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Rigorous perturbation theory versus variational methods in the spectral study of carbon nanotubes

May 1st, 2007

Horia D. Cornean[1], **Thomas G. Pedersen**[2], **Benjamin Ricaud** [3]

Abstract

Recent two-photon photo-luminescence experiments give accurate data for the ground and first excited excitonic energies at different nanotube radii. In this paper we compare the analytic approximations proved in [CDR], with a standard variational approach. We show an excellent agreement at sufficiently small radii.

1 Introduction

Recent experimental results on carbon nanotubes using two photon photo luminescence [Sc02], [W], [MPR] reveal the energy levels of the excitons, especially the ground and first excited states, and point out the dependence of these energies on the radius of the nanotube. As it is, this technique appears to be a promising way to sort out nanotubes. But on the other hand, theoretical results seem to require heavy ab initio calculation like in [MPR] [CBRM], to cite the most recent, in order to find the absorption peaks due to excitons. Nevertheless, a simple formula for the optical response based on excitons levels [HK] can give a good approximation. It has been pointed out [BGEH] [OT] that the exciton binding energy in quantum wires depends on the width of the wires by a relatively simple relation. This property is also valid for nanotubes [P1]. In the first part of the paper, we outline a rigorous justification for this latter fact and write a simple analytic formula for the energy levels of the exciton depending on the radius of the tube, based on the paper [CDR]. In the second part we compare our results with a variational numerical method and show a very good agreement between them.

2 The exciton model

As first suggested in [P1], we deal with Wannier excitons (a rigorous justification of this procedure is in preparation [R]). We take as configuration space a cylinder of radius r and infinite length, space denoted by $\mathcal{C}_r = \mathbb{R} \times rS^1$, S^1 being the unit circle. The coordinates on the cylinder are $(x, y) \in (\mathbb{R} \times rS^1)$ where x is the variable along the tube axis and y is the transverse coordinate.

The two quasi-particles live in the Hilbert space $L^2(\mathcal{C}_r \times \mathcal{C}_r)$. We formally consider the Hamiltonian

$$\bar{H}^r = -\hbar^2 \left(\frac{\Delta_{x_1}}{2m_1} + \frac{\Delta_{x_2}}{2m_2} + \frac{\Delta_{y_1}}{2m_1} + \frac{\Delta_{y_2}}{2m_2} \right) - V^r(x_1 - x_2, y_1 - y_2), \tag{2.1}$$

where

$$V^r(x, y) := \frac{-e_1 e_2}{\varepsilon \sqrt{x^2 + 4r^2 \sin^2\left(\frac{y}{2r}\right)}} \tag{2.2}$$

[1]Dept. of Mathematical Sciences, Aalborg University, Fredrik Bajers Vej 7G, 9220 Aalborg, Denmark; e-mail: cornean@math.aau.dk

[2]Dept. Phys. and Nanotech., Aalborg University, 9220 Aalborg, Denmark; e-mail: tgp@physics.aau.dk

[3]Centre de Physique Théorique UMR 6207 - Unité Mixte de Recherche du CNRS et des Universités Aix-Marseille I, Aix-Marseille II et de l'université du Sud Toulon-Var - Laboratoire affilié à la FRUMAM, Luminy Case 907, F-13288 Marseille Cedex 9 France; e-mail: ricaud@cpt.univ-mrs.fr

(x_i, y_i) are the coordinates on the cylinder of the two charged particles, m_i their masses, and e_i their charges. Here ε is the electric permittivity of the material. The potential V^r is the three dimensional Coulomb potential simply restricted to the cylinder. We justify the expression of V^r by Pythagoras's theorem. The cylinder is embedded in $\mathbb{R}^3$. The distance ρ from one particle to the other in $\mathbb{R}^3$ is:

$$\rho^2 = (x_1 - x_2)^2 + 4r^2 \sin^2\left(\frac{y_1 - y_2}{2r}\right)$$

where $|2r \sin\left(\frac{y_1-y_2}{2r}\right)|$ is the length of the chord joining two points of coordinate y_1 and y_2 on the circle.

