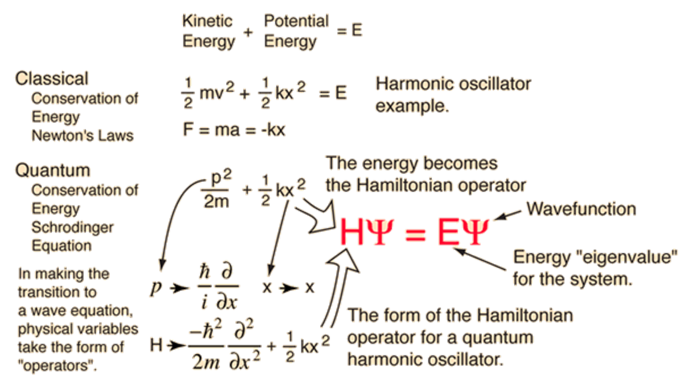
Image section - Q3

Wednesday, October 19, 2016 1:33 AM

<table>
<tr><th>Q3</th><th>D</th><th>E</th></tr>
<tr><td>1</td><td>$$[\frac{-\hbar^2}{2m}\nabla^2+V]\Psi=i\hbar\frac{\partial}{\partial t}\Psi$$</td><td>
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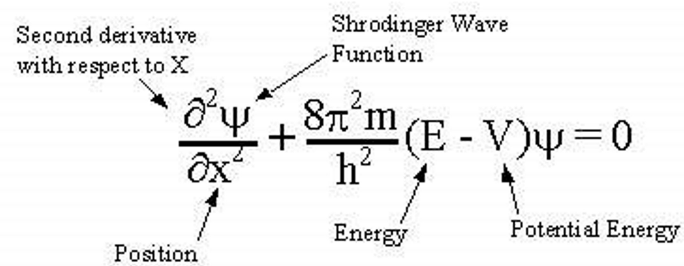
$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t)=-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r},t)+V(\mathbf{r},t)\psi(\mathbf{r},t)$$
i is the imaginary number, $\sqrt{-1}$.
$\hbar$ is Planck's constant divided by 2π: 1.05459×10^{-34} joule·second.
ψ (r,t) is the wave function, defined over space and time.
m is the mass of the particle.
∇^2 is the Laplacian operator, $\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}$.
V(r,t) is the potential energy influencing the particle.</td><td>
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4	Planck's constant Called the 'del-squared operator', this quantity describes how the wavefunction, Ψ, changes from one place to another A mathematical quantity called an 'imaginary number'. It is equal to the square root of minus one $-\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi = i\hbar\frac{\partial\Psi}{\partial t}$ The mass of the particle being described Describes the forces acting on the particle Describes how Ψ changes its shape with time	$H(t)\vert\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}\vert\psi(t)\rangle$
5	$i\hbar\frac{\partial}{\partial t} - \Psi = \hat{H}\Psi$	$H(t)\,\vert\,\psi(t)\rangle = i\hbar\frac{d}{dt}\,\vert\,\psi(t)\rangle$
6	Second derivative with respect to X Shrodinger Wave Function $\frac{\partial^2\psi}{\partial x^2} + \frac{8\pi^2 m}{h^2}(E - V)\psi = 0$ Position Energy Potential Energy	$S[\psi] = \int \frac{1}{2}(\nabla\psi)^2 + V(x)\psi^2(x)\,\mathrm{d}^3x =$ $= \int(\frac{1}{2}(\nabla(RY))^2 + V(RY)^2)\rho^2\mathrm{d}\rho\mathrm{d}\Omega =$ $= \int(\frac{1}{2}(R'^2Y^2 + R^2(\nabla Y)^2 + 2RR'(\hat{\rho}Y)\cdot\nabla Y) + V(RY)^2)\rho^2\mathrm{d}\rho\mathrm{d}\Omega =$ $= \int\left(\frac{1}{2}\left(R'^2 + R^2\frac{l(l+1)}{\rho^2}\right) + VR^2\right)\rho^2\mathrm{d}\rho =$ $= \int \frac{1}{2}\rho^2R'^2 + (\rho^2V + \frac{1}{2}l(l+1))R^2\,\mathrm{d}\rho =$
7	$\frac{\partial\psi}{\partial t} = -i\left(\frac{1}{\hbar}\hat{H}\psi\right)$ *The direction of motion of the amplitude of the wave function* = *Rotation of -90°* (*Complex energy at a particular point divided by Planck's constant*)	$\frac{-\hbar^2}{2m}\frac{\partial^2 u(x)}{\partial x^2} + V(x)u(x) = E\,u(x)$
8	**The Schrödinger Equation** $\left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x) = E\psi(x)$ Hamiltonian operator Wave function Energy	$\frac{-\hbar^2}{2\mu}\frac{1}{r^2\sin\theta}\left[\sin\theta\frac{\partial}{\partial r}\left(r^2\frac{\partial\Psi}{\partial r}\right) + \frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Psi}{\partial\theta}\right) + \frac{1}{\sin\theta}\frac{\partial^2\Psi}{\partial\phi^2}\right]$ $+U(r)\Psi(r,\theta,\phi) = E\,\Psi(r,\theta,\phi)$

