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Bound states of the one-dimensional Dirac equation for scalar and vector double square-well potentials

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ABSTRACT

We have analytically studied bound states of the one-dimensional Dirac equation for scalar and vector double square-well potentials (DSPs), by using the transfer-matrix method. Detailed numerical calculations of the eigenvalue, wave function and density probability have been performed for the three cases: (1) vector DSP only, (2) scalar DSP only, and (3) scalar and vector DSPs with equal magnitudes. We discuss the difference and similarity among results of the cases (1)–(3) in the Dirac equation and that in the Schrödinger equation. Motion of a wave packet is calculated for a study on quantum tunneling through the central barrier in the DSP.

1. Introduction

The basic physics of relativistic quantum mechanics was formulated in the Dirac equation, which elucidates the origin of spin 1/2 of an electron and predicts the existence of an antiparticle (a positron) [1]. The Dirac equation has been applied not only to realistic models like hydrogen atom but also to pedagogical models which play important roles in understanding the properties of the Dirac equation. The Dirac equation for step and square potentials has been investigated in connection to the Klein paradox [2–6]. Square-well potentials with finite and infinite depths have been studied in Refs. [7–12]. The double square-well potential (DSP) consisting of the confining potential and the central potential is more difficult than the single square-well potential [7–12]. Indeed trustworthy applications of the Dirac equation to the DSP have not been reported as far as we are aware of Ref. [13]. The DSP is a simplified model for an appropriate and realistic description of a continuous double-well potential. Extensive investigations within the nonrelativistic treatment of the Schrödinger equation have been made for double-well systems where numerous quantum phenomena have been realized (for a recent review on double-well systems, see Ref. [14]). The Schrödinger equation for the DSP with the infinite confining potential is manageable and treated in the undergraduate text, whereas the DSP with the *finite* confining potential has been investigated only in several studies [15–17]. One of the advantages of the DSP is to provide us with exact analytic expressions for eigenstates and wave functions. In the relativistic quantum theory, a combination of two types of scalar ($S(x)$) and vector ($V(x)$) potentials has been adopted. In previous studies on the single square-well potential, the vector potential was adopted in Refs. [7–9,11,12] while the scalar potential was employed in Refs. [9,10]. The purpose of this paper is to make a detailed study on the Dirac equation for scalar and vector DSPs and to make a comparison between results of the Dirac equation and the Schrödinger equation. Such a study is fundamental and inevitable for a deeper understanding of relativistic quantum double-well systems.

The paper is organized as follows. In Section 2, we obtain analytic, exact expressions for eigenvalues and wave functions of bound states in the Dirac equation for scalar and vector DSPs, by using the transfer-matrix method. In Section 3, the transcendental complex equation for the eigenvalue is numerically solved and bound-state wave functions are obtained for three cases: (1) the vector DSP only (VDSP: $S(x)=0$), (2) the scalar DSP only (SDSP: $V(x)=0$), and (3) equal scalar and vector DSPs (EDSP: $S(x)=V(x)$). In Section 4, a comparison is made among eigenvalues of the three cases (1)–(3) in the Dirac equation and that in the Schrödinger equation. Motion of a wave packet is investigated for a study on the quantum tunneling through the central barrier in the DSP. Section 5 is devoted to our conclusion. In the Appendix the transfer-matrix method is applied to the Schrödinger equation for the DSP.

2. Dirac equation for the double square-well potential

2.1. Transfer-matrix formulation

The one-dimensional Dirac equation is given by

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t)=H\Psi(x,t), \tag{1}$$

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with

$$H = c\hat{\alpha} \cdot \overline{p} + \hat{\beta} mc^2 + U(x), \tag{2}$$

where $\Psi(x,t)$ expresses the wave-vector spinor, $\hat{\alpha}$ and $\hat{\beta}$ are the Dirac matrices, $\overline{p}$ $(= -i\hbar\partial/\partial x)$ denotes the momentum operator, m is the rest mass of a particle, c is the light velocity, and the potential $U(x)$ is assumed to be given by

