Pair states in one-dimensional Dirac systems

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Analytic solutions of the quantum relativistic two-body problem are obtained for an interaction potential modeled as a one-dimensional smooth square well. Both stationary and moving pairs are considered and the limit of the δ-function interaction is studied in depth. Our result can be utilized for understanding excitonic states in narrow-gap carbon nanotubes. We also show the existence of bound states within the gap for a pair of particles of the same charge.

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I. INTRODUCTION

The analytical solutions supported by the square-well and δ potentials for the Schrödinger equation make them among the most widely used potentials in nonrelativistic quantum theory and they have given fundamental insights in the field of theoretical physics. In the relativistic case, potentials containing discontinuities or kinks are often harder to treat, since the relationship between the two components of the wave function leads to the derivative of the potential entering the wave equation. Nevertheless, the square well has been used with great success to describe the single-particle phenomenon in quasirelativistic one- and two-dimensional systems [1–3]. Here we provide a way to obtain the square-well solutions for the quasi-one-dimensional two-body relativistic problem, from the smooth analytically solvable barrier side, which foregoes the need to consider special boundary conditions. With the recent surge of Dirac materials [4] has come a renewed interest in many quasirelativistic phenomena and tabletop experiments now offer the possibility to check many relativistic theories. Currently the experimental focus is on attractive potentials to reveal the role of excitonic effects, but we show that within the same formalism, quasi-one-dimensional systems can also support bound states within the band gap for two repelling particles. In light of the ongoing extensive search of new quasiparticles in one- and two-dimensional systems, such as Majorana fermions, our result for binding same-charge particles is of significant potential importance. Indeed, of special interest is the case where both the electron-electron and the electron-hole pair binding energy correspond to the middle of the band gap, as it enforces electron-hole symmetry without the recourse to a superconductor. This state is also energetically favorable as it reduces the Fermi energy of a doped system.

Relevant examples of quasi-one-dimensional relativistic systems, for which our results are applicable, are narrow-gap carbon nanotubes and graphene nanoribbons. For these carbon-based nanostructures, the interaction potential between a pair of particles may be considered as a quasi-one-dimensional problem, averaged over the nanotube diameter or nanoribbon width. For these systems, the interaction potential is flat bottomed as it varies very little over the averaging scale. In many carbon nanotubes devices, a metallic substrate is used as the gate electrode to manipulate the Fermi level [5]. The presence of the substrate results in image charges, which make the interaction decay faster than the widely employed Coulomb potential [6], therefore the flat-bottom potential is a reasonable interaction model for a carbon nanotube or graphene nanoribbon above a metallic gate.

Charge carriers in graphene, a single monolayer of carbon in a honeycomb lattice [2], are described by the same equation used to describe two-dimensional massless Dirac fermions, the Dirac-Weyl equation. By using a simple tight-binding model, Wallace [7] demonstrated that a pristine graphene sheet has no band gap and that the conduction and valence bands are linear near the crossing points. A single-walled nanotube can be thought of as a graphene sheet rolled into a seamless cylinder. In the absence of curvature effects, within the frame of a simple tight-binding model, this rolling can result in either a semiconducting or metallic tube [8]. However, in reality all but armchair nanotubes are metallic, since nonzero curvature [9–13] gives rise to small band gaps that can be of the order of a few meV, corresponding to terahertz (THz) frequencies. The size of these gaps can be tuned by application of a magnetic field along the nanotube axis [14–17]. The diverse applications of THz radiation and its importance to fundamental science makes finding ways to generate, manipulate, and detect it one of the foremost challenges in modern applied physics [18]. One approach to fill the THz gap is to utilize narrow-gapped single-wall carbon nanotubes [19]. These tubes can exhibit strong THz optical transitions, which can be manipulated via externally applied magnetic and electric fields, giving rise to the possibility of utilizing them as highly tunable, optically active materials in THz devices [13,19–24].

In semiconductor carbon nanotubes, the existence of low-lying dark excitons drastically suppresses the photoluminescence efficiency [25–28]. However, in narrow-gap nanotubes it has been demonstrated numerically that the binding energy

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of certain potentials scales with the band gap. Therefore, undesirable effects due to dark excitons should not dominate optical processes in narrow-gap nanotubes [29,30]. However, the question of exactly how excitonic effects influence the optical processes in narrow-gap nanotube is still an outstanding problem. Excitonic effects in Dirac materials have been studied using a variety of approaches such as the Bethe-Salpeter method [31] as well as the two-body matrix Hamiltonian, based on the low-energy expansion of the tight binding [29,32–35], which will be the method employed in this study. Pair formation has been studied in Dirac materials with effective mass, such as gapped graphene [32,36–39], bilayer graphene [40], and graphene in the trigonal warping regime [41–43]. However, there is still much debate concerning the existence of coupled pairs in intrinsic graphene [34,44,45]. The two-body problem has also been the subject of study in narrow-gap carbon nanotubes and graphene nanoribbons and some analytic solutions have been found [29,30,46,47]. Numerical methods have also been used to determine exciton bound states in metallic carbon nanotubes subjected to a magnetic field [25]. Previous analytic results for finite potentials were limited to midgap states, relying on numerical methods to determine the remaining spectrum. Unlike previous studies, we calculate the full positive-energy spectrum exactly for a flat-bottomed potential, offering a powerful tool for modeling exciton energy levels.

The eigenvalues of a nonrelativistic particle, subjected to a confining potential, are obtained by first solving the Schrödinger equation and then imposing the appropriate boundary conditions upon the wave function. For the Schrödinger equation, the simplicity of the infinite square well offers many insights into quantum effects and serves as a useful approximation for more complex quantum systems. Contrastingly, the solution of the particle in a box problem in the relativistic regime is certainly nontrivial [48–54]. After solving the Dirac equation and requiring that all the components of the spinor vanish at the wells edge, the only permissible solution is the null wave function; the same is true for the cylindrical infinite well [55–57]. Supplementary boundary conditions may be employed to resolve this problem such as introducing a mass going to infinity outside the well [54,58,59]; such boundary conditions can relax the continuity of the wave function at the well's boundary yet preserve the continuity of the probability density across the well. However, different forms of quantum impenetrability may lead to different physical consequences [49]. Similar problems arise for the relativistic two-body problem. A discontinuous potential imposes many restrictions on the spinor components that are often very difficult to satisfy and demanding that the wave function and its derivative are continuous at the boundary results in the null wave function. To avoid the boundary condition issues we consider a smooth piecewise step potential that contains an adjustable parameter that can be varied such that in some limit the potential transforms into the Heaviside step function. Therefore, by symmetry one can construct a truly-flat-bottomed potential, which can be solved without the need of invoking supplementary boundary conditions. Exact solutions of the Dirac equation not only are useful in the analytic modeling of physical systems, but are also important for testing numerical, perturbation, or semiclassical methods. The smooth square well gives valuable insights in the behavior of two Dirac-like particles interacting via a short-range potential.

