Тема 4: Квантова физика

Корпускулярни свойства на ЕМ поле

$$\nu = \frac{\omega}{2\pi}, \quad \lambda = \frac{c}{\nu}, \quad \vec{k} = \frac{2\pi}{\lambda}\vec{n}$$

$$E = h\nu = \frac{h}{2\pi}\omega = \hbar\omega$$

$h = 6.6260755\,(40) \times 10^{-34}$ J.s

$\hbar = 1.05457266\,(63) \times 10^{-34}$ J.s

$\hbar = 6.58 \times 10^{-22}$ MeV.s

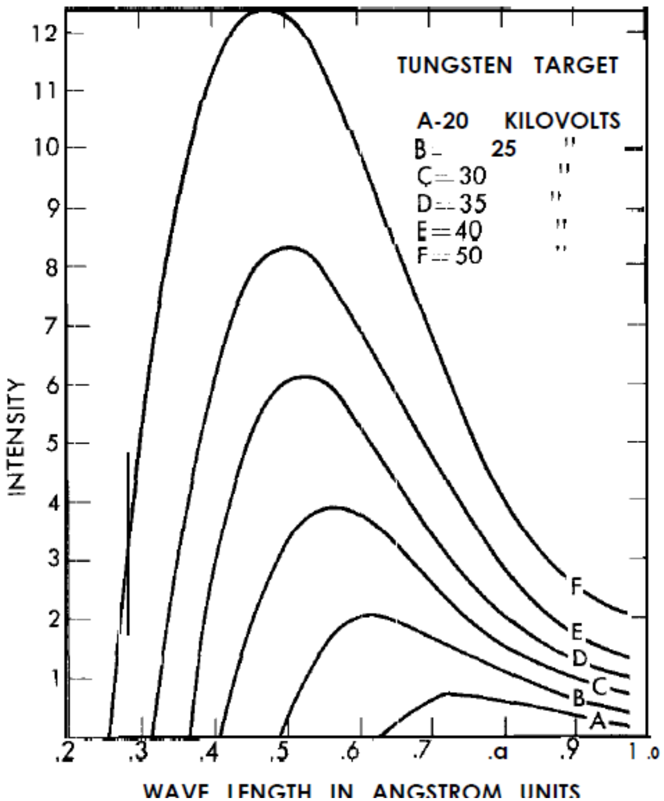
$$E^2 = \left(m_0 c^2\right)^2 + p^2 c^2 = \hbar^2 \omega^2$$

Безмасови частици с импулс p и енергия E –

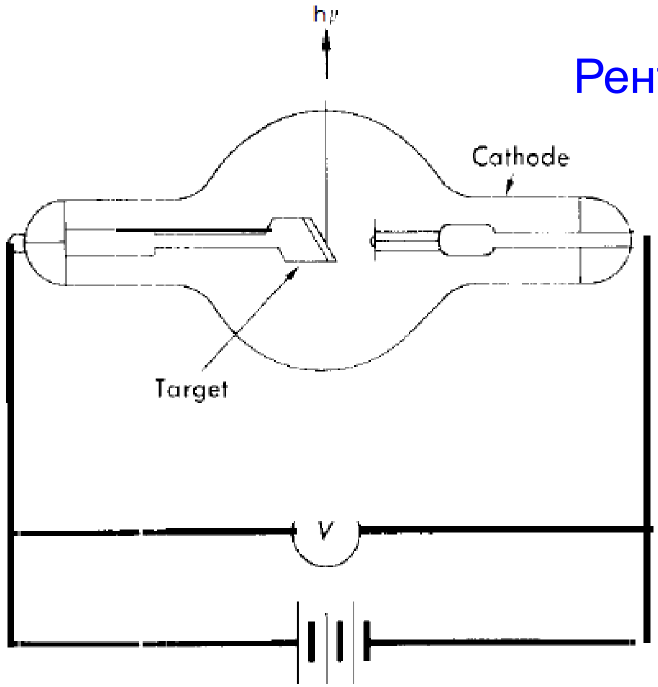
фотони

$$p = \frac{\hbar\omega}{c} = \hbar k \qquad \vec{p} = \hbar\vec{k}$$

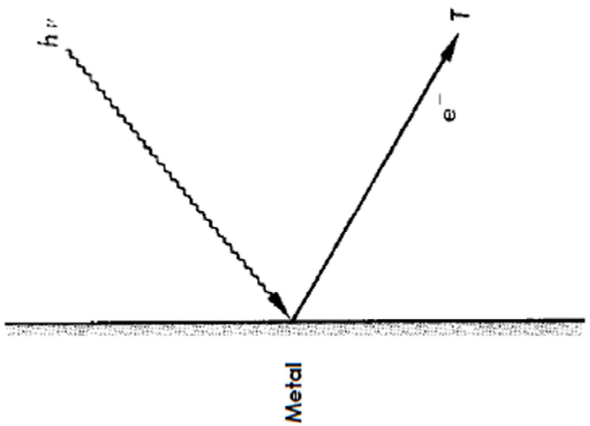
Експериментални доказателства

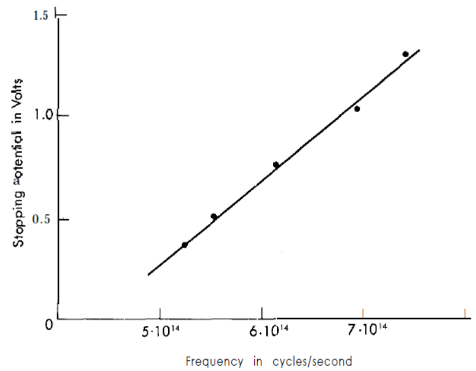


Рентгенова тръба



$$h\nu = T_{max} + \Phi$$





Вълнови свойства на частиците

$$m,\ E,\ \vec{v},\ \vec{p}$$

$$\psi = Ae \exp\left[i\left(\frac{2\pi x}{\lambda} - 2\pi\nu t\right)\right]$$

$$\Psi(\vec{r}, t) = Ae^{i\left(\vec{k}.\vec{r} - \omega t\right)}$$

Фазова скорост

$$k \cdot \frac{dr}{dt} = \omega \qquad k.u = \omega$$

Вълни на дьо Бройл (de Broglie)

