PY 502, Computational Physics, Fall 2018

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SCHRÖDINGER EQUATION IN TWO DIMENSIONS

Confining potentials can be realized in semi-conductor nano-structures by combining materials with different band gaps. In a *quantum dot*, one or several electrons are confined to a finite volume, the shape of which can be taylored using nano-fabrication technologies. Due to the confinement, the electrons exhibit discrete energy levels and are therefore some times called "artificial atoms". In this assignment you will calculate the lowest energy eigenstates and wave functions for a rectangular quantum dot with an internal structure, as shown in the figure. The dot is assumed to be very thin in the third direction, so that it is effectively two-dimensional. The shaded areas have a lower (negative) potential $-V_0$ than the rest of the structure (at potential $V = 0$), and hence an electron will be attracted to these regions.
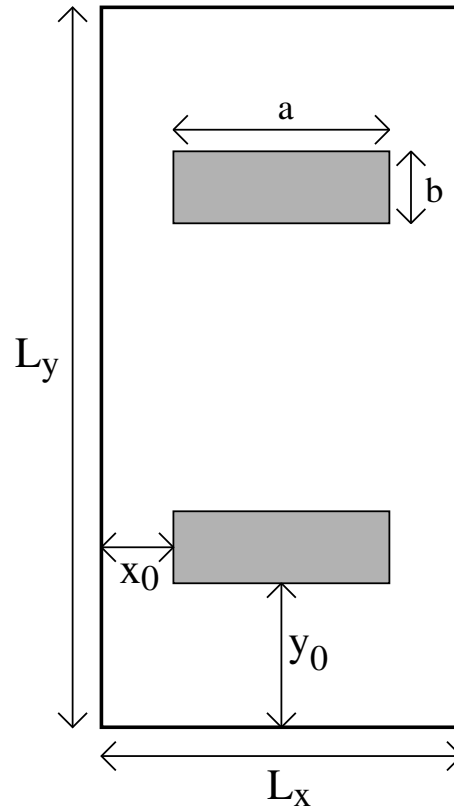

Figure 1: Geometry of the semiconductur nano-structure. The potential $V = -V_0$ in the shaded areas an $V = 0$ elsewhere inside the quantum dot. The two low-potential areas are identical and symmetrically located as shown. Outside the boundaries of the $L_x \times L_y$ structure the potential is assumed to be infinite.

We write the Schrödinger equation in two dimensions in the form

$$-\frac{1}{2}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\Psi(x,y) + \alpha V(x,y)\Psi(x,y) = \alpha E \Psi(x,y), \tag{1}$$

where $\alpha = m/\hbar^2$. It will be convenient to measure lengths in units of nm (10^{-9} m), and energies in eV ($1.602 \cdot 10^{-19}$ J). With the electron mass $m = 9.109 \cdot 10^{-31}$ kg and $\hbar = 1.055 \cdot 10^{-34}$ Js, we then get

$$-\frac{1}{2}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\Psi(x,y) + \beta V(x,y)\Psi(x,y) = \beta E \Psi(x,y), \tag{2}$$

where

$$\beta = \frac{(10^{-9}\text{m/nm})^2(1.602 \cdot 10^{-19}(\text{J/eV}) \cdot 9.109 \cdot 10^{-31}\text{kg}}{1.11302 \cdot 10^{-68}\text{J}^2\text{s}^2} = \frac{13.11}{\text{eVnm}^2}. \tag{3}$$

You should use two different methods to solve the two-dimensional Schrödinger equation approximately: A) Using a variational method with the particle-in-a-box eigenstates as a basis set, and B) using the Lanczos method to solve the real-space discretized equation. You should write your programs so that any values of the parameters defined in the figure can be studied. You should then compare results obtained with the two methods for the four lowest eigenstates of a structure explained in the figure, with the following parameters:

$L_x = 5$nm, $L_y = 10$nm, $a = 1.0$nm (corresponding to $x_0 = 2$nm), $b = 0.5$nm, $y_0 = 2$nm, and $V_0 = 0.1$eV (and note the sign; $V = -V_0$ in the regions of the attractive internal potential).

A) Variational calculation

The particle-in-a-box eigenfunctions for a rectangular infinite-wall box wiht $x \in [0, L_x]$ and $y \in [0, L_y]$ are

$$\phi_{k_x,k_y}(x,y) = f_{k_x}(x)g_{k_y}(y), \quad k_x, k_y = 1, 2. \ldots, \tag{4}$$

where

$$f_{k_x}(x) = \sqrt{\frac{2}{L_x}}\sin(k_x\pi x/L_x), \qquad g_{k_y}(y) = \sqrt{\frac{2}{L_y}}\sin(k_y\pi y/L_y). \tag{5}$$

In the variational calculation, you should use the basis set consisting of the $N = N_x N_y$ functions ϕ_{k_x,k_y} with $k_x = 1, \ldots, N_x$ and $k_y = 1, \ldots, N_y$, where N_x and N_y should be given as input to the program. Note that in the program the two indices k_x, k_y should be combined into a single index labeling the states, e.g., $k = k_x + (k_y - 1)N_x$, so that $k = 1, 2, \ldots, N$ and the hamiltonian can be constructed as an $N \times N$ matrix.

