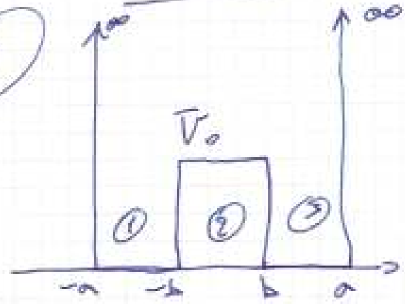
Κβαντομηχανική II

8/6/2007

(1)



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

(2) $\psi_2' = 0 \Rightarrow \psi_2'' = 0$

$E = V_0$, $\psi_2(x) = B$

(1) $-\frac{\hbar^2}{2m}\psi_1'' = E\psi_1 \Rightarrow \psi_1'' = \frac{-2mE}{\hbar^2}\psi_1 = -k^2\psi_1$

$\psi_1(x) = A\sin k(x+a)$, $\psi_1(-a) = 0$

(3) $\psi_3(x) = \Gamma \sin k(a-x)$, $\psi_3(a) = 0$

$\psi_1(-b) = \psi_2(-b) \Rightarrow A\sin k(a-b) = B$

$\psi_1'(-b) = \psi_2'(-b) \Rightarrow kA\cos k(a-b) = 0 \Rightarrow$

$\Rightarrow k(a-b) = (2n+1)\frac{\pi}{2} \Rightarrow \frac{2mE}{\hbar^2} = (2n+1)^2\frac{\pi^2}{4(a-b)^2}$

$$E_n = (2n+1)^2\frac{\pi^2\hbar^2}{8m(a-b)^2}.$$

Απόδειξη της σχέσης: $u_1(x) = A \sin k(x+a)$ (1A)

$$u_1'' = -k^2 u_1 \Rightarrow u_1(x) = A_1 e^{ikx} + A_2 e^{-ikx}$$

$$u_1(-a) = 0 \Rightarrow A_1 e^{-ika} + A_2 e^{ika} = 0$$

$$\Rightarrow A_2 = -A_1 e^{-2ika}$$

$$\Rightarrow u_1(x) = A_1 (e^{ikx} - e^{-ikx} e^{-2ika}) =$$

$$= A_1 e^{-ika} (e^{ikx} e^{ika} - e^{-ikx} e^{-ika}) =$$

$$= A_1 e^{-ika} (e^{ik(x+a)} - e^{-ik(x+a)}) =$$

$$= 2i A_1 e^{-ika} \sin k(x+a) = A \sin k(x+a)$$

με δεύτερο τρόπο $\Rightarrow$

$$u_1(x) = A_1 \sin kx + A_2 \cos kx$$

$$u_1(-a) = 0 \Rightarrow -A_1 \sin ka + A_2 \cos ka = 0$$

$$\Rightarrow A_2 = A_1 \frac{\sin ka}{\cos ka}$$

$$\Rightarrow u_1(x) = A_1 \left[\sin kx + \cos kx \frac{\sin ka}{\cos ka} \right] =$$

$$= \frac{A_1}{\cos ka} \left[\sin kx \cos ka + \cos kx \sin ka \right] =$$

$$= A \sin k(x+a) \quad .$$

(5)

(2) $H_0 = \frac{1}{2m}(p_x^2 + p_y^2) + \frac{1}{2}m\omega^2(x^2+y^2)$

(α) $H_0 = H_x + H_y \Rightarrow E = E_x + E_y$

$$E = (n_x+\tfrac{1}{2})\hbar\omega + (n_y+\tfrac{1}{2})\hbar\omega = (n+1)\hbar\omega$$

$n = n_x + n_y \Rightarrow$ εκφυλισμός $= n+1$.