$$E = h\nu = \hbar\omega$$

$$\vec{p} = \hbar\vec{k}$$

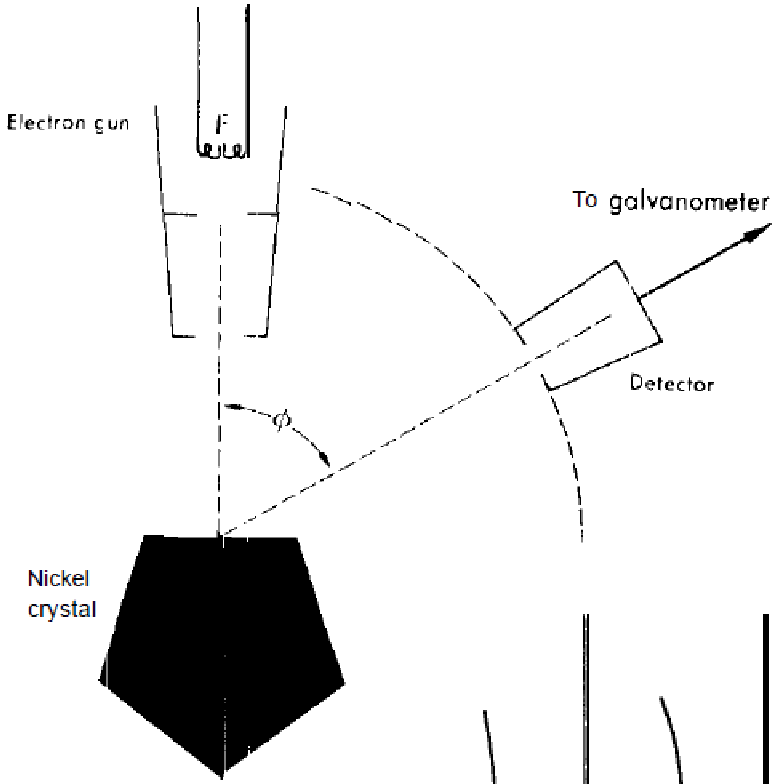
Вълна с дължина на вълната λ

и честота $\nu = E/2\pi\hbar$

$$\lambda = \frac{2\pi}{k} = \frac{2\pi\hbar}{p} = \frac{2\pi\hbar}{mv}$$

Експериментални доказателства

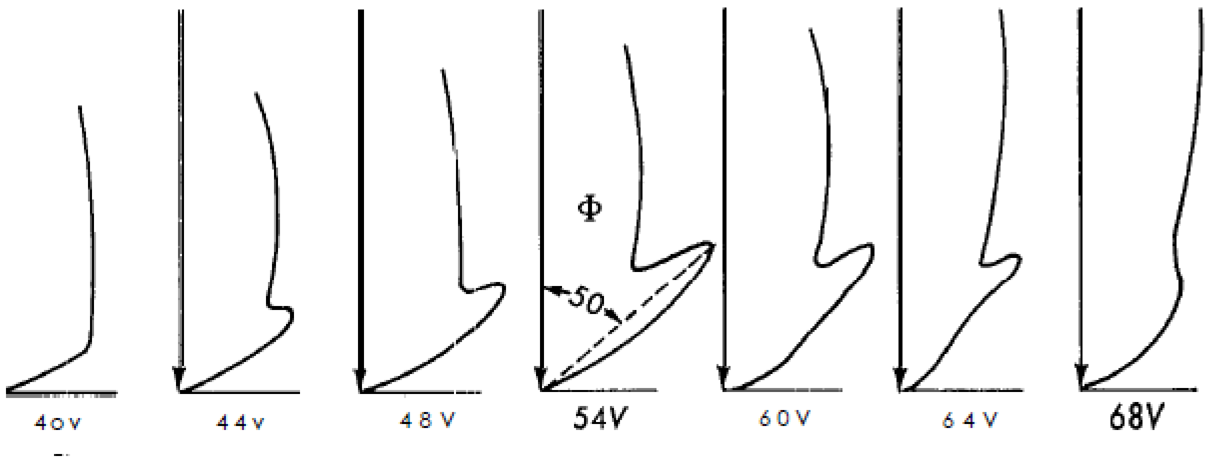
Davisson & Germer, 1927



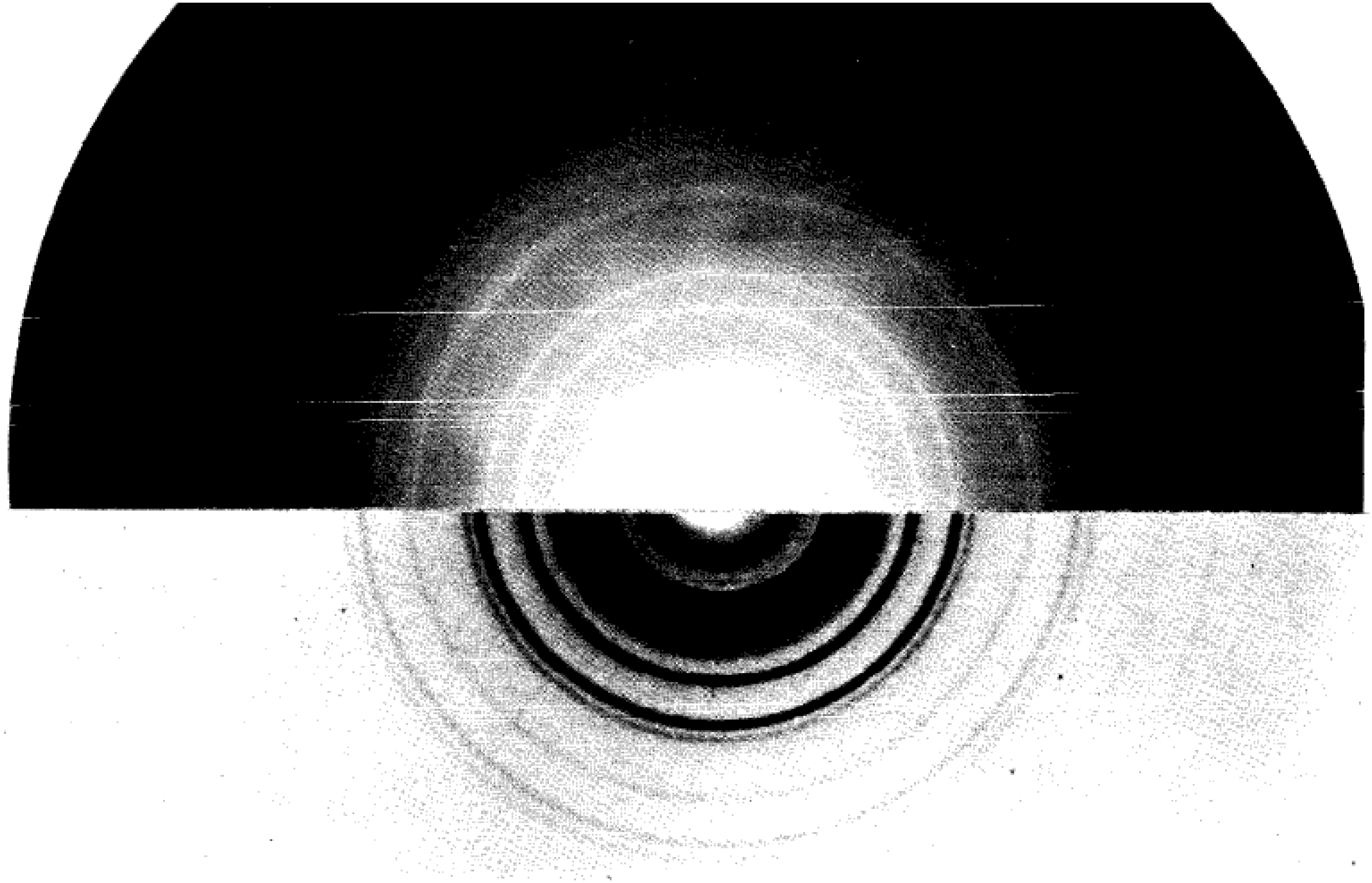
$$2d\cos\vartheta = n\lambda$$

$$\frac{p^2}{2m_0} = eV, \quad \text{or} \quad p = \sqrt{2m_0eV}$$

$$\lambda = \frac{h}{p}$$



Дифракция на електрони от алуминиев кристал



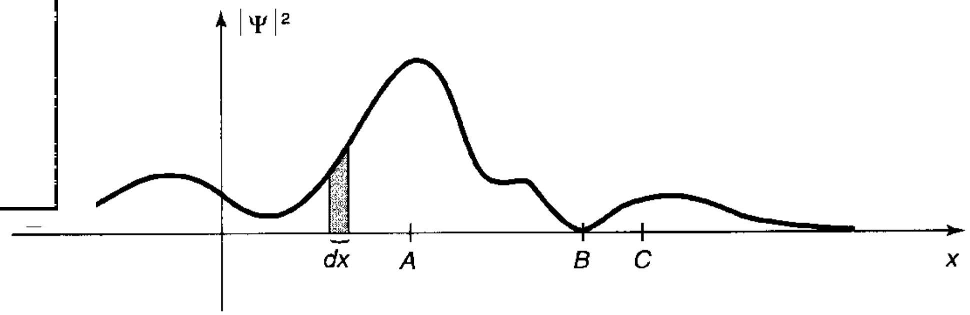
Вълнова функция и уравнение на Шрьодингер

Квантово-механически:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi.$$

Класически:

$$m\, d^2x/dt^2 = -\partial V/\partial x$$



$$|\Psi(x,t)|^2\,dx = \left\{ \begin{array}{l} \text{probability of finding the particle} \\ \text{between } x \text{ and } (x+dx), \text{ at time } t. \end{array} \right\}$$

$$\int_{-\infty}^{+\infty} |\Psi(x,t)|^2\,dx = 1.$$

Движението на квантова частица се описва с вълнова функция $\Psi(\underline{r},t)$.

Вероятността за откриване на квантовата частица, която се описва от $\Psi(\underline{r},t)$ в момент t, в елементарен обем d^3r около точка $\underline{r}$, се дава от квадрата на модула на вълнова функция:

Вълновата функция $\Psi(\underline{r},t)$ се определя от уравнението на Шродингер;

$$i\hbar \frac{\partial}{\partial t}\Psi(\vec{r},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})\right]\Psi(\vec{r},t) \equiv \hat{H}\Psi(\vec{r},t)$$

$$E \to i\hbar\frac{\partial}{\partial t} \qquad \vec{p} \to -i\hbar\nabla \qquad \vec{r} \to \vec{r}$$

На всяка физична величина се съпоставя линеен ермитов оператор. Стойностите, които физичните величини могат вземат, са собствените стойности на съответните им оператори. Между тези операторите съществуват същите съотношения и тъждества, както м/у физическите величини в класическата механика.

$$\vec{L} = \vec{r} \times \vec{p} \qquad \hat{\vec{L}} = -i\hbar\,\vec{r} \times \nabla$$

$$\{q_i, p_k\} = \delta_{ik} \qquad [\hat{r}_i, \hat{p}_k] = i\hbar\,\delta_{ik} = i\hbar\,(\hat{r}_i\partial_k - \partial_k\hat{r}_i)$$

Ако два оператора комутират, те имат обща система от собствени вектори!

Средни стойности

$$\langle x \rangle = \int_{-\infty}^{+\infty} x |\Psi(x,t)|^2 \, dx.$$

$$\frac{d\langle x \rangle}{dt} = \int x \frac{\partial}{\partial t} |\Psi|^2 \, dx = \frac{i\hbar}{2m} \int x \frac{\partial}{\partial x} \left(\Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x} \Psi \right) dx$$

$$\langle v \rangle = \frac{d\langle x \rangle}{dt}.$$

$$\frac{d\langle x \rangle}{dt} = -\frac{i\hbar}{m} \int \Psi^* \frac{\partial \Psi}{\partial x} \, dx.$$

$$\langle p \rangle = m \frac{d\langle x \rangle}{dt} = -i\hbar \int \left(\Psi^* \frac{\partial \Psi}{\partial x} \right) dx.$$

$$\mathbf{p} \to \frac{\hbar}{i} \nabla,$$

$$\langle Q(x,p) \rangle = \int \Psi^* Q(x, \frac{\hbar}{i} \frac{\partial}{\partial x}) \Psi \, dx.$$

$$\langle Q \rangle = \int \Psi(x,t)^* \hat{Q} \Psi(x,t) \, dx$$

$$\langle Q \rangle = \langle \Psi | \hat{Q} \Psi \rangle$$

Всяка механична величина
може да се представи като функция на
координатите и импулсите, т.е. да стане ***оператор***.

