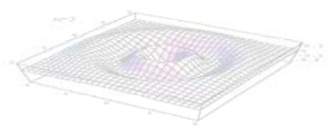


Wigner Function for an Impurity in a Parabolic Quantum Dot

Majd Mayyasi, Gary Snyder, Praveen Nittala, Tomas Materdey

University of Massachusetts Boston, Boston, MA 02125

Abstract

High sensitivity of quantum dots with impurities can be linked with phase space high sensitivity to initial conditions. We present the Wigner function for an impurity in a parabolic quantum dot obtained from a variational wavefunction.

Description

We study a nanostructure system consisting of a Gallium Arsenide (GaAs) quantum dot with an off-center donor impurity. The system is confined within an infinite spherical potential and due to the off-center impurity, will display a Columbic potential in addition to the classical parabolic potential. The resulting Hamiltonian of the system looks like:

$$H = \frac{1}{2m^*}\vec{P}^2 - \frac{e^2}{\varepsilon_0 \left|\bar{r} - \bar{r}_0\right|} + \frac{1}{2} m^* \omega_p^2 r^2 + V(\bar{r}) \qquad (1)$$

Where:

m^* = effective mass of the electron with the impurity

$\vec{r}_0$ = position of the impurity ion

ω_p = the harmonic oscillator frequency

And $V(\vec{r})$ is the spherical potential confinement defined as:

$$V(\vec{r}) = \begin{cases} 0 & 0 \le r \le R \\ \infty & r > R \end{cases} \qquad (2)$$

To simplify our calculations and analysis, all units of length are taken to be the Bohr radius $a_B = \hbar^2 \varepsilon_0 / m^* e^2$ and all units of energy are taken to be the Rydberg $R_B = m^* e^4 / 2\hbar^2 \varepsilon_0^2$. For GaAs, these values and other constants of the Hamiltonian equation can be numerically obtained: $m^* = 0.067 m_e$, $\varepsilon_0 = 12.5$, $a_B = 9.87$ nm, $R_B = 5.83$ meV. Using these simplifications, the Hamiltonian of Eq. (1) becomes:

$$H = -\nabla^2 - \frac{2}{\left|\vec{r} - \vec{r}_0\right|} + \gamma_p^2 r^2 \qquad (3)$$

Where $\gamma_p = \hbar\omega_p / 2R_B$ is the dimensionless measure of the parabolic potential. The solution to the Hamiltonian above has been found to be of the following form:

$$\psi(\vec{r}) = \begin{cases} N e^{(-\gamma_p^2/2)}\, {}_1F_1(-a_{0,} \frac{3}{2}; \gamma_p^2 r^2)\, e^{(-\lambda\left|\vec{r} - \vec{r}_0\right|)} & r \le R \\ 0 & r > R \end{cases} \qquad (4)$$

${}_1F_1$ is the confluent hypergeometric function that can be expanded into an infinite series. This series converges under certain conditions satisfied by our wave equation. Furthermore, the wave equation must satisfy boundary the conditions:

$${}_1F_1(-a_{0,} \frac{3}{2}; \gamma_p^2 R^2) = 0 \text{ , at } r = R \qquad (5)$$

The variable lambda is a variational parameter, and the resulting values for it are determined by minimizing the binding energy *Eb*, where the binding energy is the difference between the ground state energy of the system with no impurity *Eo* and the energy of the system with the impurity *E*.

