Calculating single-electron states in quantum dots

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1 Introduction

The topic of this project is the calculation of electron states confined in quantum dots. We consider two-dimensional (2D) quantum dot with harmonic oscillator potential profile, which works well for the description of semiconductor quantum dots (due to the high excitation energy in the z direction, effectively electrons are in the ground state in z, so we need to consider only the x and y dimensions).

The problem comes down to solving the Schrödinger equation

$$\hat{H}\Psi(\vec{r}) = E\Psi(\vec{r}) \tag{1}$$

and finding the eigenenergies E and eigenfunctions Ψ.

1.1 The Galerkin method

In the Galerkin method the wave function is expanded in a basis

$$\Psi(\vec{r}) = \sum_{i=1}^{N} c_i \varphi_i(\vec{r}), \tag{2}$$

where $\varphi_i(\vec{r})$ are the basis functions, and c_i the linear expansion coefficients. We require that the residual, evaluated as

$$\varepsilon = \hat{H}\Psi(\vec{r}) - E\Psi(\vec{r}), \tag{3}$$

is minimized. We convert the equation to the weak form by calculating the scalar products with the basis functions; the residual is orthogonal to each of the basis functions. We obtain the equation

$$\sum_{i=1}^{N} \langle\varphi_j|\hat{H}|\varphi_i\rangle c_i = E \sum_{i=1}^{N} \langle\varphi_j|\varphi_i\rangle c_i, \tag{4}$$

that in the matrix form reads

$$\mathbf{Hc} = E\mathbf{Sc}, \tag{5}$$

which is a generalized eigenproblem.

1.2 Calculations for two-dimensional harmonic oscillator

The 2D Hamiltonian in atomic units has the form

$$\hat{H} = -\frac{1}{2m^*}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + V(x,y), \tag{6}$$

where for 2D harmonic oscilator $V(x,y) = \frac{1}{2}m^*(\omega_x^2 x^2 + \omega_y^2 y^2)$, and m^* is the electron effective mass in a semiconductor.

We will use the Gaussian basis

$$\varphi_k(x,y) = \frac{1}{(\alpha_x\pi)^{1/4}} \exp\left(-\frac{(x-x_k)^2}{2\alpha_x}\right) \frac{1}{(\alpha_y\pi)^{1/4}} \exp\left(-\frac{(y-y_k)^2}{2\alpha_y}\right), \tag{7}$$

where $\mathbf{r}_k = (x_k, y_k)$ is the position of the center of the Gaussian function, and α_x, α_y describe its width.

For the calculation of bound states we need to calculate the elements of matrices **H** and **S**. For the Gaussian basis, it is convenient to calculate them analytically. In 2D they are given by

$$S_{kl} = \int_{-\infty}^{\infty} \varphi_k(x,y)\varphi_l(x,y)dxdy = \exp(-\tfrac{(x_k-x_l)^2}{4\alpha_x} - \tfrac{(y_k-y_l)^2}{4\alpha_y}), \tag{8}$$

$$H_{kl} = K_{kl} + V_{kl}, \tag{9}$$

$$K_{kl} = -\tfrac{1}{2m}\int_{-\infty}^{\infty} \varphi_k(x,y)\left(\tfrac{\partial^2}{\partial x^2} + \tfrac{\partial^2}{\partial y^2}\right)\varphi_l(x,y)dxdy = -\tfrac{1}{2m}\left[\tfrac{(x_k-x_l)^2-2\alpha_x}{4\alpha_x^2} + \tfrac{(y_k-y_l)^2-2\alpha_y}{4\alpha_y^2}\right] S_{kl}, \tag{10}$$

$$V_{kl} = \tfrac{1}{2}m\int_{-\infty}^{\infty} \varphi_k(x,y)\left(\omega_x^2x^2 + \omega_y^2y^2\right)\varphi_l(x,y)dxdy = \tfrac{1}{2}m\left[\omega_x^2\tfrac{(x_k+x_l)^2+2\alpha_x}{4} + \omega_y^2\tfrac{(y_k+y_l)^2+2\alpha_y}{4}\right] S_{kl}. \tag{11}$$

1.3 Tasks

We will create a grid of $n \times n$ equally spaced nodes with positions in the interval $x \in [-a, a]$, $y \in [-a, a]$. The node spacing is Δx. Each node is a center of one Gaussian function (7); there are $N = n^2$ nodes in total. Let us assume $n = 9$ and $\hbar\omega_x = 80$ meV, $\hbar\omega_y = 200$ meV (in atomic units the energy is expressed in $E_h = 27211$ meV and $\hbar = 1$, so in our program $\omega_x = 80/E_h$ etc., and the position unit is Bohr radius $a_0 = 0.0529$ nm). We will assume $\alpha_{x(y)} = \frac{\hbar}{m^*\omega_{x(y)}}$ and effective mass $m^* = 0.24$[1].