Хамилтониан

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

$$H(x, p) = \frac{p^2}{2m} + V(x)$$

$$\Psi(x,t) = \psi(x)\,f(t)$$

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

$$i\hbar\frac{1}{f}\frac{df}{dt} = -\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V$$

$$i\hbar\frac{1}{f}\frac{df}{dt} = E,$$

$$\boxed{\Psi(x,t) = \psi(x)e^{-iEt/\hbar},}$$

$$f(t) = e^{-iEt/\hbar}.$$

$$\frac{df}{dt} = -\frac{iE}{\hbar}f,$$

$$|\Psi(x,t)|^2 = \Psi^*\Psi = \psi^* e^{+iEt/\hbar}\psi e^{-iEt/\hbar} = |\psi(x)|^2$$

$$-\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V = E,$$

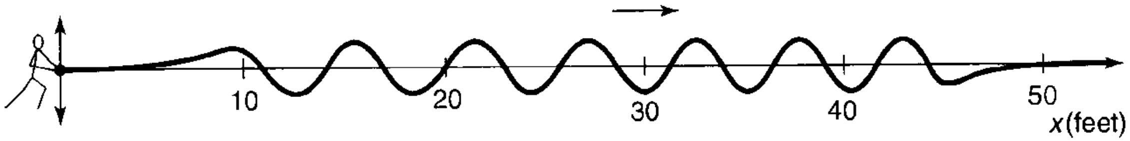
$$\hat{H}\psi = E\psi,$$

Общото решение е линейна комбинация:

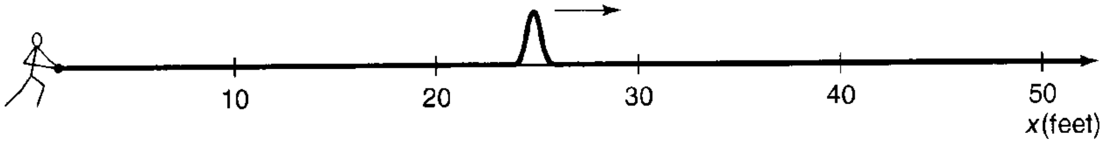
$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n\psi_n(x)e^{-iE_nt/\hbar}.$$

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi.}$$

Съотношение за неопределеност



$$p = \frac{h}{\lambda} = \frac{2\pi\hbar}{\lambda}$$



$$\sigma_x \sigma_p \geq \frac{\hbar}{2},$$

$$\sigma_Q^2 = \langle(\hat{Q} - \langle Q\rangle)^2\rangle = \langle\Psi|(\hat{Q} - \langle Q\rangle)^2\Psi\rangle$$

неравенство на Шварц:

$$|\langle\alpha|\beta\rangle|^2 \leq \langle\alpha|\alpha\rangle\langle\beta|\beta\rangle$$

$$\cos\theta = (\mathbf{a}\cdot\mathbf{b})/|\mathbf{a}||\mathbf{b}|$$

$$\sigma_A^2 \sigma_B^2 \geq \left(\frac{1}{2i}\langle[\hat{A}, \hat{B}]\rangle\right)^2.$$

$$\cos\theta = \sqrt{\frac{\langle\alpha|\beta\rangle\langle\beta|\alpha\rangle}{\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle}}$$

Вълнова функция и вероятността интерпретация

1) Движението на квантова частица се описва с вълнова функция $\Psi(\underline{r},t)$;

2) Вероятността за откриване на квантовата частица, която се описва от $\Psi(\underline{r},t)$ в момент t, в елементарен обем d^3r около точка $\underline{r}$, се дава от квадрата на модула на вълнова функция:
$$P(\vec{r},t)\,d^3r = \Psi^*(\vec{r},t)\,\Psi(\vec{r},t)\,d^3r$$

3) Вълновата функция $\Psi(\underline{r},t)$ може да се представи като сума от вълни Ψ_1, Ψ_2, Ψ_3,…, всяка от които описва определено състояние на движението: $\Psi(\vec{r},t) = \sum_i \Psi_i$

Какво е положението на частица с маса m и импулс $\underline{p}$ ако я разглеждаме като вълна?

$$\Psi(\vec{r},t) = A\,e^{\frac{i}{\hbar}(\vec{p}.\vec{r}-E.t)} \qquad P(\vec{r},t)\,d^3r = \left|A e^{\frac{i}{\hbar}(\vec{p}.\vec{r}-E.t)}\right|^2 d^3r = |A|^2 d^3r$$

Не зависи от $\underline{r}$ $\Longrightarrow$ всички точки в пространството са равновероятни!

Какъв е импулсът $\underline{p}$ на частица с маса m, локализирана в точка, ако я разглеждаме като вълна‘

Безсмислен въпрос! $\lambda = h/p$ Каква е дължината на вълната в точка?!

Едновременното познаване на $\underline{p}$ и $\underline{r}$ за квантовите системи е невъзможно – точното измерване на една от тези величини внася неопределеност в другата!

$$\Delta x\Delta p \geq \frac{\hbar}{2} \qquad \Delta E\Delta t \geq \frac{\hbar}{2} \qquad \Delta l_z\,\Delta\varphi \geq \frac{\hbar}{2}$$

Съотношения за неопределеност на Хайзенберг

$$\Psi(\vec{r}) = \frac{1}{(2\pi)^{3/2}}\int A(\vec{k})\,e^{i\vec{k}.\vec{r}}\,d^3k \qquad A(\vec{k}) = \frac{1}{(2\pi)^{3/2}}\int \Psi(\vec{r})\,e^{-i\vec{k}.\vec{r}}\,d^3r$$

$$\left|A(\vec{k}_0)\right|^2$$

Едномерен случай

Нерелативиско приближение $\longrightarrow$ уравнение на Шродингер – частица с маса m в потенциал V(x)

$$i\hbar \frac{\partial}{\partial t}\Psi(x,t) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi(x,t) \equiv \hat{H}\,\Psi(x,t)$$

$$\Psi(x,t)=\psi(x)T(t) \quad \Longrightarrow \quad \frac{1}{\psi}\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\,\psi(x)\right] = \frac{i\hbar \frac{d}{dt}T(t)}{T(t)} = E$$

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

от граничните условия $\Longrightarrow$ $\{\psi_n(x)\}$ – собствени вектори; $\{E_n\}$ – собствени стоиности

$$i\hbar\frac{d}{dt}T(t) = T(t)\,E \quad \Longrightarrow \quad T(t) = e^{-iEt/\hbar}$$

$$\mathrm{Lim}_{\varepsilon\to 0}\left[\psi(a+\varepsilon) - \psi(a-\varepsilon)\right] = 0$$

$$\mathrm{Lim}_{\varepsilon\to 0}\left[\left(\frac{d\psi(x)}{dx}\right)_{x=a+\varepsilon} - \left(\frac{d\psi(x)}{dx}\right)_{x=a-\varepsilon}\right] = 0$$

$$\Psi(x,t) = \psi(x)\,e^{-iEt/\hbar} = \sum_n C_n\,\psi_n(x)\,e^{-iE_n t/\hbar}$$

$$P(x)\,dx = \Psi^*(x,t)\,\Psi(x,t)\,dx \qquad P(x_1,x_2) = \int_{x_1}^{x_2}\Psi^*\,\Psi\,dx \qquad \int_{-\infty}^{+\infty}\Psi^*\,\Psi\,dx = 1 \qquad \langle f\rangle = \int_{-\infty}^{+\infty}\Psi^*\,f\,\Psi\,dx$$

Свободна частица V(x)=0

$$\frac{d^2}{dx^2}\psi(x) + \frac{2mE}{\hbar^2}\psi(x) = 0$$

$$\psi(x) = A'.\cos(\kappa x) + B'.\sin(\kappa x)$$

$$\psi(x) = A.e^{ikx} + B.e^{-ikx}, \quad k^2 = \frac{2mE}{\hbar^2}$$

$$\Psi(x,t) = A.e^{i(kx-\omega t)} + B.e^{-i(kx+\omega t)}$$

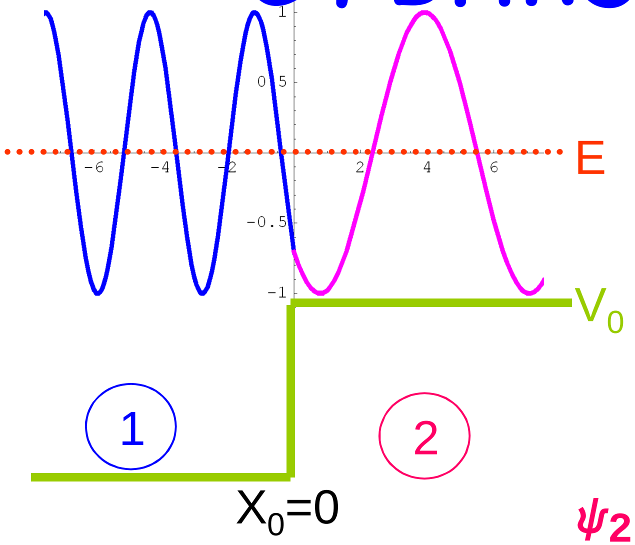
Нормиране

приемаме, че в x=-∞ имаме източник на частици с интензитет *I* (p/s) $\Longrightarrow$ B=0

$$j = \frac{\hbar}{i2m}\left(\Psi^* \frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\Psi^*}{\partial x}\right)$$

$$j = \frac{\hbar k}{m}\left|A\right|^2 = I \qquad A = \sqrt{mI/\hbar k}$$

Стъпков потенциал, $E>V_0$



$$V(x) = \begin{cases} 0 & x<0 \\ V_0 & x>0 \end{cases}$$

$$\psi_1(x) = A.e^{ik_1x} + B.e^{-ik_1x},\ k_1 = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\frac{d^2\psi_2(x)}{dx^2} = -\frac{2m(E-V_0)}{\hbar^2}\psi_2(x)$$

$$\psi_2(x) = C.e^{ik_2x} + D.e^{-ik_2x},\ k_2 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$$

$$\mathrm{Lim}_{\varepsilon\to0}[\psi(0+\varepsilon)-\psi(0-\varepsilon)] = 0 \qquad A + B = C + D$$

$$\mathrm{Lim}_{\varepsilon\to0}\left[\left(\frac{d\psi(x)}{dx}\right)_{x=0+\varepsilon} - \left(\frac{d\psi(x)}{dx}\right)_{x=0-\varepsilon}\right] = 0 \qquad k_1(A-B) = k_2(C-D)$$