In what follows we consider excitons formed by relativistic one-dimensional electrons and holes interacting via a flat-bottomed piecewise potential. We first focus on excitons possessing zero total momentum along the nanotube axis. A solution to the two-body Dirac problem in the rest frame for a smooth step potential is presented. The wave functions are expressed in terms of Heun confluent functions and all the spinor components and their derivatives are continuous throughout space. The solutions are then analyzed in the limit in which the potential transforms into a true step potential and via symmetry conditions the quantized energy spectrum of the square well is attained. This potential is then used to model the interaction potential between an electron and hole in a one-dimensional Dirac system and the binding energy is shown to scale with the band gap. The true square-well problem is then revisited. By analyzing the wave function of the smooth square well, appropriate boundary conditions are obtained for the true square well. This enables one to obtain the energy spectrum of an exciton possessing finite total momentum along the nanotube axis. Finally, the model potential is analyzed in the δ-function limit for both the nonrelativistic and relativistic regimes.

II. SOLUTION OF THE FLAT-BOTTOM INTERACTION POTENTIAL PROBLEM FOR TWO DIRAC PARTICLES

In the absence of curvature effects, the single-particle Hamiltonian of a nanotube may be obtained from graphene by applying the periodic boundary condition along the direction of the circumference. Curvature effects are equivalent to introducing an effective flux along the tube, which is equivalent to shifting the momentum of charge carriers in an unrolled graphene sheet. Therefore, the effect of curvature and applied magnetic fields are directly analogous to the one-dimensional graphene problem where the curvature-induced gap plays the role of fixed transverse momentum. In general, the single-particle Hamiltonian of a narrow-gap carbon nanotube, of band gap $2\hbar v_{\mathrm{F}}\kappa_y$, is given in the vicinity of the band-gap edge by $\hbar v_{\mathrm{F}}(\sigma_x\hat{\kappa}+\sigma_y\kappa_y)$, where $\sigma_{x,y}$ are the Pauli spin matrices, v_{F} is the Fermi velocity in graphene, and $\hat{\kappa}$ is the operator of the wave vector along the nanotube axis (x axis). The corresponding eigenvalues are given by $\varepsilon=\pm\hbar v_{\mathrm{F}}\sqrt{\kappa^2+\kappa_y^2}$. For an electron-hole pair, the Hamiltonian can be written as [29]

$$\hat{H}=\hbar v_{\mathrm{F}}\begin{pmatrix} 0 & \hat{\kappa}_e-i\kappa_y & -\hat{\kappa}_h+i\kappa_y & 0\\ \hat{\kappa}_e+i\kappa_y & 0 & 0 & -\hat{\kappa}_h+i\kappa_y\\ -\hat{\kappa}_h-i\kappa_y & 0 & 0 & \hat{\kappa}_e-i\kappa_y\\ 0 & -\hat{\kappa}_h-i\kappa_y & \hat{\kappa}_e+i\kappa_y & 0\end{pmatrix}, \tag{1}$$

where the indices e and h correspond to the electrons and holes with $\hat{\kappa}_{e,h}=-i\partial/\partial x_{e,h}$, where x_e and x_h are the positions of the electron and hole along the nanotube. This Hamiltonian acts on the basis $|\Psi_{ij}\rangle=|\psi_i^e\rangle|\psi_j^h\rangle$, where the indices i and j correspond to the carbon atoms of the two different sublattices in the honeycomb lattice. In the absence of interaction and band-filling effects, this Hamiltonian yields four energy eigenvalues corresponding to a pair of noninteracting quasiparticles:

$$\varepsilon=\hbar v_{\mathrm{F}}\big(\pm\sqrt{\kappa_y^2+\kappa_e^2}\pm\sqrt{\kappa_y^2+\kappa_h^2}\big). \tag{2}$$

In this formalism, when considering a system containing a single electron and a single hole, one should only consider the solution with positive signs and the band gap of the two-particle system is given by $E_g = 2\hbar v_F \kappa_y$. It should also be noted that there also exists a possibility of binding a pair of same-charge particles. This case corresponds to the solutions with negative signs, interacting via a repulsive potential. In what follows we will restrict ourselves to the single-valley regime. However, the complete treatment of the problem requires that all valley and spin quantum numbers be taken into account; in this instance the number of different types of excitons associated with a given carbon nanotube spectrum branch rises to 16 [60]. The full treatment of the problem is beyond the scope of the present paper.

The interaction potential $U(x_e - x_h)$ is a function of the relative separation between the particles only, therefore it is convenient to move to the center of mass and relative motion coordinates: $X = (x_e + x_h)/2$, $x = x_e - x_h$. Therefore, the operators can be expressed as $\hat{\kappa}_e = \hat{K}/2 + \hat{k}$ and $\hat{\kappa}_h = \hat{K}/2 - \hat{k}$, where $\hat{k} = -i\partial/\partial x$. The wave function of the interacting particles can by written as $\Psi_{ij}(X,x) = e^{iKX}\phi_{ij}(x)$, allowing the operator $\hat{K}$ to be replaced with the constant K, which represents the wave vector of the interacting particles center of mass. Upon separating relative and center of mass motion, it is more convenient to move to the symmetrized wave functions:

$$\psi_1 = \phi_{BA} - \phi_{AB}, \quad \psi_2 = \phi_{AA} - \phi_{BB},$$
$$\psi_3 = \phi_{AA} + \phi_{BB}, \quad \psi_4 = \phi_{BA} + \phi_{AB}. \tag{3}$$

This enables the eigenvalue problem to be expressed as

$$\hbar v_F \hat{M}_{nm}\psi_m = [\varepsilon - U(x_e - x_h)]\psi_n, \tag{4}$$

where

$$\hat{M} = \begin{pmatrix} 0 & K & i2\kappa_y & 0 \\ K & 0 & 0 & 0 \\ -i2\kappa_y & 0 & 0 & 2\hat{k} \\ 0 & 0 & 2\hat{k} & 0 \end{pmatrix}. \tag{5}$$

