Time-independent Schrödinger Equation in 2D

Particle in a Box

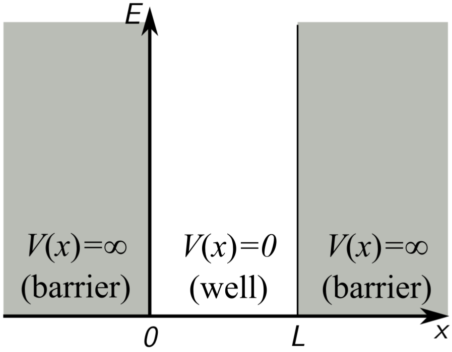
Julien

Math/ECE 697NA, Spring 2017

1D Problem

Infinite potential well

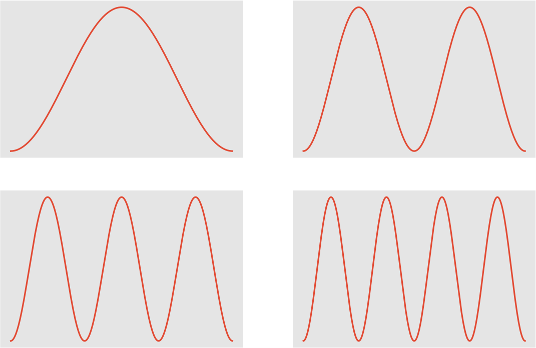
Particle trapped in a 1D well, with walls of infinite potential to either side. Size of problem $L = 1 \times 10^{-9}\ m$



1D Problem

Infinite potential well

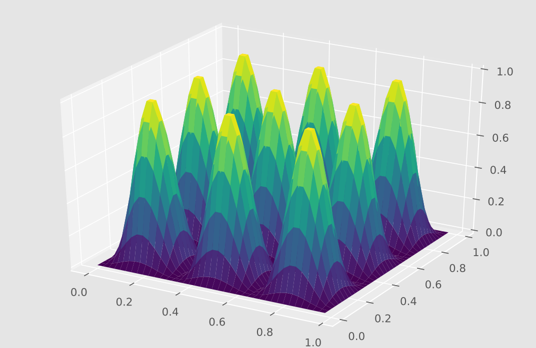
Particle has probability distribution for each energy level. For a $1 \times N$ grid we get N^2 entries in our matrix.



2D Problem

Particle in a box

The problem is the same in 2D, we get probability distributions for a particle in the well. For a $N \times N$ grid our matrix is size N^4.



Schrödinger Equation

The wave function is given by the Schrödinger equation, which can be viewed as an eigenvalue problem.

$$-\frac{\hbar}{2m_e}\Delta\Psi + U\Psi = E\Psi$$

$$\left[-\frac{\hbar}{2m_e}\Delta + U\right]\Psi = E\Psi$$

$$A\Psi = E\Psi$$

Schrödinger Equation

1D Analytical Solution

For a constant zero potential in the well $U = 0$, the equation is separable and we can find an analytical solution.

$$E_i = \frac{(i\pi\hbar)^2}{2m_e L^2}$$

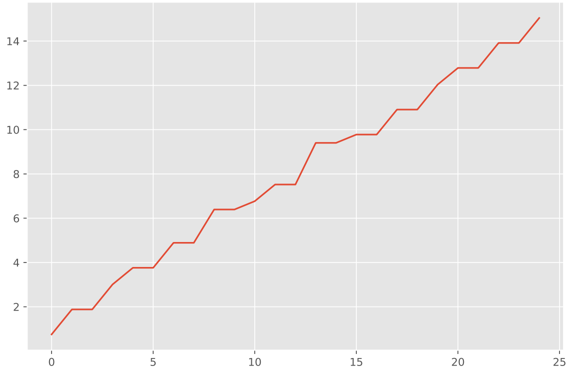
$$\psi_i(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{i\pi x}{L}\right)$$

For a constant zero potential in the well $U = 0$, the equation is separable and we can find an analytical solution.

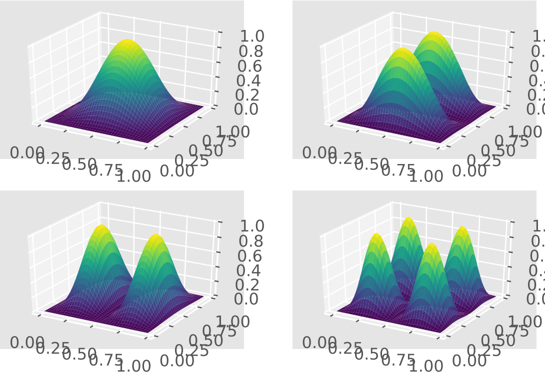
$$E_{i,j} = \frac{(i\pi\hbar)^2}{2m_e L^2} + \frac{(j\pi\hbar)^2}{2m_e L^2}$$

$$\psi_{i,j}(x) = \sqrt{\frac{4}{L^2}} \sin\left(\frac{i\pi x}{L}\right) \sin\left(\frac{j\pi x}{L}\right)$$

First 25 Eigenvalues. Since the pairs are symmetric, values appear more than once.



First 4 eigenvectors. We take $|\psi_{i,j}(x)|^2$ to get the probability distribution.



