} (1 + \cos pa) + \left( \frac{E + V_0}{E + V_0 + m} a + \frac{m}{E + V_0 + m p} \varepsilon \sin pa \right)
\]

(47)

for \(\psi^{(0)} = \psi_1, I, and \)

\[
\varepsilon^{(1)}_{II} = \frac{4V_0}{a^2} \left[ \frac{E + V_0}{E + V_0 + m} \frac{1}{12} a^3 - m \left( \frac{a^2}{4p} \sin pa + \frac{a}{2p^2} \cos pa - \frac{1}{2p^3} \sin pa \right) \right]
\]

\[
\frac{m}{E + m \kappa} (1 - \cos pa) + \left( \frac{E + V_0}{E + V_0 + m} a - \frac{m}{E + V_0 + m p} \varepsilon \sin pa \right)
\]

(48)

for \(\psi^{(0)} = \psi_1, II\).

The wave function for one-well potential has been calculated up to the first order iterative approximation. The results are

\[
\psi^{(1)}_I = \left( \begin{array}{c} u \\ v \end{array} \right)_{I}^{(1)} = \left( \begin{array}{c} \frac{1}{\kappa} (-Ey + m 2\kappa) \\ -\frac{1}{m + E} (Ey + m 2\kappa) \end{array} \right) \varepsilon^{(1)} u_A e^{\kappa y} \theta \left( -y - \frac{a}{2} \right) +
\]

\[
\left( \frac{1}{p} \left[ \varepsilon^{(1)} \left( A \cos py + C \sin py \right) - \frac{4V_0}{a^2} \left( B \cos py + D \sin py \right) \right] \right) u_B.
\]

\[
\theta \left( y + \frac{a}{2} \right) \theta \left( -y + \frac{a}{2} \right) + \left( \frac{1}{m + E} \left( Ey + m 2\kappa \right) \right) \varepsilon^{(1)} u_D e^{-\kappa y} \theta \left( y - \frac{a}{2} \right) + C^{(1)} \psi_1
\]

(49)

for \(\psi^{(0)} = \psi_1, I, and \)

\[
\psi^{(1)}_{II} = \left( \begin{array}{c} u \\ v \end{array} \right)_{II}^{(1)} = \left( \begin{array}{c} \frac{1}{\kappa} (-Ey + m 2\kappa) \\ -\frac{1}{m + E} (Ey + m 2\kappa) \end{array} \right) \varepsilon^{(1)} u_A e^{\kappa y} \theta \left( -y - \frac{a}{2} \right) +
\]

\[
\left( \frac{1}{p} \left[ \varepsilon^{(1)} \left( A \cos py - C \sin py \right) - \frac{4V_0}{a^2} \left( B \cos py - D \sin py \right) \right] \right) u_C.
\]

\[
\theta \left( y + \frac{a}{2} \right) \theta \left( -y + \frac{a}{2} \right) + \left( \frac{1}{m + E} \left( Ey + m 2\kappa \right) \right) \varepsilon^{(1)} u_D e^{-\kappa y} \theta \left( y - \frac{a}{2} \right) + C^{(1)} \psi_1
\]

(50)
for $\psi(0) = \psi_1$, II where

$$A \equiv -\lambda \frac{m}{2p} \cos 2p$$

$$B \equiv -\lambda \left(\frac{m}{2p} y^2 \cos 2p y - \frac{m}{2p^2} y \sin 2p y - \frac{m}{4p^3} \cos 2p y\right)$$

$$C \equiv - \left[ (E + V_0) y + \lambda \frac{m}{2p} \sin 2p y \right]$$

$$D \equiv - \left[ \frac{1}{3} (E + V_0) y^3 + \lambda \left(\frac{m}{2p} y^2 \sin 2p y + \frac{m}{2p^2} y \cos 2p y - \frac{m}{4p^3} \sin 2p y\right) \right]$$

and

$$\lambda = \begin{cases} +1 & \text{(for } \psi(0) = \psi_1, \text{ I)} \\ -1 & \text{(for } \psi(0) = \psi_1, \text{ II)} \end{cases}$$

$C^{(1)}$ is determined by normalization condition.
4 Double-Well Potential

The 1D Schrödinger equation with double-well potential has been investigated by FLZ method [3], WDA and variational method [7] previously. We now apply the EWDA to the double-well potential of the 1D Dirac equation and give the energy eigenvalues to the first order approximation.

