Wigner Function for a Quantum Wire with an Impurity

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Abstract

We present the Wigner function for a Gallium Arsenide (GaAs) quantum wire subjected to a magnetic field with an off-center donor impurity. The Wigner function is more sensitive to detecting changes than the variational wavefunction for smaller scale differences in the radial position of the impurity a the quantum wire. We used an infinite potential at the boundary of the quantum wire.

Introduction

A system consisting of an electron bound to a donor ion, with infinite potential barrier at the surface is present in a magnetic field parallel to the wire axis. Its Hamiltonian is given by

$$H = \frac{[\vec{p} + \frac{e}{c}\vec{A}]^2}{2m^*} - \frac{e^2}{\varepsilon_0 |\vec{r} - \vec{r}_0|} + V(\rho, \phi) \qquad (1)$$

where $|\vec{r} - \vec{r}_0| = \sqrt{\rho^2 + \rho_0^2 - 2\rho\rho_0 \cos(\phi - \phi_0) + z^2}$

$V(\rho,\phi) = \begin{cases} 0, & 0 \le \rho \le R \\ \infty, & \rho > R \end{cases}$ is confining potential

Z is the separation of the electron from the ion along the wire axis

$\vec{r}_0$ is the impurity ion position

$\vec{A}(\vec{r})$ is the magnetic-field potential

For a magnetic field parallel to the wire axis

$$\vec{A}(\vec{r}) = A_\phi = \frac{B\rho}{2}$$

Following Branis, Li, and Bajaj[1] and Brown and Spector[2], we can get wavefunction

$$\psi(\vec{r}) = \begin{cases} N \exp[-\frac{\xi}{2}]\, {}_1F_1(-a_{01}, 1, \xi) \times \exp[-\lambda\sqrt{(\rho-\rho_0)^2 + z^2}] & 0 \le \rho \le R \\ 0 & \rho > R \end{cases} \qquad (2)$$

where $N^{-2} = -2\pi \frac{dA}{d\lambda}$

$$A = \int_o^R \rho \exp(-\frac{\rho^2}{2\alpha_c^2}) \times {}_1F_1^{\,2}(-a_{01}, 1; \frac{\rho^2}{2\alpha_c^2}) K_0(2\lambda|\rho - \rho_0|)\, d\rho$$

$$\xi = \frac{\rho^2}{2\alpha_c^2}$$

$$\alpha_c^2 = \sqrt{\frac{\hbar c}{eB}}$$

λ is a variational parameter

K_0 is the modified Bessel function of the second kind of order zero

${}_1F_1(-a_{01}, 1, \xi)$ is the general form of the confluent hypergeometric function. We can calculate a_{01} according to the boundary condition

$$\psi(\rho = R) = 0$$

The binding energy $E_b(R,B)$ of the hydrogenic impurity is

$$E_b(R,B) = -\frac{\hbar^2}{2m^*}\lambda - \frac{2e^2}{\varepsilon_0}\frac{A}{dA/d\lambda} \qquad (3)$$

For computational purposes, we normalize the expression for the binding energy $E_b(R,B)$ in units of impurity Rydberg:

$$R_B = \frac{m^* e^4}{2\varepsilon_o^2 \hbar^2} = \frac{e^2}{2\varepsilon_o a_B} \qquad (4)$$

Where $a_B = \frac{\varepsilon_0 \hbar^2}{m^* e^2}$ (5)

is the electron Bohr radius

And let

$$\rho = tR \quad ; \quad \rho_0 = t_0 R$$

Sensitivity of Wigner Function

When the donor impurity is placed at different positions off the quantum wire axis, the wavefunction will change. As we can see in the figure, Wigner Function is very sensitive to detecting changes at smaller scale differences.