2.1 "Separation of the center of mass"

Due to the restrictions imposed by the cylindrical geometry, the usual separation of the center of mass does not work here.

The standard separation with Jacobi coordinates only works for the longitudinal variable, and introducing $M := m_1 + m_2$ and $\mu := m_1 m_2/(m_1 + m_2)$, we denote $X := (m_1 x_1 + m_2 x_2)/M$ and $x := x_1 - x_2$. For the transverse variable, we change to atomic coordinates $Y = y_2$ and $y = y_1 - y_2$. Let us also define the effective Rydberg $Ry^* = \mu e^4/2\hbar^2\varepsilon^2$ and Bohr radius $a_B^* = \hbar^2\varepsilon/\mu e^2$, where we set $e = e_1 = e_2$. By a scaling, the new energy and radius will be expressed in multiple of these units. This gives us the Hamiltonian:

$$H^r = -\frac{1}{M}\partial_X^2 - \frac{1}{m_2}\partial_Y^2 - \frac{1}{\mu}\partial_x^2 - \frac{1}{\mu}\partial_y^2 + \frac{2}{m_2}\partial_y\partial_Y - 2V^r(x, y).$$

First, we can separate the partial center of mass with coordinate X. Second, since on the Y variable there are periodic boundary conditions, let us consider the orthonormal basis of eigenvectors of $-\partial_Y^2$,

$$-\partial_Y^2 = \sum_{n=-\infty}^{\infty} E_n^r |\chi_n^r\rangle\langle\chi_n^r|$$

where

$$\chi_n^r(Y) = \frac{1}{\sqrt{2\pi r}} e^{in\frac{Y}{r}} \text{ and } E_n^r = \frac{n^2}{r^2},\ n \in \mathbb{Z}.$$

One can see that for small radii, the separation between different transverse levels of energy is high. A recent theoretical study based on ab initio calculations [MPR] shows that the probability density of the exciton is constant along the circumference. So it is reasonable to assume that the radius is so small that the system stays in the ground state of $-\partial_Y^2$, where $n = 0$ and the density of probability is constant along the circumference. (Note that this has been rigorously proved in [CDR]). As a consequence, we can approximate the eigenfunctions ψ of H as:

$$\psi(x, y, Y) = \phi(x, y) \cdot \chi_0^r(Y) = \phi(x, y) \cdot \frac{1}{\sqrt{2\pi r}}.$$

After this restriction to the lowest transverse mode, we only have to study the following operator:

$$\widetilde{H}^r = -\frac{1}{\mu}\partial_x^2 - \frac{1}{\mu}\partial_y^2 - 2V^r(x, y),$$

which is two dimensional and acts on $L^2(\mathcal{C}_r)$.

2.2 An effective one dimensional operator for the low lying spectrum

It will turn out that the limit $r \to 0$ is too singular and $\widetilde{H}^r$ does not have a "nice" limit. It is suitable at this point to introduce the quadratic form associated to $\widetilde{H}^r$, defined on the Sobolev space $\mathcal{H}^1(\mathcal{C}_r)$:

$$t_{\widetilde{H}}(\psi, \phi) = \frac{1}{\mu}\langle\partial_x\psi, \partial_x\phi\rangle + \frac{1}{\mu}\langle\partial_y\psi, \partial_y\phi\rangle - 2\langle\sqrt{V^r(x, y)}\psi, \sqrt{V^r(x, y)}\phi\rangle.$$