(β) $\phi_0(\vec r) = \psi_0(x)\psi_0(y)$

$$\phi_1(\vec r) = \begin{cases} \psi_0(x)\psi_1(y) \\ \psi_1(x)\psi_0(y) \end{cases}$$

(γ) $\psi(\vec r,t) = N x\, e^{-bx^2} e^{-by^2}\, e^{-i\frac{Et}{\hbar}} = \phi(\vec r)\, e^{-i\frac{Et}{\hbar}}$

$$H_0\psi = i\hbar\frac{d\psi}{dt} = (i\hbar)(-\tfrac{i}{\hbar})\psi E = E\psi$$

$$H_0\phi = E\phi \Rightarrow \frac{-\hbar^2}{2m}\left[\frac{d^2\phi}{dx^2} + \frac{d^2\phi}{dy^2}\right] + \frac{m\omega^2}{2}(x^2+y^2)\phi = E\phi$$

$$\frac{d\phi}{dx} = Ne^{-bx^2}e^{-by^2} - 2Nbx^2 e^{-bx^2}e^{-by^2}$$

$$\frac{d^2\phi}{dx^2} = -2Nbx e^{-bx^2}e^{-by^2} - 4Nbx e^{-bx^2}e^{-by^2} + 4Nb^2x^3 e^{-bx^2}e^{-by^2}$$

$$\frac{d\phi}{dy} = -2Nby\,x e^{-bx^2}e^{-by^2}, \quad \frac{d^2\phi}{dy^2} = -2Nbx e^{-bx^2}e^{-by^2} + 4Nb^2y^2x\, e^{-bx^2}e^{-by^2}$$

$$\Rightarrow -\frac{\hbar^2}{2m}\left[-2bx-4bx+4b^2x^3-2bx+4b^2xx^2\right]$$

$$+\frac{1}{2}m\omega^2(x^3+x^2x)=Ex$$

βγάζουμε κοινό παράγοντα το: $Ne^{-bx^2}e^{-bx^2}$

εξισώνουμε ίδιες δυνάμεις των x, x $\Rightarrow$

$$\frac{8b\hbar^2}{2m}=E \quad , \quad \left.\begin{array}{l}-\frac{\hbar^2}{2m}4b^2+\frac{m\omega^2}{2}=0\\ -\frac{\hbar^2}{2m}4b^2+\frac{m\omega^2}{2}=0\end{array}\right\}\Rightarrow \boxed{b^2=\frac{m^2\omega^2}{4\hbar^2}}$$

$$\boxed{E=4\frac{\hbar^2}{m}\cdot\frac{m\omega}{2\hbar}=2\hbar\omega}.$$

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(5) $\Phi_{11}=\psi_0(x)\psi_1(x)$, $\Phi_{12}=\psi_1(x)\psi_0(x)$

$$V_{11}=\int dx\,dx\,\Phi_{11}^*\,ax^4\,\Phi_{11}=\int dx\,\psi_0^*(x)\,ax^4\,\psi_0(x)\int\psi_1^*\psi_1\,dx$$

$$\int\psi_1^*\psi_1\,dx=1\Rightarrow \boxed{V_{11}=aV_0}$$

$$V_{12}=\int dx\,dx\,\Phi_{11}^*\,ax^4\,\Phi_{12}=a\int dx\,\psi_0^*(x)x^4\psi_1(x)\int dx\,\psi_1^*(x)\psi_0(x)=0$$

όμοια $V_{21}=0$

$$\boxed{V_{22}=\int dx\,dx\,\Phi_{12}^*\,ax^4\,\Phi_{12}=aV_1} \quad \Rightarrow V=\begin{pmatrix}aV_0 & 0\\ 0 & aV_1\end{pmatrix}$$

$$\Rightarrow \quad E_{11}=2\hbar\omega+aV_0 \quad , \quad E_{12}=2\hbar\omega+aV_1.$$

(3) (a) $J^2 = L^2 + S^2 + 2\vec{L}\cdot\vec{S}$ (4)

