Constructing 3D matrix Hamiltonians

Kronecker (direct) matrix product "$\otimes$":

Example:

$$\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \otimes \begin{bmatrix} a & b \\ c & d \end{bmatrix} = \begin{bmatrix} 1\begin{bmatrix} a & b \\ c & d \end{bmatrix} & 2\begin{bmatrix} a & b \\ c & d \end{bmatrix} \\ 3\begin{bmatrix} a & b \\ c & d \end{bmatrix} & 4\begin{bmatrix} a & b \\ c & d \end{bmatrix} \end{bmatrix}$$

(2×2) (2×2) (4×4)

A $3\times 3\times 3$ matrix Hamiltonian

$$\hat{H}_x = \begin{bmatrix} -2(t_x+t_y+t_z) & t_x & 0 \\ t_x & -2(t_x+t_y+t_z) & t_x \\ 0 & t_x & -2(t_x+t_y+t_z) \end{bmatrix}, \quad \hat{H}_y = t_y \hat{I}_3, \quad H_z = t_z \hat{I}_9$$

$$\hat{H}_{xy} = \hat{I}_3 \otimes \hat{H}_x + \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \otimes \hat{H}_y$$

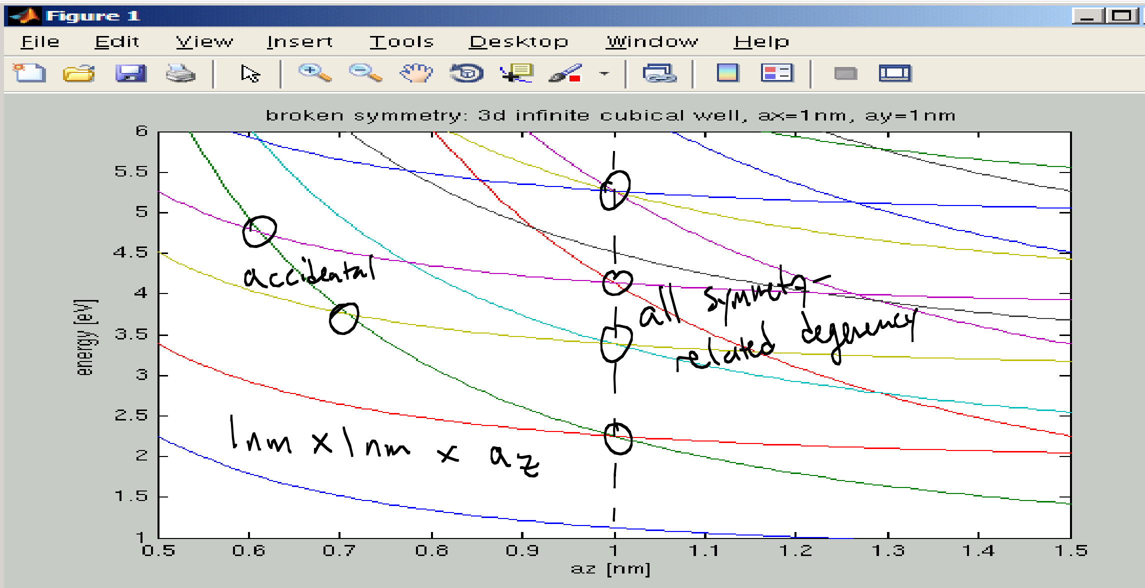
$$\hat{H} = \hat{I}_3 \otimes \hat{H}_{xy} + \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \otimes \hat{H}_z$$