Reasoning as in the previous subsection, a good approximation of the behavior of eigenfunctions along the transverse variable when the radius is small is given by the ground state of the free Laplacian with periodic boundary conditions. If we restrict the above quadratic form to functions of the type:

$$\phi(x,y) = \varphi(x) \cdot \frac{1}{\sqrt{2\pi r}}, \tag{2.3}$$

we have:

$$\begin{aligned} t_{\widetilde{H}}(\phi,\phi) &= \frac{1}{2\pi r\mu}\langle \partial_x\varphi, \partial_x\varphi\rangle - \frac{1}{\pi r}\int_{-\infty}^{\infty}\int_{-\pi r}^{\pi r} \frac{1}{\sqrt{x^2+4r^2\sin^2\frac{y}{2r}}}\varphi(x)\overline{\varphi}(x)dydx \\ &= \frac{1}{\mu}\int_{-\infty}^{\infty} \overline{(\partial_x\varphi)}(x)(\partial_x\varphi)(x)dx - 2\int_{-\infty}^{\infty} V^r_{\text{eff}}(x)\varphi(x)\overline{\varphi}(x)dx \end{aligned}$$

where

$$V^r_{\text{eff}}(x) = \frac{1}{2\pi r}\int_{-\pi r}^{\pi r} \frac{1}{\sqrt{x^2+4r^2\sin^2\frac{y}{2r}}}dy.$$

For the sake of simplicity, we will put $\mu = 1$. Let us introduce what will be our effective one-dimensional comparison operator:

$$H^r_{\text{eff}} := -\frac{d^2}{dx^2} - 2V^r_{\text{eff}}(x). \tag{2.4}$$

We now have reduced our problem of two particles on a cylinder to a one dimensional problem describing a particle interacting with an external potential. A complete and detailed mathematical justification of these steps can be found in [CDR].

2.3 The one dimensional Coulomb Hamiltonian

2.3.1 Approximation of H^r_{eff}

We now try to approximate as accurate as possible the eigenfunctions and eigenvalues of H^r_{eff} when the radius is small. Using the notation $Y_r(x) = \frac{1}{\sqrt{x^2+4r^2}}$, it was shown in [CDR] that if $r \leq 1$ and f, g are two smooth functions

$$\langle f, V^r_{\text{eff}} g\rangle = \langle f, Y_r g\rangle + \ln(4) f(0)\overline{g(0)} + O(r^{4/9})||f||_{\mathcal{H}^1(\mathbb{R})}||g||_{\mathcal{H}^1(\mathbb{R})}. \tag{2.5}$$

One can recognize in Y_r a form of the regularized one dimensional Coulomb potential. In the following, our approach will be quite similar to the one of Loudon [L] in the sense that we let the regularizing parameter tend to zero. Note though that our parameter has a clear physical interpretation being given by the radius of the nanotube, and it is not just an artifact as in Loudon's case. Hence this will give us the exciton energies as functions of r, and allow us to estimate the errors we make using this approximation.

Define the quadratic form $C_0(.,.)$ by[1]

$$\begin{aligned} C_0(f,f) &:= -\int_0^{\infty} \ln(x)\cdot(|f|^2)'(x)dx + \int_{-\infty}^{0} \ln(-x)\cdot(|f|^2)'(x)dx \\ &= \int_{-\varepsilon}^{0} \ln(-x)\cdot(|f|^2)'(x)dx - \int_0^{\varepsilon} \ln(x)\cdot(|f|^2)'(x)dx \\ &+ \ln(\varepsilon)\left(|f(\varepsilon)|^2 + |f(-\varepsilon)|^2\right) + \int_{\mathbb{R}\setminus[-\varepsilon,\varepsilon]} \frac{1}{|x|}\cdot|f(x)|^2dx. \end{aligned} \tag{2.6}$$

[1] Notice that this definition of C_0 differs from the one of [CDR] in which there is an additional term: $2\ln 2|f(0)|^2 = \int_{-\infty}^{0} \ln 2\cdot(|f|^2)'(x)dx + \int_0^{\infty} \ln 2\cdot(|f|^2)'(x)dx$. This term is here put together with the other term depending on the function at zero.