$\vec{L}\cdot\vec{S} = L_x S_x + L_y S_y + L_z S_z$

$[L_x, L_y] = i\hbar L_z \quad , \quad [S_x, S_y] = i\hbar S_z$

$[J^2, J_z] = [J^2, L_z] + [J^2, S_z] = ? = 0$

$[J^2, L_z] = [L^2 + S^2 + 2\vec{L}\cdot\vec{S}, L_z] = 2[\vec{L}\cdot\vec{S}, L_z] =$

$= 2[L_x S_x, L_z] + 2[L_y S_y, L_z] + 0 =$

$= 2[L_x, L_z]S_x + 2[L_y, L_z]S_y = -2i\hbar L_y S_x + 2i\hbar L_x S_y$

$[J^2, S_z] = \dots = 2[L_x S_x, S_z] + 2[L_y S_y, S_z] =$

$= -2i\hbar L_x S_y + 2i\hbar L_y S_x$

(b) $H = \frac{L_x^2 + L_y^2}{2I_1} + \frac{L_z^2}{2I_2} = \frac{L^2}{2I_1} - \frac{L_z^2}{2I_1} + \frac{L_z^2}{2I_2}$

$H Y_l^m = \left\{ \frac{\hbar^2 l(l+1)}{2I_1} + \frac{\hbar^2 m^2}{2I_2} - \frac{\hbar^2 m^2}{2I_1} \right\} Y_l^m$

$I_1 = 5I_2 \Rightarrow E_{lm} = \left\{ \frac{\hbar^2 l(l+1)}{10 I_2} - \frac{\hbar^2 m^2}{10 I_2} + \frac{\hbar^2 m^2}{2I_2} \right\}$

$E_{lm} = \frac{\hbar^2}{10 I_2} \left\{ l(l+1) + 4m^2 \right\}$

$$E_{00} = 0 \quad , \quad E_{10} = \frac{2\hbar^2}{10 I_2} = \frac{\hbar^2}{5 I_2}$$

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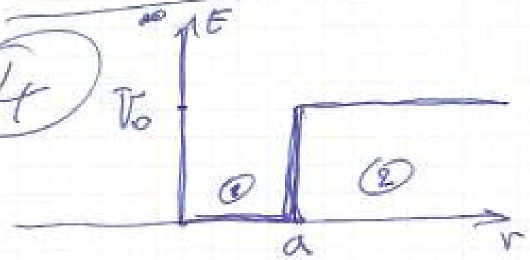
$$E_{1,\pm 1} = \frac{\hbar^2}{10 I_2}\{2 + 4\} = \frac{3\hbar^2}{5 I_2}$$

$$E_{20} = \frac{6\hbar^2}{10 I_2} = \frac{3\hbar^2}{5 I_2}$$

Τρίτη στάθμη εκφυλισμός = 3

$E_{2\pm 1}$ και $E_{2\pm 2}$ έχουν μεγαλύτερη ενέργεια

4



$$H = -\frac{\hbar^2}{2m}\nabla^2 + V(r)$$

$$\vec{L}^2 = -\hbar^2\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right\}$$

(α)

$$H\psi = -\frac{\hbar^2}{2m}\frac{1}{r}\frac{d^2}{dr^2}(r\psi) + \frac{\vec{L}^2\psi}{2mr^2} + V(r)\psi = E\psi$$

$$\psi = R(r)\, Y_{lm}(\theta,\varphi)$$

$$H\psi = -\frac{\hbar^2}{2m}\frac{1}{r}(rR)'' Y_{lm} + \frac{\hbar^2 l(l+1) R Y_{lm}}{2mr^2} + V(r) R Y_{lm}$$

(β) Χαμηλότερη στάθμη για $l=0 \rightarrow Y_{00} = \frac{1}{\sqrt{4\pi}}$

(Απόδειξη στο τέλος)

Γράφουμε την εξίσωση μόνο για το R.

$$-\frac{\hbar^2}{2m}\frac{1}{r}(rR'') + V(r)R = ER$$

ορίζουμε $u(r) = r R(r)$

$\Rightarrow -\frac{\hbar^2}{2m} u'' + V(r) u = E u$

με την συνθήκη $u(0) = 0$.

