Effect of axial electric field on the binding energy of a shallow hydrogenic impurity in a Quantum Well Wire

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Abstract: We present a study of the effect of an electric field on the binding energy of a shallow hydrogenic impurity in GaAs/Ga\textsubscript{1-x}Al\textsubscript{x}As quantum well wires. The wire is considered to be of length \(L\) and radius \(R\) and the electric field \(F\) is applied along the \(z-\)axis, the axis of the wire.

1 Introduction

The development of the epitaxial crystal growth techniques such as molecular beam epitaxy and metal-organic chemical vapor deposition has made the growth of the quasi-two-dimensional (quantum well), quasi-one-dimensional (quantum well wire), or quasi-zero-dimensional (quantum dot) become possible [1,2,3].

Several studies have investigated the optical and transport properties based on the calculated electronic structure of these systems in the presence of shallow impurities (see for example references [4-9]).

Regarding the quantum well wire (QWW), the binding energy of hydrogenic impurities in a QWW has been calculated as a function of the wire radius in case of no fields applied[7,8]. Also, Branis et al [10] considered the case of a magnetic field applied parallel to the wire axis. They found that for a given value of the magnetic field, the binding energy is larger than that of the zero-field case.

In this work we have considered the case of an electric field applied along the wire axis, we have calculated the binding energy of the ground state of a hydrogenic impurity located at the wire axis. A variational approach has been utilized with a trail wave function containing a hydrogenic part. The
other part of the variational function which represents the wave function in the absence of the impurity has been calculated analytically in terms of Bessel and Airy functions.

2 Electron Eigenstates

Consider a quantum well wire of length L and radius R (of dimension comparable to de Broglie’s wavelength), with an electric field of strength F applied along the axis of the wire. The Hamiltonian for such a system is given by:

\[ H = -\frac{\hbar^2}{2m_e} \nabla^2 + |e|Fz + V(\rho, z), \]  

(1)

where

\[ V(\rho, z) = \begin{cases} 
0, & \rho \leq R \text{ and } |z| \leq \frac{L}{2} \\
\infty, & \rho > R \text{ or } |z| > \frac{L}{2}, 
\end{cases} \]  

(2)

We have used the cylindrical coordinates such that the origin is taken at the mid point of the wire axis, which is considered as z-axis.

The Schrödinger equation takes the form

\[ \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial \psi}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2 \psi}{\partial \phi^2} + \frac{\partial^2 \psi}{\partial z^2} - \frac{2m_e|e|F}{\hbar^2} z \psi = -\frac{2m_eE_0}{\hbar^2} \psi. \]  

(3)

Assuming that

\[ \psi = \Phi(\phi)\zeta(z)\Re(\rho), \]  

(4)

and noting that the problem is rotational invariant (\( \Phi(\phi) = e^{im\phi} \)), then Eq. (3) takes the form

\[ \frac{1}{\Re \rho \frac{d}{d\rho}} \left( \rho \frac{d}{d\rho} \right) - \frac{m^2}{\rho^2} + \frac{1}{\zeta} \frac{d^2 \zeta}{dz^2} - \frac{2m_e|e|F}{\hbar^2} z = -\frac{2m_eE_0}{\hbar^2}. \]  

(5)

The radial part is

\[ \Re(\rho) = J_m(k_{nm}\rho), \]  

(6)

where \( J_m \) is the ordinary Bessel function.

Accordingly the axial part \( \zeta(z) \) is found to satisfy the equation

\[ \frac{1}{\zeta} \frac{d^2 \zeta}{dz^2} - \frac{2m_e|e|F}{\hbar^2} z + \frac{2m_eE_0}{\hbar^2} - k_{nm}^2 = 0. \]  

