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Exciton States in Narrow-Gap Carbon Nanotubes

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Abstract. Quasi-exact solutions to the quantum relativistic two-body problem are obtained for a one-dimensional Woods-Saxon-like potential. The quantised positive energy spectrum is obtained in the square well potential limit in terms of a set of simple transcendental equations. This potential is used to calculate excitonic states in narrow-gap single-walled carbon nanotubes and the binding energy is shown to scale with the band gap.

INTRODUCTION

Confining a particle to a region in space results in the quantization of the energy spectrum. For a non-relativistic particle the quantized energy levels are obtained by solving the Schrodinger equation for a particular potential and then applying the necessary boundary conditions which are defined by the physical considerations of the problem. The simplicity of the infinite square well offers many insights into quantum effects and serves as a useful approximation for more complex quantum systems. To obtain energy quantization in the relativistic regime for the case of the infinite square well is certainly non-trivial [1, 2, 3, 4], 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 wavefunction, the same is true for the cylindrical infinite well [5, 6, 7]. Supplementary boundary conditions may be employed to resolve this problem such as giving spacial dependence to the rest mass, letting it be constant inside the well and tend to infinity outside the well [4, 8, 9], such boundary conditions can relax the continuity of the wavefunction at the well's boundary yet preserve the continuity of the probability density across the well.

Similar problems arise for the square well in the two body problem. For a single Dirac particle, confined to a one dimensional well, one must solve a system of two first order differential equations in order to obtain the quantized energy spectrum. For the two body problem, the system of equations grows from two to four, with this increased level of complexity it is natural to try to solve the most simple case that of a square well. However a discontinuous potential imposes many restrictions on the spinor components which are often very difficult to satisfy, and demanding that the wavefunction and its derivative are continuous at the boundary results in the null wavefunction. To avoid the boundary condition issues we consider a solvable potential which contains a single discontinuity in the potentials derivative, but with an adjustable parameter which can be varied such that in some limit the discontinuity vanishes allowing approximate analytic answers to be obtained. Such a smooth square well gives valuable insights in the behavior of two Dirac-like particles interacting via a short-range potential. Exact solutions of the Dirac equation are not only useful in the analytic modeling of physical systems, but they are also important for testing numerical, perturbative or semi-classical methods. The hyperbolic tangent potential which shall be the subject of discussion in this paper, belongs to a class of quantum models which are quasi-exactly solvable [10, 11, 12, 13, 14, 15], where only some of the eigenfunctions and eigenvalues are found explicitly. However in the limit that the hyperbolic tangent potential transforms to the Klein step it can be used to obtain the the quantized energy spectrum for the square well.

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Graphene, a single monolayer of carbon in a honey comb lattice [16], charge carriers are described by the same equation used to describe two dimensional massless Dirac-fermions, the Dirac-Weyl's equation [17]. Electron-electron interactions plays an important role Dirac materials [18] and it has been predicted that graphene may undergo a metalinsulator transition [19, 20, 21]. Therefore knowledge of the two body problem is an important step in the understanding of excitonic systems such as Bose-Einstein condensation [22, 23, 24] and Superfluidity [25, 26]. However, a common consensus has not been met regarding the formation of coupled pairs in intrinsic graphene. Some claim that excitons do not exist in intrinsic graphene [27, 28] while others shows that pairing can occur at zero-energy for different or same charge quasiparticles [29]. The inclusion of trigonal warping effects also gives rise to the possibility pair formation [30, 31, 32]. Pair formation has also been studied in gapped graphene [33, 34, 35, 24] and the two body problem was considered in bilayer graphene quantum dots [36]. Excitonic effects in Dirac materials have been studied using a variety of approaches such as the Bethe-Salpeter method [37] as well as the two-body tight-binding matrix Hamiltonian [35, 38, 39, 29], we shall employ the later method.