Note the last equality is obtained by an integration by parts, and holds for all $\varepsilon > 0$; also note the appearance of a Coulomb potential in one dimension. Again from [CDR] we have

$$\langle f, Y_r g\rangle = -2\ln(r) f(0)\overline{g(0)} + C_0(f,g) + O(r^{4/9})||f||_{\mathcal{H}^1(\mathbb{R})}||g||_{\mathcal{H}^1(\mathbb{R})}. \tag{2.7}$$

Now let us define a new "potential" via a quadratic form

$$\langle f, V_C g\rangle := -2\ln(\frac{r}{2}) f(0)\overline{g(0)} + C_0(f,g),$$

which is close to V_{eff}^r when r is small and is exactly the Coulomb potential when we look away from the origin. We will see in the following that this particular potential gives a solvable eigenvalue problem for the associated Hamiltonian.

2.3.2 Boundary conditions of the Coulomb Hamiltonian

The operator H_C we will now consider is given by its associated quadratic form defined on $\mathcal{H}^1(\mathbb{R})$:

$$t_C(\psi,\phi) := \int_{\mathbb{R}} \overline{\phi'(x)}\psi'(x)dx + 2\left(2\ln(\frac{r}{2})\overline{\phi(0)}\psi(0) - C_0(\phi,\psi)\right).$$

One can recognize the kinetic energy in the first term and the potential V_C in the second term. The general theory of closed symmetric quadratic forms gives us the existence of an associated operator H_C defined by

$$t_C(\phi,\psi) = \langle \phi, H_C\psi\rangle, \tag{2.8}$$

whenever ψ is in the domain of H_C. The difficulty here is that V_C is not a usual Schrödinger-type multiplication potential, but due to various Sobolev embeddings it turns out that if ψ is in the domain of H_C then ψ'' is square integrable outside the origin, and we still have:

$$(H_C\psi)(x) = -\psi''(x) - \frac{2\psi(x)}{|x|}, \quad x \neq 0. \tag{2.9}$$

Now if ψ is an eigenfunction of H_C corresponding to an energy E, then it obeys the differential equation:

$$-\psi''(x) - \frac{2\psi(x)}{|x|} = E\psi(x), \quad x \neq 0. \tag{2.10}$$

In order to get the behavior at the origin of the eigenfunctions of H_C, we integrate by parts and use (2.10). For $\varepsilon > 0$ we have:

$$\begin{aligned} &\int_{\mathbb{R}} \overline{\phi'(x)}\psi'(x)dx \\ &= \overline{\phi(-\varepsilon)}\psi'(-\varepsilon) - \int_{-\infty}^{-\varepsilon} \overline{\phi(x)}\psi''(x)dx - \overline{\phi(\varepsilon)}\psi'(\varepsilon) - \int_{\varepsilon}^{\infty} \overline{\phi(x)}\psi''(x)dx \\ &+ \int_{-\varepsilon}^{\varepsilon} \overline{\phi'(x)}\psi'(x)dx \end{aligned} \tag{2.11}$$

where the last integral will converge to zero as ε goes to zero. On the other hand,

$$\begin{aligned} C_0(\phi,\psi) &= \int_{-\varepsilon}^{0} \ln(-x)\cdot(d_x(\overline{\phi}\psi))(x)dx - \int_0^{\varepsilon} \ln(x)\cdot(d_x(\overline{\phi}\psi))(x)dx \\ &+ \ln(\varepsilon)\left(\overline{\phi(\varepsilon)}\psi(\varepsilon) + \overline{\phi(-\varepsilon)}\psi(-\varepsilon)\right) + \int_{\mathbb{R}\setminus[-\varepsilon,\varepsilon]} \frac{1}{|x|}\cdot\overline{\phi(x)}\psi(x)dx. \end{aligned} \tag{2.12}$$

