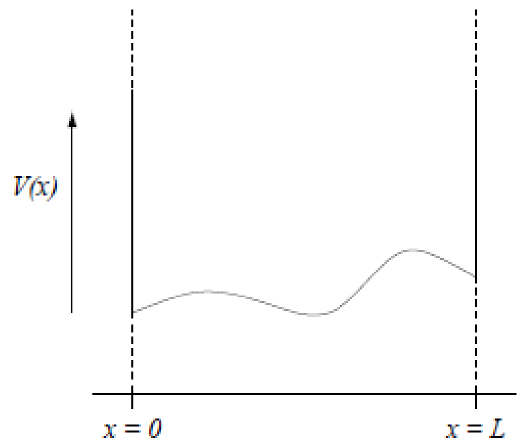
Fisi 4125 *21 de abril de 2021*

Universidad de Puerto Rico
Recinto Universitario de Mayagüez
Departamento de Física
Asignación 8

Instrucciones: Para entregar en o antes del miércoles, 28 de abril de 2021 antes de las 11:59 PM. (10 puntos = 100%).

Exercise 6.9: Asymmetric quantum well

Quantum mechanics can be formulated as a matrix problem and solved on a computer using linear algebra methods. Suppose, for example, we have a particle of mass M in a one-dimensional quantum well of width L, but not a square well like the examples you've probably seen before. Suppose instead that the potential $V(x)$ varies somehow inside the well:



We cannot solve such problems analytically in general, but we can solve them on the computer.

In a pure state of energy E, the spatial part of the wavefunction obeys the time-independent Schrödinger equation $\hat{H}\psi(x) = E\psi(x)$, where the Hamiltonian operator $\hat{H}$ is given by

$$\hat{H} = -\frac{\hbar^2}{2M}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x).$$

For simplicity, let's assume that the walls of the well are infinitely high, so that the wavefunction is zero outside the well, which means it must *go to* zero at $x = 0$ and $x = L$. In that case, the wavefunction can be expressed as a Fourier sine series thus:

$$\psi(x) = \sum_{n=1}^{\infty} \psi_n \sin\frac{\pi n x}{L},$$

where $\psi_1, \psi_2, \ldots$ are the Fourier coefficients.

a) Noting that, for m, n positive integers

$$\int_0^L \sin\frac{\pi m x}{L}\sin\frac{\pi n x}{L}\,\mathrm{d}x = \begin{cases} L/2 & \text{if } m=n, \\ 0 & \text{otherwise,} \end{cases}$$

show that the Schrödinger equation $\hat{H}\psi = E\psi$ implies that

$$\sum_{n=1}^{\infty}\psi_n\int_0^L \sin\frac{\pi m x}{L}\hat{H}\sin\frac{\pi n x}{L}\,\mathrm{d}x = \tfrac{1}{2}LE\psi_m.$$

Hence, defining a matrix $\mathbf{H}$ with elements

$$\begin{aligned} H_{mn} &= \frac{2}{L}\int_0^L \sin\frac{\pi m x}{L}\hat{H}\sin\frac{\pi n x}{L}\,\mathrm{d}x \\ &= \frac{2}{L}\int_0^L \sin\frac{\pi m x}{L}\left[-\frac{\hbar^2}{2M}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+V(x)\right]\sin\frac{\pi n x}{L}\,\mathrm{d}x, \end{aligned}$$

show that Schrödinger's equation can be written in matrix form as $\mathbf{H}\boldsymbol{\psi} = E\boldsymbol{\psi}$, where $\boldsymbol{\psi}$ is the vector $(\psi_1, \psi_2, \ldots)$. Thus $\boldsymbol{\psi}$ is an eigenvector of the *Hamiltonian matrix* $\mathbf{H}$ with eigenvalue E. If we can calculate the eigenvalues of this matrix, then we know the allowed energies of the particle in the well.

b) For the case $V(x) = ax/L$, evaluate the integral in H_{mn} analytically and so find a general expression for the matrix element H_{mn}. Show that the matrix is real and symmetric. You'll probably find it useful to know that

$$\int_0^L x\sin\frac{\pi m x}{L}\sin\frac{\pi n x}{L}\,\mathrm{d}x = \begin{cases} 0 & \text{if } m \neq n \text{ and both even or both odd,} \\ -\left(\dfrac{2L}{\pi}\right)^2\dfrac{mn}{(m^2-n^2)^2} & \text{if } m \neq n \text{ and one is even, one is odd,} \\ L^2/4 & \text{if } m = n. \end{cases}$$