$$U(x) = \hat{\beta} S(x) + V(x), \tag{3}$$

$S(x)$ and $V(x)$ expressing scalar and vector potentials, respectively. Assuming the stationary solution $\Psi(x,t) = \Psi(x)\exp(-iEt/\hbar)$, we obtain the steady-state Dirac equation $H\Psi(x) = E\Psi$ with the energy E. Among conceivable, equivalent expressions for the Dirac equation, we adopt the Dirac matrices given by

$$\hat{\alpha} = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{\beta} = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{4}$$

leading to

$$\left[c\sigma_x \left(-i\hbar \frac{\partial}{\partial x} \right) + \sigma_z [mc^2 + S(x)] \right] \Psi(x) = [E - V(x)]\Psi(x), \tag{5}$$

with

$$\Psi(x) = \begin{pmatrix} \psi_+(x) \\ \psi_-(x) \end{pmatrix}. \tag{6}$$

Two components of two-dimensional spinor of $\Psi(x)$, $\psi_+(x)$ and $\psi_-(x)$, satisfy

$$[mc^2 + V(x) + S(x)]\psi_+(x) - i\hbar c \frac{d}{dx}\psi_-(x) = E\psi_+(x), \tag{7}$$

$$-i\hbar c \frac{d}{dx}\psi_+(x) + [-mc^2 + V(x) - S(x)]\psi_-(x) = E\psi_-(x). \tag{8}$$

We consider the one-dimensional vector potential $V(x)$ expressed by

$$V(x) = \begin{cases} V_b & \text{for } x \le -b \quad \text{(region I)}, \\ 0 & \text{for } -b < x \le -a \quad \text{(region II)}, \\ V_a & \text{for } -a < x \le a \quad \text{(region III)}, \\ 0 & \text{for } a < x \le b \quad \text{(region IV)}, \\ V_b & \text{for } x > b \quad \text{(region V)}, \end{cases} \tag{9}$$

with $V_b \ge 0$ and $0 \le V_a \le V_b$. Here the x-axis is divided into five spatial regions: (I) $x \le -b$, (II) $-b \le x \le -a$, (III) $-a < x \le a$, (IV) $a < x \le b$, and (V) $x > b$; V_b expresses the confining potential in the regions I and V; V_a denotes central barrier potential in the region III (Fig. 1).

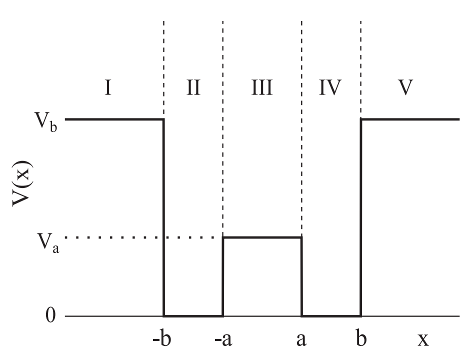

Fig. 1. Schematic vector DSP, $V(x)$, given by Eq. (9) (bold solid lines), the x-axis being divided into five regions I–V separated by dashed lines. The scalar DSP, $S(x)$, is given if we read $V_a \to S_a$ and $V_b \to S_b$.

As for the scalar potential $S(x)$, we consider

$$S(x) = \begin{cases} S_b & \text{for } x \le -b \quad \text{(region I)}, \\ 0 & \text{for } -b < x \le -a \quad \text{(region II)}, \\ S_a & \text{for } -a < x \le a \quad \text{(region III)}, \\ 0 & \text{for } a < x \le b \quad \text{(region IV)}, \\ S_b & \text{for } x > b \quad \text{(region V)}, \end{cases} \tag{10}$$

with $S_b \ge 0$ and $0 \le S_a \le S_b$ (read $V_a \to S_a$ and $V_b \to S_b$ in Fig. 1). The adopted scalar and vector DSPs are symmetric with respect to the origin. In the limit of $V_a = S_a = 0$, $a = 0$, or $a = b$, the double square-well potential reduces to the single one.