Let us first consider the case of the stationary exciton, which couples to light, i.e., $K = 0$. In this instance, $\phi_{AA} = \phi_{BB}$, which allows us to reduce Eq. (4) from a system of four equations down to three. Equation (4) can be reduced to a single second-order equation in ψ_3:

$$\frac{\partial^2\psi_3}{\partial z^2} - \frac{1}{E-V}\frac{\partial(E-V)}{\partial z}\frac{\partial\psi_3}{\partial z} + \frac{1}{4}[(E-V)^2 - 4\Delta^2]\psi_3 = 0, \tag{6}$$

where we have scaled the eigenvalue $E = \varepsilon L/\hbar v_F$, potential energy $V = UL/\hbar v_F$, and momentum $\Delta = \kappa_y L$ and made use of the variable change $z = (x - W/2)/L$, where W is the effective width of the well and L a constant. The remaining components ψ_1 and ψ_4 are found via the relations

$$\psi_1 = i\frac{2\Delta}{E-V}\psi_3, \tag{7}$$

$$\psi_4 = -i\frac{2}{E-V}\frac{\partial\psi_3}{\partial z}. \tag{8}$$

Since our primary interest is the study of optoelectronic applications of carbon nanotubes [19] we will restrict ourselves to calculations concerning electron-hole pairs. However, the approach used here can be easily generalized for the study of same-charge particle pairs [34,35]. Indeed, it can be seen that changing E to $-E$ and $V(x)$ to $-V(x)$ leaves Eq. (6) unchanged. Therefore, proving the existence of electron-hole pairs interacting via an attractive potential within the gap also demonstrates the existence of bound-state energies of same-charge pairs interacting via a repulsive potential within the gap. Notably, when the binding energy corresponds to the middle of the gap, excitons and electron-electron pairs form zero-energy states, which are currently a focus of research for the broad quantum computing community.

On first inspection is seems natural to solve for the simplest of potentials, the square well, defined by an abrupt step. However, the derivative of the potential results in Dirac δ functions, centered at the potential's walls, entering Eq. (6). Indeed, if the spinor components are a function of the potential, then any piecewise potential and its derivative should be continuous throughout the whole space to ensure that all the spinor components and their derivatives are also continuous. Therefore, it is natural to solve for either a truly smooth and continuous potential [61,62] or a piecewise potential that has a smooth derivative throughout all of space.

A smooth step potential can be defined as

$$V_1 = \begin{cases} V_0[1 - \exp(-z)], & z > 0 \\ V_0[\exp(z) - 1], & z < 0 \end{cases} \tag{9}$$

where V_0 is half the height of the step. This potential belongs to a class of quantum models that are quasiexactly solvable [62–67] and it will be shown that in the limit that the potential transforms into the Heaviside step function the wave functions can be expressed in terms of elementary functions. In Fig. 1 we plot the smooth step potential for $L = 0.1$ and 0.001. In the limit $L \to 0$ the potential tends towards the Heaviside step function and the potential becomes truly flat at the origin. It is convenient to consider one step only and take into account the second wall of the well by imposing the following wave

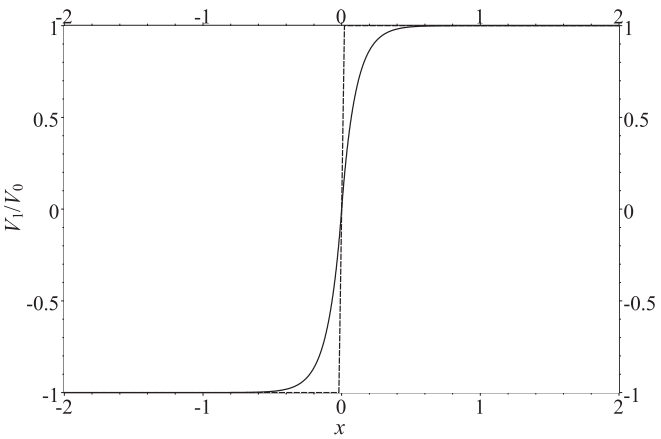

FIG. 1. Smooth Klein step for $L = 0.1$ (solid line) and $L = 0.001$ (dashed line).

function symmetry conditions at $z = -W/2L$:

$$\psi_3\left(-\frac{W}{2L}\right) = 0, \tag{10}$$

$$\left.\frac{\partial\psi_3}{\partial z}\right|_{-W/2L} = 0, \tag{11}$$

which correspond to odd and even modes of the square well, respectively. Here W is defined by the spatial extension of the interaction and the depth $2V_0$ is obtained from the electrostatic attraction between the quasiparticles. Since the two particles lie on the surface of the nanotube, the attractive interaction potential vanishing at infinity takes the form $U(x) \approx -e^2/(\varepsilon\sqrt{x^2+d^2})$. Here ε is the effective dielectric constant and d is the short-range cutoff parameter, which is of the order of the nanotube diameter. Therefore, a realistic potential should be nondivergent, thus making the square-well potential $V(x) = V_1(x) - V_0$, with $V_1(x)$ given by Eq. (9), a good first-order approximation for the short-range exciton interaction.

For $z < 0$ the solution of Eq. (6) is found to be

$$\psi_{3,\mathrm{I}} = \sum_{s_\beta} A_{s_\beta}\mathcal{H}_c(\alpha_+,\beta_+,-2,\alpha_+^2/2,1-\alpha_+^2/2;Z_+)Z_+^{\beta_+/2} \times \exp\left(\frac{1}{2}\alpha_+ Z_+\right), \tag{12}$$

where $\alpha_+ = s_\alpha i(V_0+\tilde{E})$, $\beta_+ = s_\beta\sqrt{4\Delta^2-(V_0+\tilde{E})^2}$, $s_\alpha = \pm1$, $s_\beta = \pm1$, $Z_+ = V_0\exp(z)/(V_0+\tilde{E})$, and A_{s_β} are constants. Here we introduce $\tilde{E} = E + V_0$. In addition, $\mathcal{H}_c(\alpha,\beta,\gamma,\delta,\eta;Z_+)$ is the Frobenius solution to the Heun confluent equation, which has two regular singularities at $Z_+ = 0$ and 1 and one irregular singularity located at ∞ [68]. The power series is computed about the origin and diverges at $Z_+ = 1$. It should be noted that for complex β_+, exchanging the sign of α_+ results in the same equation (12). An analytic continuation of the power series can be obtained by expanding the solution about the second regular singularity $Z_+ = 1$ and matching the two series and their derivatives in between the singularities. The second pair of independent solutions can be constructed about the point $Z_+ = 1$ via the identity [69]

$$\begin{aligned}&\mathcal{H}_c(\alpha,\beta,\gamma,\delta,\eta;Z_+)\\ &\quad= G_1\mathcal{H}_c(-\alpha,\gamma,\beta,-\delta,\eta+\delta;1-Z_+)\\ &\qquad+ G_2(-1+Z_+)^{-\gamma}\mathcal{H}_c(-\alpha,-\gamma,\beta,-\delta,\eta+\delta;1-Z_+).\end{aligned} \tag{13}$$

However, $\mathcal{H}_c(-\alpha_+,-2,\beta_+,-\alpha_+^2/2,1;1-Z_+)$ diverges since $\gamma = -2$ unless $\alpha_+^2 = \beta_+^2$, i.e., for $\Delta = 0$. Therefore, for nonzero Δ, $G_1 = 0$ and the solution to Eq. (6) can be written as

$$\psi_{3,i} = (1-Z_+)^2\sum_{s_\alpha,s_\beta} C_{s_\alpha,s_\beta}\mathcal{H}_c(-\alpha_+,2,\beta_+, -\alpha_+^2/2,1;1-Z_+)Z_+^{\beta_+/2}\exp\left(\frac{1}{2}\alpha_+ Z_+\right), \tag{14}$$

where C_{s_α,s_β} are constants. However, $\mathcal{H}_c(-\alpha_+,2,\beta_+,-\alpha_+^2/2,1;1-Z_+)Z_+^{\beta_+/2} = \mathcal{H}_c(-\alpha_+,2,-\beta_+,-\alpha_+^2/2,1;1-Z_+)Z_+^{-\beta_+/2}$; therefore we may set $c_{s_\alpha,-1} = 0$.

