

## Nonvariational approach to impurity states in quantum wires

J.F. Jan and Y.C. Lee

*Department of Physics, State University of New York at Buffalo, Amherst, New York 14260*

D.S. Chuu

*Electrophysics Department, National Chiao Tung University, Hsinchu, Taiwan 30050, Republic of China*

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While the binding energy and the ground-state wave function of a hydrogenic impurity in a strictly one-dimensional or three-dimensional system can be exactly calculated, the case of finite but small ( $a \leq a_B$ ) or large ( $a > a_B$ ) wire radius  $a$  is not amenable to an exact treatment, and is usually left to the variational method as the only resort. However, the amount of computation involved in variational calculations is large and its accuracy is sometimes difficult to assess. We have developed reliable and physically motivated perturbative approaches specifically to treat the  $a \leq a_B$  and  $a > a_B$  situations. The close agreement of our results with those from variational methods lends support for our simpler method as an alternative to the variational approach.

There has been a great deal of interest<sup>1-6</sup> in the quasi-one-dimensional (Q1D) systems or so-called quantum wires, which restrict electrons to moving in one dimension. Recent progresses<sup>5,6</sup> in growth and fabrication techniques have made possible the fabrication of quantum wires with radii less than 100 Å. Theoretically,<sup>7-16</sup> the electronic properties of a hydrogenic impurity in a quantum wire have been discussed by many researchers. Loudon<sup>7</sup> found the binding energy of a strictly one-dimensional hydrogen atom to be infinite. Brown and Spector<sup>10</sup> discussed the binding energies of impurities as a function of the well width of the quantum wire with infinite or finite potential barrier. The effect of location<sup>10,11</sup> of impurities with respect to the wire axis was also discussed. The shapes<sup>12,13</sup> of the circular or rectangular quantum wires, with equal cross sections, were found to have no significant effect on the binding energies. In the presence of a longitudinal magnetic field,<sup>17-19</sup> the binding energies were predicted to be higher than the values without magnetic fields.

Most approaches<sup>9,10</sup> to finding the ground state of an impurity in a Q1D wire depended on the variational method. However, the construction of variational trial wave functions is based entirely on physical intuition. It is difficult to estimate the accuracy of the results from variational approaches. It would be most desirable to have an alternative approach to the quantum wire problem to serve as an independent check. Yet, as soon as the radius of the wire deviates from zero (one-dimensional wire) or infinite (three-dimensional wire), the problem becomes not exactly soluble and it is often hard to devise suitable approximation scheme to get at the solution. In this paper, we shall develop two nonvariational methods to treat the small-wire and the large-wire cases separately.

The Hamiltonian for a hydrogenic impurity in a quantum wire is given by

$$H = \frac{P^2}{2m} - \frac{e^2}{\epsilon\sqrt{Z^2 + \rho^2}} + V(\rho), \quad (1)$$

where  $m$  is the electron effective mass,  $\epsilon$  is the static dielectric constant, and  $V(\rho)$  is the confining potential. In this paper, we shall use the infinite-barrier model for the confinement potential. Then  $V(\rho)$  is zero if  $\rho < a$  and infinite if  $\rho > a$ ,  $a$  being the radius of the wire. The Schrödinger equation of this system, in general, cannot be solved analytically due to the Coulomb potential. However, for a 1D quantum wire, this problem can be solved exactly with the Hamiltonian

$$H = \frac{P^2}{2m} - \frac{e^2}{\epsilon|Z|}. \quad (2)$$

The  $z$  motion is found to be extremely localized at the ion's position, producing a minus infinity ground state energy. The ground state wave function for a strictly 1D hydrogen atom is

$$\Psi_{\text{grd}}(Z) \propto \frac{1}{\sqrt{\beta a_B}} e^{-\frac{Z}{\beta a_B}}, \quad (3)$$

$$E_{\text{grd}} \propto -\frac{1}{\beta^2}, \quad \beta \rightarrow 0. \quad (4)$$

This is obtained<sup>7</sup> by solving the 1D hydrogen atom with a truncated Coulomb potential  $V = -2/(|Z| + a)$  and then letting  $a$  approach zero. The relation between  $\beta$  and  $a$  is given by  $\beta = 1/2 \ln(\frac{a_B}{a})$ .

