Calculating single-electron states in quantum dots

Simulations of quantum transport in nanoscopic systems
Nanomaterials Engineering

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Contents

Aim

The aim of this exercise is to calculate single-electron states in two-dimensional quantum dots using the Galerkin method. The potential profile of the quantum dot is modelled as a harmonic oscillator. The goal is to implement numerical methods for solving the generalized eigenvalue problem arising from the Schrödinger equation, and to analyse the resulting wavefunctions and energies.

1 Methods

Calculations were carried out in *Python* using the *NumPy* and *Matplotlib* libraries, along with *linalg* functions from *SciPy*. The complete code is available in the GitHub repository.

2 Results

The exercise is divided into four main tasks: 1) implementing and visualizing basic Gaussian functions; 2) computing eigenvalues of the Schrödinger equation and plotting the first six QD states; 3) calculating the energies of the ten lowest states as a function of ω_x; 4) determining a value of ω_y such that the lowest 5 states are only excited in the x direction.

2.1 Basic Gaussian functions

The Gaussian basis function used in the calculations is defined as:

$$\varphi_k(x,y) = \frac{1}{(\alpha_x\pi)^{1/4}} \exp\left(-\frac{(x-x_k)^2}{2\alpha_x}\right) \cdot \frac{1}{(\alpha_y\pi)^{1/4}} \exp\left(-\frac{(y-y_k)^2}{2\alpha_y}\right). \tag{1}$$

Examples of the basis functions for k = 0, 8, 9 are shown in Figure 1.

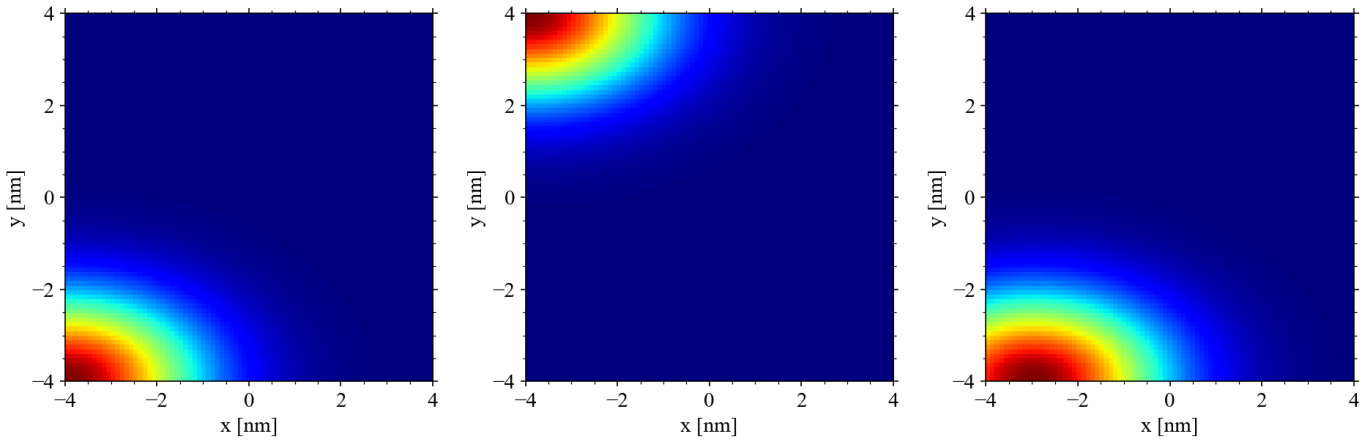

Figure 1: Maps of the three basis functions k = 0, 8, 9.

2.2 Eigenvalues of the Schrödinger equation

The first six quantum dot states were calculated using the *SciPy.linalg.eigh()* function for $\Delta x = 1$. Maps of squared modulus of the wavefunction are shown in Figure 2.