For $z > 0$ we obtain the solution

$$\psi_{3,\mathrm{II}} = \sum_{s_\beta} B_{s_\beta}\mathcal{H}_c\left(\alpha_-,\beta_-,-2,\frac{1}{2}\alpha_-^2,1-\frac{1}{2}\alpha_-^2,Z_-\right) \times Z_-^{\beta_-/2}\exp\left(\frac{1}{2}\alpha_- Z_-\right), \tag{15}$$

where $\alpha_- = s_\alpha i(V_0-\tilde{E})$, $\beta_- = s_\beta\sqrt{4\Delta^2-(V_0-\tilde{E})^2}$, $Z_- = V_0\exp(-z)/(V_0-\tilde{E})$, and the expansion about $Z_- = 1$ is given by

$$\psi_{3,\mathrm{ii}} = (1-Z_-)^2\sum_{s_\alpha} D_{s_\alpha}\mathcal{H}_c(-\alpha_-,2,\beta_-,-\alpha_-^2/2,1;1-Z_-) \times Z_-^{\beta_-/2}\exp\left(\frac{1}{2}\alpha_- Z_-\right), \tag{16}$$

where D_{s_α} are constants. It is clear from Eqs. (15) and (16) that for the function to decay at infinity we require $4\Delta^2 > (V_0-\tilde{E})^2$; therefore $D_{-1} = 0$. A real β_- means that all bound states of positive energy lie within the band gap of the two-body system.

In what follows we will restrict ourselves to analyzing bound states whose energy is above the center of the band gap, i.e., $\tilde{E} - V_0 > 0$. Paired states of negative energy will not be studied here. For photocreated electron-hole pairs, the energy range $\tilde{E} - V_0 > 0$ is sufficient. Indeed, variational calculations [70] of the binding energy in semiconductor nanotubes supported by experimental data give a value for the exciton binding energy of approximately 30% of the band gap. For the Frobenius solutions to converge we require that their arguments be less than 1. At the boundary $Z_+(0) = V_0/(V_0+\tilde{E})$ and $Z_-(0) = V_0/(V_0-\tilde{E})$. Therefore, $0 < Z_+(0) \leqslant 1/2$, whereas $Z_-(0) < 0$. Hence, for $z > 0$, we restrict ourselves to the Frobenius solutions of argument Z_-, whereas for $z < 0$, the Frobenius solutions of arguments Z_+ and $1 - Z_+$ are valid at the boundary $z = 0$. However, the Frobenius solution of argument $1 - Z_+$ diverges as $z \to 0$, which occurs rapidly for $|z| > L$ as L tends towards zero.

At the boundary the Frobenius solutions about $Z_\pm = 0$ may be expanded as a power series in $\alpha_\pm$ and $\beta_\pm$. By considering first-order powers of L only, one may write

$$\mathcal{H}_c(\alpha_\pm,\beta_\pm,-2,\alpha_\pm^2/2,1-\alpha_\pm^2/2;Z_\pm(0))\exp\left[\tfrac{1}{2}\alpha_\pm Z_\pm(0)\right] \times [Z_\pm(0)]^{\beta_\pm/2} \approx 1 + \tfrac{1}{2}\beta_\pm\{\ln[Z_\pm(0)] - Z_\pm(0)\} \tag{17}$$

and in the limit $z \to \infty$, $Z_+ \to 0$ and the Heun function of argument zero has a value of unity, which therefore allows the asymptotic wave function to be written as

$$\lim_{L\to 0}(\psi_{3,\mathrm{I}}) = A_1\exp\left(\tfrac{1}{2}\beta_+ z\right) + A_{-1}\exp\left(-\tfrac{1}{2}\beta_+ z\right). \tag{18}$$

Using the approximation (17) and equating Eqs. (12) and (14) and their derivatives at $z = 0$ allows Eq. (18) to be

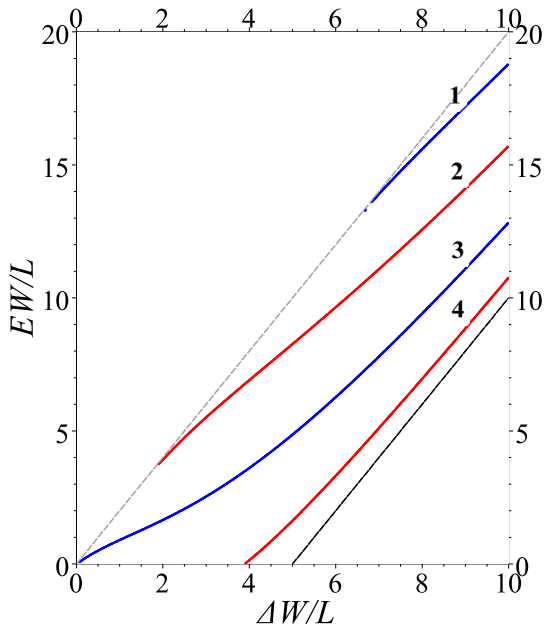

FIG. 2. Energy spectrum of an electron-hole pair interacting via a one-dimensional smooth square well as a function of $\Delta W/L$ for $2WV_0/L = 10$. The gray dashed (topmost) and black dashed (bottommost) lines represent $E = 2\Delta$ and $E - 2V_0 = 2\Delta$, respectively. Lines 2 and 4 (in red) correspond to the even modes, while lines 1 and 3 (in blue) correspond to the odd modes.