In a real but small wire system of radius  $a$ , the potential energy  $V$  is approximately given by  $\frac{-e^2}{\sqrt{Z^2 + a^2}}$ , which is qualitatively similar to the truncated potential. Then the factor  $\beta$  can be rewritten as  $\beta = 1/2 \ln(\frac{a_B}{a})$ . Accordingly,<sup>7</sup> based on Eq. (3) the potential energy  $\langle V \rangle$  is roughly  $-\frac{4\hbar^2}{ma_B^2} [\ln(\frac{a_B}{a})]^2$  and the kinetic energy is still given by the virial theorem,  $\langle T_Z \rangle = -\frac{1}{2}\langle V \rangle$ . A cautionary remark about the uncertainty relation for  $z$  motion is in order here. With kinetic energy  $\langle T_Z \rangle = (\Delta P_Z)^2/2m$ , we identify  $\Delta P_Z \sim \frac{2\hbar}{a_B} [\ln(\frac{a_B}{a})]$ . From Eq. (3), the wave function spread is  $\Delta Z \sim \beta a_B \sim a_B/2 \ln(\frac{a_B}{a})$ . Hence the uncertainty relation  $\Delta Z \Delta P_Z \sim \hbar$  is satisfied. On the other hand, if we write as usual  $\langle T_Z \rangle \sim \Delta P_Z^2/2m$ ,

$\langle \Delta Z \rangle \sim \hbar / \Delta P_Z$ , and the potential energy  $\langle V \rangle$  naively as  $\frac{e^2}{\langle \Delta Z \rangle}$ , minimization of  $\langle T_Z \rangle + \langle V \rangle$  by adjusting  $\langle \Delta Z \rangle$  would lead to a wrong result because  $V \sim \langle \frac{-1}{\Delta Z} \rangle \neq \frac{-1}{\langle \Delta Z \rangle}$  due to the fluctuation in Q1D systems.

Physically, along the radial ( $\rho$ ) direction, the wave function is dominated by the behavior of a particle confined in an infinitely deep but narrow well. The radial motion then includes the kinetic energy  $\langle T_\rho \rangle \sim \hbar^2 / 2ma^2$  and the ground state wave function  $J_0(\frac{X_{01}}{a}\rho)$ , where  $X_{01}$  corresponds to the first root of the zeroth order Bessel function  $J_0$ . The  $\rho$ -motion energy  $\langle T_\rho \rangle \sim \frac{1}{a^2}$  will go to infinity much faster than the above mentioned  $Z$ -motion energy  $\langle T_Z \rangle \sim (\ln \frac{a_B}{a})^2$ . Similarly, the binding Coulomb potential energy in the  $Z$  motion,  $\langle V \rangle \sim -(\ln \frac{a_B}{a})^2$ , is also much weaker than  $\langle T_\rho \rangle$ . Accordingly, we are motivated by the above physical considerations to first average out the fast  $\rho$  motion and then treat the remaining  $Z$  motion. To implement this idea, it is then reasonable to assume a factorized form for the ground-state wave function

$$\Psi(Z, \rho) \propto J_0\left(\frac{X_{01}}{a}\rho\right) \psi(Z). \quad (5)$$

The validity of such a factorized form in the limit of  $\lambda a \ll 1$ , implied by the variational trial function  $\Psi(\rho, Z) \propto \cos(\frac{\pi Z}{L})e^{-\lambda\sqrt{\rho^2+Z^2}}$  was pointed out by Bastard in a quasi-two-dimensional problem.<sup>20</sup> However, as we shall see, the averaging out of the fast  $\rho$ -motion based on  $\Psi(\rho, Z)$  of Eq. (5) will effectively extend its range of validity to beyond  $a \sim a_B$ , seen later to be consistent with the variational result in this range. This is not totally unexpected, since a physical averaging generally irons out the inaccuracies in the wave function. In fact, when we compare the  $\rho$ -component kinetic energy  $T_\rho = \frac{\hbar^2 X_{01}^2}{2ma^2}$  to the  $Z$ -component kinetic energy  $T_z \approx \frac{1}{2}|V| = \frac{2\hbar^2}{ma_B}(\ln \frac{a_B}{a})^2$  we see that  $T_\rho > T_z$  for  $a < 1.89a_B$ , which constitutes the range of validity for the averaging process.