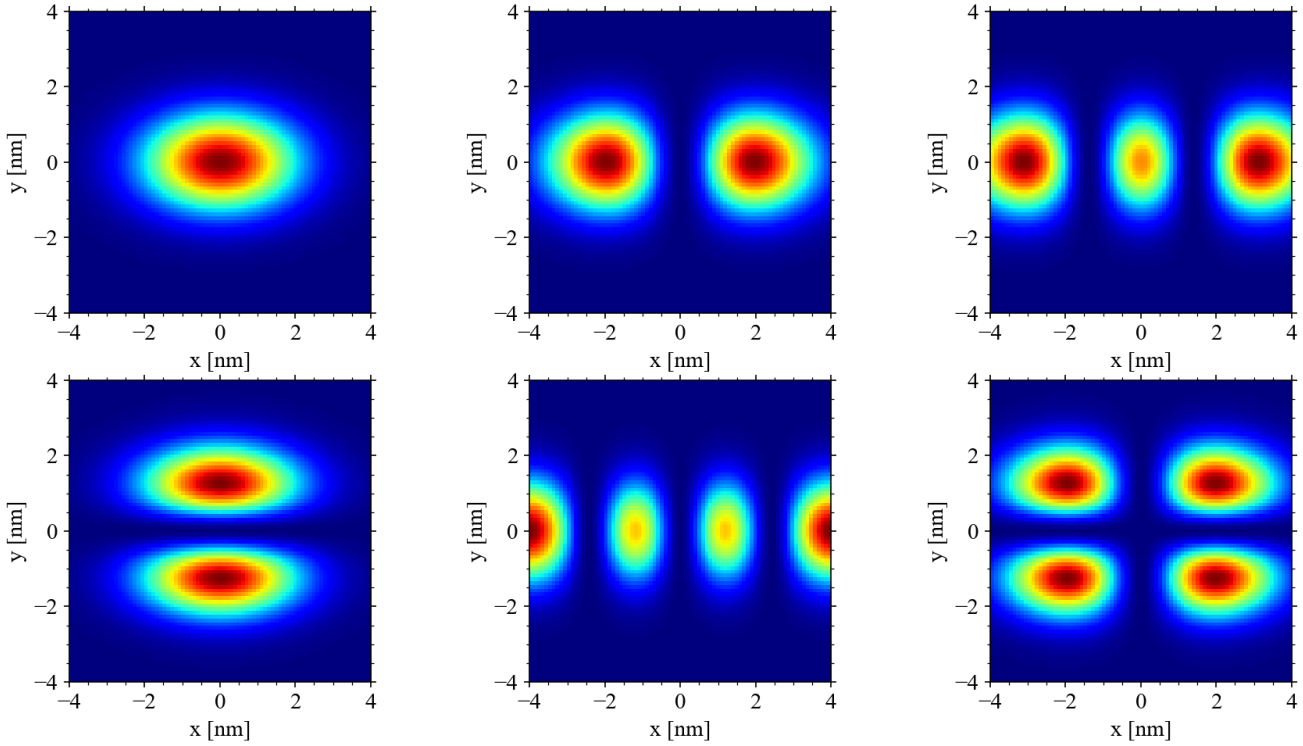

Figure 2: Maps of squared modulus of the wavefunction of 6 lowest states for Δx = 1 nm.

2.3 Energies

The calculated energies of the ten lowest quantum dot states as a function of ω_x are shown in Figure 3. Distinct energy jumps can be observed, which are associated with excitations in the y-direction. The ground state energy follows a smooth, linear trend, indicating no excitations in the perpendicular direction.

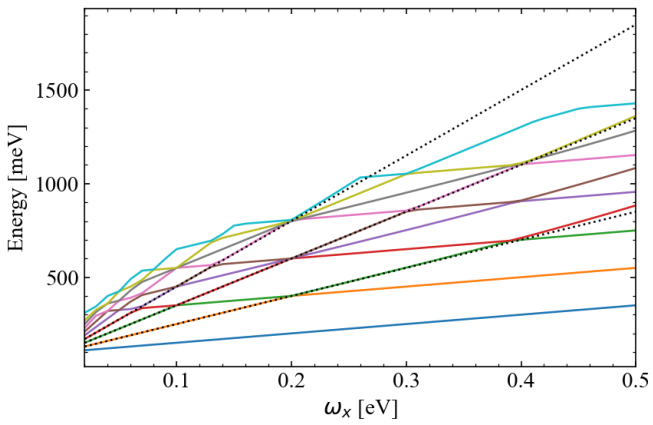

Figure 3: Energies of 10 lowest states as a function of ω_x for ω_y = 200 meV and Δx = 1 nm. Dotted black lines show selected analytical energies.