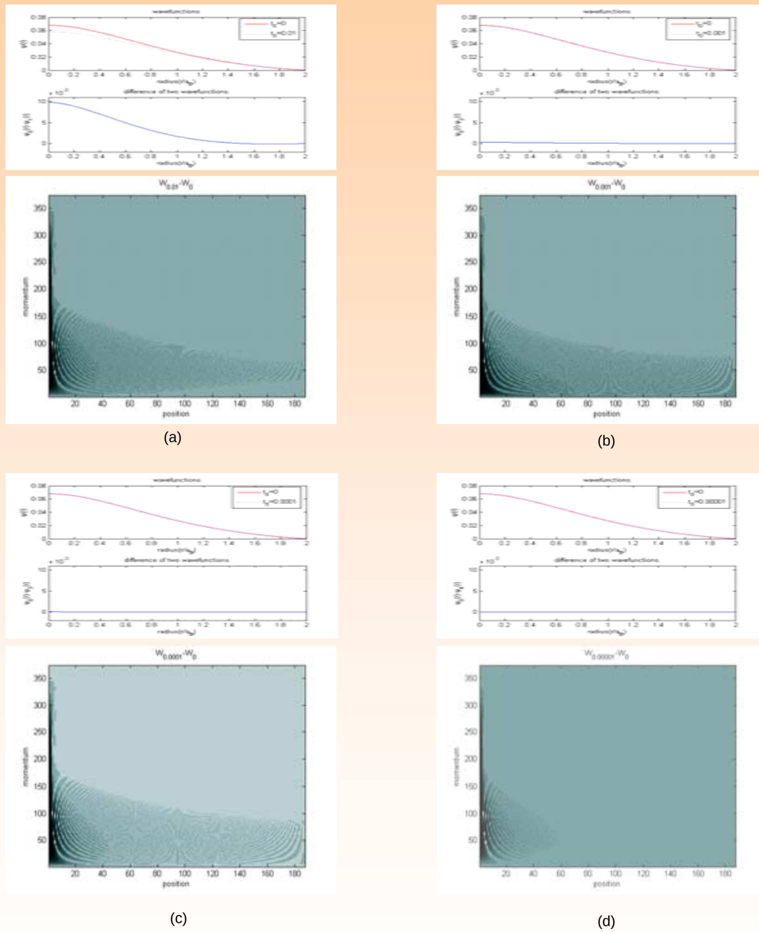

Figure 1: Variational wavefunctions and the Wigner functions for different impurity locations in a quantum wire (a)t0 =0 ; 0.01; (b) t0 =0;0.001; (c) t0=0.0;0.0001; (d) t0=0.0;0.00001.
In (a) and (b) the wavefunctions are different while the Wigner functions look nearly the same; the opposite happens in (c) and (d) when the variations are smaller by one or two orders of magnitude.

In that way binding energy is

$$E_b(R,B) = -(\lambda a_B)^2 - 4a_B \frac{C}{dC/d\lambda} \qquad (6)$$

Where

$$C = \int_0^1 t \exp(-t^2 \xi_R) K_0(2\lambda R t)\, dt$$

Now we can search for a lower bound of the binding energy with respect to λ using numerical method.

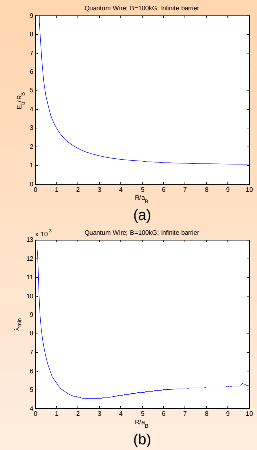

Figure 2: Binding Energy (a) and variational parameter λ (b) vs quantum wire radius when B=100KG, a_B=98A, R_B=5.8meV

Conclusions

The Wigner function is more sensitive to detecting changes than the wavefunction for smaller scale differences in a quantum wire with an off-center impurity. Also, varying the relative separation along the quantum wire axis between the ion impurity and the electron just changes the scale of the wavefunction.

References

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