With the factorized wave function in Eq. (5) and the Hamiltonian in Eq. (1), the Schrödinger equation  $H\Psi(Z, \rho) = E\Psi(Z, \rho)$  takes the form

$$\left[ \frac{P_\rho^2}{2m} + V(\rho) + \frac{P_Z^2}{2m} - \frac{e^2}{\sqrt{Z^2 + \rho^2}} \right] J_0\left(\frac{X_{01}}{a}\rho\right) \psi(Z) = EJ_0\left(\frac{X_{01}}{a}\rho\right) \psi(Z). \quad (6)$$

Multiplying by  $J_0(\frac{X_{01}}{a}\rho)$  and integrating over  $\rho$  from  $\rho = 0$  to  $\rho = a$ , we get

$$\left[ -\frac{d^2}{dZ^2} + N^2 \int_0^a \frac{-2}{\sqrt{Z^2 + \rho^2}} \rho J_0^2\left(\frac{X_{01}}{a}\rho\right) d\rho \right] \psi(Z) = \left( E - \frac{X_{01}^2}{a^2} \right) \psi(Z). \quad (7)$$

Hence, we define

$$V_{\text{eff}}(Z) = N^2 \int_0^a \frac{-2}{\sqrt{Z^2 + \rho^2}} \rho J_0^2\left(\frac{X_{01}}{a}\rho\right) d\rho \quad (8)$$

with  $a_B = \epsilon \hbar^2 / me^2$  as unit length, and  $\mathcal{R} = e^2 / 2\epsilon a_B$  as unit energy. The factor  $N$  is the normalization constant defined by

$$\frac{1}{N^2} = \int_0^a \rho J_0^2\left(\frac{X_{01}}{a}\rho\right) d\rho. \quad (9)$$

This equation can be considered as for a 1D atom in an effective Coulomb potential  $V_{\text{eff}}(Z)$ , which is seen to be an average of 3D Coulomb attraction over the fast  $\rho$  motion of the electron. Due to the finite value of the averaged  $\rho^2$ , this  $V_{\text{eff}}$  is weaker than the 1D Coulombic  $-\frac{e^2}{Z}$ .

An advantage of the effective potential is that there is no singularity in  $V_{\text{eff}}$  for all  $Z$ . It leads to a much simpler mathematic problem. Note that once the factorized form of  $\Psi(Z, \rho)$  in Eq. (5) is established for finite wire radius  $a$ , the concept of the effective potential  $V_{\text{eff}}(Z)$  of Eqs. (7),(8) is exactly valid, containing no more mathematical approximation. The results of solving Eqs. (7),(8) directly by numerical method are shown in Fig. 1. The binding energy was found to be larger and larger for smaller and smaller well width  $a$ , which agrees with the results of other works.<sup>9</sup> In the large well width limit, however, our method of effective potential ceases to be valid because the decoupled wave function is no longer viable.

To gain more insight into  $V_{\text{eff}}(Z)$  of Eq. (8) and its relation to the decoupled wave function in Eq. (5), we approximate the effective potential  $V_{\text{eff}}$  by a simple form

$$V'_{\text{eff}}(Z) \approx \frac{-2}{\sqrt{Z^2 + \bar{\rho}^2}}, \quad (10)$$

which serves to define  $\bar{\rho}$ , the average position in  $\rho$  direction. For a given radius  $a$ , the value of  $\bar{\rho}$  is calculated to make the simple effective potential  $V'_{\text{eff}}(Z)$  of Eq. (10) best resemble the averaged potential  $V_{\text{eff}}(Z)$  of Eq. (8). In our calculation listed in Table I, the average position  $\bar{\rho}$  is found to be considerably smaller than the well width  $a$ , validating thus the factorized form in the limit  $\lambda \bar{\rho} < 1$ ,