(7)
To solve this equation, we assume that
\[
\tilde{z} = G \tilde{\bar{z}} \left( G \bar{z} - \frac{2m_e E_0}{\hbar^2} + k_{nm}^2 \right),
\] (8)
where
\[
G = \frac{2m_e |e| F}{\hbar^2}.
\] (9)
Substituting from Eq. (8) into Eq. (7) we obtain the equation
\[
\frac{d^2 \zeta}{d \tilde{z}^2} = \tilde{z} \zeta,
\] (10)
which is Airy’s equation. The solution of Eq. (10) is a linear combination of the Airy functions \(Ai(\tilde{z})\) and \(Bi(\tilde{z})\). (Cetina and Montenegro [12]) Thus, the final form of \(\psi(\underline{r})\) is taken as
\[
\psi_{nm}(\underline{r}) = Ne^{i\varphi} J_m(k_{nm} \rho) \left[ Bi(\tilde{z}) - \frac{Bi(\xi_l)}{Ai(\xi_l)} Ai(\tilde{z}) \right],
\] (11)
where \(\xi_l = \tilde{z} (z = \frac{-L}{2})\). The form of \(\zeta(z)\) in Eq. (11) has been chosen so that \(\psi\) vanishes at \(z = \frac{-L}{2}\). We still need to satisfy the boundary conditions (Vanishing of the wave function at the boundaries)
\[
\psi(\rho = R) = 0, \quad \psi \left( z = \frac{L}{2} \right) = 0.
\] (12)
The first gives
\[
J_m(k_{nm} R) = 0.
\] (13)
For the ground state \((m = 0, \ n = 1)\), which is considered in this work, the above equation implies
\[
k_{10} R = 2.4048,
\] (14)
where the R.H.S. is the first root of \(J_0(x) = 0\). Also, the second condition in Eq.(12) yields
\[
Bi(\xi_h)Ai(\xi_l) = Bi(\xi_l)Ai(\xi_h),
\] (15)
where \(\xi_h = \tilde{z} (z = \frac{L}{2})\).

The energy states can consequently be obtained by solving the transcendental Eq. (15). The energy of the ground state will be denoted by \(E_0\).
2.1 Impurity Eigenstates

We consider the problem of a hydrogenic impurity located at $\rho = z = 0$. The trial wave function for the ground state is taken as

$$\psi = NJ_0(k_{10}R)(Bi(\tilde{z}) - \frac{Bi(\xi)}{Ai(\xi)}Ai(\tilde{z}))e^{-\lambda\sqrt{\rho^2+z^2}}. \quad (16)$$

The normalization condition leads to

$$N^{-2} = 2\pi \int_{\rho=0}^{R} \int_{z=-L}^{L} d\rho dz \rho J_0^2(k_{10}\rho)\left(\frac{Bi(\xi)}{Ai(\xi)}Ai(\tilde{z})\right)^2 e^{-2\lambda\sqrt{\rho^2+z^2}} \quad (17)$$

The potential energy $\langle V \rangle$ is

$$\langle V \rangle = \langle \psi | \frac{-e^2}{\epsilon_0 \sqrt{\rho^2+z^2}} | \psi \rangle = 2\pi N^2 \left(\frac{e^2}{\epsilon_0}\right) \int_{\rho=0}^{R} \int_{z=-L}^{L} d\rho dz \rho J_0^2(k_{10}\rho) \sqrt{\rho^2+z^2} \times \left(\frac{Bi(\tilde{z})}{Ai(\xi)}\right)^2 e^{-2\lambda\sqrt{\rho^2+z^2}}. \quad (18)$$

Putting the potential energy in unit of Rydberg $R_b$ and length in unit of Bohr radius $a_B$, $\langle V \rangle$ takes the form

$$\langle V \rangle = -4\pi N^2 \int_{\rho=0}^{R} \int_{z=-L}^{L} d\rho dz \rho e^{-2\lambda\sqrt{\rho^2+z^2}} \times J_0^2(k_{10}\rho) \left(\frac{Bi(\tilde{z})}{Ai(\xi)}\right)^2. \quad (19)$$

To calculate the kinetic energy $\langle T \rangle$ we first calculate $\nabla^2 \psi$ as

$$\psi = \psi_1 \psi_2,$$

where

$$\psi_1 = e^{-\lambda\sqrt{\rho^2+z^2}}$$

and

$$\psi_2 = J_0(k_{10}\rho) \left(\frac{Bi(\tilde{z})}{Ai(\xi)}\right).$$
Hence
\[ \nabla^2 \psi = (\nabla^2 \psi_1)\psi_2 + \psi_1(\nabla^2 \psi_2) + 2(\nabla \psi_1)(\nabla \psi_2), \tag{20} \]
but
\[ (\nabla^2 - Gz)\psi_2 = -\frac{2m_e E_0}{\hbar^2}\psi_2 \tag{21} \]
and
\[ \nabla^2 \psi_1 = \left( \lambda^2 - \frac{2\lambda}{\sqrt{\rho^2 + z^2}} \right)\psi_1. \tag{22} \]