The two body problem has also been the subject of study in narrow gap carbon nanotubes and some analytic solutions have been found [38, 40]. Previous analytic results for finite width potentials were limited to mid-gap states, relying on numerical methods to determine the remaining spectrum. Unlike previous studies we calculate the full positive energy spectrum exactly, offering a powerful tool for modeling exciton energy levels. Numerical methods have also been used to determine exciton bound states in metallic carbon nanotubes subjected to a magnetic field [41]. It has also been demonstrated that the binding energy of certain short range potentials scale with the bandgap and therefore excitonic effects should not dominant optical processes in narrow-gap nanotubes [38, 40]. Indeed the typical curvature-induced band gap lies in the desirable terahertz frequency range which has led to a variety of promising proposals of utilizing them in terahertz applications [42, 43, 44, 45].

In what follows we consider excitons formed by relativistic quasi one-dimensional electrons and holes interacting via a Woods-Saxon-like potential. We focus on excitons possessing zero total momentum along the nanotube axis and positive energy. It should be noted that this model potential is also analyzable for finite momentum excitons which will be a subject of future study. A method for computing the quantized energy spectrum of the Woods-Saxon-like potential is presented. The Woods-Saxon-like potential is then analyzed in the limit in which it transforms into the square well, and the the quantised energy spectrum of the square well is attained, and the binding energy is shown to scale with the band gap.

SOLUTION OF THE DIRAC EQUATION FOR THE HYPERBOLIC TANGENT POTENTIAL

In what follows we shall consider theoretically the exciton formed by an electron and a hole excited across a narrow gap quasi-metallic carbon nanotube. The Hamiltonian for a single free electron in this case can be written as

$$\hbar v_{\mathrm{F}}\left(\sigma_x \hat{\kappa} + \sigma_y \kappa_y\right) \tag{1}$$

where $\sigma_{x,y}$ are the Pauli spin matrices and $\hat{\kappa}$ is the operator of the wave vector along the nanotube axis. We use the basis $|\psi_{\mathrm{A}}\rangle$, $|\psi_{\mathrm{B}}\rangle$ with the indices A, B corresponding to the carbon atoms of the two different sub-lattices in the honeycomb lattice. Here v_{F} is the Fermi velocity in graphene which is approximately 300^{th} that of the speed of light. Equation (1) results in the dispersion $\varepsilon = \pm\hbar v_{\mathrm{F}}\sqrt{\kappa_y^2 + \kappa^2}$ and the size of the band gap is given by $2\hbar v_{\mathrm{F}} \mid \kappa_y \mid$.

For a narrow gap carbon nanotube this gap is a result of the intrinsic curvature [46], the size of which can be tuned by a magnetic field [47, 45]. The Hamiltonian is also of the same form for certain types of graphene nanoribbons [48] or an armchair carbon nanotubes subjected to an external magnetic field applied along the axis of the tube [49]. For a pair of interacting electron and hole the total Hamiltonian can be written in the form of the 4×4 matrix, and the stationary Schrodinger equation for determining the binding energy written in the basis $|\Psi_{ij}\rangle = |\psi_i^e\rangle\,|\psi_j^h\rangle$ reads

$$\hbar v_{\mathrm{F}}\begin{pmatrix} 0 & \hat{\kappa}_x^e - i\kappa_y & -\hat{\kappa}_x^h + i\kappa_y & 0 \\ \hat{\kappa}_x^e + i\kappa_y & 0 & 0 & -\hat{\kappa}_x^h + i\kappa_y \\ -\hat{\kappa}_x^h - i\kappa_y & 0 & 0 & \hat{\kappa}_x^e - i\kappa_y \\ 0 & -\hat{\kappa}_x^h - i\kappa_y & \hat{\kappa}_x^e + i\kappa_y & 0 \end{pmatrix}\begin{pmatrix} \Psi_{\mathrm{AA}} \\ \Psi_{\mathrm{BA}} \\ \Psi_{\mathrm{AB}} \\ \Psi_{\mathrm{BB}} \end{pmatrix} = \left[\varepsilon - U\left(x_e - x_h\right)\right]\begin{pmatrix} \Psi_{\mathrm{AA}} \\ \Psi_{\mathrm{BA}} \\ \Psi_{\mathrm{AB}} \\ \Psi_{\mathrm{BB}} \end{pmatrix} \tag{2}$$