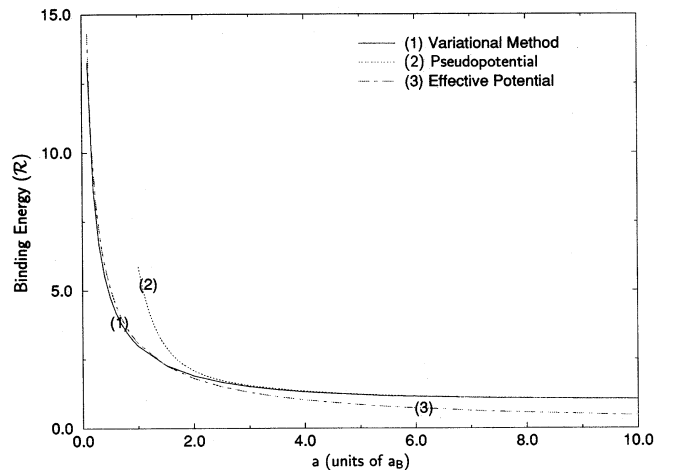


FIG. 1. The binding energies are plotted as a function of the well width  $a$  for (1) variational method, (2) pseudopotential method, (3) effective-potential method.

TABLE I. Averaged  $\rho$  position in  $V_{\text{eff}}$ .

$a(a_B)$	$\bar{\rho}(a_B)$
0.01	0.0037
0.05	0.0155
0.10	0.0463
0.50	0.2222
1.00	0.4153
1.50	0.5765
2.00	0.7077

instead of merely  $\lambda a < 1$ . Our numerical results in Fig. 1 indeed show that the effective potential gives rise to results in close agreement with the variational method up to  $a \sim 2a_B$ .

Figure 2 shows the effective potentials and the ground-state energies for different values of well width. For finite well widths, the effective potentials are truncated due to the nonzero value of  $\bar{\rho}$ , and hence there is no pole for the entire range of  $Z$ . However, the effective potentials become the 1D Coulomb potential as the well radius  $a$  approaches zero. The square of the ground state wave function  $\psi(Z)$  is plotted in Fig. 3 which shows the gradual spreading and flattening of  $\psi(Z)$  as the radius  $a$  increases. The wave functions we obtained are consistent with Loudon's result,<sup>7</sup> Eq. (5).

The variational trial wave function used by many researchers<sup>9,10</sup> is

$$\Psi(\rho, Z) \propto J_0\left(\frac{X_{01}}{a}\rho\right) e^{-\lambda\sqrt{Z^2+\rho^2}}, \quad (11)$$

where  $\lambda$  is the variational parameter. The binding energies obtained by such variational methods are also shown in Fig. 1 for comparison. When the well width  $a$  is smaller than  $a_B$ , the results from the variational method is indeed very close to that of our method of effective potential. Thus, the decoupling of the wave function which is expected to be more valid in the range  $a < a_B$ , is amply justified by the agreement of these two results. The

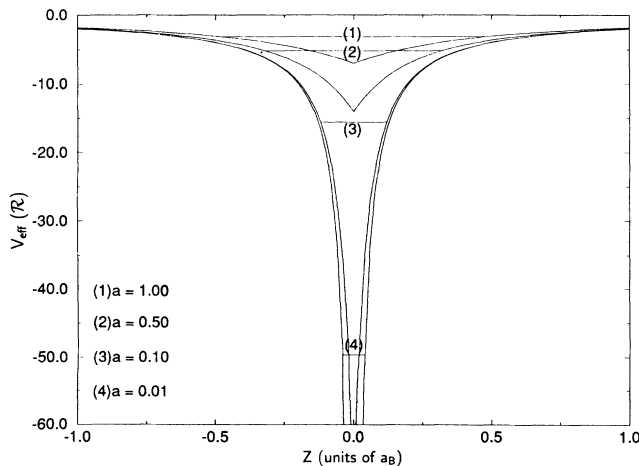


FIG. 2. Effective potential of Eq. (13) for the well width (1)  $a = 1.00$ , (2)  $a = 0.50$ , (3)  $a = 0.10$ , (4)  $a = 0.01$  ( $a_B$ ). The ground-state energies are also shown in this figure.