2.4 Excitation in the x direction

Using formula for eigenenergies[1]:

$$E_n = \hbar\omega_x(\frac{1}{2} + n_x) + \hbar\omega_y(\frac{1}{2} + n_y), \quad n_x, n_y \geq 0, \tag{2}$$

it can be calculated that for $\omega_y = 350$ meV, the energies of the first five states are oriented in the x-direction. This phenomenon is shown in Figure 4. Similar images are presented in the cited article, which confirms that QD states can be successfully described using the harmonic oscillator model.

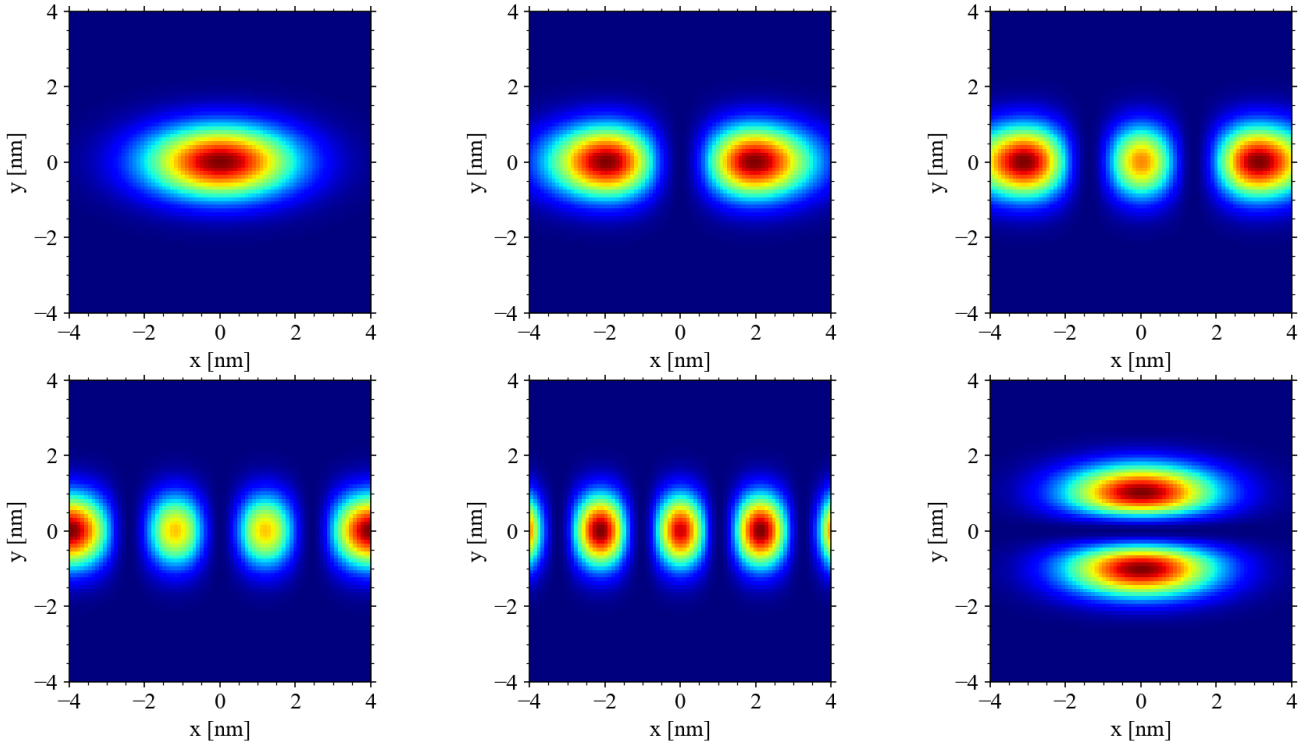

Figure 4: Maps of squared modulus of the wavefunction of 6 lowest states for $\omega_y = 350$ meV.

[1]Teichmann, K., Wenderoth, M., Prüser, H., Pierz, K., Schumacher, H. W., & Ulbrich, R. G. (2013). Harmonic Oscillator Wave Functions of a Self-Assembled InAs Quantum Dot Measured by Scanning Tunneling Microscopy. Nano Letters, 13(8), 3571–3575. doi:10.1021/nl401217q