Tutorial 3 Solutions

T3.1

$$(2E - V_0) \sin\left[\frac{\sqrt{2mE}\, l}{\hbar}\right] = 2\sqrt{V_0 E - E^2}\,\cos\left[\frac{\sqrt{2mE}\, l}{\hbar}\right] \rightarrow ①$$

$$\psi_I = C\, e^{\left[\frac{\sqrt{2m(V_0 - E)}}{\hbar} x\right]} \rightarrow ②$$

$$\psi_{II} = A\cos\left[\frac{\sqrt{2mE}}{\hbar} x\right] + B\sin\left[\frac{\sqrt{2mE}}{\hbar} x\right] \rightarrow ③$$

$$\psi_{III} = G\, e^{\left[-\frac{\sqrt{2m(V_0 - E)}}{\hbar} x\right]} \rightarrow ④$$

when $V_0 \rightarrow \infty$, ① becomes

$$-V_0 \sin\left[\frac{\sqrt{2mE}\, l}{\hbar}\right] = 2\sqrt{V_0 E}\,\cos\left[\frac{\sqrt{2mE}\, l}{\hbar}\right]$$

$$\frac{\sin\left[\frac{\sqrt{2mE}\, l}{\hbar}\right]}{\cos\left[\frac{\sqrt{2mE}\, l}{\hbar}\right]} = \frac{-2\sqrt{E}}{\sqrt{V_0}}$$

$$\tan\left[\frac{\sqrt{2mE}\, l}{\hbar}\right] = 0$$

$$\Rightarrow \frac{\sqrt{2mE}\, l}{\hbar} = n\pi$$

$$\boxed{E = \frac{n^2 h^2}{8ml^2}}$$

② becomes

$$\psi_I = C\, e^{\left[\frac{\sqrt{2m(V_0 - E)}}{\hbar} x\right]} = C e^{-\infty} = 0$$

[x is negative in region I and $V_0 \rightarrow \infty$]

④ becomes

$$\psi_{III} = G e^{-\infty} = 0$$

③

To have ψ continuous,

$\psi_{II} = 0$ at $x = 0$ and $x = l$.

Under this condition, $\psi_{II} = \sqrt{\frac{2}{l}} \sin\left(\frac{n\pi x}{l}\right)$

So, when $V_0 \rightarrow \infty$, Particle in a finite well $\longrightarrow$ Particle in a box

T3.2

YES. If the ratio of 2 lengths is an integer we will have degeneracy. For example, when $b = ka$ (k is integer),

then $\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} = \frac{1}{a^2}\left(n_x^2 + \frac{n_y^2}{k^2}\right)$

Now states with quantum numbers $(1, 2k, n_z)$ and $(2, k, n_z)$ will have the same energy.

Example Let $b = 3a$

$$E = \frac{h^2}{8m}\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right) = \frac{h^2}{8m}\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{9a^2} + \frac{n_z^2}{c^2}\right)$$

$$E = \frac{h^2}{8m}\left[\frac{1}{a^2}\left(n_x^2 + \frac{n_y^2}{9}\right) + \frac{n_z^2}{c^2}\right]$$

$$E_{1,6,3} = \frac{h^2}{8m}\left[\frac{1}{a^2}\left(1 + \frac{36}{9}\right) + \frac{9}{c^2}\right] = \frac{h^2}{8m}\left(\frac{5}{a^2} + \frac{9}{c^2}\right)$$

$$E_{2,3,3} = \frac{h^2}{8m}\left[\frac{1}{a^2}\left(4 + \frac{9}{9}\right) + \frac{9}{c^2}\right] = \frac{h^2}{8m}\left(\frac{5}{a^2} + \frac{9}{c^2}\right)$$

So $E_{1,6,3}$ and $E_{2,3,3}$ are degenerate even when $a \neq b \neq c$.

This phenomenan is called accidental degeneracy.

T3.3

$\cancel{(1-x^2)\,y''(x) \neq 2}$

$$(1-x^2)\,y''(x) - 2x\,y'(x) + 3\,y(x) = 0 \longrightarrow (1)$$

$$\text{Let } y(x) = \sum_{n=0}^{\infty} c_n x^n \longrightarrow (2)$$

$$y'(x) = \sum_{n=1}^{\infty} n c_n x^{n-1} = \sum_{n=0}^{\infty} n c_n x^{n-1} \longrightarrow (3)$$

$$y''(x) = \sum_{n=2}^{\infty} n(n-1) c_n x^{n-2} = \sum_{n=0}^{\infty} (n+2)(n+1) c_{n+2} x^n \longrightarrow (4)$$

Put (2), (3) and (4) in (1)

$$(1-x^2)\sum_{n=0}^{\infty}(n+2)(n+1)c_{n+2}x^n - 2x\sum_{n=0}^{\infty} n c_n x^{n-1} + 3\sum_{n=0}^{\infty} c_n x^n = 0$$

$$\sum_{n=0}^{\infty}(n+2)(n+1)c_{n+2}x^n - \sum_{n=0}^{\infty}(n+2)(n+1)c_{n+2}x^{n+2} - 2\sum_{n=0}^{\infty} n c_n x^n$$

$$\sum_{n=0}^{\infty}(n+2)(n+1)C_{n+2}x^n - \sum_{n=0}^{\infty} n(n-1)C_n x^n - 2\sum_{n=0}^{\infty} nC_n x^n + 3\sum_{n=0}^{\infty} C_n x^n = 0$$

$$\sum_{n=0}^{\infty}\left[(n+2)(n+1)C_{n+2} - n(n-1)C_n - 2nC_n + 3C_n\right]x^n = 0$$

$$(n+2)(n+1)C_{n+2} - (n^2 - n + 2n - 3)C_n = 0$$

$$C_{n+2} = \frac{n^2+n-3}{(n+1)(n+2)}C_n$$

$n=0$

$$C_2 = \frac{-3}{2}C_0$$

$n=2$

$$C_4 = \frac{4+2-3}{3.4}C_2 = \frac{1}{4}\left(\frac{-3}{2}\right)C_0 = \frac{-3}{8}C_0$$