where the indices *e* and *h* correspond to the electrons and holes, $\hat{\kappa}_{e,h} = -i\partial / \partial x_{e,h}$. It should be noted that one can easily modify the above system of equations for particles of the same charge and for two particles belonging to different valleys. In the absence of interaction and band-filling effects this Hamiltonian yields four energy eigenvalues corresponding to a pair of non-interacting quasi-particles: $\varepsilon = \hbar v_{\mathrm{F}}\left(\pm\sqrt{\kappa_y^2 + \kappa_e^2} \pm \sqrt{\kappa_y^2 + \kappa_h^2}\right)$; only the solution with positive signs should be taken if we consider a system containing a single electron and a single hole and the band gap of the two-particle system is given by $E_g = 4|\Delta|$. The interaction potential $U\left(x_e - x_h\right)$ 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; $X = \left(x_e + x_h\right)/2$, $x = x_e - x_h$ therefore the operators can be expressed as $\hat{\kappa}_e = \hat{K}/2 + \hat{k}$, $\hat{\kappa}_h = \hat{K}/2 - \hat{k}$. The wave function of the interacting particles can by written as $\Psi_{ij}\left(X,x\right) = e^{iKX}\phi_{ij}\left(x\right)$ allowing the operator $\hat{K}$ to be replaced with the constant *K* which represents the wave vector of the interaction particles center of mass. Upon separating relative and center of mass motion it is more convenient to move to the symmetrized wave functions:

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

Which enables Equation (2) to be expressed as

$$\hbar v_F M_{nm}\psi_n = \left[\varepsilon - U\left(x_e - x_h\right)\right]\psi_n \tag{3}$$

where

$$M_{nm} = \begin{pmatrix} 0 & K & i2\kappa_y & 0 \\ K & 0 & 0 & 0 \\ -i2\kappa_y & 0 & 0 & 2\hat{k} \\ 0 & 0 & 2\hat{k} & 0 \end{pmatrix}$$

Where $\hat{k} = -i\partial/\partial x$. Let us consider the case of the stationary exciton i.e. $K = 0$. In this instance the system of equations reduces from four in number down to three and Equation (3) can be reduced to a single second order equation in ψ_3:

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

Where $z = \left(x - \tilde{W}/2\right)/L$, $V = UL/\hbar v_F$, $E = \varepsilon L/\hbar v_F$, $\Delta = \kappa_y L$ and $W = \tilde{W}/L$ and the remaining components ψ_1 and ψ_4 are found via the relations

$$\psi_1 = i\frac{2\Delta}{\left(E-V\right)}\psi_3 \qquad \psi_4 = -i\frac{2}{\left(E-V\right)}\frac{\partial\psi_3}{\partial z} \tag{5}$$

For the case of a square well of width *W* and depth V_0, defined by an abrupt step i.e. a Heaviside function, the derivative of the potential results in Dirac delta functions, centered at the potential's walls, entering into Equation (4). To avoid this complication one may analyze the solutions inside and outside the well, however matching the wavefunctions for all components of the spinor and their derivatives is non-trivial. Therefore we seek a potential which is continuous throughout space. For a Triangular well, Equation (4) can be solved exactly in terms of Kummer functions, this solution is important when considering schemes using the WKB approximation around the classical turning points. One may envisage a combination of linear and constant potentials which would create a trapezoidal well however the derivatives of all the spinors components being continuous across an interface of adjoining potentials is hard to achieve. It is therefore natural to either solve for a truly smooth and continuous single potential or a combination of solvable potentials spanning different domains providing that $\partial V / \partial x$ be continuous throughout all space.