"A" – падаща вълна "B" – отразена вълна "C" – преминала вълна D=0

$$B = A\frac{1-k_2/k_1}{1+k_2/k_1} \qquad C = A\frac{2}{1+k_2/k_1}$$

Коефициент на отражение

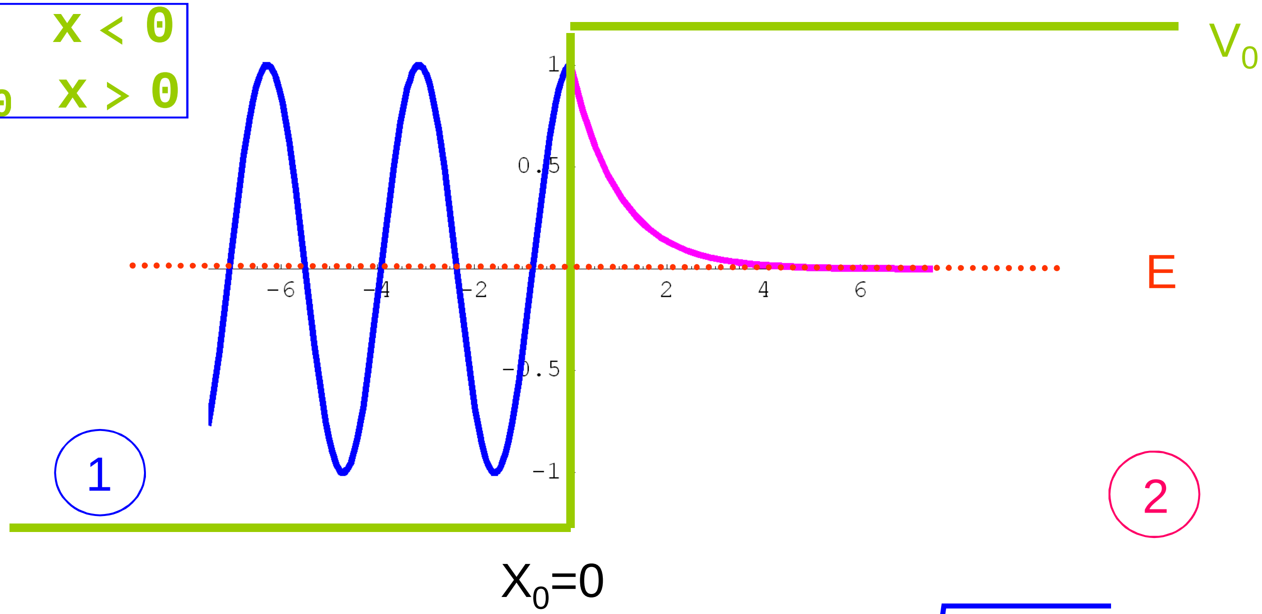
Коефициент на преминаване

$$R = \frac{j_{ref}}{j_{inc}} = \frac{|B|^2}{|A|^2} = \left(\frac{1-k_2/k_1}{1+k_2/k_1}\right)^2 \qquad T = \frac{j_{trans}}{j_{inc}} = \frac{|C|^2}{|A|^2} = \frac{4.k_2/k_1}{(1+k_2/k_1)^2}$$

$$R + T = 1$$

Стъпков потенциал, $E<V_0$

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & x > 0 \end{cases}$$



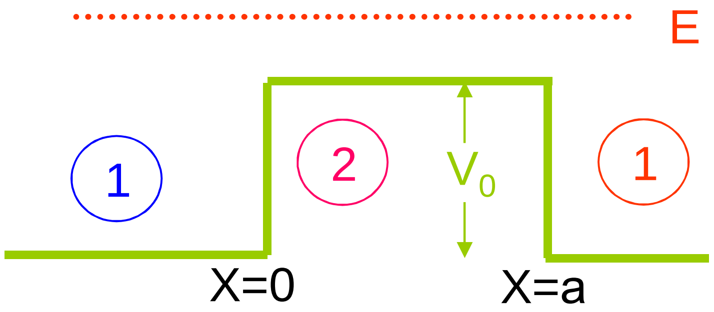
$$\psi_1(x) = A.e^{ik_1 x} + B.e^{-ik_1 x}, \quad k_1 = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\frac{d^2\psi_2(x)}{dx^2} = \frac{2m(V_0 - E)}{\hbar^2}\psi_2(x)$$

$$\psi_2(x) = C.e^{k_2 x} + D.e^{-k_2 x}, \quad k_2 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

$$\psi_2 \xrightarrow{x\to\infty} \text{const} \implies C = 0$$

Правоъгълна бариера, $E>V_0$



$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & 0 \le x \le a \\ 0 & x > a \end{cases}$$

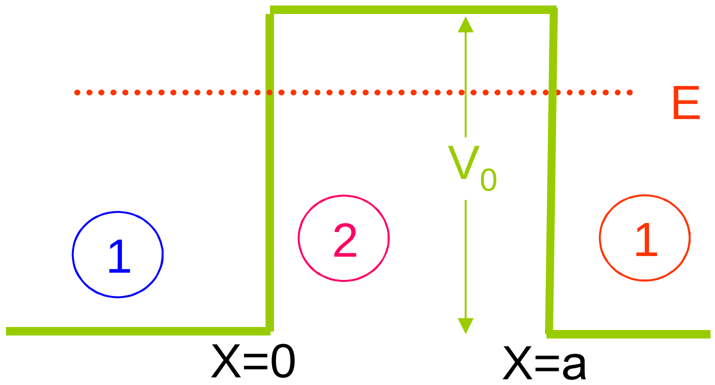
$$\psi_1(x) = A.e^{ik_1x} + B.e^{-ik_1x}, \quad k_1 = \sqrt{2mE/\hbar^2}$$

$$\psi_2(x) = C.e^{ik_2x} + D.e^{-ik_2x}, \quad k_2 = \sqrt{2m(E-V_0)/\hbar^2}$$

$$\psi_3(x) = F.e^{ik_3x}, \quad k_3 = \sqrt{2mE/\hbar^2}$$

$$T = \frac{|F|^2}{|A|^2} = \frac{1}{1 + \frac{1}{4}\frac{V_0^2}{E(E-V_0)}\sin^2(k_2 a)}$$

Правоъгълна бариера, $E<V_0$



$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & 0 \le x \le a \\ 0 & x > a \end{cases}$$

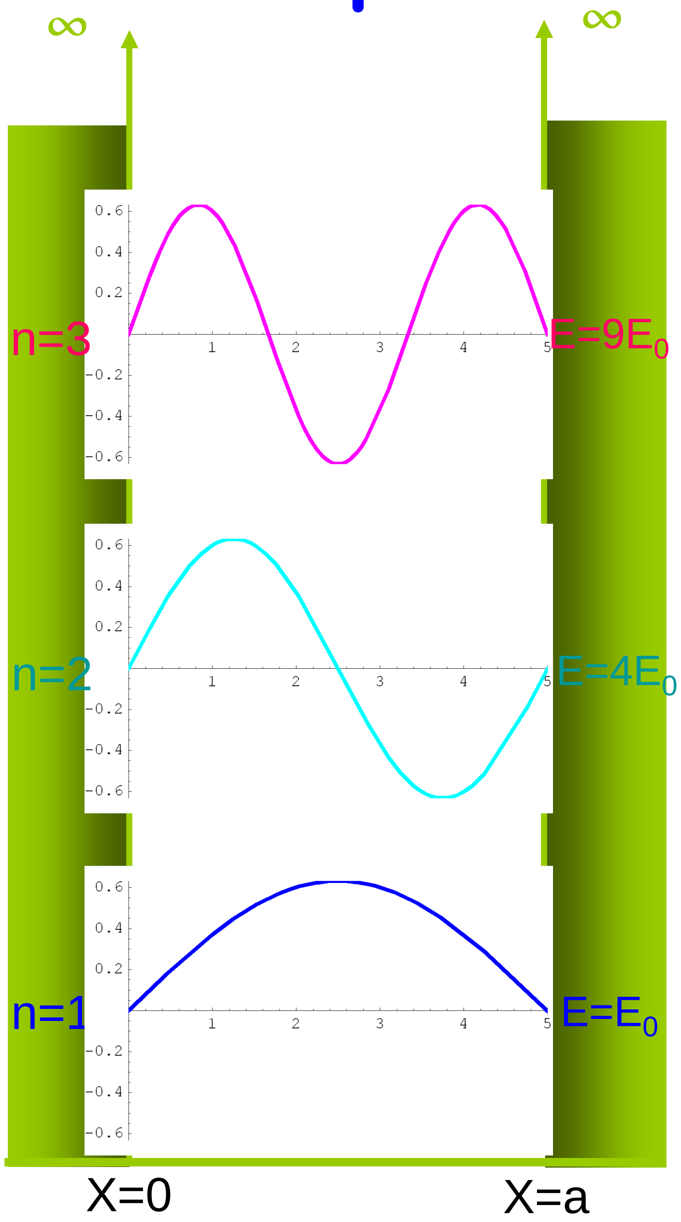
$$\psi_1(x) = A.e^{ik_1 x} + B.e^{-ik_1 x}, \; k_1 = \sqrt{2mE/\hbar^2}$$

$$\psi_2(x) = C.e^{k_2 x} + D.e^{-k_2 x}, \; k_2 = \sqrt{2m(V_0 - E)/\hbar^2}$$

$$\psi_3(x) = F.e^{ik_3 x}, \; k_3 = \sqrt{2mE/\hbar^2}$$

$$T = \frac{|F|^2}{|A|^2} = \frac{1}{1 + \frac{1}{4}\frac{V_0^2}{E(V_0-E)}\sinh^2(k_2 a)}$$

Безкрайна потенциална яма



$$V(x) = \begin{cases} \infty & x < 0,\ x > a \\ 0 & 0 \le x \le a \end{cases}$$

ψ = A.Sin(kx) + B.Cos(kx) $\qquad k^2 = \dfrac{2mE}{\hbar^2}$

Гранични условия:

$\psi(0) = 0$ $\Longrightarrow$ $B = 0$

$\psi(a) = 0$ $\qquad ka = n\pi \quad n = 1, 2, \ldots$ $\Longrightarrow$

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 \pi^2}{2ma^2} n^2$$

$$A^2 \int_0^a (\mathrm{Sin}[nx\pi/a])^2 \, dx = 1$$

$$\psi_n = \sqrt{\frac{2}{a}} \, \mathrm{Sin}\left(\frac{n\pi x}{a}\right)$$

Крайна потенциална яма

$$V(x) = \begin{cases} V_0 & |x| > a/2 \\ 0 & |x| > a/2 \end{cases}$$

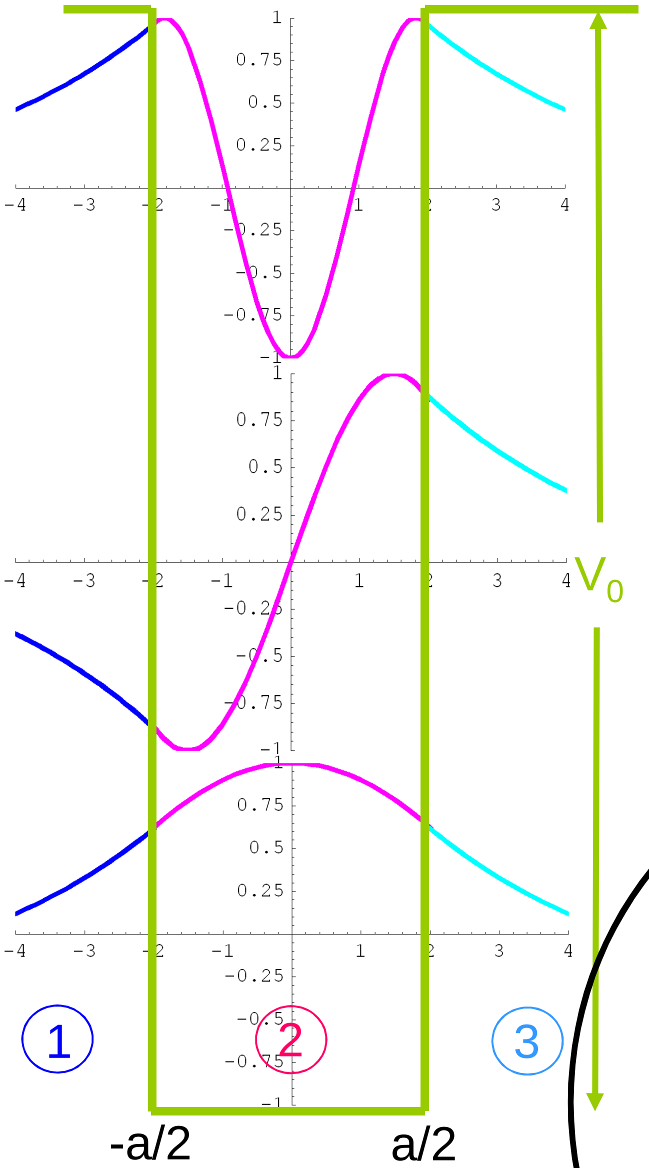
$\psi_1 = A.\,e^{k_1 x}$

$\psi_2 = C.\,e^{ik_2 x} + D.\,e^{-ik_2 x}$

$\psi_3 = G.\,e^{-k_1 x}$

$k_1 = \sqrt{2m(V_0 - E)/\hbar^2}$

$k_2 = \sqrt{2mE/\hbar^2}$



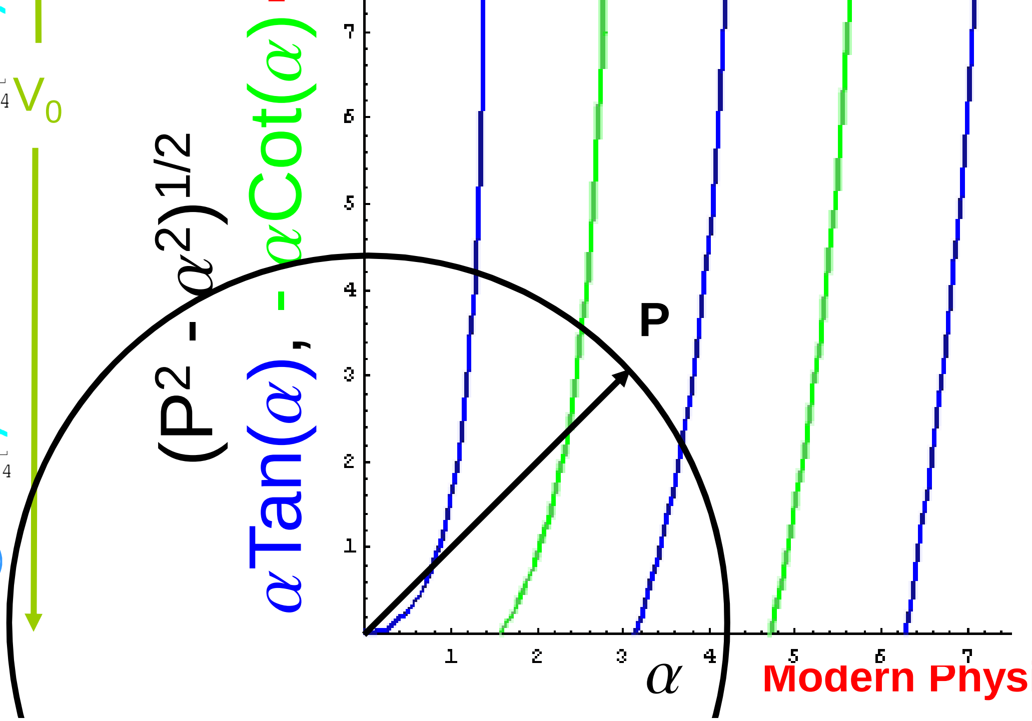
Гранични условия:

$k_2 \,\mathrm{Tan}\left(\frac{k_2 a}{2}\right) = k_1$ $\qquad \alpha.\mathrm{Tan}(\alpha) = \sqrt{P^2 - \alpha^2}$

$-k_2 \,\mathrm{Cot}\left(\frac{k_2 a}{2}\right) = k_1$ $\qquad -\alpha.\mathrm{Cot}(\alpha) = \sqrt{P^2 - \alpha^2}$

$P^2 = mV_0 a^2 / 2\hbar^2$

$\alpha = k_2 a / 2$



Хармоничен осцилатор

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{1}{2}kx^2\right)\psi = E\psi \qquad \frac{d^2\psi}{dx^2}+\frac{2m}{\hbar^2}\left(E-\frac{k}{2}x^2\right)\psi=0 \qquad \omega=\sqrt{\frac{k}{m}} \qquad \frac{d^2\psi}{dx^2}+\frac{2m}{\hbar^2}\left(E-\frac{m\omega^2}{2}x^2\right)\psi=0$$

$$\xi=\sqrt{\frac{m\omega}{\hbar}}\,x \qquad \frac{m\omega}{\hbar}\frac{d^2}{d\xi^2}\psi(\xi)+\frac{2m}{\hbar^2}\left(E-\frac{m\omega^2}{2}\frac{\hbar}{m\omega}\xi^2\right)\psi(\xi)=0 \qquad \psi''+\left(\frac{2E}{\hbar\omega}-\xi^2\right)\psi=0$$

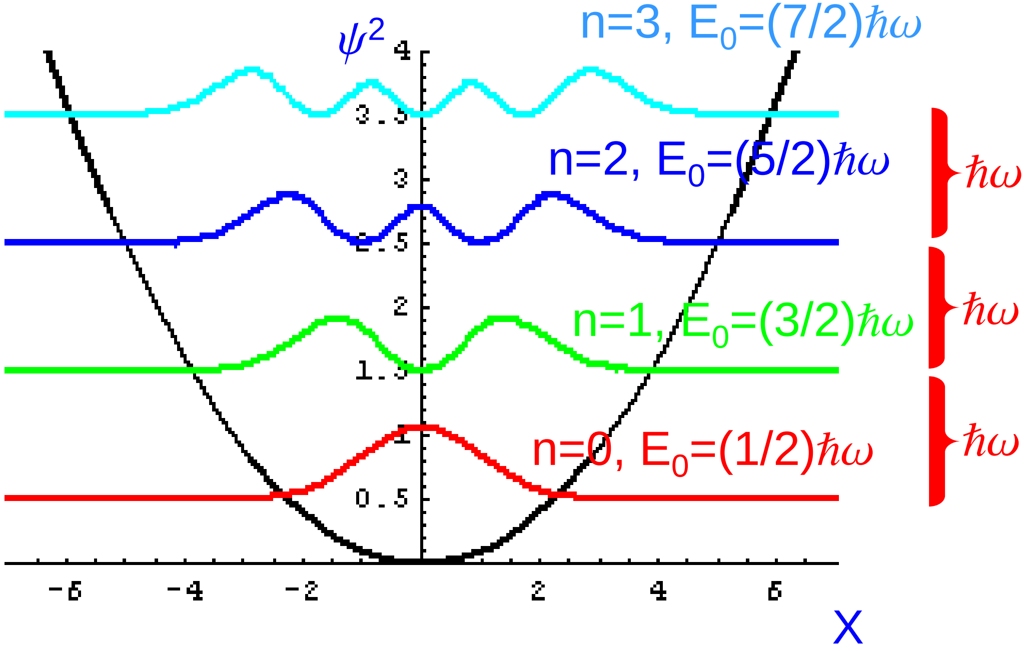
$$\chi''-2\xi\chi'+\left(\frac{2E}{\hbar\omega}-1\right)\chi=0$$

$$\xi^2\gg\frac{2E}{\hbar\omega} \qquad \psi''=\xi^2\psi \qquad \psi=e^{\pm\xi^2/2} \qquad \psi=e^{-\xi^2/2}\chi(\xi)$$

$$\chi''-2\xi\chi'+2n\chi=0$$

$$\chi(\xi)=N\,H_n(\xi) \qquad H_n(\xi)=(-1)^n e^{\xi^2}\frac{d^n}{d\xi^n}e^{-\xi^2} \qquad E_n=\hbar\omega\,(n+1/2) \qquad n=0,\,1,\,2,\,3,\;....$$

$$\psi_n(x)=N\,H_n(\alpha x)\,e^{-\alpha^2x^2/2} \qquad \alpha^2=\sqrt{km}\,/\,\hbar \qquad \int\psi_n^2(x)\,dx=1 \qquad N=\sqrt{\frac{\alpha}{2^n\,n!\,\sqrt{\pi}}}$$