(1) $-\frac{\hbar^2}{2m} u_1'' = E u_1 \Rightarrow u_1'' = -\frac{2mE}{\hbar^2} u_1 = -k_1^2 u_1$

$k_1^2 = \frac{2mE}{\hbar^2}$ και $u_1(r) = A \sin k_1 r$

(2) $-\frac{\hbar^2}{2m} u_2'' + V_0 u_2 = E u_2$

$$u_2'' = \frac{2m}{\hbar^2}(V_0 - E) u_2 = k_2^2 u_2$$

$$u_2(r) = B e^{-k_2 r}, \quad k_2^2 = \frac{2m}{\hbar^2}(V_0 - E)$$

<u>οριακές συνθήκες:</u>

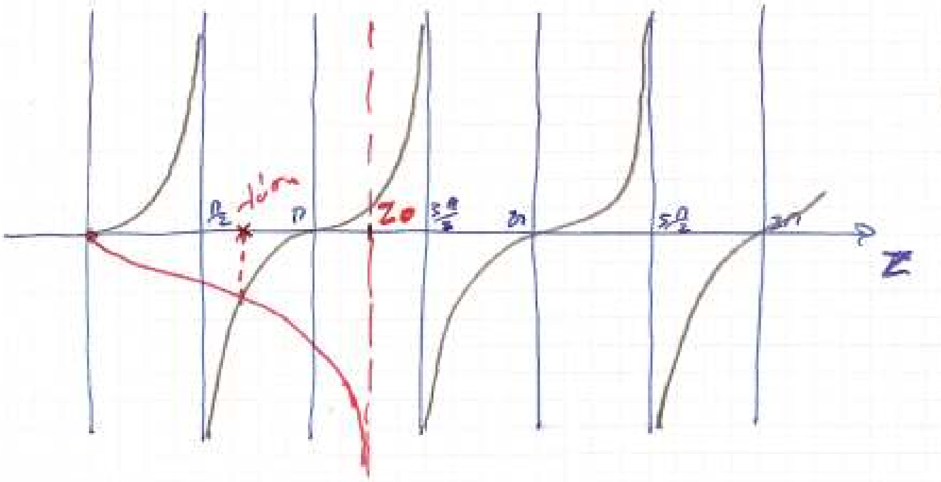
$u_1(a) = u_2(a) \Rightarrow A \sin k_1 a = B e^{-k_2 a}$

$u_1'(a) = u_2'(a) \Rightarrow k_1 A \cos k_1 a = -k_2 B e^{-k_2 a}$

$\Rightarrow \boxed{\tan k_1 a = -\frac{k_1}{k_2}}$

θέτουμε: $k_1 a = z$ $\Rightarrow k_2^2 a^2 = z_0^2 - z^2$

με $\boxed{z_0^2 = \frac{2m}{\hbar^2} V_0}$ $\Rightarrow \boxed{\tan z = -\sqrt{\frac{z^2}{z_0^2 - z^2}}}$



Μια μόνο λύση όταν $\frac{\pi}{2} < z_0 < \frac{3\pi}{2}$.

$$\frac{\pi^2}{4} < \frac{2m}{\hbar^2} V_0 < \frac{9\pi^2}{4} \Rightarrow \boxed{\frac{\hbar^2\pi^2}{8m} < V_0 < \frac{9\hbar^2\pi^2}{8m}}.$$