4.1 Double-Well and Double-Square-Well Potentials

Given a symmetrical double-well potential

\[ V = \nu \left[ \left( \frac{y}{\eta} \right)^2 - 1 \right] \left[ \left( \frac{y}{\xi} \right)^2 - 1 \right] \] (56)

(Fig. 3) with the minimum of \( V \) being \(-\mu\), define

\[ \tau \equiv \sqrt{\frac{\mu}{\nu}} + 1 + \sqrt{\frac{\mu}{\nu}} \] (57)

then we have

\[ \xi = \tau \eta \] (58)

With \( \tau \) and \( \eta \), instead of \( \eta \) and \( \xi \), \( V \) can be expressed as

\[ V = \nu \left[ \frac{1}{\tau^2} \left( \frac{y}{\eta} \right)^4 - \left( 1 + \frac{1}{\tau^2} \right) \left( \frac{y}{\eta} \right)^2 + 1 \right] \] (59)

An exactly solvable double-square-well potential, whose bound states can serve as the zeroth order wave function for iteration procedure, is chosen in the homogeneous equation as,

\[ V \equiv V_0 \theta (-y - a) - \mu \theta (y + a) \theta (-y + b) + \nu \theta (y + b) \theta (-y + b) - \mu \theta (y - b) \theta (-y + a) + V_0 \theta (y - a) \] (60)

in which

\[ V_0 = V (-a) = V (a) \] (61)

where \( a \) and \( b (0 < b < a) \) are parameters which can be adjusted to minimize the energy shift \( \varepsilon^{(1)} \).

The wave function of a bound state solution to the Dirac equation with the double-
square-well potential is

\[ \psi_1 = \begin{pmatrix} u_1 \\ v_1 \end{pmatrix} = + \left( \frac{1}{m - E + V_0} \right) u_A e^{\kappa y} \theta (-y - a) + \left( \frac{u_B \cos \lambda y + \tilde{u}_B \sin \lambda y}{m - E - \mu} \right) \frac{1}{\lambda} (u_B \sin \lambda y - \tilde{u}_B \cos \lambda y) \theta (y + b) \theta (-y - b) + \left[ \left( \frac{\cosh qy}{q} \right) u_C + \left( \frac{\sinh qy}{q} \cosh qy \right) \tilde{u}_C \right] \theta (y + b) \theta (-y + b) + \left( \frac{1}{m - E + V_0} \right) u_E e^{-\kappa y} \theta (y - a) \right] \]

where

\[ \kappa = \sqrt{m^2 - (E - V_0)^2} \quad (-m - V_0 < E < m + V_0) \]  \hspace{1cm} (62)

\[ \lambda = \sqrt{-m^2 + (E + \mu)^2} \quad (E < -m - \mu \text{ or } m - \mu < E) \]  \hspace{1cm} (63)

\[ q = \sqrt{m^2 - (E - \nu)^2} \quad (-m - \nu < E < m + \nu) \]  \hspace{1cm} (64)

If Eq. (65) dose not satisfy when \((E - \nu)^2 > m^2\), we define

\[ p = \sqrt{-m^2 + (E - \nu)^2} \quad (E < -m - \mu \text{ or } m + \mu < E) \]  \hspace{1cm} (66)

By replacing \(q\) by \(ip\) and \(\tilde{u}_C\) by \(-i\tilde{u}_C\) the wave function (62) and all the following expressions maintain their forms.

Similar to the square-well case, the coefficients \(u_A, u_B, \tilde{u}_B, u_C, \tilde{u}_C, u_D, \tilde{u}_D\) and \(u_E\) of the solution \(\psi_1, I\) with even symmetric upper component \(u_1\) and odd symmetric lower component \(v_1\) are given by

\[ u_B = u_D = \alpha u_C \]  \hspace{1cm} (67)

\[ \tilde{u}_B = -\tilde{u}_D = -\tilde{\alpha} u_C \]  \hspace{1cm} (68)

\[ u_A = u_E = \gamma u_C \]  \hspace{1cm} (69)
\[ u_C = \left[ \frac{4m}{m + E - V_0} \gamma^2 C + \frac{4m}{m + E + \mu} \left( \alpha^2 - \bar{\alpha}^2 \right) F + \frac{4(E + \mu)}{m + E + \mu} \left( \alpha^2 + \bar{\alpha}^2 \right) \frac{1}{2} (a - b) \right. \\
- \frac{4m}{m + E + \mu} \alpha \bar{\alpha} L + \frac{2m}{m + E - \nu} \frac{1}{2} \sinh 2qb + \frac{2(E - \nu)}{m + E - \nu} b^{\frac{1}{2}} \right]^{-\frac{1}{2}} \]

and the energy spectrum satisfies
\[ \tanh qb = \frac{\kappa}{m - E + V_0} \frac{m - E - \mu}{\lambda} \tan \lambda (b - a) - 1 \\
\left( \frac{\lambda}{m - E - \mu} \tan \lambda (b - a) + \frac{\kappa}{m - E + V_0} \right) \frac{m - E + \mu}{q}. \]