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$$
\begin{aligned}
\left(\vec{\sigma}\cdot[\vec{p}+\frac{e}{c}\vec{A}(\vec{r},t)]\right)^2 &= \sigma_i\sigma_j\left(p_ip_j+\frac{e^2}{c^2}A_iA_j+\frac{e}{c}(p_iA_j+A_ip_j)\right)\\
&= \frac{1}{2}(\sigma_i\sigma_j+\sigma_j\sigma_i)\left(p_ip_j+\frac{e^2}{c^2}A_iA_j\right)+\frac{e}{c}\sigma_i\sigma_j\left(A_jp_i+A_ip_j+\frac{\hbar}{i}\frac{\partial A_j}{\partial x_i}\right)\\
&= \delta_{ij}\left(p_ip_j+\frac{e^2}{c^2}A_iA_j\right)+\frac{e}{c}(\sigma_i\sigma_jA_jp_i+\sigma_j\sigma_iA_jp_i)+\frac{e\hbar}{ic}\sigma_i\sigma_j\frac{\partial A_j}{\partial x_i}\\
&= p^2+\frac{e^2}{c^2}A^2+\frac{e}{c}\{\sigma_i,\sigma_j\}A_jp_i+\frac{e\hbar}{ic}\frac{1}{2}(\sigma_i\sigma_j+\sigma_i\sigma_j)\frac{\partial A_j}{\partial x_i}\\
&= p^2+\frac{e^2}{c^2}A^2+\frac{e}{c}2\delta_{ij}A_jp_i+\frac{e\hbar}{ic}\frac{1}{2}(\sigma_i\sigma_j-\sigma_j\sigma_i+2\delta_{ij})\frac{\partial A_j}{\partial x_i}\\
&= p^2+\frac{e^2}{c^2}A^2+\frac{2e}{c}\vec{A}\cdot\vec{p}+\frac{e\hbar}{ic}(i\epsilon_{ijk}\sigma_k+\delta_{ij})\frac{\partial A_j}{\partial x_i}\\
&= p^2+\frac{e^2}{c^2}A^2+\frac{2e}{c}\vec{A}\cdot\vec{p}+\frac{e\hbar}{ic}i\epsilon_{ijk}\sigma_k\frac{\partial A_j}{\partial x_i}\\
&= p^2+\frac{e^2}{c^2}A^2+\frac{2e}{c}\vec{A}\cdot\vec{p}+\frac{e\hbar}{c}\vec{\sigma}\cdot\vec{B}
\end{aligned}
$$

$$[\frac{-\hbar^2}{2m}\nabla^2+V]\Psi = i\hbar\frac{\partial}{\partial t}\Psi$$

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Schrödinger Equation in 3d

- Consider a cubic “box” in which an electron of mass m is confined
- outside the cube, we have $U(x,y,z)=\infty$ and inside $U(x,y,z)=0$
- hence electron has $\psi(x,y,z)=0$ on all faces of the cube
- $\psi(x,y,z)=A\sin(k_1x)\sin(k_2y)\sin(k_3z)$
- $\psi(L,y,z)=0$ for all $0<y<L$ and $0<z<L$ => $k_1=n_1\pi/L$
- similarly we need $k_2=n_2\pi/L$ and $k_3=n_3\pi/L$

$$\boxed{-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right)+U\psi=E\psi}$$