5 $\chi_+ = \begin{pmatrix}1\\0\end{pmatrix}, \quad \chi_- = \begin{pmatrix}0\\1\end{pmatrix}$

$$\psi^*\psi = c^*c\,(1+4) = 5c^*c \Rightarrow c = \frac{1}{\sqrt{5}}$$

$$\boxed{\psi = \frac{1}{\sqrt{5}}\chi_+ + \frac{2}{\sqrt{5}}\chi_- = \frac{1}{\sqrt{5}}\begin{pmatrix}1\\2\end{pmatrix}}$$

$$S_n = \frac{1}{\sqrt{3}}\left(S_x + \sqrt{2}\,S_y\right) = \frac{\hbar}{2}\begin{pmatrix}0 & \frac{1-i\sqrt{2}}{\sqrt{3}}\\ \frac{1+i\sqrt{2}}{\sqrt{3}} & 0\end{pmatrix}$$

$$S_n = \frac{\hbar}{2}\begin{pmatrix}0 & a^*\\ a & 0\end{pmatrix}, \quad a = \frac{1+i\sqrt{2}}{\sqrt{3}}.$$

(α) $S_n\psi = \lambda\psi \Rightarrow \det\left(S_n - \lambda\mathbb{1}\right) = 0$

$$\begin{vmatrix} -\cancel{\tilde{\lambda}} & a^* \\ a & -\tilde{\lambda} \end{vmatrix} = 0 \quad , \lambda = \tilde{\lambda}\frac{\hbar}{2} = \pm\frac{\hbar}{2}$$ 8

$$\tilde{\lambda}^2 - aa^* = 0 \Rightarrow \tilde{\lambda}^2 - 1 = 0 \Rightarrow \tilde{\lambda} = \pm 1$$

$$aa^* = \frac{1}{3}(1+i\sqrt{2})(1-i\sqrt{2}) = \frac{3}{3} = 1$$

(b) $\langle S_u \rangle = P_+\left(\frac{\hbar}{2}\right) + P_-\left(-\frac{\hbar}{2}\right)$

$$P_+ + P_- = 1 \quad , \quad P_- = 1 - P_+$$

$$\langle S_u \rangle = 2P_+\left(\frac{\hbar}{2}\right) + \left(-\frac{\hbar}{2}\right) = \frac{\hbar}{2}\left(2P_+ - 1\right)$$

$$\langle S_u \rangle = \frac{\hbar}{2}\cdot\frac{1}{5}\,(1,2)\begin{pmatrix} 0 & a^* \\ a & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 2 \end{pmatrix} = \frac{\hbar}{10}\left(2a^* + 2a\right)$$

$$\langle S_u \rangle = \frac{2\hbar}{10}\left(\frac{2}{\sqrt{3}}\right) = \frac{4\hbar}{10\sqrt{3}} = \frac{\hbar}{2}\left(-1 + 2P_+\right)$$

$$-1 + 2P_+ = \frac{4}{5\sqrt{3}} \rightarrow 2P_+ = \frac{4}{5\sqrt{3}} + 1 = \frac{4+5\sqrt{3}}{5\sqrt{3}}$$

$$\boxed{P_+ = \frac{4+5\sqrt{3}}{10\sqrt{3}}} \qquad \boxed{P_- = \frac{5\sqrt{3}-4}{10\sqrt{3}}}$$

Δεύτερη λύση στο (β)

Βρίσκουμε τις ιδιοτιμές του $S_n \rightarrow \pm \frac{\hbar}{2}$

$$S_n = \frac{\hbar}{2}\begin{pmatrix} 0 & \frac{1-i\sqrt{2}}{\sqrt{3}} \\ \frac{1+i\sqrt{2}}{\sqrt{3}} & 0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 0 & a^* \\ a & 0 \end{pmatrix}$$

Βρίσκουμε τις ιδιοσυναρτήσεις του S_n

$$S_n \chi_1 = \frac{\hbar}{2}\chi_1 \Rightarrow \frac{\hbar}{2}\begin{pmatrix} 0 & a^* \\ a & 0 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

$$\Rightarrow \left.\begin{array}{l} c_2 a^* = c_1 \\ a c_1 = c_2 \end{array}\right\} \quad \begin{array}{l} \text{κανονικοποίηση} \\ c_1^* c_1 + c_2^* c_2 = 1 \end{array}$$

$$\Rightarrow c_2^* a a^* c_2 + c_2^* c_2 = 1 \Rightarrow 2 c_2^* c_2 = 1$$

$c_2 = \frac{1}{\sqrt{2}}$ και $c_1 = \frac{1-i\sqrt{2}}{\sqrt{6}}$, $aa^* = 1$.

