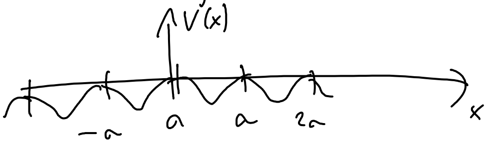
Cwiczenia 13
3 kwietnia 2014
15:08

1. Potencjały periodyczne - Kryształy

$$V(x+a) = V(x)$$



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

Operator przesunięcia: $D_a(\psi(x)) = \psi(x-a)$

Wiemy że $D_a = e^{-\frac{i\hat{p}a}{\hbar}} = e^{-a\frac{\partial}{\partial x}}$

$$D_a H D_a^{-1} = H \qquad [H, D_a] = 0$$

Czyli możemy szukać stanów własnych w ramach klasy stanów własnych D_a :

Szukamy: $D_a \psi(x) = \lambda \psi(x)$ $\quad \lambda = e^{-ika}$

$$\psi(x-a) = e^{-ika}\psi(x) \qquad k \in \mathbb{C}$$

Zdefiniujmy $\psi(x) = u(x) e^{ikx}$

$$u(x-a) e^{ik(x-a)} = e^{-ika} u(x) e^{ikx}$$

$$u(x-a) = u(x)$$

Czyli ogólna postać st. własnego op. przesunięcia

$$\boxed{\psi(x) = u(x) e^{ikx}, \quad u(x+a) = u(x)}$$

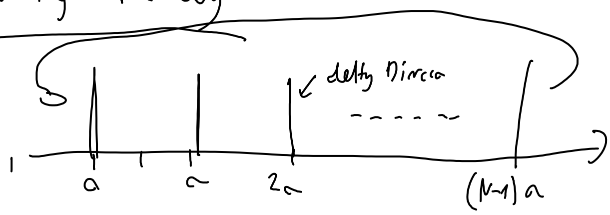
Tw. Blocha

$k \in \mathbb{R}$ inaczej f. wybucha,
Warunki brzegowe nie istotne zwykle narzucamy periodyczne warunki brzegowe:

$$\psi(x+Na) = \psi(x), \quad kNa = 2\pi n, \quad k_n = \frac{2\pi n}{Na}$$

$\hbar k$ - zwane quasipędem, dyskretyzacja k_n, dla dużych N nieistotna.

Model Kroniga-Penney



$$V(x)=\sum_{n=0}^{N-1}\lambda\,\delta(x-na)$$

Szukamy rozwiązań o energii E, postaci

$$\Psi(x)=u(x)\,e^{ikx}$$

$\psi(x)$ ciągła a w $\delta(x)$ skok:

$$\psi'_>(a)-\psi'_<(a)=\frac{2m\lambda}{\hbar^2}\psi(a)$$

Czyli:

$$u'_>(a)-u'_<(a)=\frac{2m\lambda}{\hbar^2}u(a)$$

ale pamiętamy że

$$u'_>(a)=u'_>(0)$$

czyli:

$$\begin{cases} u'_>(0)-u'_<(a)=\dfrac{2m\lambda}{\hbar^2}u(0) \\ u(a)=u(0) \end{cases}$$

Rozwiązanie pomiędzy deltami:

$$\psi(x)=Ae^{iqx}+Be^{-iqx} \qquad q=\sqrt{\frac{2mE}{\hbar^2}}$$

$$u(x)=Ae^{i(q-k)x}+Be^{-i(q+k)x}$$

$$\begin{cases} A+B=Ae^{i(q-k)a}+Be^{-i(q+k)a} \\ i(q-k)A-i(q+k)B-\left[i(q-k)Ae^{i(q-k)a}-iB(q+k)e^{-i(q+k)a}\right]=\dfrac{2m\lambda}{\hbar^2}(A+B) \end{cases}$$