Wave functions in five regions I–V may be expressed by

$$\Psi_I(x) = A_1 \begin{pmatrix} 1 \\ \beta \end{pmatrix} e^{iqx} + B_1 \begin{pmatrix} 1 \\ -\beta \end{pmatrix} e^{-iqx} \quad \text{for } x < -b, \tag{11}$$

$$\Psi_{II}(x) = A_2 \begin{pmatrix} 1 \\ \alpha \end{pmatrix} e^{ikx} + B_2 \begin{pmatrix} 1 \\ -\alpha \end{pmatrix} e^{-ikx} \quad \text{for } -b < x < -a, \tag{12}$$

$$\Psi_{III}(x) = A_3 \begin{pmatrix} 1 \\ \gamma \end{pmatrix} e^{ipx} + B_3 \begin{pmatrix} 1 \\ -\gamma \end{pmatrix} e^{-ipx} \quad \text{for } -a < x < a, \tag{13}$$

$$\Psi_{IV}(x) = A_4 \begin{pmatrix} 1 \\ \alpha \end{pmatrix} e^{ikx} + B_4 \begin{pmatrix} 1 \\ -\alpha \end{pmatrix} e^{-ikx} \quad \text{for } a < x < b, \tag{14}$$

$$\Psi_V(x) = A_5 \begin{pmatrix} 1 \\ \beta \end{pmatrix} e^{iqx} + B_5 \begin{pmatrix} 1 \\ -\beta \end{pmatrix} e^{-iqx} \quad \text{for } x < -a, \tag{15}$$

with

$$k = \frac{\sqrt{E^2 - m^2c^4}}{\hbar c}, \tag{16}$$

$$p = \frac{\sqrt{(E + mc^2 - V_a + S_a)(E - mc^2 - V_a - S_a)}}{\hbar c}, \tag{17}$$

$$q = \frac{\sqrt{(E + mc^2 - V_b + S_b)(E - mc^2 - V_b - S_b)}}{\hbar c}, \tag{18}$$

$$\alpha = \frac{\hbar ck}{E + mc^2}, \tag{19}$$

$$\beta = \frac{\hbar cq}{E + mc^2 - V_b + S_b}, \tag{20}$$

$$\gamma = \frac{\hbar cp}{E + mc^2 - V_a + S_a}, \tag{21}$$

where $\sqrt{z}$ signifies the square root of a complex z: for a real z, $\sqrt{z} = z^{1/2}\Theta(z) + i(-z)^{1/2}\Theta(-z)$ with the Heaviside function $\Theta(z)$.

Matching conditions of wave functions at boundaries at $x = \pm b$ and $x = \pm a$ yield

$$\begin{pmatrix} e^{-iqb} & e^{iqb} \\ \beta e^{-iqb} & -\beta e^{iqb} \end{pmatrix} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \begin{pmatrix} e^{-ikb} & e^{ikb} \\ \alpha e^{-ikb} & -\alpha e^{ikb} \end{pmatrix} \begin{pmatrix} A_2 \\ B_2 \end{pmatrix}, \tag{22}$$

$$\begin{pmatrix} e^{-ika} & e^{ika} \\ \alpha e^{-ika} & -\alpha e^{ika} \end{pmatrix} \begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = \begin{pmatrix} e^{-ipa} & e^{ipa} \\ \gamma e^{-ipa} & -\gamma e^{ipa} \end{pmatrix} \begin{pmatrix} A_3 \\ B_3 \end{pmatrix}, \tag{23}$$

$$\begin{pmatrix} e^{ipa} & e^{-ipa} \\ \gamma e^{ipa} & -\gamma e^{-ipa} \end{pmatrix} \begin{pmatrix} A_3 \\ B_3 \end{pmatrix} = \begin{pmatrix} e^{ika} & e^{-ika} \\ \alpha e^{ika} & -\alpha e^{-ika} \end{pmatrix} \begin{pmatrix} A_4 \\ B_4 \end{pmatrix}, \tag{24}$$

$$\begin{pmatrix} e^{ikb} & e^{-ikb} \\ \alpha e^{ikb} & -\alpha e^{-ikb} \end{pmatrix} \begin{pmatrix} A_4 \\ B_4 \end{pmatrix} = \begin{pmatrix} e^{iqb} & e^{-iqb} \\ \beta e^{ipb} & -\beta e^{-ipb} \end{pmatrix} \begin{pmatrix} A_5 \\ B_5 \end{pmatrix}. \tag{25}$$