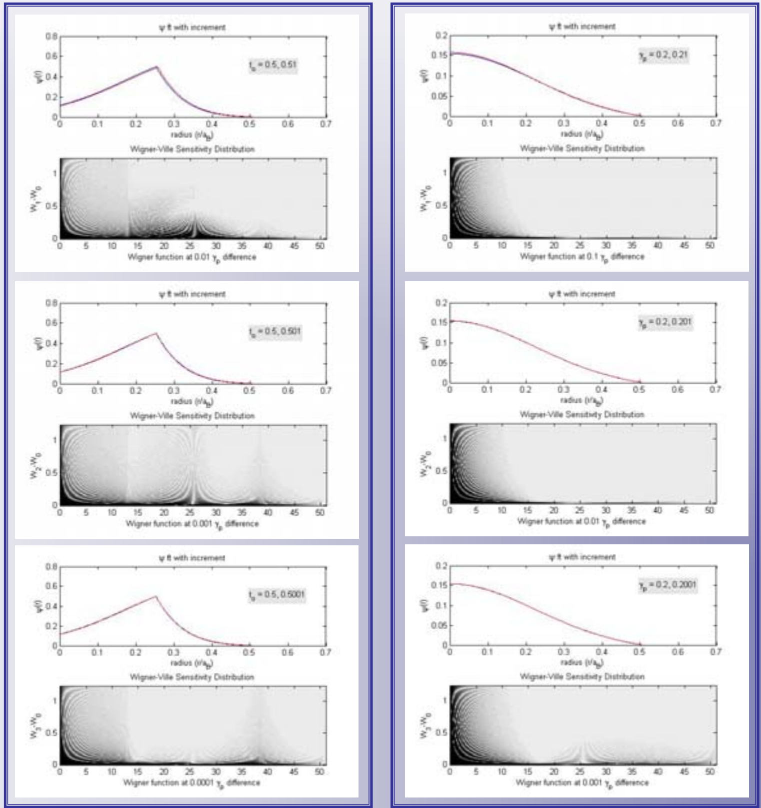
$$Eb = Eo - E \qquad (6)$$

Once a value of lambda is determined, we use the resulting Schrödinger wave equation to analyze sensitivity to small changes in impurity. We also implement the Wigner function for our case to analyze the same sensitivities and compare our results. The Wigner function resulting from a single-particle Schrödinger equation is found using the following transformation:

$$f(x, v, t) = \frac{m}{2\pi\hbar} \int_{-\infty}^{+\infty} e^{-i\frac{mv\Delta}{\hbar}} \Psi^*(x - \frac{\Delta}{2}, t)\Psi(x + \frac{\Delta}{2}, t)\, d\Delta \qquad (7)$$

Graphs and Analysis

Taking the variational analysis into consideration, we find a graphical solution to the Schrödinger wave equation. As the impurity location varies, so does the wave distribution. As the impurity dislocation decreases, the wave equation no longer conveys changes. However, when the same wave functions are filtered through the Wigner function transformation, the resulting phase space distribution demonstrates visible differences where the wave equation fails.



Conclusion

Finite differences are visible in the Wigner function transformations of a wavefunction that are otherwise invisible to the wavefunction itself. In conclusion, the Wigner function is more sensitive to detecting changes than the wavefunction for relatively smaller scale differences in GaAs quantum dots with an off-center donor impurity.

Objective

The Wigner distribution function is a mathematical transform of the density matrix which approaches the classical distribution function as the system becomes classical. This representation of the statistical state has proven to be useful in modeling quantum-effect devices. In our analysis, we show that the Wigner transformation is sensitive to minute impurity changes in a quantum nanostructure that would otherwise be hidden from the standard Schrödinger wave equation.

Procedure

The variational parameter λ is studied for minimum values of the binding energy. The two are related as follows:

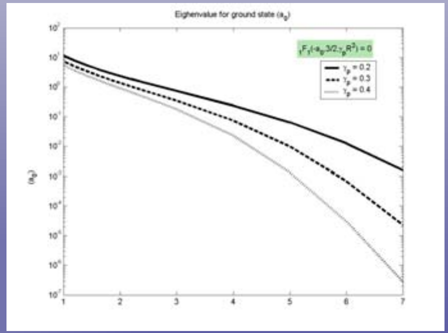
$$E_b = -\lambda^2 - 4\lambda \frac{D}{C} \qquad (8)$$

Where

$$C = \int_0^1 t e^{(-\gamma_p R^2 t^2)}\, {}_1F_1^2(-a_{0,} \frac{3}{2}; \gamma_p R^2 t^2) \left\{[2\lambda R|t - t_0| + 1] e^{(-2\lambda R|t - t_0| + 1)} - [2\lambda R(t + t_0) + 1] e^{(-2\lambda R(t + t_0))}\right\} dt$$

$$D = \int_0^1 t e^{(-\gamma_p R^2 t^2)}\, {}_1F_1^2(-a_{0,} \frac{3}{2}; \gamma_p R^2 t^2) \left\{e^{-2\lambda R(t + t_0)} - e^{-2\lambda R|t - t_0|}\right\} dt \qquad (9)$$

Ground state eigenvalues for varying values of γ_p, are plotted:



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