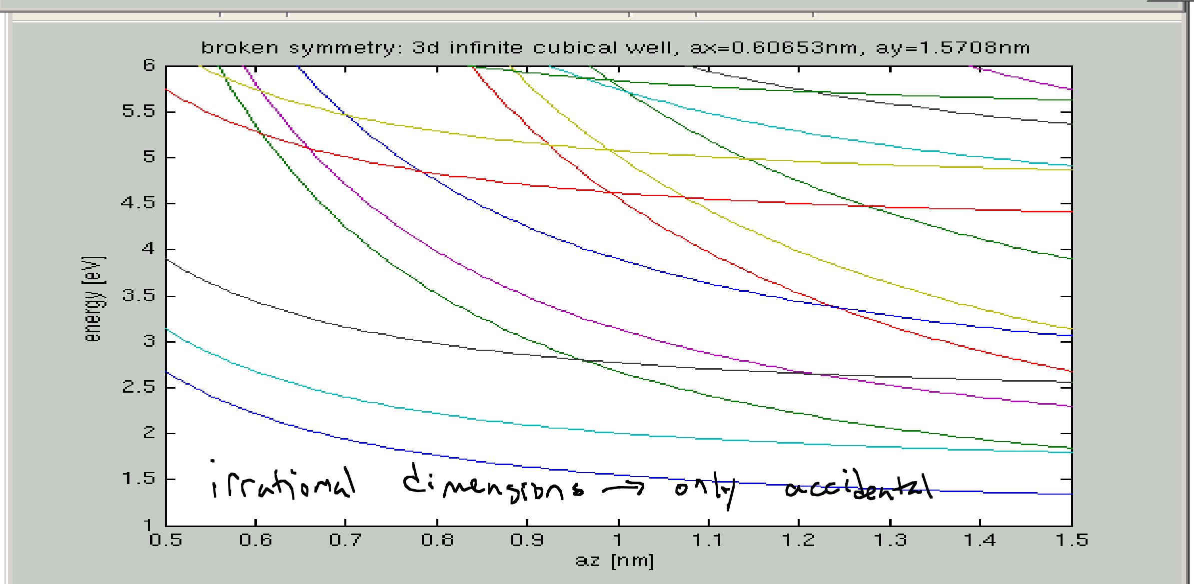
In Matlab/Octave: $A \otimes B \rightarrow$ Kron(A, B)

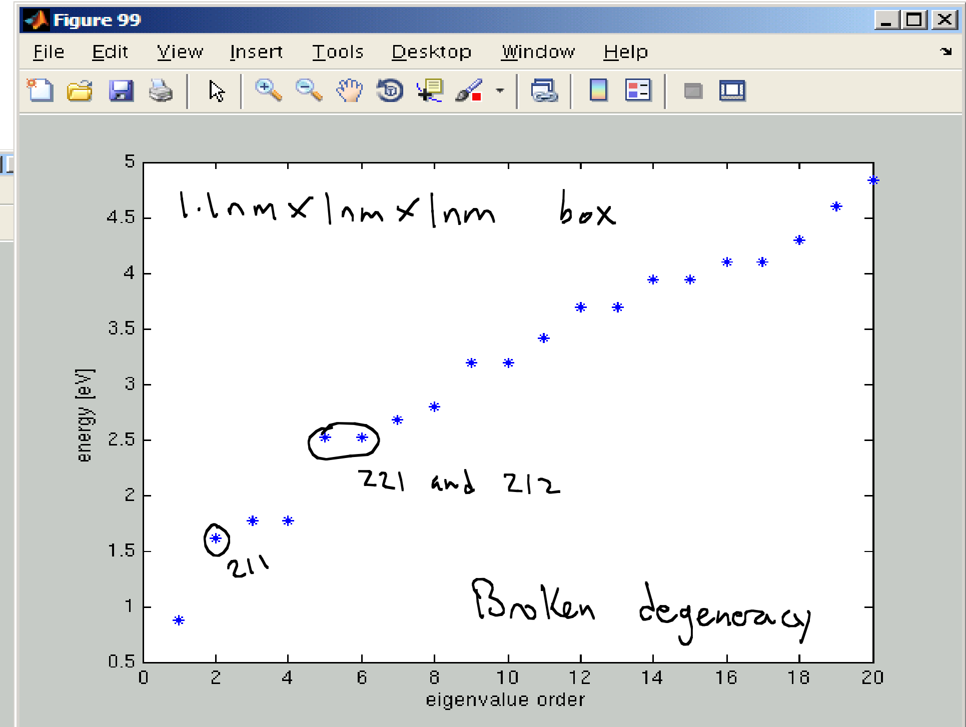
$|\Psi|^2_{3D}$ = reshape($|\Psi|^2_{1D}$, N_x, N_y, N_z)

isosurface ($|\Psi|^2_{3D}$, density)