written as

$$\lim_{L\to 0}(\psi_{3,1}) = B_1\left[\cos\left(\frac{z}{2}\sqrt{(V_0+\tilde{E})^2-4\Delta^2}\right) + \frac{V_0+\tilde{E}}{V_0-\tilde{E}}\frac{\sqrt{4\Delta^2-(V_0-\tilde{E})^2}}{\sqrt{(V_0+\tilde{E})^2-4\Delta^2}} \times \sin\left(\frac{z}{2}\sqrt{(V_0+\tilde{E})^2-4\Delta^2}\right)\right], \quad (19)$$

and for $V_0 = 0$, Eq. (19) reduces to the plane wave of the two-body wave function of wave vector $\sqrt{\tilde{E}^2-4\Delta^2}/2L$. The other components are obtained via the relationships given by Eq. (11). No further matching conditions are required since ψ_3, the potential, and their derivatives are matched at the boundary (note this is not the case if the derivative of the potential is discontinuous). For bound states, ψ_3 exponentially decays outside the well and therefore all the other spinor components will decay too, and since $\tilde{E} > V_0$ there will be no singularities in the other spinor components. The odd modes of the square well are therefore given by

$$\frac{V_0-\tilde{E}}{V_0+\tilde{E}}\frac{\sqrt{(V_0+\tilde{E})^2-4\Delta^2}}{\sqrt{4\Delta^2-(V_0-\tilde{E})^2}} - \tan\left(\frac{W}{4L}\sqrt{(V_0+\tilde{E})^2-4\Delta^2}\right) = 0 \quad (20)$$

and the even modes are given by

$$\frac{V_0-\tilde{E}}{V_0+\tilde{E}}\frac{\sqrt{(V_0+\tilde{E})^2-4\Delta^2}}{\sqrt{4\Delta^2-(V_0-\tilde{E})^2}} + \cot\left(\frac{W}{4L}\sqrt{(V_0+\tilde{E})^2-4\Delta^2}\right) = 0. \quad (21)$$

The two transcendental equations can be solved graphically or via other standard root-finding methods. In Fig. 2 we plot the obtained energy spectrum for $V_0W/L = 10$ and in Fig. 3 we show the dependence of the static exciton energy on the depth of the well for two different values $\Delta W/L = 1$ and $\Delta W/L = 0.01$ corresponding to the cases of semiconductor and narrow-gap nanotubes respectively. For both narrow-gap and semiconducting tubes, when V_0W/L is small, there is only one bound state. As V_0 increases, the binding energy, defined as $E_b = 2\Delta - \tilde{E}$, increases until it is equal to the value of the band gap, upon which the exciton enters the continuum of states and disassociates.

As mentioned in the Introduction, the question of exactly how excitonic effects influence the optical processes in narrow-gap nanotube is important for prospective THz devices. Previous works suggest that the one-dimensional Van Hove singularity is suppressed by excitonic effects for both long-range and short-range electron-hole interaction potentials [30] and prominent peaks arise in the absorption spectrum that coincide with the exciton bound-state energies. Our analytic results are therefore extremely important in determining the role of excitonic effects, since knowledge of the eigenvalues and functions at zero separation allows one, in principle, to calculate the absorption coefficient via the Elliot formula.

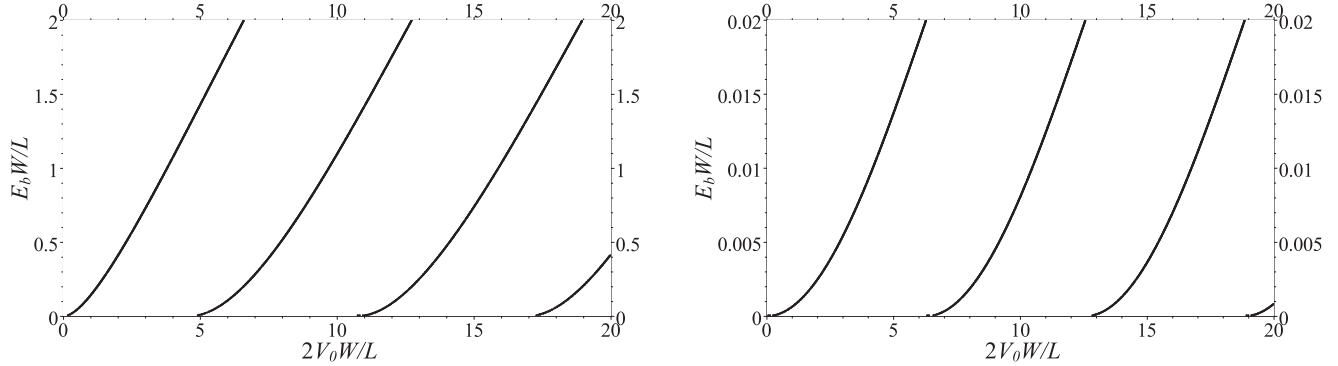

FIG. 3. Dependence of the exciton energy E_b on the interaction strength $2V_0$: The left-hand side is for a semiconductor nanotube with $\Delta W/L = 1$; the right-hand side is for a narrow-gap tube with $\Delta W/L = 0.01$. The different lines correspond to different excitonic states.

Unlike for the Gauss hypergeometric series, for the Heun functions the general formulas connecting solutions about two different singular points for arbitrary parameters are not known. To analyze the behavior of Eq. (16), we make use of the following approximation. In the limit $L \to 0$,

$$\begin{aligned}\mathcal{H}_c(-\alpha_\pm,2,\beta_\pm,0,1;1-Z_\pm)&\\ \approx {}_2F_1\left(2+\frac{1}{2}\beta_\pm,1+\frac{1}{2}\beta_\pm;3;1-Z_\pm\right)&\\ -\alpha_\pm\left[\frac{1-Z_\pm+\ln(Z_\pm)}{1-Z_\pm}\right],&\end{aligned} \tag{22}$$

where ${}_2F_1$ is the Gauss hypergeometric function. This enables Eq. (14), at the well's edge, to be written as

$$\psi_{3,i} \approx -\sum_{s_\alpha} C_{s_\alpha,1}(2+\alpha_+)[(1-Z_+)+\ln(Z_+)] \tag{23}$$

and as $Z_+ \to 0$ to be expressed as

$$\begin{aligned}\psi_{3,i} \approx -\sum_{s_\alpha} C_{s_\alpha,1}(2+\alpha_+)&\\ \times\left[\cosh\left(\frac{1}{2}\beta_+ z\right)+\frac{2}{\beta_+}\sinh\left(\frac{1}{2}\beta_+ z\right)\right].&\end{aligned} \tag{24}$$

