Scientific Computing, Homework 5

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Problem 1: Electrostatics

In this problem, the goal is to solve Laplace's equation for the setup shown in Fig. 1.

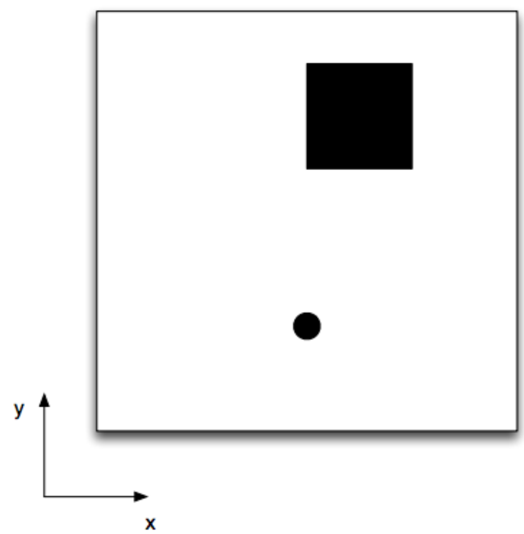

Figure 1: A box with an area within of potential V=+10, and a point charge of -2 near the bottom.

The first step to do all of this is to split up the region into a grid of locations from which to solve laplace's equation given the nearest neighbors. By enforcing a value of ϕ for each iteration, we can ensure than the boundary conditions will be honored. For the boundary condition around the point charge, we set the closest points to it equal to an analytically set value. The equation we are solving is:

$$\nabla^2 \phi = 0 \tag{1}$$

To do this, we discretize the Laplacian on the left into a sparse matrix which in general looks like:

$$\nabla^2_{m,n} = \begin{pmatrix} -4 & 1 & 0 & \cdots & 0 & 1 & 0 & \cdots & \cdots & 0 \\ 1 & -4 & 1 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \end{pmatrix}$$

and obviously square-er than this thing shown above. The ones that are directly off diagonal, and those slightly offset correspond to the nearest neighbors of the point in question.

The congugate gradient method provides us with a good way to solve for ϕ in Equation 1. The basic outline for the method is outlined below:

- set some variables
  $\nabla^2 = A$ $r_0 = A * \phi$ This is the first residual.
  $p_0 = r_0$ This is the 'search' direction for the algorithm.

- iterate the following with i:
  $\alpha_i = \frac{r_i^T r_i}{p_i^T A p_i}$
  $\phi_{i+1} = \phi_i + \alpha_i p_i$
  $r_{i+1} = A\phi_{i+1} - \alpha_i A p_i$
  $\beta_i = \frac{r_{i+1}^T r_{i+1}}{r_i^T r_i}$
  $p_{i+1} = r_{i+1} + \beta_i p_i$

- For each iteration, enforce the boundary conditions that ϕ must be a certain value at these boundaries.

The result is shown in figures 2 and 3.

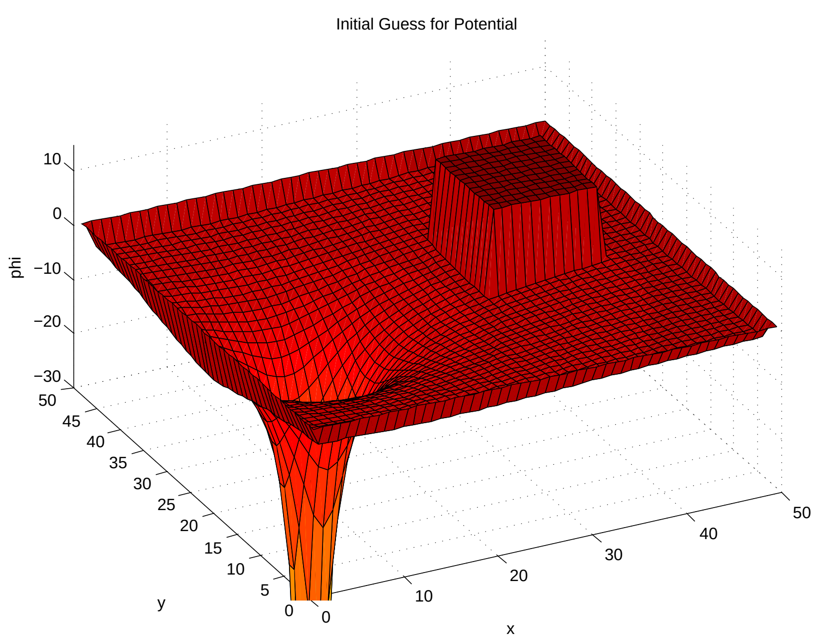

Figure 2: Initial guess for the potential ϕ using a simple 1/r.