Correspondingly, the coefficients of the alternative solution \( \psi_1, II \) with the exchanged symmetry of components are given by
\[ u_B = -u_D = -\beta \bar{u}_C \]
\[ \bar{u}_B = \bar{u}_D = \bar{\beta} \bar{u}_C \]
\[ u_A = -u_E = -\delta \bar{u}_C \]

\[ \bar{u}_C = \left[ \frac{4m}{m + E - V_0} \delta^2 C + \frac{4m}{m + E + \mu} \left( \beta^2 - \bar{\beta}^2 \right) F + \frac{4(E + \mu)}{m + E + \mu} \left( \beta^2 + \bar{\beta}^2 \right) \frac{1}{2} (a - b) \right. \\
- \frac{4m}{m + E + \mu} \beta \bar{\beta} L + \frac{2m}{m + E - \nu} \frac{1}{2} \sinh 2qb - \frac{2(E - \nu)}{m + E - \nu} b^{\frac{1}{2}} \right]^{-\frac{1}{2}} \]

and the energy spectrum satisfies
\[ \coth qb = \frac{\kappa}{m - E + V_0} \frac{m - E - \mu}{\lambda} \tan \lambda (b - a) - 1 \\
\left( \frac{\lambda}{m - E - \mu} \tan \lambda (b - a) + \frac{\kappa}{m - E + V_0} \right) \frac{m - E + \mu}{q}. \]

In the above expressions we have defined
\[ \alpha = \cosh qb \cos \lambda b + \frac{\lambda}{m - E - \mu} \frac{m - E + \nu}{q} \sinh qb \sin \lambda b \]
\[ \bar{\alpha} = \cosh qb \sin \lambda b - \frac{\lambda}{m - E - \mu} \frac{m - E + \nu}{q} \sinh qb \cos \lambda b \]
\[ \beta = \sinh qb \cos \lambda b + \frac{\lambda}{m - E - \mu} \frac{m - E + \nu}{q} \cosh qb \sin \lambda b \]
\[ \tilde{\beta} = \sinh qb \sin \lambda b - \frac{\lambda}{m - E - \mu} \frac{m - E + \nu}{q} \cosh qb \cos \lambda b \] (80)

\[ \gamma = e^{\kappa a} \left[ \cosh qb \cos \lambda (b - a) + \frac{\lambda}{m - E - \mu} \frac{m - E + \nu}{q} \sinh qb \cos \lambda (b - a) \right] \] (81)

\[ \delta = e^{\kappa a} \left[ \sinh qb \cos \lambda (b - a) + \frac{\lambda}{m - E - \mu} \frac{m - E + \nu}{q} \cosh qb \sin \lambda (b - a) \right] \] (82)

and \( C, F \) and \( L \) given later in Eqs. (90), (93) and (96).

Another linearly independent solution, though it is not necessary for deriving the first order energy shift. But it is involved in higher order calculations. The result, which can be constructed by Eq. (19), reads

\[ \psi_2 = \begin{pmatrix} u_2 \\ v_2 \end{pmatrix} = \frac{1}{2} \left( \begin{pmatrix} -m - E + V_0 \\ \kappa \end{pmatrix} \frac{1}{u_A} e^{-\kappa y} \theta (-y - a) \right. \\
+ \left( \begin{pmatrix} m + E + \mu \\ \lambda \end{pmatrix} \frac{1}{u_B} \theta (y + a) \theta (-y - b) + \sum_{C} \frac{1}{u_C} \theta (y - b) \theta (-y + a) + \frac{1}{u_E} e^{\kappa y} \theta (y - a) \right) \] (83)

where \( u_A, u_B, \tilde{u}_B, u_C, \tilde{u}_C, u_D, \tilde{u}_D \) and \( u_E \) are given by Eqs. (69-72) for \( \psi_2, I \) and Eqs. (74-77) for \( \psi_2, II \) respectively.