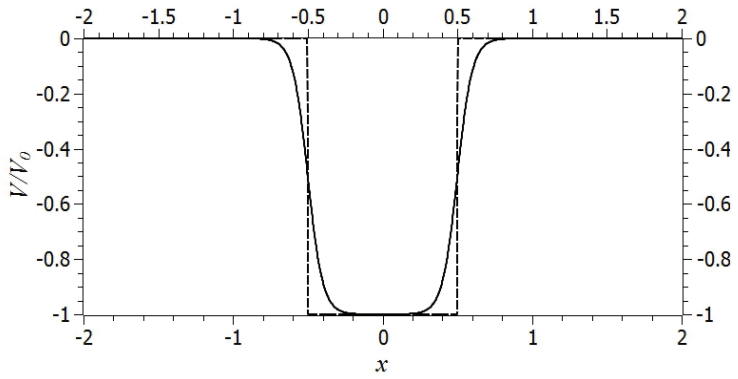

FIGURE 1. The "smooth" square well potential for $\widetilde{W}=1$ with $L = 0.1$ (solid line) and $L = 0.001$ (dashed line) respectively

We shall use the model potential

$$V=\begin{cases} -V_0\left[1-\tanh(z)\right]/2 & z\geq -\dfrac{W}{2} \\ -V_0\left[1+\tanh(z+W)\right]/2 & z\leq -\dfrac{W}{2} \end{cases} \tag{6}$$

where V_0 is the depth of the well and W is the well's width, for a barrier-like potential one must exchange $V_0 \to -V_0$. W is defined by the spatial extension of the interaction and the depth V_0 is obtained from the electrostatic attraction between the quasi particles which is given by the expression $U(x)\approx -e^2/\left(\varepsilon\sqrt{x^2+d^2}\right)$, where ε is the effective dielectric constant and d is the short-range cut-off parameter, which is of the order of the nanotube diameter. Though barely discernible in Figure (1) there is a cusp in the potential at $x = 0$, therefore we shall restrict ourselves to the the regime where $L \to 0$, in this instance the cusp vanishes and the potential transforms into a Klein step which has been solved analytically in the one-dimensional single body Dirac problem [50]. Other cusp potentials, such as the shifted one-dimensional Coulomb potential are also known to admit analytic results [51]. Since in the small L limit there is an absence of a discontinuity in the potential, we refer to the barrier as a "smooth" square well. Since the derivative vanishes at the center of the well we can therefore obtain exact solutions to the problem. Furthermore the "smooth" square well potential is a good first order approximation to an actual excitonic potential. It should be noted that a square-like exponential potential can also be solved analytically and analytic solutions were obtained for mid gap states for the hyperbolic sectant potential [38].

In what folllows we shall consider the smooth step potential

$$V=-V_0\left[\frac{1-\tanh(z)}{2}\right] \tag{7}$$

which is sufficient to obtain the complete energy spectrum of the smooth square well via symmetry conditions. For the potential defined by Equation (7) the natural choice of variable is $\xi=\left[1-\tanh(z)\right]/2$ and rewriting Equation (4) in terms of the variable ξ yields

$$\frac{\partial^2\psi_3}{\partial\xi^2}-\frac{V_0\xi^2+2\xi E-E}{\xi(1-\xi)(E+V_0\xi)}\frac{\partial\psi_3}{\partial\xi}+\frac{(E+V_0\xi)^2-(2\Delta)^2}{16\xi^2(1-\xi)^2}\psi_3=0 \tag{8}$$

We seek solutions of the form

$$\psi_3=\sum_{s_1,s_2}A_{s_1,s_2}\xi^Q(1-\xi)^R\Psi(\xi) \tag{9}$$

where $Q=s_1\sqrt{(2\Delta)^2-E^2}/4$, $R=s_2\sqrt{(2\Delta)^2-(E+V_0)^2}/4$, $s_1=\pm1$, $s_2=\pm1$ and A_{s_1,s_2} is a constant. Substitution of Equation (9) into Equation (8) allows Equation (8) to be reduced to Heun equation [52] which has singular points at $\xi=0,1,-E/V_0$ and ∞. Ψ is found to be

$$\Psi = Hl\left(-\frac{E}{V_0},-\frac{E}{V_0}(Q+R)(2Q+1)+\frac{E^2}{8}-Q;R+Q-i\frac{1}{4}V_0,R+Q+\frac{1}{4}iV_0,2Q+1,2R+1;\xi\right) \tag{10}$$