Broken Symmetry: non-cubical infinite box







3D Isotropic Harmonic Oscillator

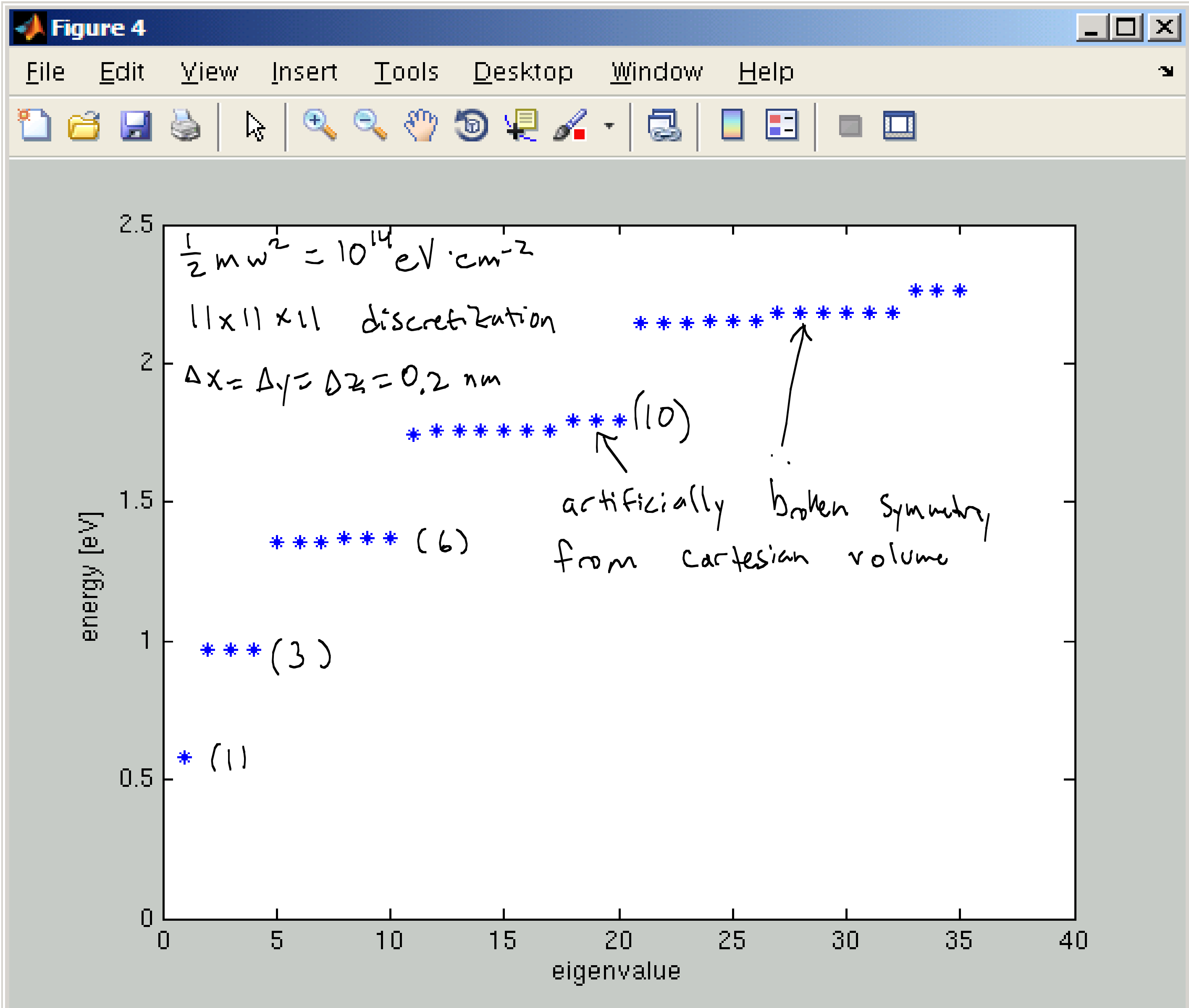
$$-\frac{\hbar^2}{2m}\nabla^2\psi + \frac{1}{2}m\omega^2 r^2\psi = E\psi, \quad r=\sqrt{x^2+y^2+z^2} \qquad \text{so} \quad V(x)=\frac{1}{2}m\omega^2(x^2+y^2+z^2)$$