### 4.2 First Order Energy Shift for the Double-Well Potential

The perturbation potential on the double-square-well potential reads

\[ w(y) = V(y) - V(y) \] (84)

Using \( \psi_1 \) as the zeroth order \( \psi^{(0)} \) in iterative procedure, and \( g^{(0)} = \binom{1}{0} \) from Eq. (20), the first order energy shift \( \varepsilon^{(1)} \) is obtained by substituting Eq. (82) and \( g^{(0)} \) into the iterative procedure.
into Eq. (30), we get

\[ \varepsilon^{(1)} = \]

\[ + \frac{4m}{m + E - V_0} u_A^2 \left[ \frac{\nu}{\tau^2 \eta^2} A - \left( 1 + \frac{1}{\tau^2} \right) \frac{\nu}{\eta^2} B + (\nu - V_0) C \right] \]

\[ + \frac{4m}{m + E + \mu} (u_B^2 - \bar{u}_B^2) \left[ \frac{\nu}{\tau^2 \eta^2} D - \left( 1 + \frac{1}{\tau^2} \right) \frac{\nu}{\eta^2} G + (\nu + \mu) F \right] \]

\[ + \frac{4(E + \mu)}{m + E + \mu} (u_B^2 + \bar{u}_B^2) \left[ \frac{\nu}{\tau^2 \eta^2} \frac{1}{4} (a^5 - b^5) - \left( 1 + \frac{1}{\tau^2} \right) \frac{\nu}{\eta^2} \frac{1}{6} (a^3 - b^3) + (\nu + \mu) \frac{1}{2} (a - b) \right] \]

\[ + \frac{4m}{m + E + \mu} u_B \bar{u}_B \left[ \frac{\nu}{\tau^2 \eta^2} J - \left( 1 + \frac{1}{\tau^2} \right) \frac{\nu}{\eta^2} K + (\nu + \mu) L \right] \]

\[ + \frac{2m}{m + E - \nu} (u_C^2 + \bar{u}_C^2) \left[ \frac{\nu}{\tau^2 \eta^2} M - \left( 1 + \frac{1}{\tau^2} \right) \frac{\nu}{\eta^2} N \right] \]

\[ + \frac{2(E - \nu)}{m + E - \nu} (u_C^2 - \bar{u}_C^2) \left[ \frac{\nu}{\tau^2 \eta^2} \frac{1}{5} b^5 - \left( 1 + \frac{1}{\tau^2} \right) \frac{\nu}{\eta^2} \frac{1}{3} b^3 \right] , \]

where

\[ A = \left( \frac{a^4}{2\kappa} + \frac{a^3}{\kappa^2} + \frac{3a^2}{2\kappa^3} + \frac{3a}{2\kappa^4} + \frac{3}{4\kappa^5} \right) e^{-2\kappa a} \]

\[ B = \frac{1}{2} \left( \frac{a^2}{\kappa} + \frac{a}{\kappa^2} + \frac{1}{2\kappa^3} \right) e^{-2\kappa a} \]

\[ C = \frac{1}{2\kappa} e^{-2\kappa a} \]

\[ D = + \frac{1}{4} \left( \frac{a^4}{\lambda} - \frac{3a^2}{\lambda^3} + \frac{3}{2\lambda^5} \right) \sin 2\lambda a + \frac{1}{4} \left( \frac{2a^3}{\lambda^2} - \frac{3a}{2\lambda^4} \right) \cos 2\lambda a \]

\[ - \frac{1}{4} \left( \frac{b^4}{\lambda} - \frac{3b^2}{\lambda^3} - \frac{3}{2\lambda^5} \right) \sin 2\lambda b - \frac{1}{4} \left( \frac{2b^3}{\lambda^2} - \frac{3b}{2\lambda^4} \right) \cos 2\lambda b \]

\[ G = + \frac{1}{4} \left( \frac{a^2}{\lambda} - \frac{1}{2\lambda^3} \right) \sin 2\lambda a + \frac{a}{4\lambda^2} \cos 2\lambda a \]

\[ - \frac{1}{4} \left( \frac{b^2}{\lambda} - \frac{1}{2\lambda^3} \right) \sin 2\lambda b - \frac{b}{\lambda^2} \cos 2\lambda b \]

\[ F = \frac{1}{4\lambda} \left( \sin 2\lambda a - \sin 2\lambda b \right) \]

\[ J = + \frac{1}{2} \left( \frac{a^4}{\lambda} - \frac{3a^2}{\lambda^3} + \frac{3}{2\lambda^5} \right) \cos 2\lambda a - \frac{1}{2} \left( \frac{2a^3}{\lambda^2} - \frac{3a}{2\lambda^4} \right) \sin 2\lambda a \]