Write a Python program to evaluate your expression for H_{mn} for arbitrary m and n when the particle in the well is an electron, the well has width 5 Å, and $a = 10\,\mathrm{eV}$. (The mass and charge of an electron are 9.1094×10^{-31} kg and 1.6022×10^{-19} C respectively.)

c) The matrix $\mathbf{H}$ is in theory infinitely large, so we cannot calculate all its eigenvalues. But we can get a pretty accurate solution for the first few of them by cutting off the matrix after the first few elements. Modify the program you wrote for part (b) above to create a 10×10 array of the elements of $\mathbf{H}$ up to $m, n = 10$. Calculate the eigenvalues of this matrix using the appropriate function from `numpy.linalg` and hence print out, in units of electron volts, the first ten energy levels of the quantum well, within this approximation. You should find, for example, that the ground-state energy of the system is around $5.84\,\mathrm{eV}$. (Hint: Bear in mind that matrix indices in Python start at zero, while the indices in standard algebraic expressions, like those above, start at one. You will need to make allowances for this in your program.)

Exercise 9.1: Write a program, or modify the one from Example 9.1, to solve Poisson's equation for the system described in Example 9.2. Work in units where $\epsilon_0 = 1$ and continue the iteration until your solution for the electric potential changes by less than 10^{-6} V per step at every grid point.

Exercise 9.2: Use the Gauss–Seidel method to solve Laplace's equation for the two-dimensional problem in Example 9.1—a square box 1 m on each side, at voltage $V = 1$ volt along the top wall and zero volts along the other three. Use a grid of spacing $a = 1$ cm, so that there are 100 grid points along each wall, or 101 if you count the points at both ends. Continue the iteration of the method until the value of the electric potential changes by no more than $\delta = 10^{-6}$ V at any grid point on any step, then make a density plot of the final solution, similar to that shown in Fig. 9.3. Experiment with different values of ω to find which value gives the fastest solution. As mentioned above, you should find that a value around 0.9 does well. In general larger values cause the calculation to run faster, but if you choose too large a value the speed drops off and for values above 1 the calculation becomes unstable.

Exercise 9.4: Thermal diffusion in the Earth's crust

A classic example of a diffusion problem with a time-varying boundary condition is the diffusion of heat into the crust of the Earth, as surface temperature varies with the seasons. Suppose the mean daily temperature at a particular point on the surface varies as:

$$T_0(t) = A + B \sin \frac{2\pi t}{\tau},$$

where $\tau = 365$ days, $A = 10°\text{C}$ and $B = 12°\text{C}$. At a depth of 20 m below the surface almost all annual temperature variation is ironed out and the temperature is, to a good approximation, a constant 11°C (which is higher than the mean surface temperature of 10°C—temperature increases with depth, due to heating from the hot core of the planet). The thermal diffusivity of the Earth's crust varies somewhat from place to place, but for our purposes we will treat it as constant with value $D = 0.1\,\text{m}^2\,\text{day}^{-1}$.

Write a program, or modify one of the ones given in this chapter, to calculate the temperature profile of the crust as a function of depth up to 20 m and time up to 10 years. Start with temperature everywhere equal to 10°C, except at the surface and the deepest point, choose values for the number of grid points and the time-step h, then run your program for the first nine simulated years, to allow it to settle down into whatever pattern it reaches. Then for the tenth and final year plot four temperature profiles taken at 3-month intervals on a single graph to illustrate how the temperature changes as a function of depth and time.

Instrucciones para Entregar sus Asignaciones

1) Prepare un archivo en pdf con la información que pide el ejercicio. Por ejemplo, si el ejercicio pide que escriba un programa, deberá mostrar su programa. Si el ejercicio pide output para un input dado, deberá mostrar el input y el output. Este archivo lo subirá a la plataforma Moodle del curso.

2) Suba también en archivos separados los programas usados para la hacer la asignación a la plataforma Moodle.