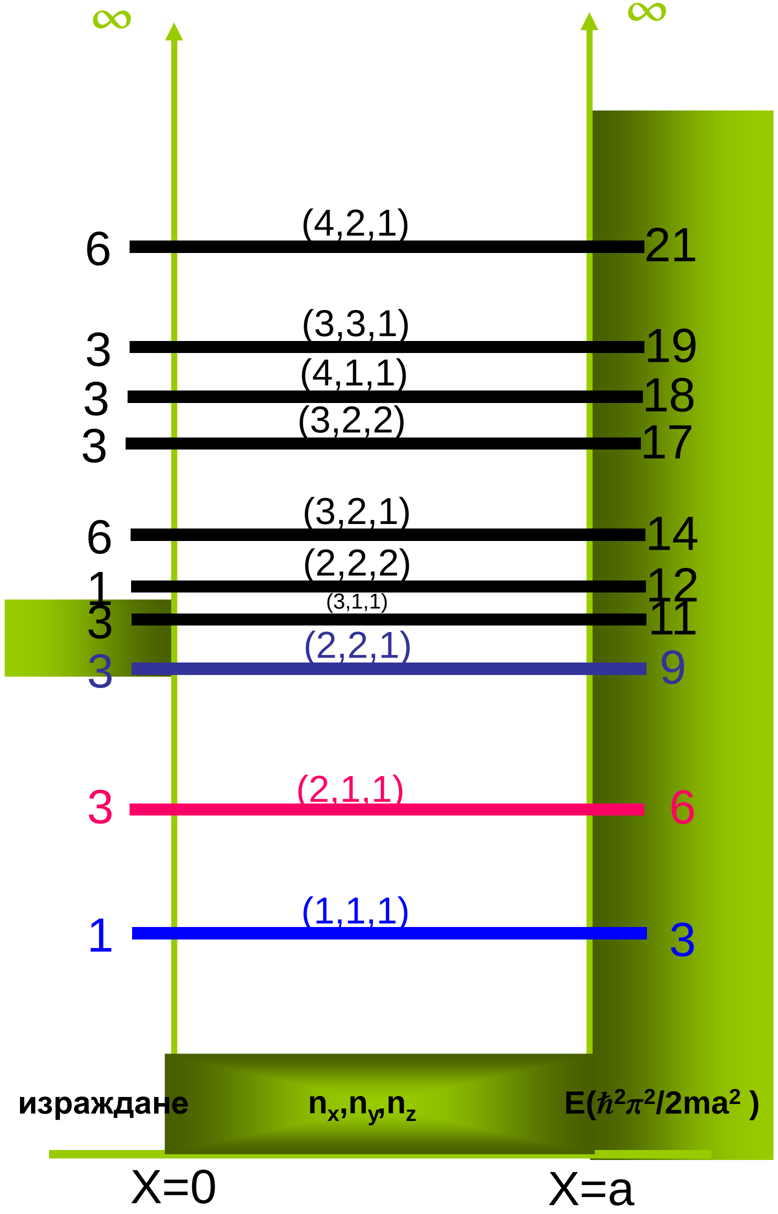


$$H_2=(4\alpha^2x^2-2)$$
$$\psi_2=2^{-3/2}\alpha^{1/2}\pi^{-1/4}(4\alpha^2x^2-2)\,e^{-\alpha^2x^2/2}$$

$$H_1=2\alpha x$$
$$\psi_1=2^{-1/2}\alpha^{1/2}\pi^{-1/4}(2\alpha x)\,e^{-\alpha^2x^2/2}$$

$$H_0=1 \qquad \psi_0=\alpha^{1/2}\pi^{-1/4}e^{-\alpha^2x^2/2}$$

Безкрайна потенциална яма - 3D



$$V(x) = \begin{cases} \infty & x, y, z < 0,\ x, y, z > a \\ 0 & 0 \le x, x, y, z \le a \end{cases}$$

$$\Psi_{n_x, n_y, n_z} = \sqrt{\left(\frac{2}{a}\right)^3} \sin\left(\frac{n_x \pi x}{a}\right) \sin\left(\frac{n_y \pi y}{a}\right) \sin\left(\frac{n_z \pi z}{a}\right)$$

$$E_{n_x, n_y, n_z} = \frac{\hbar^2 \pi^2}{2\, ma^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$

$n_x, n_y, n_z = 1, 2, 3. \ldots$

Основно състояние

$n_x = 1;\ n_y = 1;\ n_z = 1 \quad \Longrightarrow \quad E_{1,1,1} = \dfrac{3\hbar^2\pi^2}{2\, ma^2}$

Първо възбудено

$$\left.\begin{array}{l} n_x = 2;\ n_y = 1;\ n_z = 1 \\ n_x = 1;\ n_y = 2;\ n_z = 1 \\ n_x = 1;\ n_y = 1;\ n_z = 2 \end{array}\right\} \Longrightarrow \quad E_{2,1,1} = \frac{6\hbar^2\pi^2}{2\, ma^2}$$

Второ възбудено

$$\left.\begin{array}{l} n_x = 2;\ n_y = 2;\ n_z = 1 \\ n_x = 1;\ n_y = 2;\ n_z = 2 \\ n_x = 2;\ n_y = 1;\ n_z = 2 \end{array}\right\} \Longrightarrow \quad E_{2,2,1} = \frac{9\hbar^2\pi^2}{2\, ma^2}$$

Централен потенциал

$$V(\vec{r}) \equiv V(r,\theta,\varphi) = V(r)$$

Сферични координати: $\{x,y,z\} \Longrightarrow \{r.\cos(\varphi)\sin(\theta),\ r.\sin(\varphi)\sin(\theta),\ r.\cos(\theta)\}$

l^2 е интеграл на движението, т.е. $[H,l^2]=0$

$$\vec{l} = \vec{r}\times\vec{p} \qquad -i\hbar\begin{vmatrix} i & j & k \\ x & y & z \\ \partial_x & \partial_y & \partial_z \end{vmatrix} \qquad [l_x, l_y] = i\hbar l_z \qquad \vec{r}.\vec{p} = -i\hbar r\frac{\partial}{\partial r}$$

$$\vec{l} = -i\hbar\,\vec{r}\times\nabla$$

$$l^2 = (\vec{r}\times\vec{p}).(\vec{r}\times\vec{p}) = r^2p^2 - \vec{r}(\vec{r}.\vec{p}).\vec{p} + 2i\hbar\,\vec{r}.\vec{p} = r^2p^2 + \hbar^2 r^2\frac{\partial^2}{\partial r^2} + \hbar^2\,2r\frac{\partial}{\partial r}$$

$$l^2 = r^2p^2 + \hbar^2\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) \Longrightarrow T = \frac{p^2}{2m} = \frac{l^2}{2mr^2} - \frac{\hbar^2}{2mr^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)$$

$$\left[-\frac{\hbar^2}{2mr^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{l^2}{2mr^2} + V(r)\right]\psi = E\psi \qquad \psi(r,\theta,\phi) = R(r)\,\Theta(\theta)\,\Phi(\phi)$$

$$l^2\psi = \hbar^2\lambda\psi \qquad l^2 = -\hbar^2\left\{\frac{1}{\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2(\theta)}\frac{\partial^2}{\partial\phi^2}\right\}$$

$$\left\{\frac{1}{\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2(\theta)}\frac{\partial^2}{\partial\phi^2}\right\}\psi = \lambda\psi$$

Централен потенциал - ъглова част

$$\left\{\frac{1}{\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2(\theta)}\frac{\partial^2}{\partial\phi^2}\right\}\psi=\lambda\psi$$

$$Y(\theta,\phi)=\Theta(\theta)\,\Phi(\phi)$$

$$\frac{d^2\Phi}{d\phi^2}+\mu_l^2\Phi=0 \qquad \Phi_{\mu l}(\phi)=\frac{1}{\sqrt{2\pi}}e^{i\mu_l\phi}$$

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\left[\lambda-\frac{\mu_l}{\sin^2\theta}\right]\Theta=0 \qquad \lambda=l(l+1)$$

$$\Theta_{\mu l}(\theta)=\left[\frac{2l+1}{2}\frac{(l-\mu_l)!}{(l+\mu_l)!}\right]^{1/2}P_l^{\mu_l}(\theta)$$

$l=0, 1, 2, \ldots$ $\mu_l=0, \pm1, \pm2, \ldots, \pm l$

$$\Phi_{\mu_l}(\phi)\,\Theta_{\mu_l}(\theta)=Y_{l\mu_l}(\theta,\phi)$$

$$l^2\,Y_{l\mu}(\theta,\phi)=\hbar^2\,l(l+1)\,Y_{l\mu}(\theta,\phi) \qquad l_z\,Y_{l\mu}(\theta,\phi)=\hbar\,\mu\,Y_{l\mu}(\theta,\phi)$$