Then adding (2.11) with (2.12), using (2.10) and letting ε tend to zero (see [CDR] for technical details) we have:

$$\lim_{\varepsilon\to 0} t_C(\phi,\psi) = \langle\phi, E\psi\rangle + 2\lim_{\varepsilon\to 0}\overline{\phi(0)}\left[\frac{\psi'(-\varepsilon)-\psi'(\varepsilon)}{2} + 2\ln(\frac{r}{2})\psi(0) - \ln(\varepsilon)\left(2\psi(0)\right)\right].$$

Now using (2.8) and the eigenvalue equation $H_C\psi = E\psi$ we get the boundary condition:

$$\lim_{\varepsilon\to 0}\left[\frac{\psi'(-\varepsilon)-\psi'(\varepsilon)}{2} + 2\ln(\frac{r}{2})\psi(0) - 2\ln(\varepsilon)\psi(0)\right] = 0. \tag{2.13}$$

2.4 Eigenvalues and eigenfunctions

We now have to solve the equation

$$-\partial_x^2\psi - \frac{2}{|x|}\psi = E\psi, \qquad x \neq 0, \tag{2.14}$$

with the boundary condition (2.13). Similarly to Loudon in [L], we introduce a dimensionless quantity α and the change of variables

$$E = -\frac{1}{\alpha^2} \text{ and } x = \frac{\alpha}{2}z, \tag{2.15}$$

then we obtain

$$\frac{d^2}{dz^2}\widetilde{\psi} - \frac{1}{4}\widetilde{\psi} + \frac{\alpha}{|z|}\widetilde{\psi} = 0, \qquad z \neq 0. \tag{2.16}$$

The solutions are known for $z > 0$ and $z < 0$, see [AS, chap. 13] for example. The second thing is to see what condition at $z = 0$ should the eigenfunctions $\widetilde{\psi}$ obey. If we scale (2.13),

$$\lim_{\varepsilon\to 0}\left[\frac{\widetilde{\psi}'(-\varepsilon)-\widetilde{\psi}'(\varepsilon)}{2} + \alpha(\ln r - \ln(\alpha\varepsilon))\widetilde{\psi}(0)\right] = 0. \tag{2.17}$$

We only give here the results. Details of calculations can be found in [CDR]. If we take the only square integrable solution, we have two cases: If $\alpha = N$ is a positive integer, then the eigenstates are the odd functions $\widetilde{\psi}_{n_\alpha p}$ with associated eigenvalues $E_{n_\alpha p}$, where $n_\alpha = N + 1$,

$$\widetilde{\psi}_{n_\alpha p}(z) = e^{-\frac{1}{2}|z|}z\frac{1}{\sqrt{2N}}L^1_{N-1}(|z|), \qquad E_{n_\alpha p} = -\frac{1}{N^2},$$

where L^1_{N-1} is an associated Laguerre polynomial. Notice that these energies are independent of the radius of the tube. If α is not an integer, the eigenstates are the even functions $\widetilde{\psi}_{n_\alpha s}$ with associated eigenvalues $E_{n_\alpha s}$, where n_α is the smallest integer larger than α and:

$$\widetilde{\psi}_{n_\alpha s} = C_\alpha W_{\alpha,\frac{1}{2}}(|z|) = C_\alpha|z|e^{-\frac{1}{2}|z|}U(1-\alpha, 2, |z|) \qquad E_{n_\alpha s} = -\frac{1}{\alpha^2},$$

where C_α is a normalizing constant, W is the Whittaker function and U is the confluent hypergeometric function or Kummer function of the second kind. We denote with $\Gamma(z)$ and $\Psi(z) = \Gamma'(z)/\Gamma(z)$ the usual gamma and digamma functions, and we get from (2.17) that for even solutions α must satisfy the relation:

$$\Psi(1-\alpha) + 2\gamma + \frac{1}{2\alpha} - \ln\alpha + \ln r = 0. \tag{2.18}$$