For arbitrary $\tilde{E}$ and V_0 it is not possible to ensure the continuity of Eqs. (23) and (15) and their derivatives at the step edge using the approximate wave functions. However, both Frobenius solutions of arguments Z_+ and $1-Z_+$ are valid at the boundary $z=0$. Therefore, we may search for solutions that are a superposition of both Frobenius solutions inside the well. Upon substituting the approximate wave functions (17) and (23) into the boundary conditions

$$\psi_{3,\mathrm{II}}(0) = \psi_{3,\mathrm{I}}(0)+\psi_{3,i}(0), \quad \left.\frac{\partial\psi_{3,\mathrm{II}}}{\partial z}\right|_0 = \left.\frac{\partial\psi_{3,\mathrm{I}}+\psi_{3,i}}{\partial z}\right|_0 \tag{25}$$

and making use of the asymptotic expressions (18) and (24) we find that if A_1 or A_{-1} are zero, then we restore the eigenvalues obtained in Eqs. (20) and (21). For the case of nonzero A_1 and A_{-1} we find that

$$A_{\pm1} \approx \frac{1}{2}\left[1 \mp \frac{\beta_-}{\beta_+}\frac{1-Z_-}{1-Z_+}\right]B_1 \mp \frac{\omega}{\beta_+}, \tag{26}$$

where $\omega = -\sum_{s_\alpha} C_{s_\alpha,1}(2+\alpha_+)$, which allows the superposition of $\psi_{3,\mathrm{I}}(-W/2)+\psi_{3,i}(-W/2)$ to be expressed as

$$\begin{aligned}B_1\left[\cosh\left(\frac{1}{2}\beta_+ z\right)-\frac{\beta_-}{\beta_+}\frac{1-Z_-}{1-Z_+}\sinh\left(\frac{1}{2}\beta_+ z\right)\right]&\\ +\omega\cosh\left(\frac{1}{2}\beta_+ z\right).&\end{aligned} \tag{27}$$

Therefore, for the case of finite nondivergent A_1 and A_{-1}, we require that $\omega \propto L$ and in this instance the eigenvalues are restored.

III. MOVING EXCITON

The spinor components of the eigenfunctions of a square well need not necessarily be continuous at the well's edge [54] since they are solutions to a system of first-order differential equations containing a potential that is itself discontinuous. By analyzing the behavior of the wave function for our smooth potential, in the limit in which it approaches a smooth square well, one can obtain the appropriate boundary conditions for the spinor components of the true square well at the well's edge. For our model potential, as $L \to 0$ the wave function remain continuous at the well's edge; however, the derivative of the spinor components may tend to infinity, which corresponds to an abrupt jump in a square well's wave function, i.e., a discontinuity. The derivatives of the spinor components of the smooth square well are given by the expressions

$$\begin{aligned}\frac{\partial\psi_1}{\partial x} &= \frac{1}{L}\left[\pm\frac{1}{1-Z_\pm}\psi_1-\Delta\psi_4\right],\\ \frac{\partial\psi_4}{\partial x} &= -\frac{1}{2}\left[\frac{(E-V)^2-4\Delta^2}{(E-V)L}\right]\psi_3,\\ \frac{\partial\psi_3}{\partial x} &= \pm\frac{1}{L}\frac{\partial\psi_3}{\partial Z_\pm}.\end{aligned}$$

From Eq. (17) $\partial\psi_3/\partial Z_\pm|_{z=0} \propto L$, hence it can be seen from the above expressions that when evaluated at the well's edge $\partial\psi_1/\partial x$ diverges as $L \to 0$, while all the other components and their derivatives remain finite. Away from the well's edge, all the spinor components of positive-energy bound states are nondivergent. Therefore, when solving the same problem for an abrupt step potential and analyzing to the left and to the right of the well's wall, the wave functions to be matched are ψ_3 and ψ_4 and not ψ_1. However, though ψ_3 and ψ_4 are continuous across the square well, their derivatives are not since they are functions of the potential derivative.

For the case of the square well, of depth $\tilde{V}_0$ and width W, centered about the origin, Eq. (6) becomes

$$\frac{\partial^2\psi_3}{\partial x^2}+\lambda\psi_3 = 0, \tag{28}$$

where $L^2\lambda = [E^2-4\Delta^2]/4$ inside the well and $L^2\lambda = [(E+\tilde{V}_0)^2-4\Delta^2]/4$ outside the well, which admits the solution

$$\psi_3 = \begin{cases} A_{\mathrm{I}}\cos\left(\frac{\sqrt{(E+\tilde{V}_0)^2-4\Delta^2}}{2L}x\right)+A_{\mathrm{II}}\sin\left(\frac{\sqrt{(E+\tilde{V}_0)^2-4\Delta^2}}{2L}x\right), & x < \left|\frac{W}{2}\right| \\ \pm B\exp\left(-\frac{\sqrt{4\Delta^2-E^2}}{2L}|x|\right), & x > \left|\frac{W}{2}\right|, \end{cases} \tag{29}$$

where A_{I}, A_{II}, and B are constants and for odd modes $A_{\mathrm{I}} = 0$ while for even $A_{\mathrm{II}} = 0$. Using the continuity of the functions ψ_3 and ψ_4 at the well's edge, one restores the result obtained for the smooth square well. However, unlike the smooth square

well one may obtain exact solutions with finite K for the true square well. For the case of an exciton possessing finite total momentum along the nanotube axis, ψ_2 cannot be eliminated and both $\partial\psi_1/\partial x$ and $\partial\psi_2/\partial x$ diverge at the well's edge. By matching ψ_3 and ψ_4 at the well's edge one obtains the following eigenvalue relations:

$$\tan\left(\frac{W}{4L}\sqrt{\frac{(E+\tilde{V}_0)^2-\tilde{K}^2-4\Delta^2}{(E+\tilde{V}_0)^2-\tilde{K}^2}}(E+\tilde{V}_0)^2\right)+\frac{E}{E+\tilde{V}_0}\sqrt{\frac{(E^2-\tilde{K}^2)(E+\tilde{V}_0)^2[(E+\tilde{V}_0)^2-\tilde{K}^2-4\Delta^2]}{E^2[(E+\tilde{V}_0)^2-\tilde{K}^2][4\Delta^2-(E^2-\tilde{K}^2)]}}=0, \quad (30)$$

$$\cot\left(\frac{W}{4L}\sqrt{\frac{(E+\tilde{V}_0)^2-\tilde{K}^2-4\Delta^2}{(E+\tilde{V}_0)^2-\tilde{K}^2}}(E+\tilde{V}_0)^2\right)-\frac{E}{E+\tilde{V}_0}\sqrt{\frac{(E^2-\tilde{K}^2)(E+\tilde{V}_0)^2[(E+\tilde{V}_0)^2-\tilde{K}^2-4\Delta^2]}{E^2[(E+\tilde{V}_0)^2-\tilde{K}^2][4\Delta^2-(E^2-\tilde{K}^2)]}}=0, \quad (31)$$

where $\tilde{K}=KL$ and we restrict ourselves to the case where $(E+\tilde{V}_0)^2-\tilde{K}^2>0$ to ensure that there are no singularities in the spinor components and that $4\Delta^2-(E^2-\tilde{K}^2)>0$ and $E^2-\tilde{K}^2>0$ for the states to decay outside the well. Here Eq. (30) is for odd ψ_3 and Eq. (31) is for even ψ_3. It should be noted that in the δ-function limit considered in the next section Eqs. (30) and (31) give the same result as for the δ function of small strength. In general, Eqs. (30) and (31) can be solved graphically or via other standard root-finding methods. In Fig. 4 we plot the obtained energy spectrum as a function of $\Delta W/L$ for $\tilde{V}_0 W/L=10$ for a range of K values and it can be seen that as K increases, the bands blueshift. In Fig. 5 we show the dependence of the dynamic exciton energy on the depth of the well for a narrow-gap nanotube defined by $\Delta W/L=0.01$. The increase of K naturally shifts the excitonic states to higher energies.