$n=1$

$$C_3 = \frac{1+1-3}{2.3}C_1 = \frac{-1}{6}C_1$$

$n=3$

$$C_5 = \frac{9+3-3}{4.5}C_3 = \frac{9}{20}\left(\frac{-1}{6}\right)C_1 = \frac{-3}{40}C_1$$

T3.4

$$H = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m} + \frac{k_x x^2}{2} + \frac{k_y y^2}{2} + \frac{k_z z^2}{2}$$

Hamiltonian operator

$$\hat{H} = \frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + \frac{k_x}{2}\hat{x}^2 + \frac{k_y}{2}\hat{y}^2 + \frac{k_z}{2}\hat{z}^2$$

Schrödinger equation

$$\frac{-\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right) + \left(\frac{k_x}{2}\hat{x}^2 + \frac{k_y}{2}\hat{y}^2 + \frac{k_z}{2}\hat{z}^2\right)\psi = E\psi \longrightarrow 1$$

Let $\psi(x,y,z) = f(x)\, g(y)\, h(z) \longrightarrow 2$

2 in 1

$$-\frac{\hbar^2}{2m}\frac{d^2f}{dx^2}gh - \frac{\hbar^2}{2m}f\frac{d^2g}{dy^2}h - \frac{\hbar^2}{2m}fg\frac{d^2h}{dz^2} + \left(\frac{k_x x^2}{2} + \frac{k_y y^2}{2} + \frac{k_z z^2}{2}\right)fgh = Efgh$$

Divide by fgh

$$-\frac{\hbar^2}{2m}\frac{1}{f}\frac{d^2f}{dx^2}-\frac{\hbar^2}{2m}\frac{1}{g}\frac{d^2g}{dy^2}-\frac{\hbar^2}{2m}\frac{1}{h}\frac{d^2h}{dz^2}+\frac{k_x x^2}{2}+\frac{k_y y^2}{2}+\frac{k_z z^2}{2}=E \quad (4)$$

$$-\frac{\hbar^2}{2m}\frac{1}{f}\frac{d^2f}{dx^2}+\frac{k_x x^2}{2}=E+\frac{\hbar^2}{2m}\frac{1}{g}\frac{d^2g}{dy^2}+\frac{\hbar^2}{2m}\frac{1}{h}\frac{d^2h}{dz^2}-\frac{k_y y^2}{2}-\frac{k_z z^2}{2}$$

$$-\frac{\hbar^2}{2m}\frac{1}{f(x)}\frac{d^2f(x)}{dx^2}+\frac{k_x x^2}{2}=E_x$$

Similarly,

$$\left.\begin{aligned}-\frac{\hbar^2}{2m}\frac{1}{g(y)}\frac{d^2g(y)}{dy^2}+\frac{k_y y^2}{2}&=E_y\\-\frac{\hbar^2}{2m}\frac{1}{h(z)}\frac{d^2h(z)}{dz^2}+\frac{k_z z^2}{2}&=E_z\end{aligned}\right\} \longrightarrow (3)$$

Equ. (3) corresponds to three independent Harmonic Oscillators and they can be solved separately.

Finally,

$$\psi_{v_x,v_y,v_z}(x,y,z)=\frac{1}{\sqrt{2^{v_x+v_y+v_z}(v_x!)(v_y!)(v_z!)}}\left(\frac{\alpha}{\pi}\right)^{\frac{3}{4}}e^{-\frac{\alpha}{2}(x^2+y^2+z^2)}H_{v_x}(\sqrt{\alpha}x)H_{v_y}(\sqrt{\alpha}y)H_{v_z}(\sqrt{\alpha}z) \longrightarrow (4)$$

$$E_{v_x,v_y,v_z}=\left(v_x+\frac{1}{2}\right)h\nu_x+\left(v_y+\frac{1}{2}\right)h\nu_y+\left(v_z+\frac{1}{2}\right)h\nu_z$$

$v_x=0,1,2,\ldots$
$v_y=0,1,2,\ldots$
$v_z=0,1,2,\ldots$

when $k_x=k_y=k_z$, we will have degeneracy

$$\nu_x=\nu_y=\nu_z=\nu$$

$$E_{v_x,v_y,v_z}=\left(v_x+v_y+v_z+\frac{3}{2}\right)h\nu$$

$$H=\frac{p_x^2}{2m}+\frac{p_y^2}{2m}+\frac{p_z^2}{2m}+\frac{1}{2}k_x x^2+\frac{1}{2}k_y y^2+\frac{1}{2}k_z z^2+xy^2\sqrt{z}$$

For the above Hamiltonian, seperation of variables is not possible because of the $xy^2\sqrt{z}$ term. Hence solutions of form equ. (4) cannot be obtained and one has to use approximation methods.