From this relation, which contains an implicit expression for $\alpha(r)$, one can deduce several important facts. For all integers N and for α in between N and $N + 1$, there is only one solution of (2.16) satisfying the boundary condition. Furthermore, the energies associated with the non integer α tend to their closest lower integer when r tends to zero. A special case is the one of the ground state E_{1s} of the exciton which tends to minus infinity as the radius tends to zero. The behavior for small r is

$$E_{1s} \overset{r\to 0}{=} -4(\ln r)^2.$$

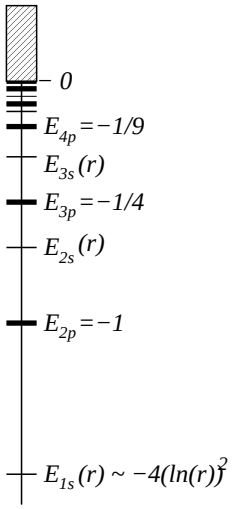

Figure 1: Energy of the bound states of the exciton. Energies are expressed in multiples of the effective Rydberg of the exciton.

Notice that equation (2.18) is exactly what one gets by explicitly calculating the condition requiring the derivative of even states to vanish at the origin, relation (3.22) in Loudon's paper, and replacing his parameter a by $r \cdot a_0/2$, for small r. We can also compare with the result from [BGEH] where Banyai et al. found numerically $a = 0.3a_0 \cdot r$ for the exciton problem in a quantum wire of radius r. The energies associated to the exciton are drawn on figure 1 and we calculated numerically the lowest four eigenvalues with respect to the radius on figure 3, along with a comparison of the ground state given by the variational method of [P1]. On figure 4 a zoom was made around the first and second excited states.

One can notice that the odd states possess a constant energy, independent of the radius. This is due to the fact that the odd states vanish at zero where there is the singularity of the potential. Indeed, the potential becomes, for an odd function f:

$$\langle f, V^r_{\text{eff}} f\rangle \simeq C_0(f, f),$$

which is independent of r.

3 Variational approach and comparison

The variational method operates by minimizing the energy of a trial function and is therefore usually applied to approximate the ground state. However, by restricting the trial function to forms that are orthogonal to the ground state, low lying excited states can be obtained variationally as well. In Ref. [P1], the variational method was applied to the ground state and in Ref. [P3] a similar approach was applied to calculate the $2p$ oscillator strength of interest for two-photon absorption. The $2p$ state is especially important because this state is used for excitation in two-photon fluorescence measurements [W]. By recording the energy of photons emitted from the lowest ($1s$) exciton, a direct measure of the $2p - 1s$ energy difference is obtained. In turn, the $1s$ exciton binding energy (i.e the 1s excitation energy measured relative to the band gap) can be derived if a reliable model for the exciton energy spectrum is invoked.

In the present work, we wish to compare results of the relatively complicated variational approach to the straight-forward and analytical Coulomb model. Hence, in the following we briefly explain the reasoning behind our variational estimate of the lowest excited ($2p$) state. In practical applications, the trial function must be sufficiently simple that calculation of the energy is manageable. This implies that relatively few adjustable parameters should be considered. At

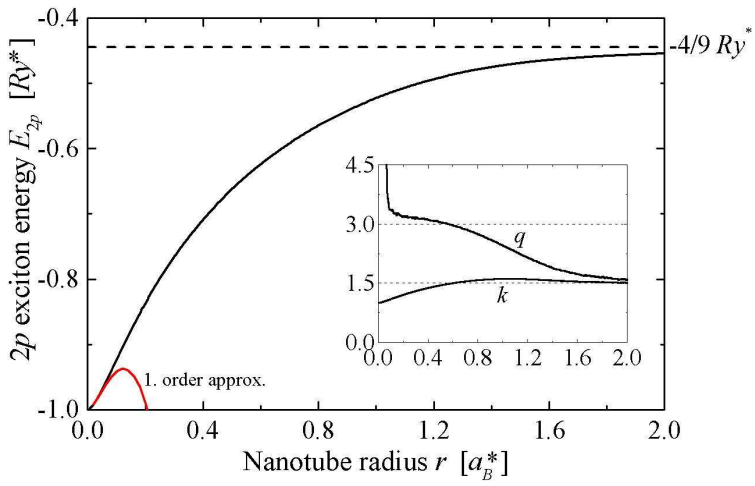

Figure 2: Variational $2p$ state energy as a function of nanotube radius. Inset: the r-dependence of decay lengths k and q of the trial wave function.