$$A\left(1-e^{i(q-k)a}\right)=B\left(e^{-i(q+k)a}-1\right)$$

$$\begin{cases} A\left[i(q-k) - i(q-k)e^{i(q-k)a} - \frac{2m\lambda}{\hbar^2}\right] = \\ \qquad = B\left[i(q+k) - i(q+k)e^{-i(q+k)a} + \frac{2m\lambda}{\hbar^2}\right] \end{cases}$$

$$=-A e^{i\frac{(q-k)a}{2}}\, \cancel{2i}\, \sin\left(\frac{q-k}{2}a\right) = B e^{-i\frac{(q+k)a}{2}}\, \cancel{2i}\, \sin\left(\frac{q+k}{2}a\right)$$

$$A e^{iqa} \sin\left[\frac{q-k}{2}a\right] = B \sin\left[\frac{q+k}{2}a\right]$$

$$A e^{i\left(\frac{q-k}{2}\right)a}\left[-i(q-k)\,2i\sin\left(\frac{q-k}{2}a\right) - \frac{2m\lambda}{\hbar^2}e^{-i\left(\frac{q-k}{2}\right)a}\right] =$$

$$= B e^{-i\frac{(q+k)a}{2}}\left[i(q+k)\,2i\sin\left(\frac{q+k}{2}a\right) + \frac{2m\lambda}{\hbar^2}e^{i\left(\frac{q+k}{2}\right)a}\right]$$

$$A e^{iqa}\left[2(q-k)\sin\left(\frac{q-k}{2}a\right) - \frac{2m\lambda}{\hbar^2}e^{-i\frac{(q-k)a}{2}}\right]$$

$$= B\left[-2(q+k)\sin\left(\frac{q+k}{2}a\right) + \frac{2m\lambda}{\hbar^2}e^{i\left(\frac{q+k}{2}\right)a}\right]$$

$$\sin\left(\frac{q+k}{2}a\right)\left[2(q-k)\sin\left(\frac{q-k}{2}a\right) - \frac{2m\lambda}{\hbar^2}e^{-i\frac{(q-k)a}{2}}\right] =$$

$$= \sin\left(\frac{q-k}{2}a\right)\left[-2(q+k)\sin\left(\frac{q+k}{2}a\right) + \frac{2m\lambda}{\hbar^2}e^{i\frac{q+k}{2}a}\right]$$

$$2(q-k) - \frac{2m\lambda}{\hbar^2}\frac{e^{-i\frac{(q-k)a}{2}}}{\sin\left(\frac{q-k}{2}a\right)} = -2(q+k) + \frac{2m\lambda}{\hbar^2}\frac{e^{i\left(\frac{q+k}{2}\right)a}}{\sin\left(\frac{q+k}{2}a\right)}$$

$$4q - \frac{2m\lambda}{\hbar^2}\left[\operatorname{ctg}\left(\frac{q-k}{2}\right)a + \operatorname{ctg}\left(\frac{q+k}{2}\right)a\right] = 0$$

$$\frac{2q\hbar^2}{m\lambda} = \underbrace{\frac{\cos\frac{q-k}{2}a}{\sin\frac{q-k}{2}a} + \frac{\cos\frac{q+k}{2}a}{\sin\frac{q+k}{2}a}}_{\parallel}$$

$$\begin{cases} \dfrac{\cos\frac{q-k}{2}a\,\sin\frac{q+k}{2}a + \cos\frac{q+k}{2}a\,\sin\frac{q-k}{2}a}{\sin\frac{q-k}{2}a\,\sin\frac{q+k}{2}a} = \\ = \dfrac{\sin qa}{\qquad} \qquad \left\{ \sin\alpha\sin\beta = \right. \end{cases}$$

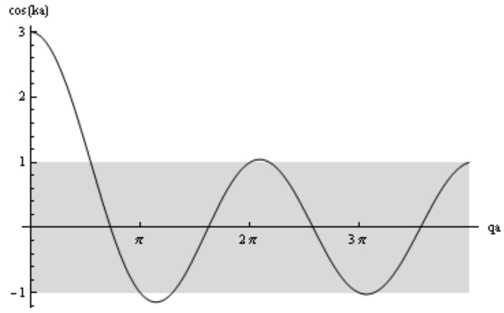
$$\Big| = \frac{\sin qa}{\frac{1}{2}(\cos ka - \cos qa)}$$