where $Hl = Hl(a,q;\alpha,\beta,\gamma,\delta;\xi)$ is the Heun function, defined by [52]

$$\sum_{j=0}^{\infty} c_j \xi^j$$

where $\widetilde{R}_j c_{j+1} - (\widetilde{Q}_j + q)c_j + \widetilde{P}_j c_{j-1} = 0$ with $\widetilde{P}_j = (j+\alpha-1)(j+\beta-1)$, $\widetilde{Q}_j = j[(j-1+\gamma)(1+a)+a\delta+\varepsilon]$, $\widetilde{R}_j = a(j+1)(j+\gamma)$, $\varepsilon = \alpha+\beta-\gamma-\delta+1$, $c_0 = 1$ and $a\gamma c_1 - qc_0 = 0$. The Heun series, $\sum_{j=0}^{\infty} c_j \xi^j$, converges to $Hl(a,q;\alpha,\beta,\gamma,\delta;\xi)$ within the disk defined by $|\xi| < |\xi_0|$ where ξ_0 is the location of the singularity closest to the origin, which is either *a* or 1. An analytic continuation of Hl is obtained through identities, relating the values of the function in different regions, or by expanding the solution about the other singularities *a*, 1 or ∞ [53]. From the above consideration two situations may arise depending on the values of the ratio E/V_0. Firstly, the Heun series $\sum_{j=0}^{\infty} c_j \xi^j$ converges within the range $0 \le \xi < 1$ and secondly the discontinuity, *a*, falls within the range of z.

Let us first consider the case where the discontinuity, *a*, falls outside the range of z. In this instance if $V_0 > 0$ then the range of permissible *E* is $E > 0$ and $E < -V_0$ or if $V_0 < 0$ then the range of permissible *E* is $E < 0$ and $E > V_0$. In the limit that $z \to \infty$, $\xi \to 0$ and Equation (10) has a value of unity therefore for the wave function, Equation (9), to decay to zero we require that $Q > 0$. Therefore all bound states with positive energy must be located within the band gap i.e. $|E| < |2\Delta|$. To analyze Equation (10) in the limit of $z \to -\infty$ i.e. $\xi \to 1$ an analytic continuation is obtained using the Frobenius solutions about $\xi = 1$. In the two domains $0 \le \xi < 1$ and $0 < \xi \le 1$ Equation (10) can be expressed as

$$\Psi_{\mathrm{I}} = Hl(a,q;\alpha,\beta,\gamma,\delta;\xi), \qquad 0 \le \xi < 1 \tag{11}$$

$$\Psi_{\mathrm{II}} = C_1 Hl(1-a,-q+\alpha\beta;\alpha,\beta,\delta,\gamma;1-\xi) + C_2(1-\xi)^{1-\delta} Hl(1-a,-q+(\delta-1)\gamma a+(\beta-\delta+1)(\alpha-\delta+1);\beta-\delta+1,\alpha-\delta+1,2-\delta,\gamma;1-\xi), \quad 0 < \xi \le 1 \tag{12}$$

and we require

$$\Psi_{\mathrm{I}}(\xi_0) = \Psi_{\mathrm{II}}(\xi_0) \qquad \left.\frac{\partial \Psi_{\mathrm{I}}}{\partial \xi}\right|_{\xi_0} = \left.\frac{\partial \Psi_{\mathrm{II}}}{\partial \xi}\right|_{\xi_0} \tag{13}$$

where $0 < \xi_0 < 1$. Using Equation (12) the energy eigenvalues can be found by solving $\psi_3\left(z = -\frac{W}{2}\right) = 0$ for the odd modes and $\left.\frac{\partial \psi_3}{\partial z}\right|_{z=-\frac{W}{2}} = 0$ for the even modes. However in the limit that *L* « 0 the eigenvalues can be obtained via the solution of a simple set of transcendental equations.