the same time, a certain flexibility is required to provide reasonable accuracy. A useful strategy consists in constructing trial functions so that they correctly accommodate the known solutions in limiting cases of the general problem. Thus, we are guided by the analytical solution for the plane, i.e. for nanotube radii much larger than the effective Bohr radius. In our units, this state is simply $\varphi_{2p} \propto x \exp\{-2/3(x^2+y^2)^{1/2}\}$. On the other hand, in the extreme 1D limit we expect $\varphi_{2p} \propto x \exp\{-|x|\}$. To accommodate both limits, we consequently suggest the (un-normalized) trial form

$$\varphi_{2p}(x,y) = x \exp\{-(x^2/k^2 + y^2/q^2)^{1/2}\}, \tag{3.1}$$

where q and k are variational parameters to be determined by minimizing the expectation value of the energy . This expectation value is found as $E_{2p} = (K - V)/N$, where K, V and N are the kinetic energy, potential energy and normalization constant, respectively. The integrations are quite cumbersome and only K and N can be obtained in closed form in terms of Struve and modified Bessel functions. The potential energy V is evaluated numerically using Gaussian quadrature.

The minimized energy as a function of radius r is illustrated in Fig. 2. The limiting values are $E_{2p} = -1$ and $E_{2p} = -4/9$ for small and large r, respectively, in agreement with the analytic solutions in these limits. In between these limits, the curve interpolates smoothly between the limiting values and the dominant correction at small r is $-8(1+\gamma+\ln(r))r^2$.

In order to judge the usefulness of the different approaches used in the present work it is essential to determine the appropriate nanotube radius r in excitonic units, i.e. in units of a_B^*. An important point in this respect is that, in fact, a_B^* varies between different nanotubes. The relation needed for conversion is $a_B^* = 0.529\text{Å}\varepsilon/\mu$, where ε is the dielectric constant screening the Coulomb interaction and μ is the reduced effective mass. Whereas ε may be assumed the same for all nanotubes, μ must be derived from the curvature of the band structure and, hence, depends on both radius and chirality of the nanotube. However, detailed studies [P2] show that a_B^* is roughly proportional to the nanotube diameter and as a consequence r (in units of a_B^*) is nearly constant and given by $r \approx 0.1 a_B^*$ if $\varepsilon \approx 3.5$. It should be noted, though, that in media with little screening a larger r/a_B^* is expected. The smallness of r means that approximations based on expansion around $r = 0$ are expected to be accurate.

In figure 3 and 4, a comparison of variational energies and the results of the Coulomb model is given. In both the $1s$ and $2p$ cases, reasonable agreement between the two approaches is found