- $E=(\square/2m)(k_1^2+k_2^2+k_3^2) = (\square\pi^2/2mL^2)(n_1^2+n_2^2+n_3^2)$
  $=E_1(n_1^2+n_2^2+n_3^2)$
- where E_1 is ground state energy of 1-d well

$$i\hbar\frac{\partial}{\partial t}\Psi = H\Psi$$

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$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V(x)\psi = E\psi$$

$$
\begin{aligned}
\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial z^2}\psi(z)+mgz\,\psi(z) &= E\,\psi(z)\\
\frac{-\hbar^2}{2m}\frac{1}{l^2}\frac{\partial^2}{\partial z'^2}\psi(z')+mgz'l\,\psi(z') &= E'e\,\psi(z')\\
-A\frac{1}{(A/B)^{\frac{2}{3}}}\frac{\partial^2}{\partial z'^2}\psi(z')+Bz'(A/B)^{\frac{1}{3}}\psi(z') &= E'(AB^2)^{\frac{1}{3}}\psi(z')\\
-\frac{\partial^2}{\partial z'^2}\psi(z')+z'\,\psi(z') &= E'\,\psi(z')\\
-\frac{\partial^2}{\partial z'^2}\psi(z')+(z'-E')\,\psi(z') &= 0\\
-\frac{\partial^2}{\partial z''^2}\psi(z'')+z''\,\psi(z'') &= 0
\end{aligned}
$$

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$$-\frac{\hbar^2}{2m}?\Delta\psi+V\psi = i\hbar\frac{f\psi}{ft}$$

$$\frac{\hbar^2}{2m}\nabla^2\psi+U\psi=-i\hbar\frac{\partial\psi}{\partial t}$$

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$$H(t)\,|\,\psi(t)\rangle = i\hbar\frac{d}{dt}\,|\,\psi(t)\rangle$$

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$$\begin{aligned}\frac{\partial\rho}{\partial t} &= \sum_{\alpha=1}^{z}\left[\left(\frac{\partial}{\partial t}|\Psi^{(\alpha)}(t)\rangle\right)\langle\Psi^{(\alpha)}(t)| + |\Psi^{(\alpha)}(t)\rangle\left(\frac{\partial}{\partial t}\langle\Psi^{(\alpha)}(t)|\right)\right]\\ &= \frac{1}{i\hbar}\sum_{\alpha=1}^{z}\left[\left(H|\Psi^{(\alpha)}(t)\rangle\right)\langle\Psi^{(\alpha)}(t)| - |\Psi^{(\alpha)}(t)\langle\left(\langle\Psi^{(\alpha)}(t)|H\right)\right]\\ &= \frac{1}{i\hbar}(H\rho - \rho H)\\ &= \frac{1}{i\hbar}[H,\rho]\end{aligned}$$

$$\frac{\partial\rho}{\partial t} = \frac{1}{i\hbar}[H,\rho]$$

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$$\hat{H}\psi = E\psi$$

The Schrodinger equation was discovered in 1926 by Erwin Schrodinger, an Austrian theoretical physicist.
It is an important equation that is fundamental to quantum mechanics.

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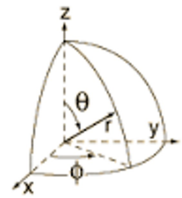

$$\frac{\hbar^2}{2I}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Psi}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2\Psi}{\partial\phi^2}\right] + E\Psi = 0$$

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$$\psi(x) = Axe^{-\frac{x^2}{L^2}}$$

$$\frac{\delta\psi}{\delta x} = Ae^{-\frac{x^2}{L^2}} - \frac{2Ax^2}{L^2}e^{-\frac{x^2}{L^2}}$$

$$= \left(1 - \frac{2x^2}{L^2}\right)\frac{\psi}{x}$$

$$\frac{\delta^2\psi}{\delta x^2} = \left(-\frac{4x}{L^2}\right)\left(\frac{\psi}{x}\right) + \left(1 - \frac{2x^2}{L^2}\right)\left(-\frac{2\psi}{L^2}\right)$$

$$-\frac{2m}{\hbar^2}(E-U)\psi = \psi\left(-\frac{4}{L^2} - \frac{2}{L^2} + \frac{4x^2}{L^2}\right)$$

$$U(x) = \frac{\hbar^2}{2mL^2}\left(\frac{4}{L^2}x^2 - 6\right)$$

$$= \frac{4\hbar^2}{2mL^4}x^2 - \frac{6\hbar^2}{2mL^2}$$

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Problem 1: Schrodinger's Equation - "Particle in a box"

The time independent Schrodinger Equation has the form:

$$\frac{\partial^2\psi}{\partial x^2} = \frac{2m}{\hbar^2}\left[U(x) - E\right]\psi$$

a) Considering the *boundary conditions* for an infinite potential (length, *L* - particle in a box) demonstrate the validity of this equation.

b) Determine the Energy of the confined levels in this system.

c) What is the Normalization constant for the *n=2* state.

d) What is i) the probability of finding a particle in the confined *n=2* state? And ii) What is the most likely position to find the particle?

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