The Square Well Limit

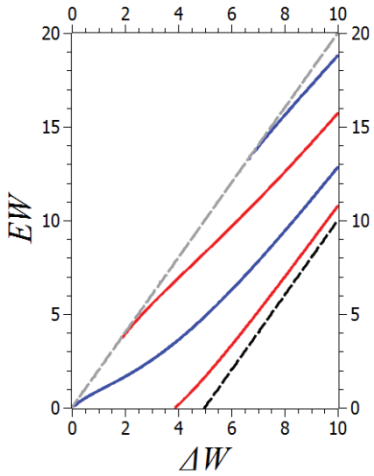

FIGURE 2. The energy spectrum of excitonic states in a one-dimensional smooth square well as a function of ΔW for $V_0 W = 10$. The gray and black lines represent $E = \Delta$ and $E + V_0 = \Delta$ respectively while the blue and red lines correspond to odd and even modes respectively

In the square well potential limit i.e. as $L \to 0$, $\xi \to 0$ rapidly for all values of x above $W/2$, retaining only first order terms in L, for $\xi < 1/2$ the asymptotic expression reads

$$\lim_{L\to 0}\left(\Psi_{\mathrm{I}}\right) \approx \left[1 - \frac{q}{a}\ln\left(1-\xi\right)\right] \tag{14}$$

where $q \approx a\left(Q+R\right) - Q$. Similarly as $L \to 0$, $\xi \to 1$ rapidly for all values of x below $W/2$, and the asymptotic expression for $\xi > 1/2$ is

$$\lim_{L\to 0}\left(\Psi_{\mathrm{II}}\right) \approx C_1\left[1 + \frac{q}{(1-a)}\ln\left(\xi\right)\right] + C_2\left(1-\xi\right)^{-2R}\left[1 + \frac{q-2Ra}{(1-a)}\ln\left(\xi\right)\right] \tag{15}$$

In the limit that $L \to 0$, the only meaningful place to match the two functions is at the wells boundary i.e. $\xi_0 = 1/2$. Applying these approximate functions to the boundary conditions Equation (13) yield

$$\frac{q}{2aR} = C_2 \qquad \left(1 - \frac{q}{2aR}\right) = C_1 \tag{16}$$

The eigenvalues are obtained by analyzing Equation (9) in the limit that $\xi \to 1$. Substituting Equation (15) and Equation (16) into Equation (9) and noting that

$$Hl\left(a,q;\alpha,\beta,\gamma,\delta;\xi\right) = \left(1-\xi\right)^{1-2\delta} Hl\left(a,q-\left(\delta-1\right)\gamma a;\beta-\delta+1,\alpha-\delta+1,\gamma,2-\delta;\xi\right)$$

allows the asymptotic function to be written as

$$\lim_{\xi\to 1}\left(\psi_3\right) \propto \left[\cosh\left(2Rz\right) - \frac{Q\left(a-1\right)}{aR}\sinh\left(2Rz\right)\right] \tag{17}$$

Therefore the odd and even bound energy eigenvalues are found via the relations

$$\frac{E}{\left(E+V_0\right)}\frac{\sqrt{\left(E+V_0\right)^2 - 4\Delta^2}}{\sqrt{4\Delta^2 - E^2}} + \tan\left[\frac{W}{4}\sqrt{\left(E+V_0\right)^2 - \left(2\Delta\right)^2}\right] = 0 \tag{18}$$

and

$$\frac{E}{\left(E+V_0\right)}\frac{\sqrt{\left(E+V_0\right)^2 - 4\Delta^2}}{\sqrt{4\Delta^2 - E^2}} - \cot\left[\frac{W}{4}\sqrt{\left(E+V_0\right)^2 - 4\Delta^2}\right] = 0 \tag{19}$$

which can be solved graphically or via other standard root-finding methods. In Figure (2) we plot the obtained energy spectrum as a function of ΔW for $V_0 W = 10$. It should be noted that for $V_0 > 0$ the above relations are only

