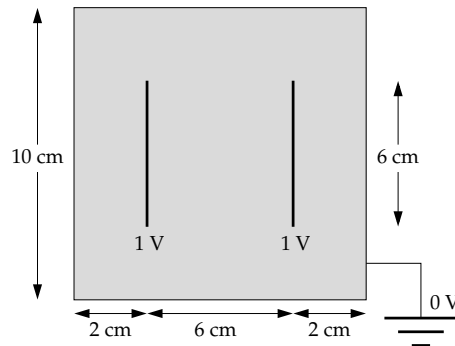


### Homework 3: Partial Differential Equation

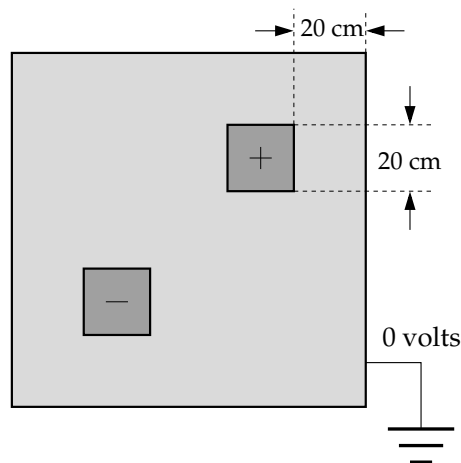
**Exercise 3.1:** Consider the following simple model of an electronic capacitor, consisting of two flat metal plates enclosed in a square metal box:



For simplicity let us model the system in two dimensions. Using any of the methods we have studied, write a program to calculate the electrostatic potential in the box on a grid of  $100 \times 100$  points, where the walls of the box are at voltage zero and the two plates (which are of negligible thickness) are at voltages  $\pm 1$  V as shown. Have your program calculate the value of the potential at each grid point to a precision of  $10^{-6}$  volts and then make a density plot of the result.

Hint: Notice that the capacitor plates are at fixed *voltage*, not fixed charge. In effect, the capacitor plates are part of the boundary condition in this case: they behave the same way as the walls of the box, with potentials that are fixed at a certain value and cannot change.

**Exercise 3.2:** Write a program to solve Poisson's equation for the system described below. 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.



Two square charges are placed inside a square two dimensional box. The potential is zero on the walls and the squares have charge densities  $+1C\ m^{-2}$  and  $-1C\ m^{-2}$

### Exercise 3.3: Thermal diffusion in the Earth's crust

An 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,  $A = 10^\circ\text{C}$  and  $B = 12^\circ\text{C}$ . 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  $11^\circ\text{C}$  (which is higher than the mean surface temperature of  $10^\circ\text{C}$ —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 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  $10^\circ\text{C}$ , 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.

### Exercise 3.4: The Schrödinger equation and the spectral method

This exercise uses the spectral method to solve the time-dependent Schrödinger equation

$$-\frac{\hbar^2}{2M} \frac{\partial^2 \psi}{\partial x^2} = i\hbar \frac{\partial \psi}{\partial t}$$

for a single particle in one dimension in a box of length  $L$  with impenetrable walls. The wavefunction in such a box necessarily goes to zero on the walls and hence one possible (unnormalized) solution of the equation is

$$\psi_k(x, t) = \sin\left(\frac{\pi k x}{L}\right) e^{iEt/\hbar},$$

where the energy  $E$  can be found by substituting into the Schrödinger equation, giving

$$E = \frac{\pi^2 \hbar^2 k^2}{2ML^2}.$$

We can write a full solution as a linear combination of such individual solutions, which on the grid points  $x_n = nL/N$  takes the value

$$\psi(x_n, t) = \frac{1}{N} \sum_{k=1}^{N-1} b_k \sin\left(\frac{\pi k n}{N}\right) \exp\left(i \frac{\pi^2 \hbar k^2}{2ML^2} t\right),$$

where the  $b_k$  are some set of (possibly complex) coefficients that specify the exact shape of the wavefunction and the leading factor of  $1/N$  is optional but convenient.

Since the Schrödinger equation is first order in time, we need only a single initial condition on the value of  $\psi(x, t)$  to specify the coefficients  $b_k$ , although, since the coefficients are in general complex, we will need to calculate both real and imaginary parts of each coefficient.

We consider an electron (mass  $M = 9.109 \times 10^{-31} \text{ kg}$ ) in a box of length  $L = 10^{-8} \text{ m}$ . At time  $t = 0$  the wavefunction of the electron has the form

$$\psi(x, 0) = \exp\left[-\frac{(x - x_0)^2}{2\sigma^2}\right] e^{ikx},$$

where

$$x_0 = \frac{L}{2}, \quad \sigma = 1 \times 10^{-10} \text{ m}, \quad \kappa = 5 \times 10^{10} \text{ m}^{-1},$$

and  $\psi = 0$  on the walls at  $x = 0$  and  $x = L$ .

- a) Write a program to calculate the values of the coefficients  $b_k$ , which for convenience can be broken down into their real and imaginary parts as  $b_k = \alpha_k + i\eta_k$ . Divide the box into  $N = 1000$  slices and create two arrays containing the real and imaginary parts of  $\psi(x_n, 0)$  at each grid point. Perform discrete sine transforms on each array separately and hence calculate the values of the  $\alpha_k$  and  $\eta_k$  for all  $k = 1 \dots N - 1$ .

(Note that the first element of the input array should in principle always be zero for a sine transform. Similarly the first element of the returned array is always zero, since the  $k = 0$  coefficient of a sine transform is always zero. So in effect, the sine transform really only takes  $N - 1$  real numbers and transforms them into another  $N - 1$  real numbers. In some implementations of the discrete sine transform, therefore the first element of each array is simply omitted, since it's always zero anyway, and the arrays are only  $N - 1$  elements long.)

- b) Putting  $b_k = \alpha_k + i\eta_k$  in the solution above and taking the real part we get

$$\text{Re } \psi(x_n, t) = \frac{1}{N} \sum_{k=1}^{N-1} \left[ \alpha_k \cos\left(\frac{\pi^2 \hbar k^2}{2ML^2} t\right) - \eta_k \sin\left(\frac{\pi^2 \hbar k^2}{2ML^2} t\right) \right] \sin\left(\frac{\pi kn}{N}\right)$$

for the real part of the wavefunction. This is an inverse sine transform with coefficients equal to the quantities in the square brackets. Extend your program to calculate the real part of the wavefunction  $\psi(x, t)$  at an arbitrary time  $t$  using this formula and the inverse discrete sine transform. Test your program by making a graph of the wavefunction at time  $t = 10^{-16}$  s.

- c) Extend your program further to make an animation of the wavefunction over time. A suitable time interval for each frame of the animation is about  $10^{-18}$  s.
- d) Run your animation for a while and describe what you see. Write a few sentences explaining in physics terms what is going on in the system.