$$Y_{00}=\frac{1}{\sqrt{4\pi}}$$

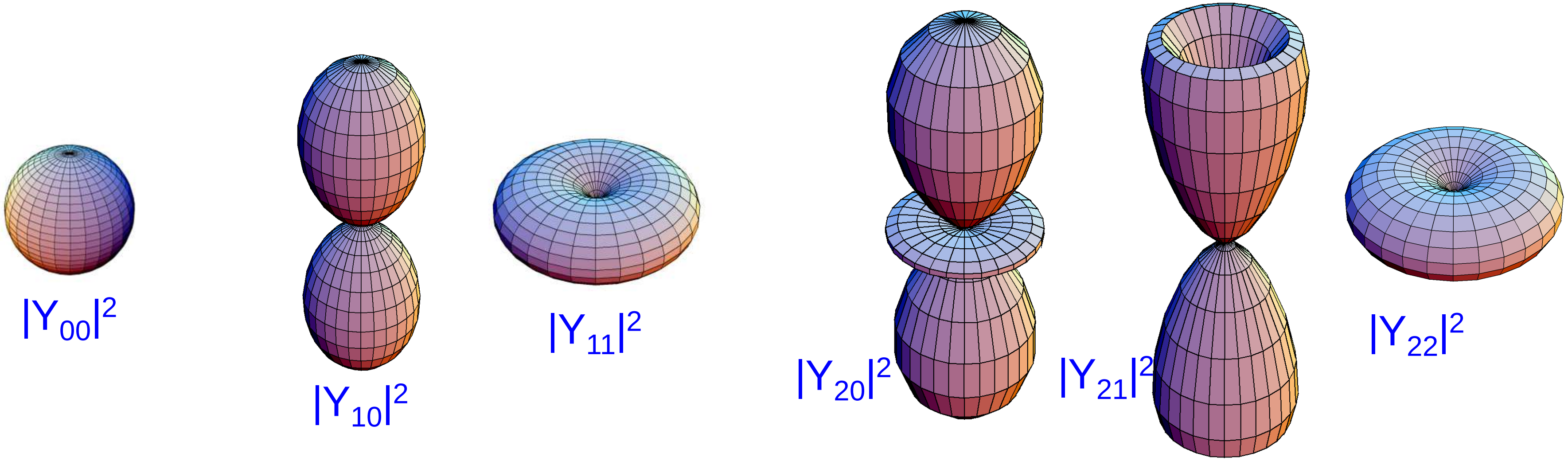
$$Y_{1-1}=\sqrt{\frac{3}{8\pi}}\,e^{-i\phi}\sin(\theta) \qquad Y_{10}=\sqrt{\frac{3}{4\pi}}\cos(\theta) \qquad Y_{1+1}=-\sqrt{\frac{3}{8\pi}}\,e^{+i\phi}\sin(\theta)$$

$$Y_{2-2}=\sqrt{\frac{15}{32\pi}}\,e^{-2i\phi}\sin^2(\theta) \qquad Y_{2-1}=\sqrt{\frac{15}{8\pi}}\,e^{-i\phi}\cos(\theta)\sin(\theta) \qquad Y_{20}=\sqrt{\frac{5}{16\pi}}\left(3\cos^2(\theta)-1\right)$$

$$Y_{2+1}=-\sqrt{\frac{15}{8\pi}}\,e^{i\phi}\cos(\theta)\sin(\theta) \qquad Y_{2+2}=\sqrt{\frac{15}{32\pi}}\,e^{2i\phi}\sin^2(\theta)$$

За всяка стойност на орбиталното квантово число (l) съществуват $2l+1$ решения свързани с магнитното квантово число (m_z)

Плътност, определена от ъгловата част



• За всеки централен потенциал големината на орбиталния ъглов момент е *добро* квантово число: $\langle l^2 \rangle = \hbar^2\, l(l+1),\ l=0, 1, 2, \ldots.$

Спектрометрични означения

l	0	1	2	3	4	5	6
символ	s	p	d	f	g	h	i

•Възможно е да познаваме само една от компонентите на орбиталния ъглов момент

$$l_z = \hbar m_l,\ m_l=0, \pm1, \pm2, \ldots.\pm l$$

Пълен ъглов момент и четност

Нуклоните (протони и неутрони) имат вътрешен спин 1/2

$\langle s^2 \rangle = \hbar^2 s(s+1)$ $\qquad \vec{j} = \vec{l} + \vec{s}$

$\langle s_z \rangle = \hbar m_s \qquad m_s = \pm 1/2$

$\langle j^2 \rangle = \hbar^2 j(j+1)$

$\langle j_z \rangle = \langle l_z + s_z \rangle = \hbar m_j \qquad m_j = -j,\ -j+1,\ \ldots,\ j-1,\ j$

$m_j = m_l + m_s = m_l \pm 1/2 \qquad m_j = \pm 1/2,\ \pm 3/2,\ \pm 5/2,\ \ldots \qquad j = l + 1/2$ или $l - 1/2$

Означения: $n\, l_j$ $\quad 1s_{1/2}\ 1p_{3/2}\ 1p_{1/2}\ 1d_{5/2}\ 1d_{3/2}\ 2s_{1/2}\ 1f_{7/2}\ 1f_{5/2}\ 2p_{3/2}\ 2p_{1/2}\ 1g_{9/2}\ 2d_{5/2}$

$$\vec{r} = -\vec{r} \qquad \begin{pmatrix} x \to -x \\ y \to -y \\ z \to -z \end{pmatrix} \quad \begin{pmatrix} r \to r \\ \theta \to \pi - \theta \\ \phi \to \pi + \phi \end{pmatrix} \qquad V(\vec{r}) = V(-\vec{r}) \quad |\psi(\vec{r})|^2 = |\psi(-\vec{r})|^2$$

$$\Pi \psi(\vec{r}) = \pi \psi(-\vec{r}) \qquad \Pi^2 \psi(\vec{r}) = \pi^2 \psi(\vec{r}) \qquad \pi = \pm$$

$$\psi(r,\theta,\phi) = R(r)\, Y_{lm_l}(\theta,\phi) \qquad \Pi\, Y_{lm_l}(\theta,\phi) = Y_{lm_l}(\pi-\theta, \phi+\pi) = (-1)^l\, Y_{lm_l}(\theta,\phi)$$

Централен потенциал - радиална част

$$\left[-\frac{\hbar^2}{2mr^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{l^2}{2mr^2}+V(r)\right]\psi=E\psi$$

$$\psi(r,\theta,\phi)=R(r)\,\Theta(\theta)\,\Phi(\phi)$$

$$\psi(r,\theta,\phi)=R(r)\,Y(\theta,\phi)$$

$$-\frac{\hbar^2}{2m}\left(\frac{d^2R}{dr^2}+\frac{2}{r}\frac{dR}{dr}\right)+\left[V(r)+\frac{l(l+1)\hbar^2}{2mr^2}\right]R=ER$$

Алтернативен подход

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2\,\mathrm{Sin}(\theta)}\frac{\partial}{\partial\theta}\left(\mathrm{Sin}(\theta)\frac{\partial}{\partial\theta}\right)+\frac{1}{r^2\,\mathrm{Sin}^2(\theta)}\frac{\partial^2\psi}{\partial\phi^2}+\frac{2\mu}{\hbar^2}(V(r)-E)\psi=0$$

$$\psi(r,\theta,\phi)=R(r)\,Y(\theta,\phi)$$

$$\frac{Y}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{R}{r^2\,\mathrm{Sin}(\theta)}\frac{\partial}{\partial\theta}\left(\mathrm{Sin}(\theta)\frac{\partial Y}{\partial\theta}\right)+\frac{R}{r^2\,\mathrm{Sin}^2(\theta)}\frac{\partial^2Y}{\partial\phi^2}+\frac{2\mu}{\hbar^2}(V(r)-E)RY=0$$

$$Y(\theta,\phi)=\Theta(\theta).\Phi(\phi)$$

$$\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{2\mu}{\hbar^2}(V(r)-E)R-AR=0$$

$$\frac{1}{\mathrm{Sin}(\theta)}\frac{\partial}{\partial\theta}\left(\mathrm{Sin}(\theta)\frac{\partial Y}{\partial\theta}\right)+\frac{R}{\mathrm{Sin}^2(\theta)}\frac{\partial^2Y}{\partial\phi^2}+AY=0$$

$$A=l(l+1)$$

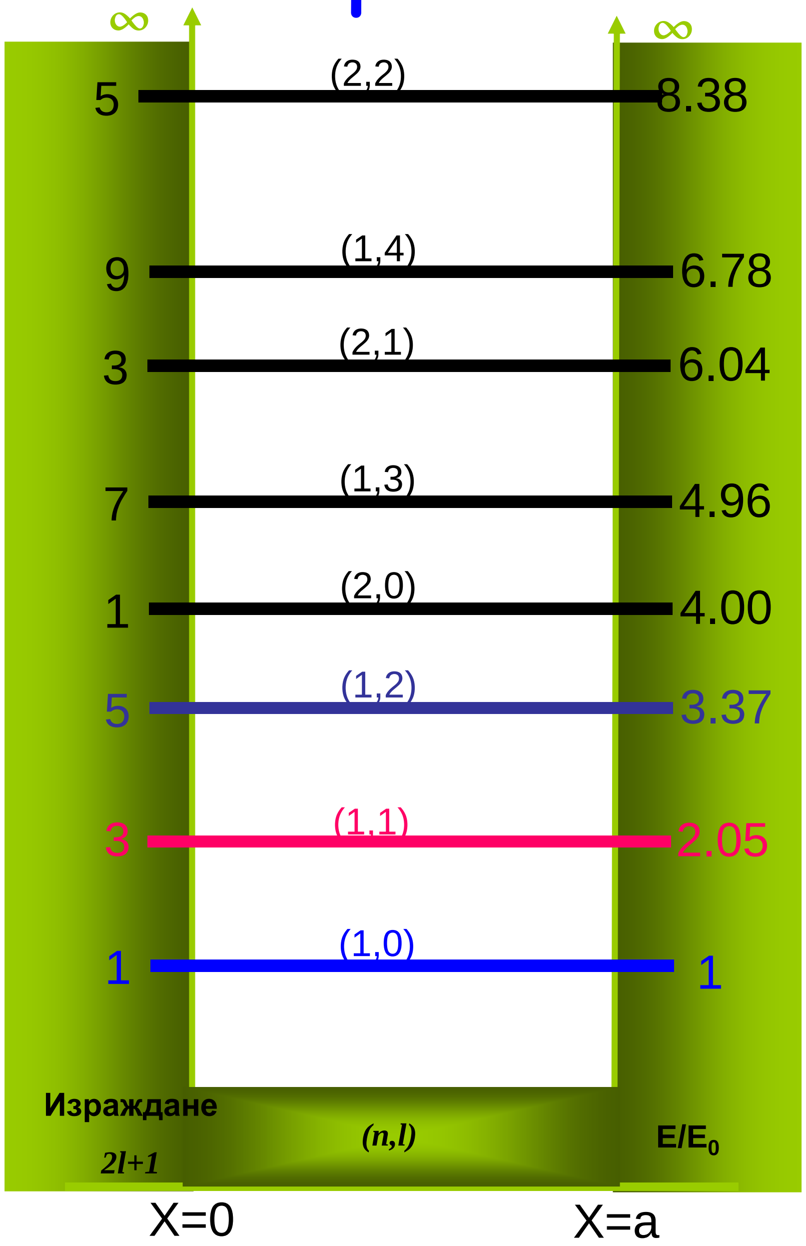
$$\frac{\mathrm{Sin}(\theta)}{\Theta}\frac{d}{d\theta}\left(\mathrm{Sin}(\theta)\frac{d\Theta}{d\theta}\right)+\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}+A.\mathrm{Sin}^2(\theta)=0$$

$$\frac{\mathrm{Sin}(\theta)}{\Theta}\frac{d}{d\theta}\left(\mathrm{Sin}(\theta)\frac{d\Theta}{d\theta}\right)+A.\mathrm{Sin}^2(\theta)-B=0$$

