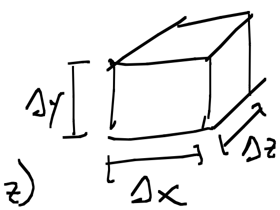
Finite differences in 3-d

$$-\frac{\hbar^2}{2m}\nabla^2\psi_{ijk} + V_{ijk}\psi_{ijk} = E\psi_{ijk}$$

(integer
i : index along $\hat{x}$
j : index along $\hat{y}$
k : index along $\hat{z}$)

Volume element: at location $(x,y,z) = (i\Delta x, j\Delta y, k\Delta z)$

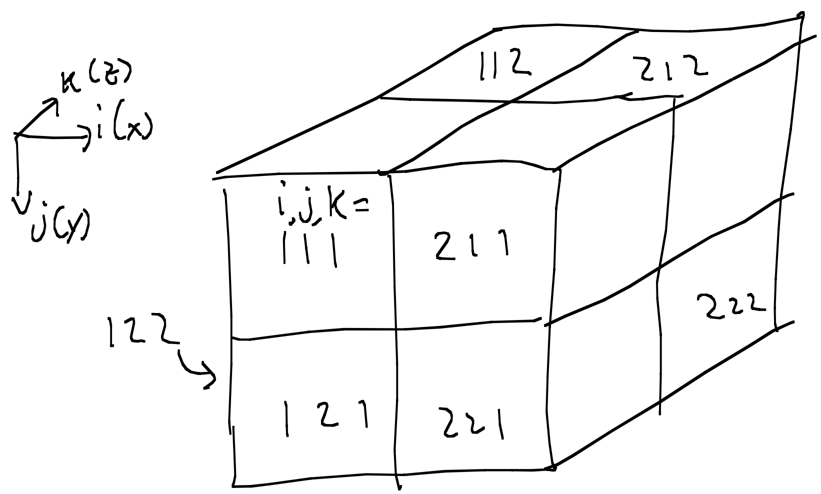


System of linear equations:

$$t_x\left(\psi_{i+1,j,k} - 2\psi_{i,j,k} + \psi_{i-1,j,k}\right) + t_y\left(\psi_{i,j+1,k} - 2\psi_{i,j,k} + \psi_{i,j-1,k}\right) + t_z\left(\psi_{i,j,k+1} - 2\psi_{i,j,k} + \psi_{i,j,k-1}\right) + V_{i,j,k}\psi_{i,j,k} = E\psi_{i,j,k}$$

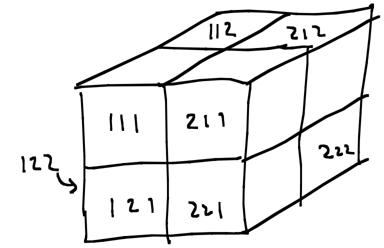
$$\left(t_x \equiv \frac{-\hbar^2}{2m\Delta x^2} \qquad t_y \equiv -\frac{\hbar^2}{2m\Delta y^2} \qquad t_z \equiv \frac{-\hbar^2}{2m\Delta z^2}\right)$$

Example: $2\times 2\times 2$ discretization of infinite cubical well



Application of finite differences results in 8×8 matrix eigenvalue problem

Matrix Hamiltonian (just $H = -\frac{\hbar^2}{2m}\nabla^2$ Kinetic energy term)



$$
\begin{array}{c|c}
ijk & \begin{array}{cccccccc} ijk=111 & 211 & 121 & 221 & 112 & 212 & 122 & 222 \end{array} \\
\begin{array}{c} 111 \\ 211 \\ 121 \\ 221 \\ 112 \\ 212 \\ 122 \\ 222 \end{array} &
\left[\begin{array}{cc:cc:cc:cc}
-2(t_x+t_y+t_z) & t_x & t_y & 0 & t_z & 0 & 0 & 0 \\
t_x & -2(t_x+t_y+t_z) & 0 & t_y & 0 & t_z & 0 & 0 \\
\hdashline
t_y & 0 & -2(t_x+t_y+t_z) & t_x & 0 & 0 & t_z & 0 \\
0 & t_y & t_x & -2(t_x+t_y+t_z) & 0 & 0 & 0 & t_z \\
\hdashline
t_z & 0 & 0 & 0 & -2(t_x+t_y+t_z) & t_x & t_y & 0 \\
0 & t_z & 0 & 0 & t_x & -2(t_x+t_y+t_z) & 0 & t_y \\
\hdashline
0 & 0 & t_z & 0 & t_y & 0 & -2(t_x+t_y+t_z) & t_x \\
0 & 0 & 0 & t_z & 0 & t_y & t_x & -2(t_x+t_y+t_z)
\end{array}\right]
\end{array}
$$

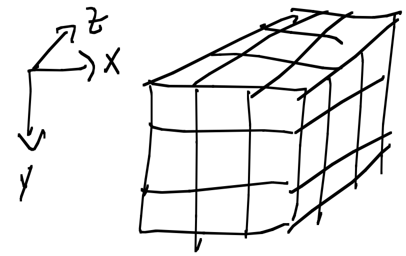
BLOCK

tridiagonal!