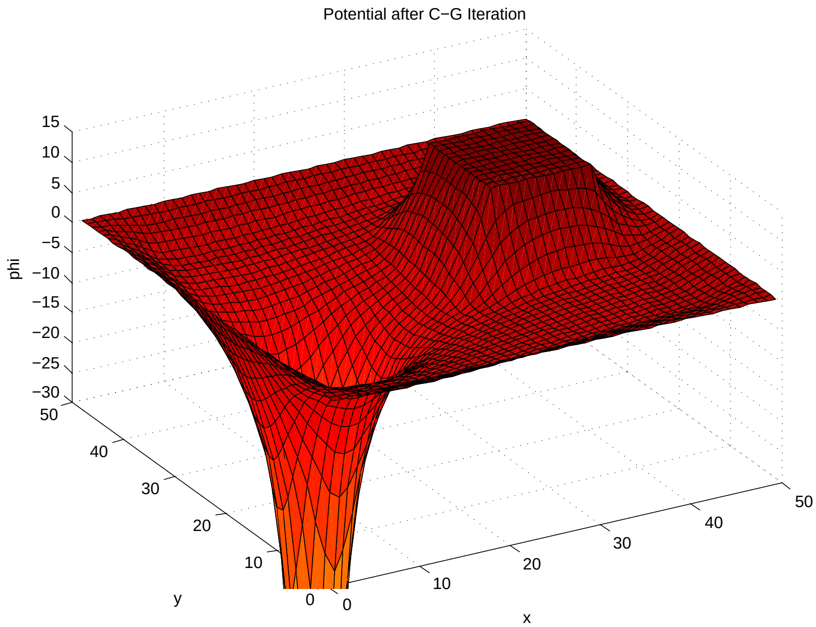

Figure 3: Solution for ϕ after Congugate Gradient solving of Laplace's equation for the region.

Problem 2: Quantum Mechanics

This problem had us solve the situation above, but for schrodinger's equation. So there is a change to the Laplacian operator in that we divide by a factor of $-2m$, and we are now solving the equation:

$$-\frac{\nabla^2}{2m}\psi = E\psi, \tag{2}$$

where $\hbar = 1$ So we are solving the eigenvalue equation.

For part (a), there was no point charge, and we find the three lowest eigenvalues to be:

$$E_1 = 158.6, E_2 = 284.4, E_3 = 385.6$$

Plotting the corresponding square of Eigenvectors, we produce the figures of probability below:

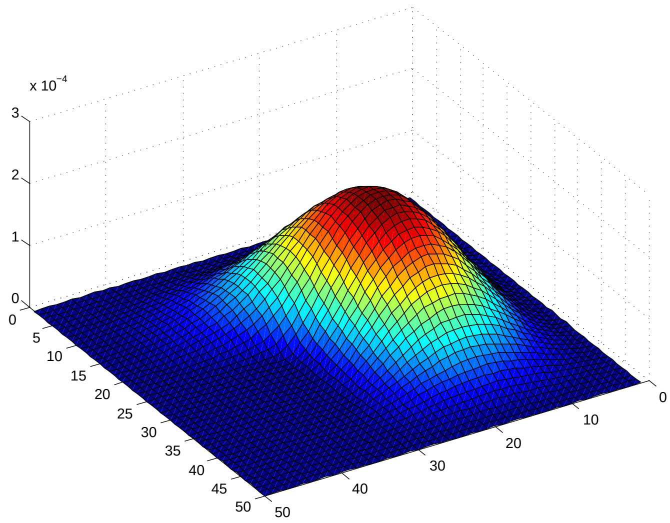

Figure 4: Lowest Energy Eigenvalue.

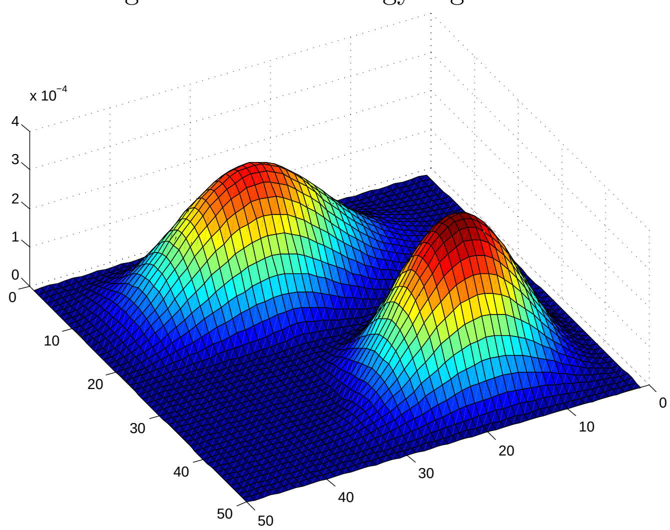

Figure 5: n=2 Eigenvalue.