\[ - \frac{1}{2} \left( \frac{b^4}{\lambda} - \frac{3b^2}{\lambda^3} + \frac{3}{2\lambda^5} \right) \cos 2\lambda b + \frac{1}{2} \left( \frac{2b^3}{\lambda^2} - \frac{3b}{2\lambda^4} \right) \sin 2\lambda b \]
\begin{align*}
K &= + \frac{1}{2} \left( \frac{a^2}{\lambda} - \frac{1}{2\lambda^3} \right) \cos 2\lambda a - \frac{a}{2\lambda^2} \sin 2\lambda a \\
&\quad - \frac{1}{2} \left( \frac{b^2}{\lambda} - \frac{1}{2\lambda^3} \right) \cos 2\lambda b + \frac{b}{2\lambda^2} \sin 2\lambda b \\
(93) \\
L &= \frac{1}{2\lambda} (\cos 2\lambda a - \cos 2\lambda b) \\
(94) \\
M &= \frac{1}{2} \left( \frac{b^4}{q} + \frac{3b^3}{q^3} + \frac{3}{2q^5} \right) \sinh 2qb - \frac{1}{2} \left( \frac{2b^3}{q^2} + \frac{3b}{2q^4} \right) \cosh 2qb \\
(95) \\
N &= \frac{1}{2} \left( \frac{b^2}{q} + \frac{1}{2q^3} \right) \sinh 2qb - \frac{b}{2q^2} \cosh 2qb \\
(96)
\end{align*}
5 Discussion and Conclusion

In summary, a new method, namely, the Extended Wronskian Determinant Approach has been suggested to calculate the energy spectra and the wave functions of 1D Dirac equation. An integral equation which can be solved by iterative procedure has been established to study the inhomogeneous Dirac equation with perturbation potential. Using the solution of the corresponding homogeneous Dirac equation as the zeroth wave function, we can calculate the wave function and energy spectrum of the perturbative Dirac equation up to any order in principle. Two kinds of exact solutions including solution of one square-well potential and double-square-well potential have been employed as the zeroth approximations to study the one-well potential and double-well potential respectively. For one-well case, the first order iterative approximation to the energy levels and the wave functions has been obtained. For double-well case, we have got the energy level approximation up to the first order. These two examples confirm that the EWDA is a successful method to investigate the 1D Dirac equation.

In fact, it is not necessary to adopt the exact solutions of homogeneous 1D Dirac equation as the zeroth order wave functions. Instead of exact solution, we can use a trial wave function. And we can use the variational method for the non-perturbative Hamiltonian to determine the best choice of the parameters in the trial wave function first, and then use the trial wave function with the best parameters as the zeroth order wave function to study the perturbative Dirac equation by EWDA.
Acknowledgments

We thank J. Qiu and Prof. W. Q. Zhao for helpful discussions. This work was supported in part by National Natural Science Foundation of China under Grant NOS. 10047005, 10235030, 19947001.
References

[1] R. Friedberg, T. D. Lee and W. Q. Zhao, IL Naovo Cimento A112(1999)1195
[2] R. Friedberg, T. D. Lee and W. Q. Zhao, Ann. of Phys. 288(2001)52
[3] R. Friedberg, T. D. Lee, W. Q. Zhao and A. Cimenser, Ann. of Phys. 294(2001)67
[4] W. Q. Zhao, Commun. Theor. Phys. 38(2002)15
[5] W. Q. Zhao and C. S. Ju, Commun. Theor. Phys. 38(2002)271
[6] A. Messiah, Quantum Mechanics, ChIII, Dunod, Paris(1973)
[7] J. Qiu and R. K. Su, Commun. Theor. Phys. 39(2003)21
[8] J. Zinn-Justin, Nucl. Phys. B192(1981)125
[9] E. Shuryak, Nucl. Phys. B302(1985)601
[10] S. V. Faleev and P. G. Silverstov, Phys. Lett. A197(1995)372
[11] T. D. Lee, Particle Physics and Introduction to Field, Harwood Academic Pub.(1981)
[12] W. A. Bardeen, M. S. Chanowitz, S. D. Drell, M. Weinstein and T. M. Yan, Phys. Rev. D11(1975)1094
[13] W. Greiner, B. Müller and J. Rafelski, Quantum Electrodynamics of Strong Fields, Ch. 2, Springer-Verlag(1985)
Figure Captions

Figure 1: one-well potential
Figure 2: perturbed one-well potential
Figure 3: square-double-well and double-well potentials