$\sin\alpha \sin\beta = \frac{1}{2}[\cos(\alpha-\beta) - \cos(\alpha+\beta)]$

$\sin(\alpha+\beta) = \sin\alpha\cos\beta + \sin\beta\cos\alpha$

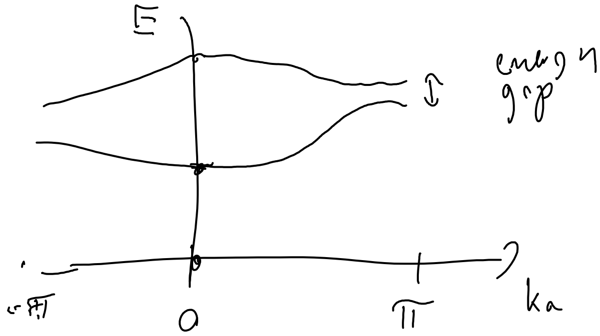
$$\frac{\sin qa \; m\lambda}{q\hbar^2} = \cos ka - \cos qa$$

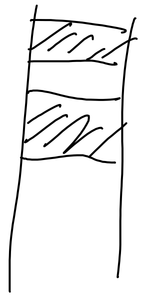
$$\frac{\sin qa}{qa}\underbrace{\frac{m\lambda a}{\hbar^2}}_{F} + \cos qa = \cos ka$$



Teraz wykres E(k)

$$E(k) = \frac{\hbar^2 q^2}{2m} \qquad k \in [0, \tfrac{\pi}{a}]$$





$k = \frac{2n\pi}{Na}$, mamy N różnych stanów k dostępnych w danym paśmie.
(jeśli uwzględnić spin 2N) - czyli atomy z dwoma el. walencyjnymi wypełniają pasmo w pełni ≈ izolatory.

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1. Znaleźć stany własne i energie w sferycznej studni potencjału

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

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

$$\psi_{n,l,m}(r,\theta,\varphi) = R_{n,l}(r)\, Y_{l,m}(\theta,\varphi)$$

harmoniki sferyczne

$$\begin{cases} L_z Y_{l,m} = \hbar m Y_{l,m} \\ \hat{L}^2 Y_{l,m} = \hbar^2 l(l+1) Y_{l,m} \\ Y_{0,0} = \frac{1}{\sqrt{4\pi}} \qquad Y_{1,0} = \frac{1}{2}\left(\frac{3}{\pi}\right)^{\frac{1}{2}}\cos\theta, \quad Y_{1,\pm 1} = \frac{1}{2}\left(\frac{3}{2\pi}\right)^{\frac{1}{2}}\sin\theta\, e^{\pm i\varphi} \\ \int d\varphi\, d\theta \sin\theta\, Y_{l,m}(\theta,\varphi)\, Y^*_{l',m'}(\theta,\varphi) = \delta_{m,m'}\delta_{l,l'} \end{cases}$$

$$\frac{\hbar^2}{2m}\frac{1}{r}\frac{d^2}{dr^2}(rR) + \left\{\frac{\hbar^2 l(l+1)}{2mr^2} + V(r) - E\right\}R = 0$$

Weźmy $V(r)=0$ i zmienną $\rho = k\cdot r$ $\quad R'(\rho) = R'(kr) = R(r)$

$$-\frac{\hbar^2 k^2}{2m}\frac{1}{\rho}\frac{d^2}{d\rho^2}(\rho R') + \left(\frac{\hbar^2 l(l+1)k^2}{2m\rho^2} - E\right)R' = 0$$

$$\frac{1}{\rho}\frac{d^2}{d\rho^2}(\rho R') + \left(\frac{2mE}{\hbar^2 k^2} - \frac{l(l+1)}{\rho^2}\right)R' = 0$$

$$E = \frac{\hbar^2 k^2}{2m}$$

$$\frac{d^2 R'}{d\rho^2} + \frac{2}{\rho}\frac{dR'}{d\rho} + \left[1 - \frac{l(l+1)}{\rho^2}\right]R' = 0$$