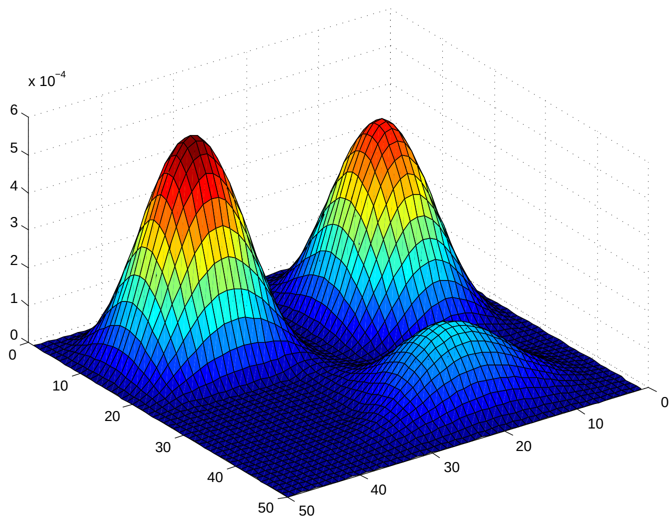

Figure 6: n=3 Eigenvalue.

For part (b), we put the point charge back in and solve for the ground state wavefunction, and plot the probability. For the charge = -15, we get figure 7.

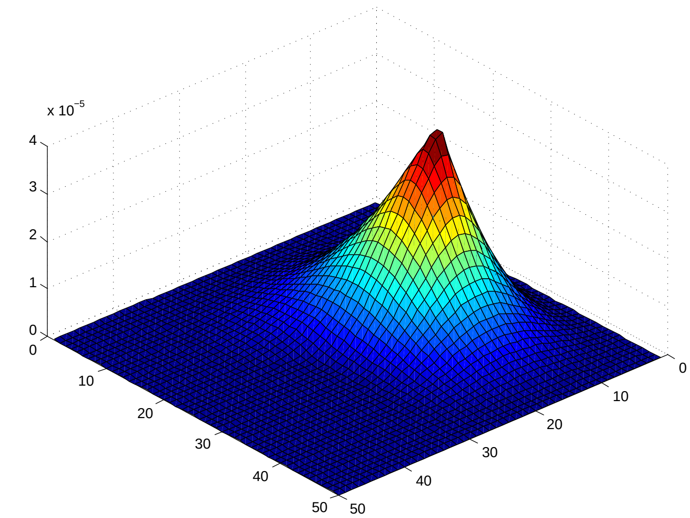

Figure 7: Probability for the q=-15.

To get 90% of the probability in the lower half of the setup, I tested values of q, and checked the probability that the particle will be in the lower half. I find that q = -143. The result is in figure 8.

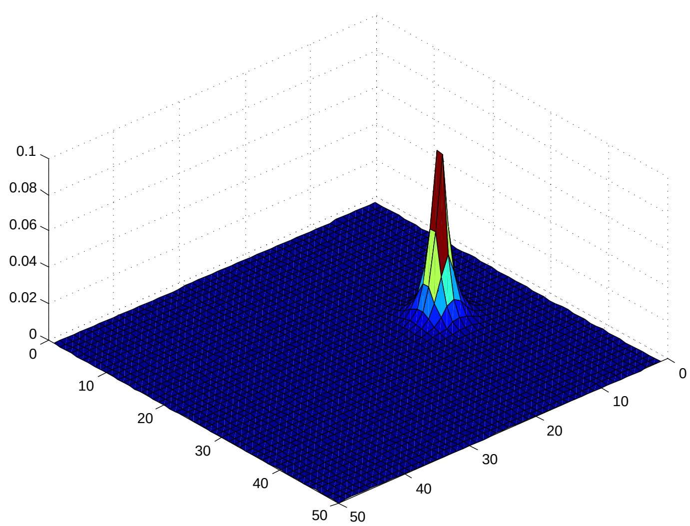

Figure 8: Probability for the q=-143.