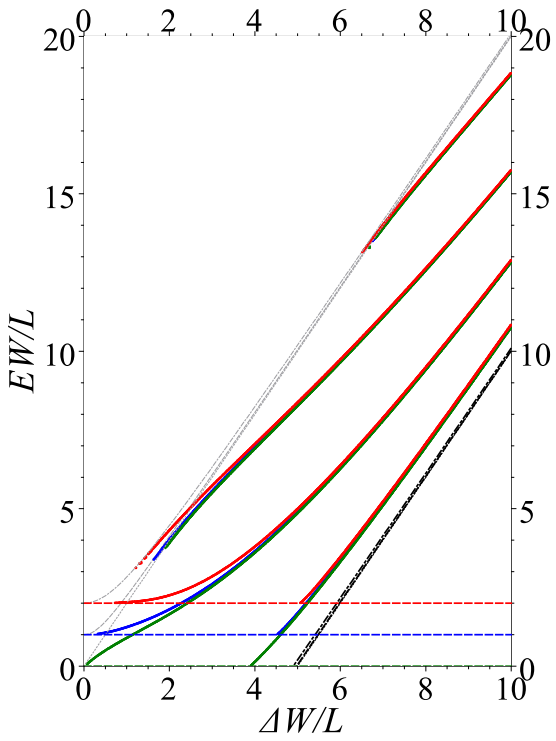

FIG. 4. Thick gray dotted, dashed, and dot-dashed lines denote $E=\sqrt{\tilde{K}^2+4\Delta^2}$ for $\tilde{K}=0$, 1, and 2, respectively, while their black counterparts denote $E=\sqrt{\tilde{K}^2+4\Delta^2}-V_0$. The solid green, blue, and red lines (the lowest, second from the bottom, and top lines in each set of lines, respectively) correspond to the eigenvalues of $\tilde{K}=0$, 1, and 2, respectively, and their dashed counterparts mark $E=\tilde{K}$.

IV. THE δ-FUNCTION POTENTIAL

Let us now consider the limit of very weak electron-hole attraction in the nonrelativistic regime $|2V_0|\ll\Delta$. In this limit approximate solutions to Eqs. (20) and (21) can be obtained for small binding energies. We find that for small binding energies $E_b=\Delta V_0^2W^2/L^2$. Therefore, for a very narrow deep well where $2V_0/L\gg W$, with $2V_0W/L=\alpha$, the binding energy is $E_b=\Delta\alpha^2/4$, thus we recover the nonrelativistic solution for an attractive δ-function potential of strength α. The strength of the potential α, i.e., $V=-\alpha L\delta(x)$, can be estimated as a product of the strength of the realistic potential and its width.

We will now consider the case when the interaction potential (9) tends towards the δ-function potential $V_1(x)=-\alpha L\delta(x)+V_0$ in the nonclassical regime. In the limit that $2V_0/L\to\infty$ and $W\to 0$ such that $2V_0W/L=\alpha$ and $\Delta W/L\ll 1$, Eqs. (20) and (21) admit the approximate solutions

$$E=-2\Delta\frac{\tan\left(\frac{\alpha}{4}\right)}{\sqrt{1+\tan^2\left(\frac{\alpha}{4}\right)}} \quad (32)$$

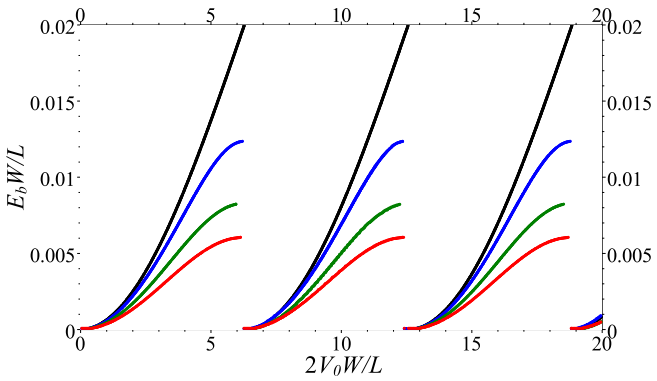

FIG. 5. Dependence of the exciton binding energy E_b on the interaction strength $2V_0$ with $\Delta W/L=0.01$ for $K=0$ (black topmost line in each set), $K=\Delta$ (blue line, second from top in each set), $K=2\Delta$ (green line, third from top in each set), and $K=3\Delta$ (red bottommost line in each set).

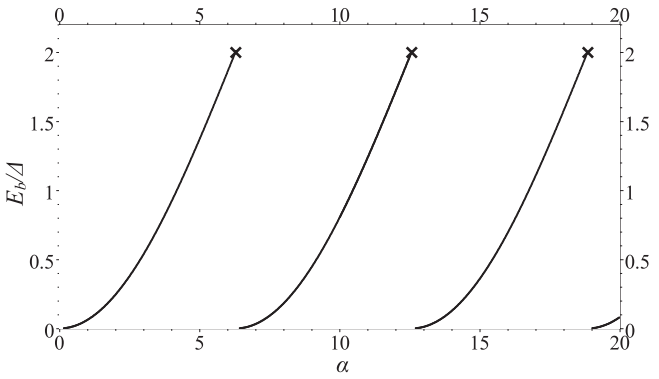

FIG. 6. Dependence of the exciton binding energy E_b on the interaction strength α, for an electron-hole pair interacting via the interaction potential (9) in the δ-function limit. The different lines correspond to different excitonic states. The crosses indicate when $E_b = 2\Delta$, which occurs at $\alpha = 2(1+n)\pi$, where $n = 0,1,2,3,\ldots$.

and

$$E = 2\Delta \frac{\cot\left(\frac{\alpha}{4}\right)}{\sqrt{1+\cot^2\left(\frac{\alpha}{4}\right)}} \tag{33}$$

for odd and even modes, respectively. For a given Δ, if Eq. (32) is negative, Eq. (33) is positive and vice versa. Therefore, the δ function can at most contain one bound state of positive energy. This can be seen in Fig. 6, where the appearance of a higher-order solutions coincides with the dissociation of the lower-order one. In the limit of very weak electron-hole attraction we find that for small binding energies, $E_b \approx \Delta\alpha^2/16$.