→ This symmetry extends to arbitrary matrix sizes!

(in a general 3-d problem, V_{ijk} will appear along the diagonal)

Larger Hamiltonian (Ex. 3x3x3)



$$\begin{bmatrix} \begin{matrix} H_x & t_y\hat{I}_3 & \hat{O}_3 \\ t_y\hat{I}_3 & H_x & t_y\hat{I}_3 \\ \hat{O}_3 & t_y\hat{I}_3 & H_x \end{matrix} & t_z\hat{I}_9 & \hat{O}_9 \\ t_z\hat{I}_9 & & t_z\hat{I}_9 \\ \hat{O}_9 & t_z\hat{I}_9 & \end{bmatrix}$$

$$\hat{H}_x = \begin{bmatrix} -2(t_x+t_y+t_z) & t_x & 0 \\ t_x & -2(t_x+t_y+t_z) & t_x \\ 0 & t_x & -2(t_x+t_y+t_z) \end{bmatrix}$$

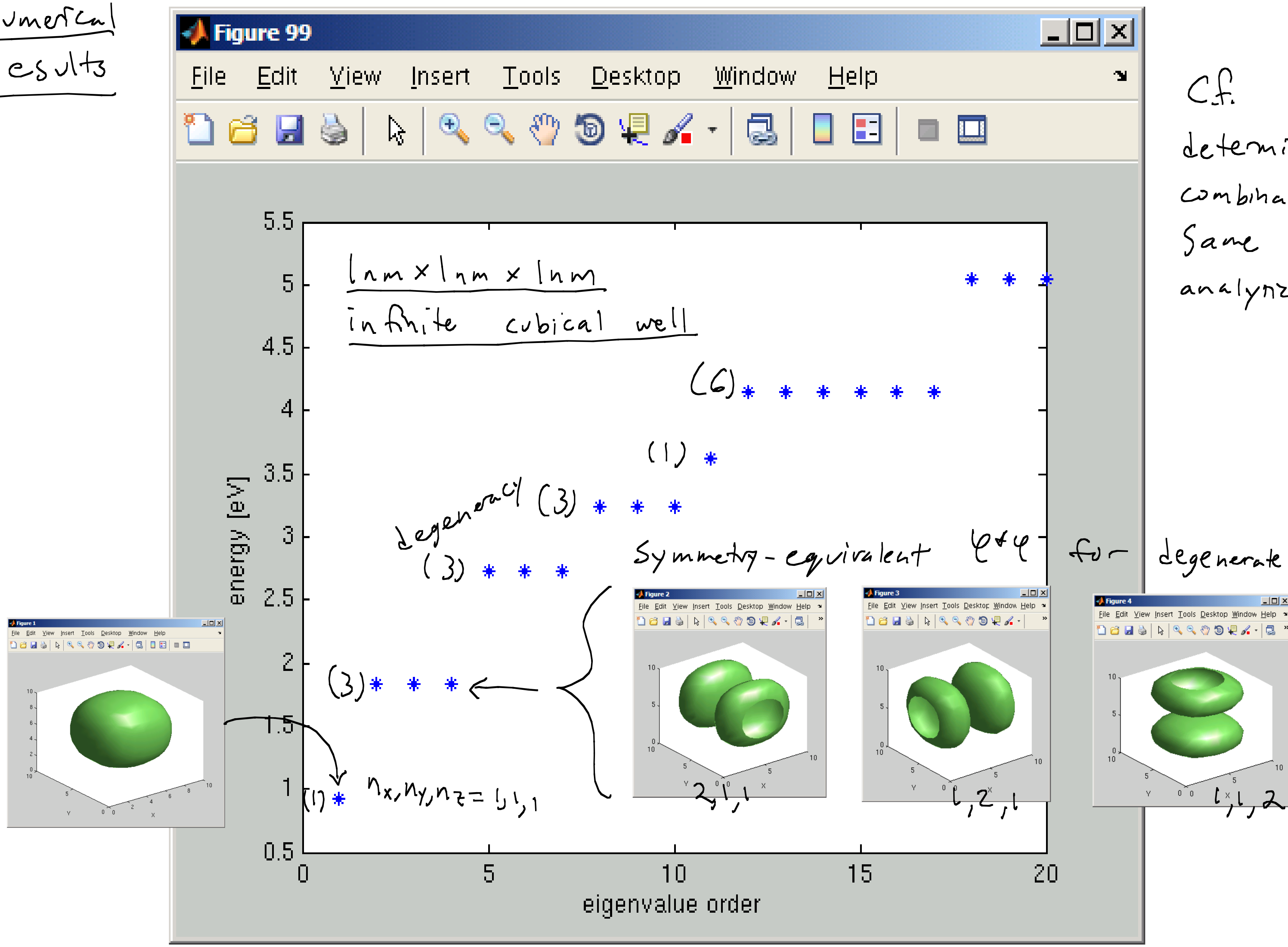
$\hat{I}_3$ = 3x3 identity

$\hat{I}_9$ = 9x9 identity

$\hat{O}_3$ = 3x3 zeros

$\hat{O}_9$ = 9x9 zeros

Numerical Results



Cf. degeneracy determined by combinatorics, same as analytic case!