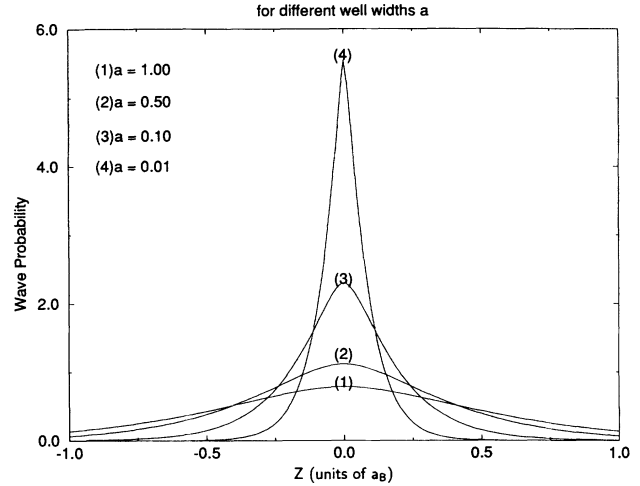


FIG. 3. The square of wave function  $w(z)$  in arbitrary units by solving Eq. (12) for (1)  $a = 1.00$ , (2)  $a = 0.50$ , (3)  $a = 0.10$ , (4)  $a = 0.01$  ( $a_B$ ).

probability densities for the trial functions for different well widths are shown in Fig. 4. The wave functions obtained by the variational method and by our method are again very close. However, the wave function by our effective-potential method is slightly sharper than the function by the variational method. This is because the variational function was devised to fit the full range of the well width, while our effective potential is specifically devised for  $a < a_B$ . This difference could affect the optical transition matrix elements for slender quantum wires. On the other hand, the close agreement of our results to that of the variational calculation even in the range  $a_B < a \leq 2a_B$  as shown in Fig. 1 is a pleasant surprise. This is attributed to the ironing out of the inaccuracies of the decoupled wave function Eq. (5) in this range as a consequence of the averaging that yields  $V_{\text{eff}}(Z)$  of Eq. (8).

In the large well width limit ( $a > a_B$ ), the boundary

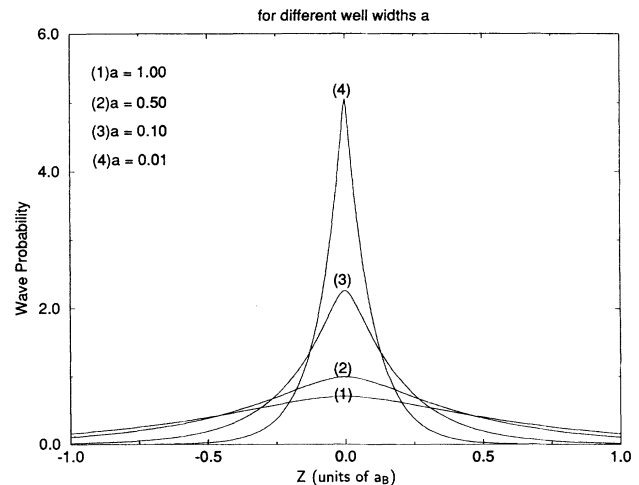


FIG. 4. The square of the  $z$ -component wave function in arbitrary units in Eq. (16) for (1)  $a = 1.00$ , (2)  $a = 0.50$ , (3)  $a = 0.10$ , (4)  $a = 0.01$  ( $a_B$ ).