$$S_n \chi_2 = -\frac{\hbar}{2}\chi_2 \Rightarrow \frac{\hbar}{2}\begin{pmatrix} 0 & a^* \\ a & 0 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = -\frac{\hbar}{2}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

$$\Rightarrow \left.\begin{array}{l} a^* c_2 = -c_1 \\ a c_1 = -c_2 \end{array}\right\} \quad \begin{array}{l} c_1^* c_1 + c_2^* c_2 = 1 \\ c_2^* a a^* c_2 + c_2^* c_2 = 1 \end{array}$$

$$\Rightarrow c_2 = \frac{1}{\sqrt{2}}, \quad c_1 = -\frac{1-i\sqrt{2}}{\sqrt{6}}.$$

$$\chi_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} \frac{1-i\sqrt{2}}{\sqrt{3}} \\ 1 \end{pmatrix}, \quad \chi_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} -\frac{1-i\sqrt{2}}{\sqrt{3}} \\ 1 \end{pmatrix}$$

$$P_+ = |\langle \chi_1 | \psi \rangle|^2, \quad P_- = |\langle \chi_2 | \psi \rangle|^2$$

$$\langle x_+|\psi\rangle = \frac{1}{\sqrt{10}}\left(\frac{1-i\sqrt{2}}{\sqrt{3}}+2\right) = \frac{1}{\sqrt{10}}\left(\frac{1+2\sqrt{3}-i\sqrt{2}}{\sqrt{3}}\right)$$

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$$P_+ = \frac{1}{10}\left\{\frac{(1+2\sqrt{3})^2+2}{3}\right\} = \frac{1}{10}\,\frac{1+12+4\sqrt{3}+2}{3}$$

$$P_+ = \frac{1}{10}\,\frac{15+4\sqrt{3}}{3} = \frac{5\sqrt{3}+4}{10\sqrt{3}}$$

Άσκηση 4 Απόδειξη ότι για $\ell=0$ έχουμε την ελάχιστη ενέργεια:

Έστω ότι η $u_\ell(r)$ ελαχιστοποιεί την μέση τιμή της ενέργειας για την στροφορμή ℓ

$$E_\ell^{min} = \int dr\, u_\ell^* H_\ell u_\ell$$

όπου $H_\ell = -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r) + \frac{\hbar^2\ell(\ell+1)}{2mr^2}$

και η $u_{\ell+1}(r)$ ελαχιστοποιεί την ενέργεια για $\ell+1$

$$E_{\ell+1}^{min} = \int dr\, u_{\ell+1}^* H_{\ell+1} u_{\ell+1}, \quad H_{\ell+1} = -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r) + \hbar^2\frac{(\ell+1)(\ell+2)}{2mr^2}$$

$$\Rightarrow E_{\ell+1}^{min} = \int dr\, u_{\ell+1}^*\left[H_\ell + \frac{\hbar^2\, 2(\ell+1)}{2mr^2}\right]u_{\ell+1}, \quad (\ell+1)(\ell+2) = (\ell+1)\ell + (\ell+1)2$$

και $\int dr\, u_{\ell+1}^* u_{\ell+1}\left[\frac{2\hbar^2(\ell+1)}{2mr^2}\right] > 0 \Rightarrow$

$$E_{\ell+1}^{min} > \int dr\, u_{\ell+1}^* H_\ell u_{\ell+1} \geq E_\ell^{min}$$

$\Rightarrow$ γενικά έχουμε $E_{\ell+1}^{min} > E_\ell^{min} \Rightarrow \ell=0$ θα αντιστοιχεί στην ελάχιστη ενέργεια.