applicable for $E > 0$ since for $E < 0$ Equation (16) becomes invalid, and deviates successively more from the true values as E becomes increasingly negative, this is due to the presence of a singularity appearing at $\xi = a$. Indeed for negative energies one must take special care and attention to include all possible solutions to obtain the correct negative energy spectrum and this shall be a topic of future study. An analogous case was found in the two dimensional problem [35] which was later resolved in [39]. However in our case only positive solutions are needed since we are considering a system containing a single electron above the Dirac point and a single hole below it. It should also be noted that under certain conditions the Heun function can be reduced to a finite polynomial of order n, this occurs when two conditions are met, firstly when $\alpha = -n$, where n is a positive integer and when the $n^{th}+1$ coefficient in the series expansion is a polynomial in q of order $n + 1$ such that q is a root of that polynomial. Under these circumstances the coefficient is zero and the series truncates and providing that Q and R are positive and real, then these modes will be bound for the Klein step. Another interesting case is when the Heun equation loses a singular point and becomes the hypergeometric equation, which may occur but not limited to when $a = 0$, 1/2 and 1. In these instances the solutions are congruent with the eigenvalues obtained above. It should be noted that for the case of the square barrier potential bound states are also possible, however in this instance Equations (18) and (19) are only valid for $E < 0$.

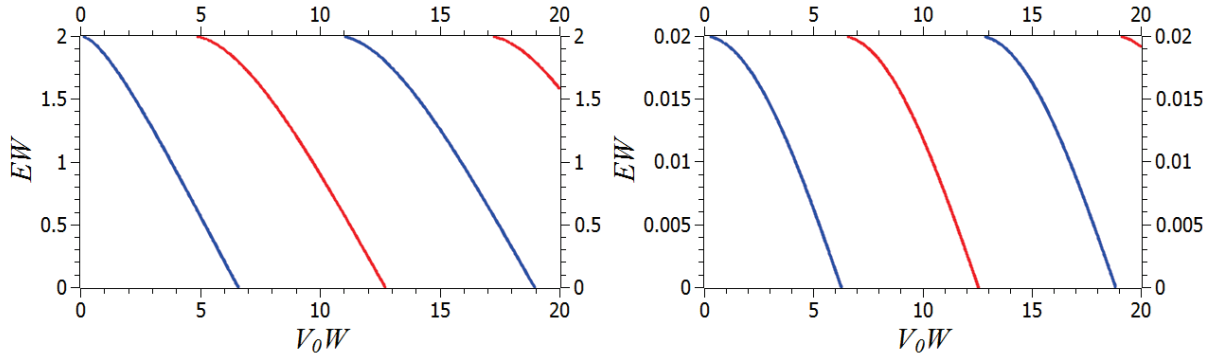

FIGURE 3. The dependence of the exciton energy E on the interaction strength V_0 : The left-hand side is for a semiconductor nanotube with $\Delta W = 1$; The right-hand side is for a narrow-gap tube with $\Delta W = 0.01$.

In Figure (3) we show the dependence of the static exciton energy on the depth of the well for two different values: $\Delta W = 1$ and $\Delta W = 0.01$ corresponding to the cases of semiconductor and narrow-gap nanotubes respectively. The increase of V_0 leads to the appearance of higher order solutions, corresponding to *p*, *d*, etc excitons. As the band gap decreases the higher order modes emerge at correspondingly lower potential strengths, however the difference between large and narrow gap tubes is slight. In the above consideration we have only considered the one valley regime, the full 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 [54]. In principle this can be accommodated into the above model by modifying the parameters of the potential, consequently all excitons be them dark or bright should have a binding energy within the band gap, ergo for narrow gap tubes, at room temperature, they should be fully ionized and the direct inter-band transitions [42, 43, 49, 45] will govern the emission in the terahertz range.

CONCLUSION

We have calculated the static exciton energy levels in a narrow-gap single-walled carbon nanotube, accounting for the quasi-relativistic dispersion of electrons and holes. Analytic solutions were obtained for a smooth square well and the eigenvalues are obtained via the solution of a simple set of transcendental equations. It has been show that the exciton binding energy scales with the band gap.

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