The energies of these wavefunctions are, keeping the constant β as defined in the Schrödinger equation (2),

$$\beta E_{kx,k_y} = \frac{\pi^2}{2}\left[\left(\frac{k_x}{L_x}\right)^2 + \left(\frac{k_y}{L_y}\right)^2\right]. \tag{6}$$

The integrals needed for the potential-energy part of the variational Hamiltonian are

$$V_{k_x,k_y}^{p_x,p_y} = \int\int dxdy \, \phi_{p_x,p_y}(x,y)V(x,y)\phi_{k_x,k_y}(x,y), \tag{7}$$

which can be easily calculated analytically since the potential inside the box is non-zero only in rectangular regions. To this end, you will need the following indefinite integrals:

$$\int \sin^2(ax)dx = \frac{1}{2}x - \frac{1}{4a}\sin(2ax), \tag{8}$$

$$\int \sin(ax)\sin(bx)dx = \frac{\sin[(a-b)x]}{2(a-b)} - \frac{\sin[(a+b)x]}{2(a+b)}, \quad |a| \neq |b|. \tag{9}$$

In addition to the eigenvalues βE_n obtained by diagonalizing the Hamiltonian, you should also extract the eigenfunctions corresponding to the four lowest eigenvalues. They are linear combinations of the basis functions, with weights given by the eigenvectors H that are obtained in the form of a transformation matrix in the diagonalization. Chose a reasonable grid, e.g., 100×200 (x, y) points, for writing the wave functions to files.

B) Lanczos calculation

In the real-space discretized 2D Schrödinger equation the kinetic energy acting on a localized state gives

$$K|j\rangle = \frac{2}{\Delta^2}|j\rangle - \frac{1}{2}\frac{1}{\Delta^2}\sum_{\delta[j]} |\delta[j]\rangle, \tag{10}$$

where $\delta[j]$ is a nearest-neighbor of element j. For interior elements there are 4 neighbors, but on the edges there can be no "hopping" out of the dot. The potential energy is diagonal;

$$\beta V|j\rangle = -\beta V_0|j\rangle, \quad \text{if } (x_j, y_j) \text{ inside low}-\text{potential region}, \quad 0 \text{ else.} \tag{11}$$

From these expressions the matrix elements $\langle j|K|l\rangle$ and $\langle j|V|l\rangle$ are obtained.

The discretization Δ should be chosen in a such a way that the system dimensions are integer multiples of Δ; $L_x = N_x\Delta$, $L_y = N_y\Delta$.

Use the variant of the lanczos method where the normalized basis states $|\phi_m\rangle$ are generated directly. This avoids problems with large numbers when computing the normalization constants of the unnormalized states $|f_m\rangle$.

Your program should write all the Lanczos eigenvalues to disk, and also produce the wave functions corresponding to the four lowest energies.

Specific instructions

You should test your program, and write a short report on the results (for the structure with parameters specified above). Consider the four lowest energy eigenvalues and the corresponding states. Give all energies in eV (i.e., divide out the constant β from the calculated eigenvalues βE_n—note that with the units we are using the unit of βE is nm^{-2}).

You should check the energy convergence as the size of the basis is increased in the variational calculation. You should carry out the Lanczos calculation for different discretizations Δ (e.g., $\Delta = 0.2, 0.1, 0.05, 0.025$ and smaller if you can with your computer resources) and check the convergence of the energies as the number of Lanczos iterations is increased. You may not be able to completely converge the calculations before the computational effort becomes too large, or instabilities related to non-orthogonality (due to build-up of numerical truncation errors) start to plague the Lanczos calculation. Mention any numerical problems you encounter in the report.

You should produce graphs showing your energy convergence tests. You should also produce plots showing the probability densities (square of the wavefunctions) inside the quantum dot for the four lowest states (resulting from the most accurate calculations you are able do in the variational as well as the Lanczos calculation)). You can use the 2D color plotting program available on the course web site, or any other graphing software if you prefer (you don't have to print the graphs in color).

You can use elements from the programs 'sqvar.f90' and 'lanczos.f90' on the course web sites. You will also need the LAPAC diagonalization routines DSYEV and DSTEV available on the web site.