1. Create arrays of the node positions $x_k, y_k, k = 0, \ldots, N-1$. The grid is two dimensional with indices (i, j), so we map the two indices to a single index $(i, j) \to k$, e.g. by $k = i \cdot n + j$, $i, j = 0, \ldots, n-1$. Conversion of k to $i, j : i = k/n$ (integer number division – in Python `k // n`), $j = k\%n$.

   $$x_k = x_{i(k)} = -a + \Delta x \cdot i, \quad i = 0, \ldots, n-1,$$

   $$y_k = y_{j(k)} = -a + \Delta x \cdot j, \quad j = 0, \ldots, n-1.$$

   Implement the functions (7) returning the kth Gaussian, centered at x_k, y_k, as a function of (x, y). For a test, we will plot maps of a few basis functions with $\Delta x = 1$ nm i $n = 9$, and $a = \Delta x \cdot (n-1)/2$. (Note that the (x, y) points should be on a denser grid, e.g. with the spacing 0.1 nm). Plot three of the basis functions, e.g. $k = 0, 8, 9$.

2. Implement the calculation of arrays of matrix elements of the overlap integral matrix **S** and the Hamiltonian **H** using (8-11), for general ω_x, ω_y, etc., passed as function parameters. Solve the generalized eigenproblem numerically using a library of your choice (in Python you can use `scipy.linalg.eigh`, in C e.g. z `gsl_eigen_gensymmv` of the GSL library, in C++ also e.g. `GeneralizedSelfAdjointEigenSolver` from the `Eigen` library).

3. For $\Delta x = 1$ nm calculate the squared modulus of the wave functions of 6 lowest states and plot their maps (use the functions (7) you implemented and the expansion coefficients c_i obtained as the eigenvectors from the generalized eigenvalue problem).

4. Calculate energies of 10 lowest states as a function of $\hbar\omega_x \in [0, 500]$ meV and $\omega_y = 200$ meV, and plot them. With dashed lines plot analytical energies for a few lowest states.

5. Compare the results with the experimental work [2]; the STM measurement results for the states confined in a quantum dot are shown in Fig. 1. Try to choose a value of ω_y such that the lowest 5 states are only excited in the x direction and calculate the wave functions again (task 3).

[1] This is the effective mass measured in the publication Nano Letters for InAs quantum dots embedded in AlAs.

[2] K. Teichmann *et al*, *Harmonic oscillator wave functions of a self-assembled InAs quantum dot measured by scanning tunneling microscopy*,Nano Lett. 13, 8 (2013).

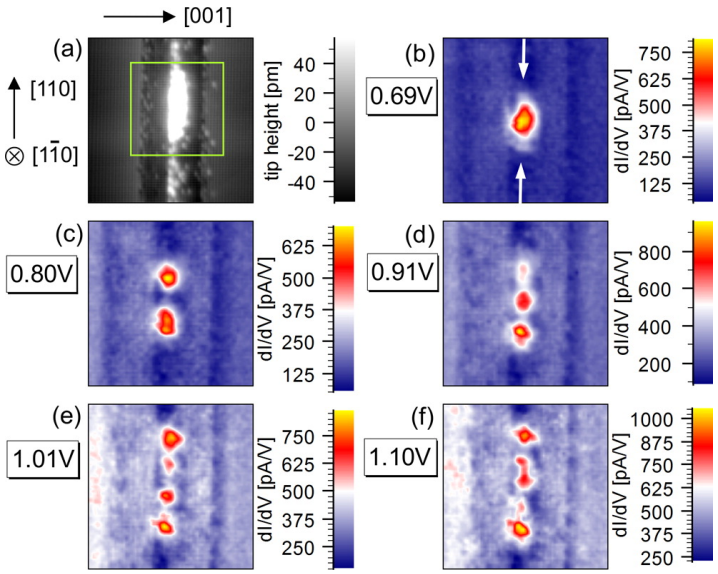

Figure 1: STM maps for various gate voltages measured in the work in Nano Letters.