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}+B=0$$

$$B=m^2$$

Безкрайна потенциална яма - 3D



$$-\frac{\hbar^2}{2m}\left(\frac{d^2R}{dr^2}+\frac{2}{r}\frac{dR}{dr}\right)+\left[V(r)+\frac{l(l+1)\hbar^2}{2mr^2}\right]R = ER$$

$$u(r) = rR(r)$$

$$-\frac{\hbar^2}{2m}u'' + \frac{\hbar^2 l(l+1)}{2mr^2}u = Eu \qquad \rho = kr = \sqrt{\frac{2mE}{\hbar^2}}\,r$$

$$-\frac{d^2u(\rho)}{d\rho^2}+\frac{l(l+1)}{\rho^2}u(\rho) = u(\rho) \qquad u(\rho) = \sqrt{\rho}\,J(\rho)$$

$$\rho^2\frac{d^2J(\rho)}{d\rho^2}+\rho\frac{dJ(\rho)}{d\rho}+\left[\rho+\left(l+\frac{1}{2}\right)^2\right]J(\rho) = 0$$

$$J_\nu(\rho),\ \nu = l+\frac{1}{2}$$

$$R_l = \frac{u}{r} = N_l\, j_l(kr) \qquad j_l(kr) = \sqrt{\frac{\pi}{2kr}}\,J_{l+\frac{1}{2}}(kr)$$

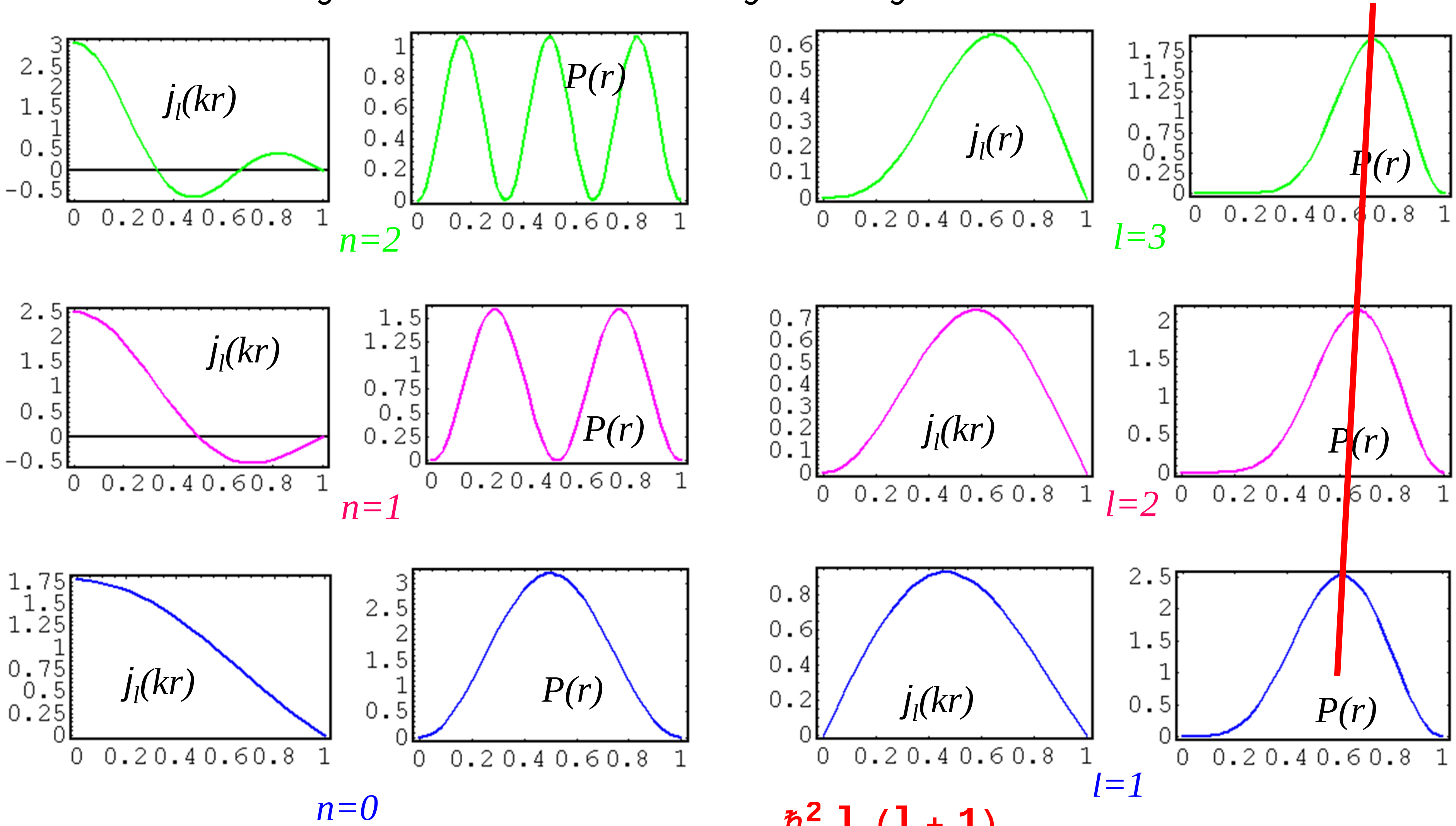
$$j_l(ka) = 0 \quad \{\xi_n^l\} \qquad E_{nl} = \frac{\hbar^2}{2ma^2}\left(\xi_n^l\right)^2$$

n	=	1	2	3	4	....
$l=0$ $\{\xi_n^0\}$	=	3.14,	6.28,	9.42,	12.56,	....
$l=1$ $\{\xi_n^1\}$	=	4.49,	7.72,	10.90,	14.06,	....

$2l+1$ изразждане по m_l

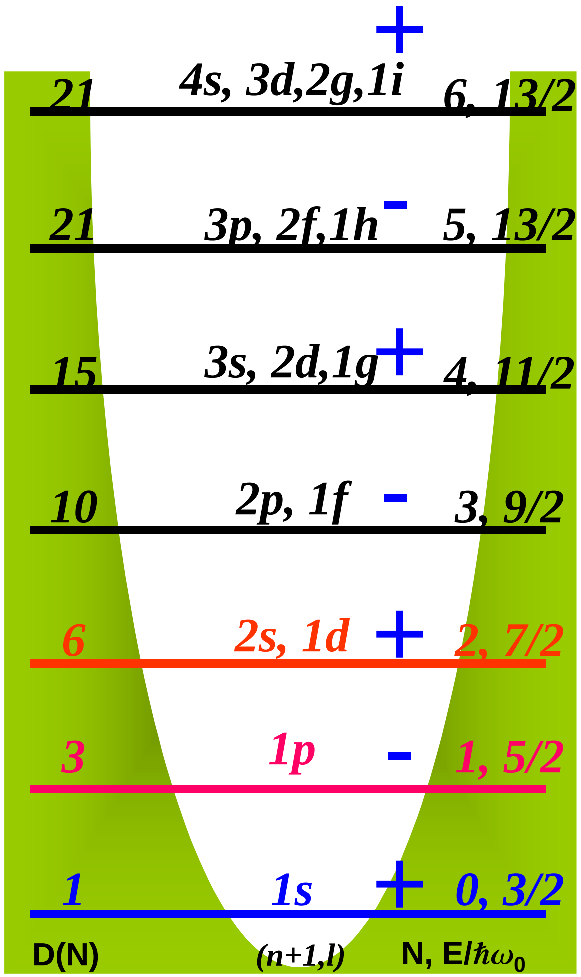
Центробежен потенциал

$$P(r)\,dr = \int |\psi|^2 dV = r^2 |R(r)|^2 dr \int \sin\theta\, d\theta \int |Y_{lm}|^2 d\phi = r^2 |R(r)|^2 dr$$



$l=0$ - const $\qquad V_{eff} = V(r) + \dfrac{\hbar^2\, l\,(l+1)}{2\,mr^2}$ $\qquad n=0$ - const

Сферичен хармоничен осцилатор



$$V(r) = \frac{1}{2} m \omega_0^2 r^2$$

$$\frac{d^2 R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \left[\frac{2mE}{\hbar^2} - \frac{m\omega_0^2}{\hbar^2} r^2 - \frac{l(l+1)}{r^2}\right] R = E R$$

$$R \propto F\left(-n,\ l + \frac{3}{2};\ \frac{m\omega_0}{\hbar^2} r^2\right)$$

$$E_{nl} = \hbar\omega_0\left(2n + l + \frac{3}{2}\right) = \hbar\omega_0\left(N + \frac{3}{2}\right)$$

$n = 0, 1, 2, 3, \ ....$ – радиално квантово число

N – главно квантово число – осцилаторен слой;

N – четно (нечетно) $\Longrightarrow$ l четно (нечетно) 0(1), 2(3) ….N

$\Longrightarrow$ N определя четността на състоянията в него

за дадено l имаме $(2l+1)$ израждане по m_l

$\Longrightarrow$ пълното израждане за дадено квантово число N

$$D(N) = \sum_{l=0,1}^{N} (2l+1) = \frac{1}{2}(N+1)(N+2)$$