Separation of variables

1D → 3D

$\psi(x;t) \rightarrow \psi(x,y,z;t)$

Prob. $(x \ldots x+\Delta x) =$
$|\psi(x,t)|^2 \cdot \Delta x$ → Prob $(x \ldots x+\Delta x, y \ldots y+\Delta y, z \ldots z+\Delta z)$
(inside a 3-D volume $\Delta\tau = \Delta x \Delta y \Delta z$)
$|\psi(x,y,z;t)|^2 \cdot \Delta x \Delta y \Delta z$

Req.: $\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx = 1$ → $\iiint dx\,dy\,dz\, |\psi(x,y,z;t)|^2 = 1$

3 Position operators X, Y, Z

$(X\psi)(x,y,z) = x\,\psi(x,y,z)$

$(Y\psi)(x,y,z) = y \cdot \psi(x,y,z)$

$Z \qquad\qquad =$

$P_x \quad \frac{\hbar}{i}\frac{\partial}{\partial x}$

$P_y \quad \frac{\hbar}{i}\frac{\partial}{\partial y}$

$P_z \quad \frac{\hbar}{i}\frac{\partial}{\partial z}$

$\vec{P} = \frac{\hbar}{i}\vec{\nabla}$

$$H = \frac{p_x^2 + p_y^2 + p_z^2}{2m} + V(x,y,z)$$

$$H\varphi = -\frac{\hbar^2}{2m}\underbrace{\left(\frac{\partial^2 \varphi \cdot\cdot}{\partial x^2} + \frac{\partial^2 \varphi \cdot\cdot}{\partial y^2} + \frac{\partial^2 \varphi \cdot\cdot}{\partial z^2}\right)}_{\vec{\nabla}^2 = \Delta} + V(x,y,z)\cdot\varphi(x,y,z)$$

To Do:

i) find eigenStates $H\varphi_E(x,y,z) = E\varphi_E(x,y,z)$

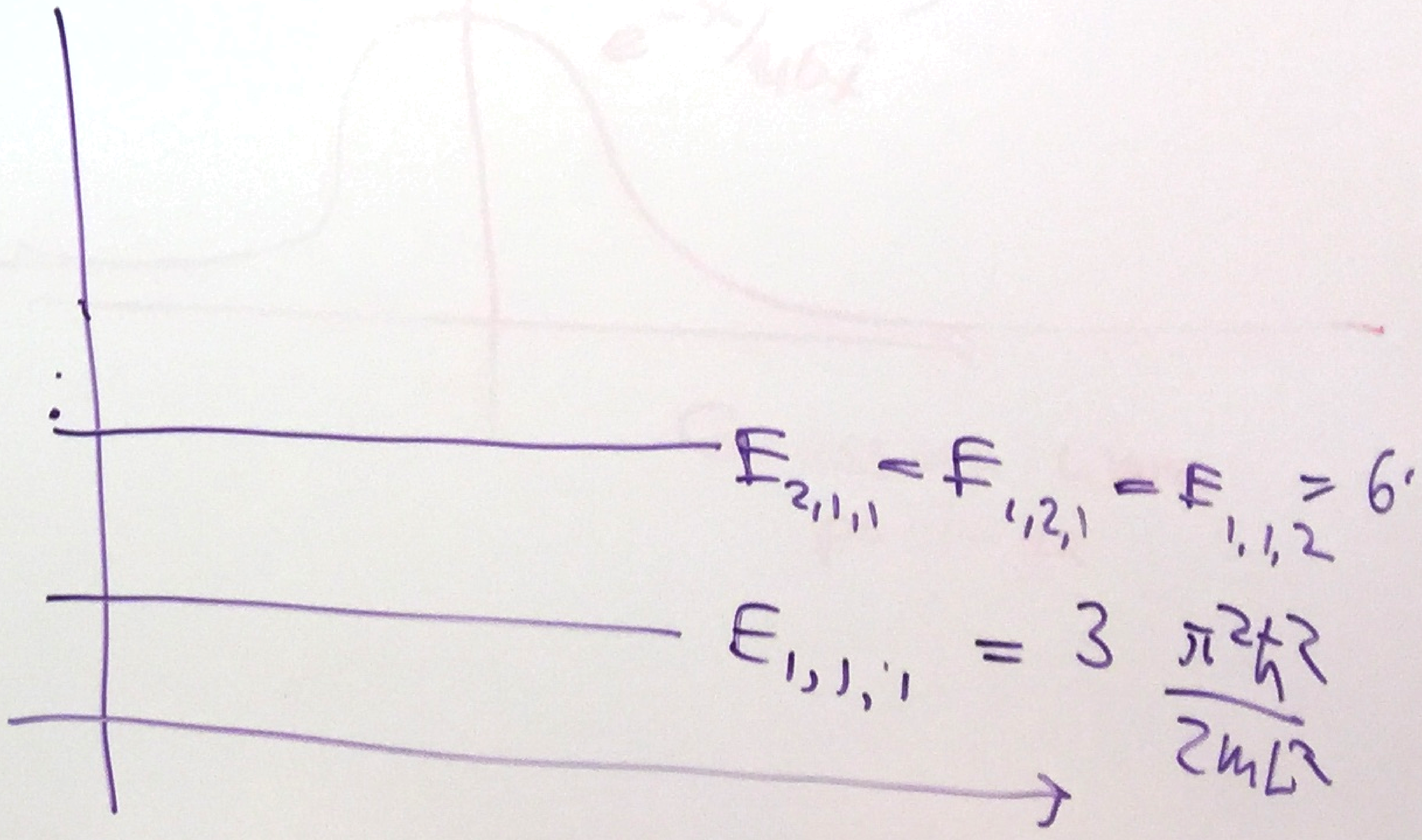
ii) write full solution to Schrödinger Eq.:

$$\Psi_E(x,y,z;t) = \varphi_E(x,y,z)\cdot e^{-\frac{i}{\hbar}Et}$$

$$\varphi_{n,m,k}(x,y,z) = A \sin\frac{n\pi x}{L}\sin\frac{m\pi y}{L}\sin\frac{k\pi z}{L}$$

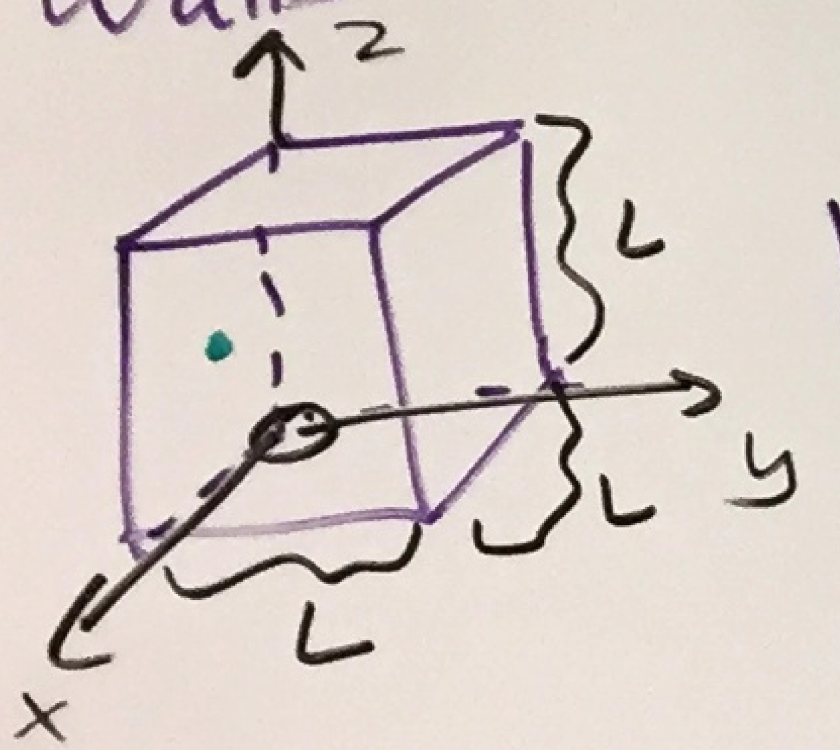
Quantum numbers $n, m, k = 1, 2, 3 \ldots$

$$E_{n,m,k} = \frac{\pi^2\hbar^2}{2mL^2}\left(n^2 + m^2 + k^2\right)$$



Particle in a box

hard walls



$$V(x,y,z) = \begin{cases} 0 & \text{if } 0\le x\le L \text{ and } 0\le y\le L \text{ and } 0\le z\le L \\ \infty & \text{else} \end{cases}$$

Separation of variables: $\varphi_E(x,y,z) \overset{\text{ansatz}}{=} \varphi_1(x)\,\varphi_2(y)\,\varphi_3(z)$

$$-\frac{\hbar^2}{2m}\left\{\frac{1}{\varphi_1(x)}\frac{\partial^2\varphi_1}{\partial x^2}\cancel{\varphi_2\varphi_3} + \cancel{\varphi_1}\frac{1}{\varphi_2}\frac{\partial^2\varphi_2}{\partial y^2}\cancel{\varphi_3} + \cancel{\varphi_1\varphi_2}\frac{1}{\varphi_3}\frac{\partial^2\varphi_3}{\partial z^2}\right) = + -V\cdot\cancel{\varphi_1\varphi_2\varphi_3} \overset{+}{=} E\,\cancel{\varphi_1\varphi_2\varphi_3}$$

Genius $\rightarrow$: divide by $\varphi_1\varphi_2\varphi_3$

$f(x)=E_1 \qquad g(y)=E_2 \qquad h(z)=E_3$

3 Eq.: $-\frac{\hbar^2}{2m}\frac{\partial^2\varphi(x)}{\partial x^2} = E_1\varphi_1(x) \rightarrow \varphi_1(x) = A\sin\left(\frac{n\pi x}{L}\right)$ $\quad E_1 = \frac{n^2\pi^2\hbar^2}{2mL^2}$ $\quad 0\le x\le L \quad$ 0 else

$\varphi_2(x) = \sin\left(\frac{m\pi y}{L}\right) \quad E_2 = \frac{m^2\pi^2\hbar^2}{2mL^2}$