11.4 (a)

Taking u(x,y,z,t) = X(x)Y(y)Z(z)T(t)

for solution to $-\frac{\hbar^2}{2m}\nabla^2 u = i\hbar\frac{\partial u}{\partial t}$, $\hbar$ is Plank's constant divided by π

Verify u is a solution (note no y dependence)

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2}\right] = i\hbar\frac{\partial u}{\partial t}$$

$$-\frac{\hbar^2}{2m}\left[X''YZT + XY''ZT + XYZ''T\right] = i\hbar XYZ\dot{T}$$

or

$$-\frac{\hbar^2}{2m}\left[\frac{X''}{X}+\frac{Y''}{Y}+\frac{Z''}{Z}\right] = i\hbar\frac{\dot{T}}{T}$$

Let $\frac{X''}{X} = -k_x^2$, solving gives $X = e^{ik_x x}$, similar for y and z

Then $X(x)Y(y)Z(z) = e^{ik_x x}e^{ik_y y}e^{ik_z z} = e^{i(k\cdot r)}$

where $k = k_x\hat{i} + k_y\hat{j} + k_z\hat{k}$ and $r = x\hat{i} + y\hat{j} + z\hat{k}$ ($\hat{i},\hat{j},\hat{k}$ are unit direction vectors)

deBroglie relation for matter wave is p(momentum) = $\hbar$k, k is wave number

Now substituting $\frac{X''}{X} = -k_x^2$ and similar for y and z in equation above gives

$$-\frac{\hbar^2}{2m}\left[-k_x^2 + -k_y^2 + -k_z^2\right] = i\hbar\frac{\dot{T}}{T}$$

Rearranging (don't forget $i^2 = -1$)

$$-\frac{\hbar i}{2m}\left[k_x^2 + k_y^2 + k_z^2\right] = \frac{\dot{T}}{T}$$

Then with $p_x = \hbar k_x$ similar for y and z. Substitution gives

$$-\frac{\hbar i}{2m}\left[\frac{p_x^2}{\hbar^2}+\frac{p_y^2}{\hbar^2}+\frac{p_z^2}{\hbar^2}\right] = \frac{\dot{T}}{T} \text{ or } -\frac{i}{\hbar}\left[\frac{p_x^2+p_y^2+p_z^2}{2m}\right] = \frac{\dot{T}}{T}$$

Now $\frac{p_x^2+p_y^2+p_z^2}{2m} = \frac{p^2}{2m} = E$. but also for quantum mechanics $E = \hbar\omega$

Therefore

$$-\frac{i}{\hbar}[\hbar\omega] = \frac{\dot{T}}{T} \text{ or } \frac{dT}{T} = -i\omega dt \quad \text{Solving gives } T = e^{-i\omega t}$$

Therefore

$$u(x,y,z,t) = AX(x)Y(y)Z(z)T(t) = Ae^{i(k\cdot r)}e^{-i\omega t} = Ae^{i(k\cdot r-\omega t)}$$

For part (b) we have specific boundary conditions since confined to box for x we have u(0,y,z,t)=u(a,y,z,t)=0, similar in y and z. Thus in particular X(0)=X(a)=0, and similar for y and z.

Solving the separated equations, eg. For X,

Let $\frac{X''}{X} = -k_x^2$, with $X(0) = X(a) = 0$ since this is a periodic boundary codition we choose $X(x) = A\cos k_x x + B\sin k_x x$

Using the boundary conditions gives (as usual) $X(x) = B\sin k_x \left(\frac{n_x \pi}{a}\right) x$

where $k_x = \frac{n_x \pi}{a}$, similar for y and z

As before $E = \frac{p_x^2 + p_y^2 + p_z^2}{2m}$ and $p_x = \hbar k_x$ similar for y and z gives

$$E = \frac{(\hbar k_x)^2 + (\hbar k_y)^2 + (\hbar k_z)^2}{2m} = \frac{\hbar^2}{2m}[k_x{}^2 + k_y{}^2 + k_z{}^2]$$

Finally using $k_x = \frac{n_x \pi}{a}$, $k_y = \frac{n_y \pi}{a}$, $k_z = \frac{n_z \pi}{a}$ we get

$$E = \frac{\hbar^2 \pi^2}{2ma^2}[n_x{}^2 + n_y{}^2 + n_z{}^2]$$