This is a separable potential, giving

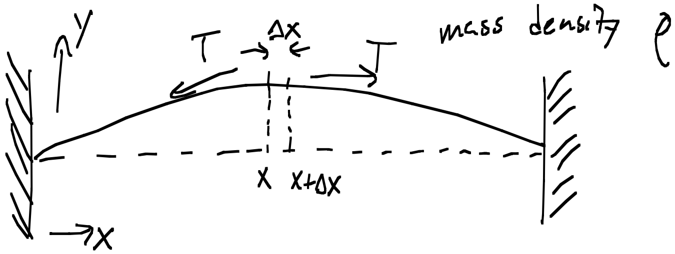
$$E = E_x + E_y + E_z = \hbar\omega(n_x+\tfrac{1}{2}) + \hbar\omega(n_y+\tfrac{1}{2}) + \hbar\omega(n_z+\tfrac{1}{2}) = \hbar\omega(n_x+n_y+n_z+\tfrac{3}{2}), \quad n_x, n_y, n_z = 0, 1, 2, \ldots$$

n_x	n_y	n_z	$E\ (\hbar\omega)$	degeneracy
0	0	0	3/2	1
1	0	0	5/2	3
0	1	0		
0	0	1		
2	0	0	7/2	6
0	2	0		
0	0	2		
1	1	0		
1	0	1		
0	1	1		

Finite differences calculation of 3D HO Spectrum



Classical waves in one dimension (review)

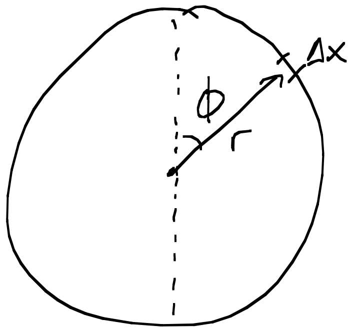


$$F = ma \longrightarrow T\frac{\partial y(x+\Delta x)}{\partial x} - T\frac{\partial y(x)}{\partial x} = (\rho\Delta x)\frac{\partial^2 y}{\partial t^2}$$

$$\sim T\left(\frac{\partial}{\partial x}\left(y(x) + \Delta x\frac{\partial y(x)}{\partial x}\right)\right) - T\frac{\partial y(x)}{\partial x} = \rho\Delta x\frac{\partial^2 y}{\partial t^2}$$

$$\frac{\partial^2 y}{\partial x^2} = \frac{\rho}{T}\frac{\partial^2 y}{\partial t^2} = \frac{1}{c^2}\frac{\partial^2 y}{\partial t^2} \qquad \left(\frac{1}{c^2} \equiv \frac{T}{\rho}\right)$$

Classical wave on a circle



$$\Delta x = r\Delta\phi \longrightarrow dx = r\,d\phi$$

$$\frac{1}{c^2}\frac{\partial^2 y}{\partial t^2} = \frac{\partial^2 y}{r^2\partial\phi^2}$$

$$y(\phi,t) = T(t)\,\varphi(\phi)$$

$$\frac{\frac{1}{c^2}\ddot{T}\cancel{\varphi}}{T\cancel{\varphi}} = \frac{\frac{1}{r^2}\cancel{T}\varphi''}{\cancel{T}\varphi} = -k^2$$

$$\ddot{T} = -k^2c^2T \longrightarrow T = A_\pm\, e^{\pm ikct} \qquad \varphi'' = -k^2r^2\varphi \rightarrow \varphi = Be^{\pm ikr\phi}$$

Apply periodic B.C.'s:

$$\varphi(\phi) = \varphi(\phi + 2\pi) \qquad e^{ikr\phi} = e^{ikr(\phi+2\pi)} = e^{ikr\phi}\underbrace{e^{ikr2\pi}}_{=1}$$

So $kr = n$, $n = 0, \pm 1, \pm 2, \ldots$

$$\varphi \propto e^{in\phi}$$