has only a slight effect on the exponentially decaying electronic wave function of the impurities. The physical reason is the following. In the absence of an attraction center (an ionic core at the origin), the electron wave function is a standing wave which vanishes at  $\rho = a$ . When the well width shrinks, the standing-wave-like eigenfunction will be much affected by the changing of the well width. On the other hand, a hydrogenlike ground-state function will not be influenced too much due to the exponentially decaying behavior of the wave function ( $e^{-\sqrt{Z^2+\rho^2}}$ ) at large  $\rho$  ( $a_B \ll \rho \ll a$ ). The ground-state energy  $E_{\text{grd}}(e^2 \neq 0)$  associated with such a decaying wave function will not change much by decreasing  $a$ . Being the difference of the energies in the above two situations, the binding energy will thus be slightly larger than the usual  $1 \mathcal{R}$  (for  $a = \infty$ ) for large but finite wells ( $a_B < a < \infty$ ).

Conventional perturbation theories, however, cannot be readily adapted to obtain the energy correction as the radius  $a$  decreases from  $\infty$  to finite but large values. Here, we use the pseudopotential method<sup>21</sup> specifically devised for such problems. The boundary condition for the wave function is  $\Psi(Z, \rho) = 0$  for  $\rho \geq a$ . This condition can be shown to be exactly reproduced by a pseudopotential  $H' = -\delta(\rho - a)(\frac{\partial}{\partial \rho})|_{\rho=a^-}$ . Hence, the Schrödinger equation becomes an ordinary second order differential equation but with the added pseudopotential term

$$\left( -\nabla^2 + \frac{-2}{\sqrt{Z^2 + \rho^2}} - E \right) \Psi(\rho, Z) = \delta(\rho - a) \left( \frac{\partial \Psi}{\partial \rho} \right) \Big|_{\rho=a^-}, \quad (12)$$

which now is valid for all values of  $\rho$ . As long as the boundary potential barrier is not located too close as to jam the ionic Coulombic well significantly, it is physically clear that the modifications to the eigenenergy and wave functions will not be major ones. Perturbation treatment based on the pseudopotential  $H'$  should be then valid. However, the ordinary perturbation theory again cannot

be applied to such an artificial perturbative term. This is because the total energy correction is given by

$$\Delta E = \frac{\langle \psi^0 | H' | \psi^0 + \Delta \psi^0 \rangle}{\langle \psi^0 | \psi^0 + \Delta \psi^0 \rangle} \quad (13) \\ \approx \langle \psi^0 | H' | \psi^0 \rangle + \langle \psi^0 | H' | \Delta \psi^0 \rangle,$$

in which the wave function correction term  $|\Delta \psi^0\rangle$  cannot be neglected since it is approximately equal to  $|\psi^0\rangle$  at the boundary  $\rho = a$ , where  $H'$  is dominant. In contrast to the conventional perturbation theory, the actual first order correction due to  $H'$  is then given by<sup>21</sup>

$$\Delta E \approx 2 \langle \psi^0 | H' | \psi^0 \rangle. \quad (14)$$

The binding energies calculated by using Eqs. (12) and (14) is also plotted in Fig. 1. We note that in the range  $a > 2a_B$  our result practically coincides with that from the variational method, thereby attesting to the reliability of both methods. Indeed, it is amazing to see how the variational result bridges our two results, one for small  $a$ , the other for large  $a$  as shown in Fig. 1.

In this paper, we have calculated the binding energies and ground-state wave functions for quantum wire systems by the use of physically motivated perturbation methods specifically designed to treat quantum wires of small ( $a \leq a_B$ ) or large ( $a > a_B$ ) radii. The averaged effective potential method is especially suited to the narrow quantum wire problem, and the pseudopotential method is tailored to the large wire system ( $a > a_B$ ). The implementation is much simpler than the variational method as far as the amount of computation is concerned. These methods provide clear physical descriptions for the electron behaviors in both the small and large wire limits in that the electrons in a small wire are seen perturbatively to be extremely localized, while in a large wire they naturally behave like a 3D hydrogen atom. The excellent agreement between our results and those from the variational method lends comforting support for our method as an alternative to the variational approach.

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