$\}$ rów. Bessla

$$R_l^1(\rho) = A\, j_l(\rho) + B\, n_l(\rho)$$

kul. f. Bessla — kul. f. Neumana

$$j_l(\rho) = (-\rho)^l \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^l \left(\frac{\sin\rho}{\rho}\right)$$

$$n_l(\rho) = -(-\rho)^l \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^l \left(\frac{\cos\rho}{\rho}\right)$$

dla małych ρ:

$$j_l(\rho) \approx \frac{2^l l!}{(2l+1)!}\rho^l \qquad n_l(\rho) = \frac{-(2l)!}{2^l l!}\rho^{-(l+1)}$$

dla dużych ρ:

$$j_l(\rho) = \frac{1}{\rho}\sin\left(\rho - \frac{l\pi}{2}\right), \quad n_l(\rho) = -\frac{1}{\rho}\cos\left(\rho - \frac{l\pi}{2}\right)$$

$$l=0 \qquad j_0(\rho) = \frac{\sin\rho}{\rho}, \quad n_0(\rho) = \frac{\cos\rho}{\rho}$$

$$l=1 \quad j_1(\rho) = -\frac{d}{d\rho}\left(\frac{\sin\rho}{\rho}\right) = -\frac{\cos\rho}{\rho} + \frac{\sin\rho}{\rho^2}, \quad n_1(\rho) = \frac{-\sin\rho}{\rho} - \frac{\cos\rho}{\rho^2}$$

$\vdots$

W $\rho \to 0$ $n_l(\rho)$ wybucha czyli bierzemy

$$R_l(r) = A\, j_l(kr) = j_l\left(\sqrt{\frac{2mE}{\hbar^2}}\, r\right)$$

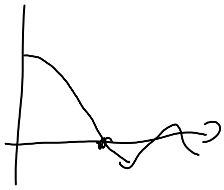
Warunek zszycia $R_l(a) = 0$ czyli dyskretne energie:

$$\sqrt{\frac{2mE_{n,l}}{\hbar^2}}\, a = z_{n,l} \qquad \text{- n-te zero } j_l$$

$$\boxed{E_{n,l} = \frac{z_{n,l}^2 \hbar^2}{2ma^2}}$$

Dla $l=0$

$$R_0(r) = A\,\frac{\sin kr}{kr}$$



$$\frac{1}{\rho}\frac{d^2}{d\rho}(rR') + \frac{2mE}{\hbar^2 k^2} R' = 0$$

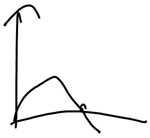
$$\frac{d^2}{d\rho^2}(\rho R') = -(\rho R')$$

$$\rho R' = A\sin\rho + B\cos\rho \qquad ak$$

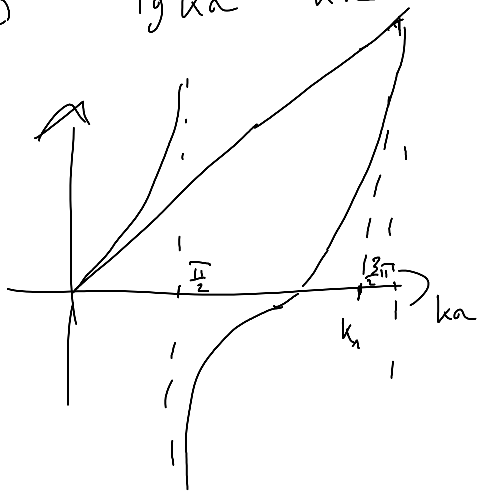
$ka = n\pi$ $\qquad E_{n,0} = \frac{\hbar^2 n^2 \pi^2}{2ma^2}$ $\qquad n = 1, \ldots$