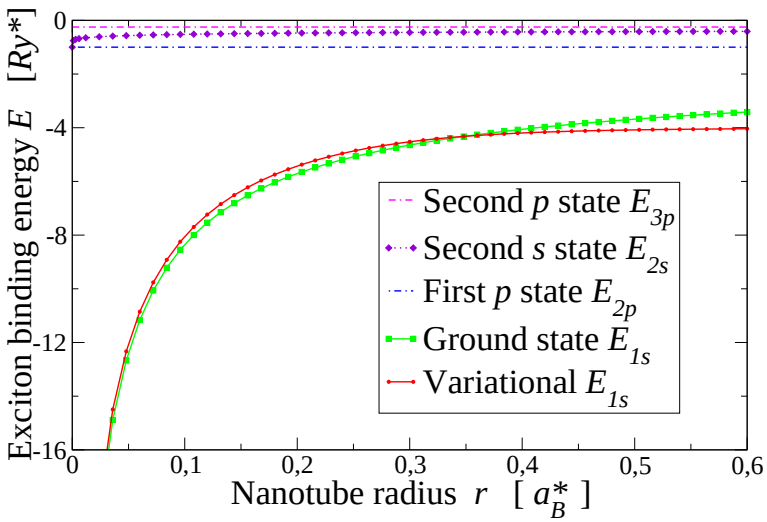

Figure 3: Energy of the four lowest bound states of the exciton with respect to the radius. Even states were calculated numerically using (2.18). Notice that the energy of the second s state is equal to the one of the first p state at zero. In red: graph of the ground state computed with the variational method on the cylinder from [P1].

around $r \approx 0.1a_B^*$. Also, in both cases, the variational result lies slightly higher than the Coulomb model. The ground state has deviated by more than 100% from the plane value for radii around $0.1a_B^*$. An error of less than 5% is seen between the curves at this point. Note that if the curve from the Coulomb model is lower in energy than the variational one, this does not means that the approximation is better. Although in the variational approach the lower is the better since the exact solution is always below the variational result, in the Coulomb model the exact value is somewhere around the approximation, bounded by an error bound. In this work the error bound was not calculated because, unfortunately, the compromises made to get a simple formula implied a difficult calculus to optimize on the bound, even by numerical computations. For the first excited state, the Coulomb model approximation for the energy is independent of the radius of the tube. This must be a good approximation for very small radii. However, this approximation becomes increasingly inaccurate as the radius increases, as the exact value should tend to the energy of the problem on the plane with energy equal to $-4/9a_B^*$ as do the variational curve.

4 Conclusion

The Coulomb model applied to excitons in carbon nanotubes demonstrates that the energy associated with each even state decreases to the energy of its closest odd state as the radius tends to zero. Since each odd state energy is independent of the size of the tube in this approach, all energies associated to excited states stay in the range $(-1, 0)$ (in effective Rydberg energy units). So only the ground state diverges when the radius gets smaller. This is confirmed by the behavior of the first variational excited state which converges to -1. The simple exciton model proposed in this paper and studied both by means of rigorous perturbation theory and by a variational approach is a good starting point for attacking the difficult problem of electron-electron interactions in low dimensional structures such as carbon nanotubes.

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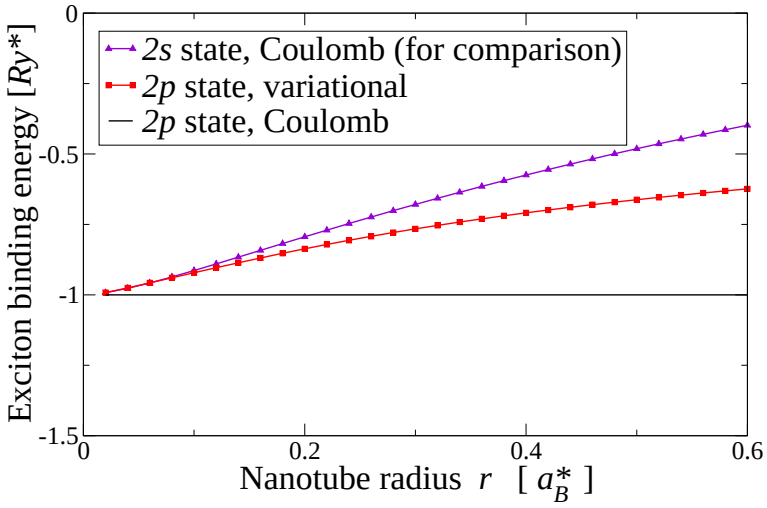

Figure 4: Zoom around the energy of the $2p$ state showing both variational and Coulomb model results. In addition, the $2s$ state obtained with Coulomb model is included for comparison.

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