There are many other smooth analytic approximations to the δ function. The hyperbolic secant potential $V = -\alpha/\pi \cosh(x/L)$ is known to admit analytical expressions for zero energy when $\alpha = (1+2n)\pi + \sqrt{1+4\Delta^2}\pi$ [29]. In the δ-function limit, i.e., as $L \to 0$, the condition becomes $\alpha = 2(1+n)\pi$, where $n = 0,1,2,\ldots$. Restricting ourselves to the modes of relevant parity, we find that the same conditions hold true for Eqs. (32) and (33) at zero energy.

It should be noted that for odd solutions of ψ_3, the δ function can be solved by imposing that ψ_3 is discontinuous at the origin, whereas ψ_4 is continuous but its derivative is not. Let us consider the potential $V = -\alpha L\delta(x)$; expressing Eq. (4) in terms of ψ_4 and integrating across the interval $[0_-;0_+]$ yields

$$E\left(\left.\frac{\partial\psi_4}{\partial\tilde{x}}\right|_{0_+} - \left.\frac{\partial\psi_4}{\partial\tilde{x}}\right|_{0_-}\right) + \frac{1}{4}\alpha(E^2-4\Delta^2)\psi_4(0) = 0, \tag{34}$$

where $\tilde{x} = x/L$. A second relation can be found in the regions $x > 0$ and $x < 0$, $\frac{\partial^2\psi_4}{\partial\tilde{x}^2} - \frac{1}{4}(4\Delta^2 - E^2)\psi_4 = 0$, which admits the solution $\psi_4 = G_4 \exp(-\sqrt{4\Delta^2-E^2}|\tilde{x}|/2)$. Substituting the definition of ψ_4 into Eq. (34) results in the eigenvalue $E = -2\Delta\alpha/\sqrt{16+\alpha^2}$, which for small values of α [when $\tan(\alpha/4) \approx \alpha/4$] is in agreement with Eq. (32). Since ψ_4 is even, it follows that ψ_1 and ψ_3 are odd. For even ψ_3 we must solve Eq. (6). Integrating Eq. (6) across the interval $[0_-;0_+]$ yields

$$\frac{1}{E}\left(\left.\frac{\partial\psi_3}{\partial\tilde{x}}\right|_{0_+} - \left.\frac{\partial\psi_3}{\partial\tilde{x}}\right|_{0_-}\right) + \frac{1}{4}\alpha\psi_3(0) - \int_{0_-}^{0_+}\frac{\Delta^2}{(E-V)}\psi_3 d\tilde{x} = 0, \tag{35}$$

and in the regions $x > 0$ and $x < 0$ we find that $\psi_3 = G_3 \exp(-\sqrt{4\Delta^2-E^2}|\tilde{x}|/2)$. After regularization, the integral containing the δ function becomes zero and the resulting eigenvalue is found to be $E = 8\Delta/\sqrt{\alpha^2+16}$, which in the limit of small α agrees with Eq. (33).

We will now consider the case of an exciton possessing finite total momentum along the nanotube axis formed by an electron-hole pair interacting via a δ-function potential. Repeating the same procedure for finite K, we find for even ψ_4, $\psi_4 = G_4 \exp(-\frac{1}{2}\sqrt{\frac{4\Delta^2+\tilde{K}^2-E^2}{E^2-\tilde{K}^2}}|E\tilde{x}|)$ and

$$E = \pm\sqrt{\tilde{K}^2 + \frac{4\alpha^2\Delta^2}{16+\alpha^2}}, \tag{36}$$

where $\tilde{K} = KL$. We also require that $4\Delta^2 + \tilde{K}^2 > E^2$ to ensure that the state is bound. For even ψ_3, we integrate Eq. (6) across the interval $[0_-;0_+]$ to obtain

$$\frac{1}{E}\left(\left.\frac{\partial\psi_3}{\partial\tilde{x}}\right|_{0_+} - \left.\frac{\partial\psi_3}{\partial\tilde{x}}\right|_{0_-}\right) + \frac{1}{4}\alpha\psi_3(0) + \int_{0_-}^{0_+}\frac{(E-V)\Delta^2}{\tilde{K}^2-(E-V)^2}\psi_3 d\tilde{x} = 0. \tag{37}$$

Regularizing the δ function requires that the denominator be nonsingular; this imposes the requirement that $\tilde{K}^2 - (E-V)^2 > 0$. Since $\psi_3 = G_3 \exp(-\frac{1}{2}\sqrt{\frac{4\Delta^2+K^2-E^2}{E^2-K^2}}|E\tilde{x}|)$ the integral containing the δ function becomes zero and the resulting eigenvalue is found to be

$$E = \pm\sqrt{\tilde{K}^2 + \frac{64\Delta^2}{16+\alpha^2}}. \tag{38}$$

Comparing the rest frame to the moving frame and treating the transverse momentum as an effective mass, one restores the energy-momentum relation given by special relativity.

V. CONCLUSION

Solutions were obtained in the rest frame for the quasi-one-dimensional two-body Dirac problem, for a smooth step interaction potential, in terms of Heun confluent functions. By symmetry, this potential was used to obtain the eigenvalues of a smooth square well, which are found by solving a set of transcendental equations. Such a potential can be used to approximate the interaction potential between an electron-hole pair in a narrow-gap nanotube. The binding energy of these pairs was found to never exceed the band gap and therefore at room temperature the electron-hole pairs should be fully ionized. Hence, undesirable effects due to dark excitons should not dominate optical processes in narrow-gap nanotubes. By analyzing the smooth square well's stationary excitonic

wave functions, the appropriate boundary conditions were obtained for an abrupt square well, which in turn enables the dynamic exciton energy levels to be found. We also consider δ-function interaction, a highly nontrivial problem for relativistic particles, and show that different approximations for the δ function give the same result. Many of our results can be generalized for a pair of particles of the same charge, which, as we have shown, can have bound states within the gap.

The question of exactly how excitonic effects influence the optical processes in a narrow-gap nanotube is still an outstanding problem. Not only does this piecewise potential serve as an important tool for analyzing the excitonic energy levels in a narrow gap nanotube, but the simplicity of the asymptotic forms of the wave function in the square limit coupled with their easily determinable eigenvalues is extremely useful in determining the optical absorption spectra due to excitons in narrow-gap carbon nanotubes [30]. It should also be noted that the Hamiltonian used in this paper is of the same form as certain types of graphene nanoribbons or armchair carbon nanotubes subjected to an external magnetic field applied along the tube axis [13,21,22] and therefore the results obtained herein are relevant to a broad range of quasi-one-dimensional Dirac systems.

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