Dla $l=1$

$$R_1(r) = A\left(\frac{\sin kr}{(kr)^2} - \frac{\cos kr}{(kr)}\right)$$



$R_1(a) = 0$ $\qquad \operatorname{tg} ka = ka$ $\qquad k = \sqrt{\frac{2mE}{\hbar^2}}$



$$\pi < ka < \frac{3}{2}\pi$$

najmniejsza energia $\qquad \sqrt{\frac{2mE}{\hbar^2}} < \frac{3\pi}{2a}$

$$E_{1,1} < \frac{\hbar^2}{2ma^2}\left(\frac{3\pi}{2}\right)^2$$

$$E_{1,1} < E_{2,0}$$

Czyli dwie najniższe energie $E_{1,0}$, $E_{1,1}$

jeden $\qquad$ 3 stany

jeden stan ↑ 3 stany ↑

$$\Psi_{1,0,0} = A \cdot \frac{\sin \frac{\pi r}{a}}{\frac{\pi r}{a}} \cdot Y_{0,0}(\theta,\varphi) \qquad (E_{1,0})$$

$$\Psi_{1,1,m} = A\left(\frac{\sin k_1 r}{k_1 r} - \frac{\cos k_1}{(k_1 r)^2}\right) Y_{1,m}(\theta,\varphi) \qquad (E_{1,1})$$

3. $V(r) = \begin{cases} -V_0, & r \le a \\ 0 & r > a \end{cases}$

Dla $l=0$

Szukamy stanów związanych $E<0$

$r<a$

$$R_I(r) = A\,\frac{\sin kr}{r} \qquad k = \sqrt{\frac{2m(E+V_0)}{\hbar^2}}$$

$r>a$

$$R_{II}(r) = \underbrace{B\,\frac{e^{k'r}}{r}}_{\text{odrzucamy}} + C\,\frac{e^{-k'r}}{r} \qquad k' = \sqrt{\frac{2m|E|}{\hbar^2}}$$

$$A \sin ka = Ce^{-k'a}$$

$$Ak \cos ka = -k'C e^{-k'a}$$

$$\operatorname{tg} ka = -\left(\frac{k}{k'}\right)$$

$$-ka \operatorname{ctg} ka = k'a \qquad k'a = \sqrt{\frac{2mV_0a^2}{\hbar^2} - k^2a^2}$$

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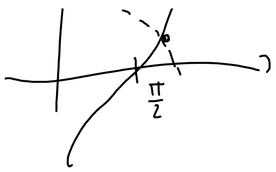

Są stany związane pod warunkiem że

$$\sqrt{\frac{2mV_0a^2}{\hbar^2}} > \frac{\pi}{2}$$

Stany rozproszeniowe $E > 0$

W obszarze $r \le a$, $l=0$

$$R_I(r) = A\frac{\sin kr}{r} \qquad k=\sqrt{\frac{2m(E+V_0)}{\hbar^2}}$$

W obszarze $r \geq a$

$$R_{II} = B\frac{\sin k'r}{r} + C\frac{\cos k'r}{r} \qquad k' = \sqrt{\frac{2mE}{\hbar^2}}$$

Szukamy st. rozproszeniowych $E \geq 0$

$$R_{II} = B\frac{\sin(k'r+\delta)}{r}$$

$$\begin{cases} A\sin ka = B\sin(k'a+\delta) \\ Ak\cos ka = Bk'\cos(k'a+\delta) \end{cases}$$

$$\frac{k'}{k}\tan ka = \tan(k'a+\delta)$$

Szukamy δ

$$\left\{ \tan(\alpha+\beta) = \frac{\tan\alpha+\tan\beta}{1-\tan\alpha\tan\beta} \right.$$

$$\left(\frac{k'}{k}\right)\tan ka = \frac{\tan k'a+\tan\delta}{1-\tan k'a\tan\delta}$$

$$\tan\delta \cdot \left(1 + \tan k'a \tan ka \left(\frac{k'}{k}\right)\right) = \left(\frac{k'}{k}\right) \tan ka - \tan k'a$$

$$\tan\delta = \frac{\left(\frac{k'}{k}\right) \tan ka - \tan k'a}{1 + \tan k'a \tan ka \left(\frac{k'}{k}\right)}$$