Finite Difference Method

We can solve this by using a finite difference method to approximate the Laplacian.

$$A = \frac{1}{h^2}\begin{pmatrix} 4+U & -1 & 0 & \dots & -1 & 0 & \dots & \\ -1 & 4+U & -1 & 0 & \dots & -1 & 0 & \dots \\ 0 & -1 & 4+U & -1 & 0 & \dots & \ddots & \\ \vdots & 0 & -1 & 4+U & -1 & 0 & \dots & \\ -1 & 0 & \dots & -1 & 4+U & -1 & 0 & \dots \\ 0 & -1 & \dots & & & \ddots & & \\ \vdots & 0 & \ddots & & & & \ddots & \end{pmatrix}$$

Finite Difference Method

We can solve this by using a finite difference method to approximate the Laplacian.

$$A = \frac{1}{h^2}\begin{pmatrix} B & -I & 0 & \dots \\ -I & B & \ddots & \\ 0 & \ddots & \ddots & -I \\ \vdots & & -I & B \end{pmatrix}$$

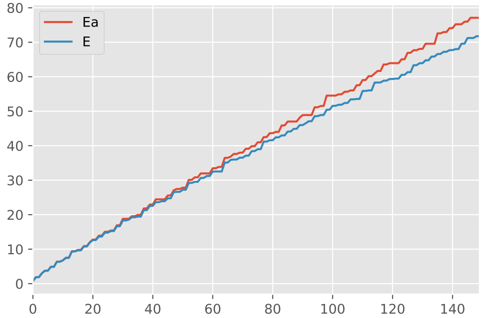
Finite Difference Method

Since the problem is the same in both dimensions, the 2D Laplacian can be computed as a tensor product of 1D Laplacians.

$$L_2 = L_1 \oplus L_1 = L_1 \otimes I + I \otimes L_1$$

Finite Difference Method

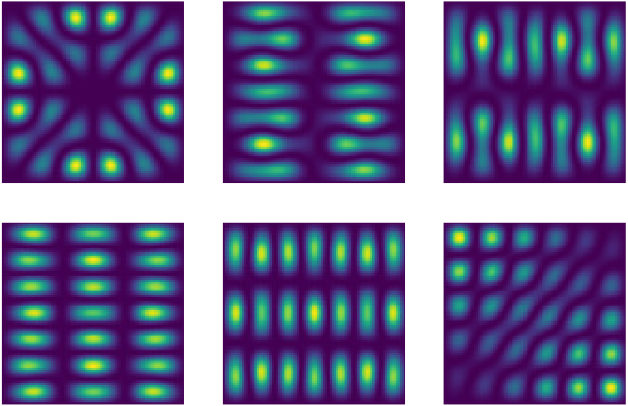
We can then solve $A\psi = E\psi$ using FEAST, ARPACK, Lanczos algorithm, or other sparse eigenvalue methods. The error increases for larger eigenvalues.



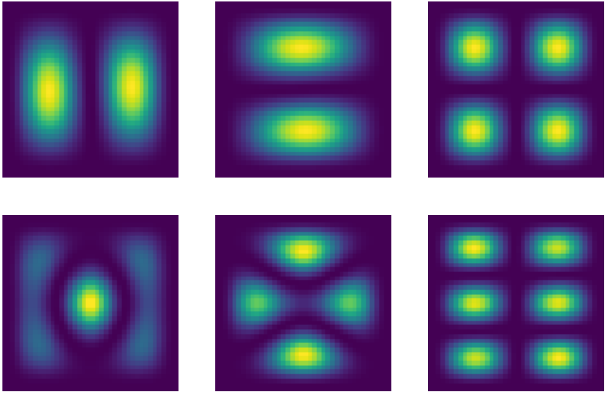
Lanczos Algorithm

$v_1 \leftarrow$ `random vector of norm 1`
$v_0 \leftarrow 0$
$\beta_1 \leftarrow 1$
for $j = 1, 2, \ldots, m$ **do**
  $w'_j \leftarrow Av_j - \beta_j v_{j-1}$
  $\alpha_j \leftarrow {w'_j}^T \cdot w_j$
  $w_j \leftarrow w'_j - \alpha_j v_j$
  $\beta_{j+1} \leftarrow ||w'_j||$
  $v_{j+1} \leftarrow w'_j / \beta_{j+1}$
end for

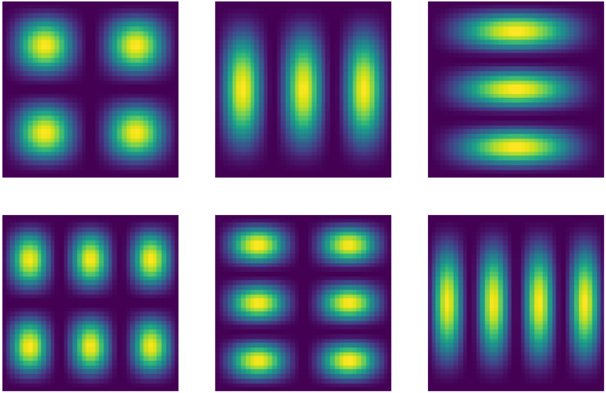
Summary



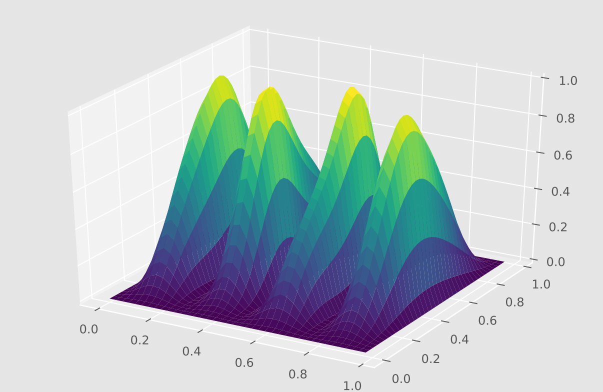
Summary



Summary



Summary



Summary