We then evaluate the term
\[
2\langle \psi | \nabla \psi_1 \nabla \psi_2 \rangle = 2 \int d\phi dz d\rho \rho (\partial_{\psi_1}^2 \partial_{\psi_2}^2 + \partial_{\psi_1} \partial_{\psi_2}) \\
= \frac{1}{2} \int d\phi dz d\rho \rho \left( \frac{-\lambda \rho}{\sqrt{\rho^2 + z^2}} \right) \partial_{\psi_2}^2 \\
+ \frac{1}{2} \int d\phi dz d\rho \rho \left( \frac{-\lambda z}{\sqrt{\rho^2 + z^2}} \right) \partial_{\psi_2}^2. \tag{23} \]

Integrating the first term by parts with respect to \( \rho \) and the second term by parts with respect to \( z \) and using the boundary conditions (vanishing of \( \psi_2 \) at the boundary) we get
\[
2\langle \psi | \nabla \psi_1 \nabla \psi_2 \rangle = -2\lambda^2 \int d\phi dz d\rho \rho \psi_2^2 + 2\lambda \int d\phi dz d\rho \rho \sqrt{\rho^2 + z^2} \psi_1^2 \psi_2^2. \tag{24} \]

Using Eq. (21), Eq. (22), and Eq. (24), we get
\[
-\frac{\hbar^2}{2m_e} \langle \psi | \nabla^2 - Gz | \psi \rangle = E_0 + \frac{\hbar^2 \lambda^2}{2m_e}. \tag{25} \]

Putting Eq. (25) in units of Rydberg \( R_b \) and length in units of Bohr radius \( a_B \) and adding to \( \langle V \rangle \), the total energy is
\[
\langle H(R, L, F) \rangle = E_0 + \lambda^2 + \frac{4A}{\Delta T} \tag{26} \]

where
\[
A = \int_{\rho = 0}^{R} \int_{z = -L}^{L} d\rho dz \rho e^{-2\lambda \sqrt{\rho^2 + z^2}} J_0^2(K_{10}\rho) \left( Bi(\tilde{z}) - \frac{Bi(\tilde{\xi})}{Ai(\tilde{\xi})} Ai(\tilde{\xi}) \right)^2. \tag{27} \]
Minimizing $\langle H(R, F, L) \rangle$ with respect to $\lambda$, we obtain the total energy, and the binding energy is thus

$$E_b = E_0 - \langle H(R, F, L) \rangle = -\lambda^2 - \frac{4A}{d\lambda}$$  \hfill (28)

3 Results and Discussions

The variation of the binding energy with the electric field strength $F$ and the wire radius $R$ are given in figures (1) and (2) respectively. The results displayed in Figure(1) show that for a wire of fixed dimensions $L$ and $R$ the binding energy decreases as the strength of the applied electric field increases. This is due to the fact that the increase of the electric field causes the electron to be less confined to the impurity and accordingly reduces the binding energy. Also the results in figures (1), (2) indicate that for a fixed electric field the binding energy increases as the wire radius decreases until it diverges as $R \to 0$. The divergence of the binding energy occurs since the infinite confining potential of the well forces the electron and the impurity to become very close as $R \to 0$. The same behavior has been previously pointed out in the absence of the electric field (ref[7]).

4 Conclusions

The binding energy of the hydrogenic donor impurity decreases as the strength of the applied electric field increases. It behaves with the variation of the wire radius in a similar manner to the case of no electric field applied.

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Figure 1: Variation of the binding energy in Rydberg ($R_b$) units as a function of the electric field strength $F$ (kV/cm). The wire length $L = 3\ a_B$, while three values of the wire radius are considered $0.50\ a_B$, $0.75\ a_B$, and $1.00\ a_B$.

Figure 2: Variation of the binding energy $E_b$ in Rydberg $R_b$ units as a function of the wire radius $R$ in Bohr radius $a_B$ units, where, $F = 10kV/cm$, and $L = 3a_B$. 