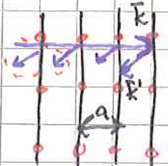
31/1-2013 Rep NFEM.

(6)

FEM $H^0 \phi_n^0 = E_n^0 \phi_n^0$

$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$ e^{ikx} $\frac{\hbar^2 k_n^2}{2m}$

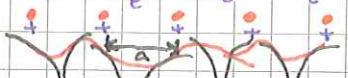


$V(x)$ (periodisk) $\Rightarrow \bar{k} \curvearrowright \bar{k}'$

Braggspridnings $n\lambda = 2a$ (normalt infall)

↑ V(x) periodisk (kvasi)

$V(x) = -V_0 \cos\left(\frac{2\pi}{a}x\right)$ e^- e^- e^- e^- e^- e^- e^-



$H = H^0 + V(x)$ svag störning.

egenfunktioner: $\phi_n^0 \propto e^{ik_n x}$ ← ortogonal: $\int \phi_n^{0*}\phi_m^0 dx = \delta_{nm}$

egenenergier: $E_n^0 = \frac{\hbar^2 k_n^2}{2m}$ ϕ_n^0 inte egenfunktioner till H.

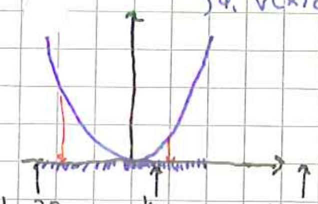
$\phi(x) = c_1\phi_1^0 + c_2\phi_2^0 + \ldots$

$H\phi(x) = E\phi(x)$. multiplicera fr. v. med ϕ_1^{0*} & $\int_0^L \ldots dx$

$c_1 E_1^0 + c_2\left(-\frac{V_0}{2}\right) = c_1 E$

URVALSREGEL

$\int \phi_1^{0*} V(x)\phi_2^0 dx = \begin{cases} -V_0/2 & \text{om } k_1 = k_2 \pm \frac{2\pi}{a} \\ 0 & \text{annars} \end{cases}$



$k_1 - \frac{2\pi}{a}$ k_1 $k_1 + 2\pi/a$.

Samma procedur (mult. fr. v. med ϕ_2^{0*} + $\int_0^L \ldots dx$

$\Rightarrow c_1(-V_0/2) + c_2 E_2^0 = c_2 E$

$$\begin{pmatrix} E_1^0 & -V_0/2 \\ -V_0/2 & E_2^0 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = E\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

$Ax = \lambda x$

$|A - \lambda I| = 0$ linj. alg. lösningar

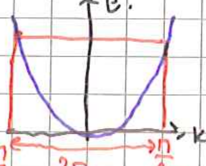
$$E = \frac{E_1^0 + E_2^0}{2} \pm \sqrt{\frac{(E_1^0 - E_2^0)^2}{4} + \left(\frac{V_0}{2}\right)^2}$$

Inte exakta egenenergier. - approximationer.

Välj ett (special)-fall $E_1^0 = E_2^0 \Rightarrow E = E_1^0 \pm \frac{V_0}{2}$

Om ϕ_1^0 & ϕ_2^0 har samma energi och skiljer sig i k-värde med $\frac{2\pi}{a}$.

- $E_1 = \boxed{E_1^0} - \boxed{V_0/2} \Rightarrow c_1 = c_2$
- $\phi_1(x) = \frac{1}{\sqrt{2L}}\left(e^{i\pi/a x} + e^{-i\pi/a x}\right) = \sqrt{\frac{2}{L}}\cos\left(\frac{\pi x}{a}\right)$ ← lägre pot. energi



$-\frac{\pi}{a}$ $\frac{2\pi}{a}$ $\frac{\pi}{a}$

$E_2 = \boxed{E_2^0} + \boxed{V_0/2} \Rightarrow c_1 = -c_2$.

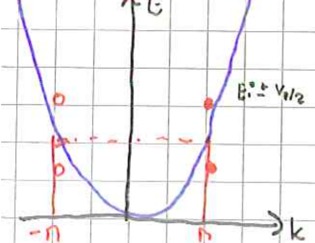
$\phi_2(x) = \frac{1}{\sqrt{2L}}\left(e^{i\pi/a x} - e^{-i\pi/a x}\right) = \sqrt{\frac{2}{L}}\, i\sin\left(\frac{\pi x}{a}\right)$ Stående vågor. $\langle p \rangle = 0$

högre pot. energi.

Tidsberoendet. $\left(e^{-iEt/\hbar}\right)$

kin energ. pot energ.

Se fig. 5.8 sid 119!



$E_1^0 \pm V_0/2$

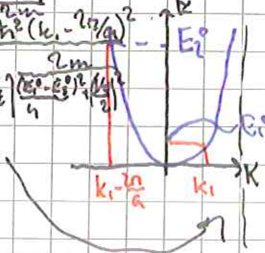
$-\frac{\pi}{a} < k \leq \frac{\pi}{a}$ → 1:a Brillouinzonen.

Annat fall: $E_1^0 \neq E_2^0$

$E_1^0 = \frac{\hbar^2 k_1^2}{2m}$

$E_2^0 = \frac{\hbar^2 (k_1 - 2\pi/a)^2}{2m}$

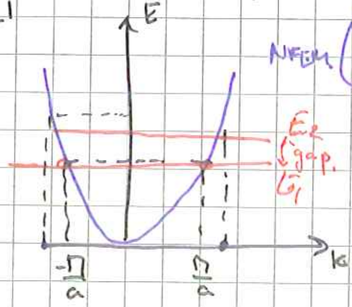
$E = \frac{E_1^0 + E_2^0}{2} \pm \sqrt{\frac{(E_1^0 - E_2^0)^2}{4} + \left(\frac{V_0}{2}\right)^2}$



$|E_1^0 - E_2^0| \gg V_0$: $E \to \frac{E_1^0 + E_2^0}{2} \pm \sqrt{\frac{(E_1^0 - E_2^0)^2}{4}}$ → E_1^0 → E_2^0

"Tätare" E_1^0 & E_2^0 ⇒ Större störning av FEM.

$|c_1| \neq |c_2|$



NFEM: $E_1^0 = E_2^0$, $k_1 = \frac{\pi}{a}$, $k_2 = -\frac{\pi}{a}$

$E_1 = E_1^0 - V_0/2$ $c_1 = c_2$

$E_2 = E_2^0 + V_0/2$ $c_1 \neq c_2$

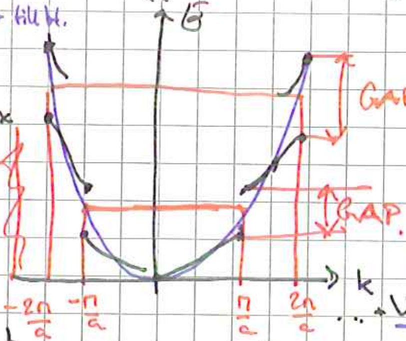
$\phi_1 \sim e^{i\pi/a x} + \ldots \sim \cos\left(\frac{\pi}{a}x\right)$

E_2, gap, E_1

$H\phi = E\phi$.

Bragg $n\lambda = 2a \Rightarrow k = \frac{\pi}{a} \cdot n$ $e^{i\pi/a x} \leftrightarrow e^{-i\frac{\pi}{a}x}$ $k = \pm\frac{\pi}{a}$

$e^{i\frac{2\pi}{a}x} \leftrightarrow e^{-i\frac{2\pi}{a}x}$



GAP

GAP.

Mer generell potential.

$V(x) = \sum_p V_p e^{i\left(\frac{2\pi}{a}\right)px}$

tillför på $p = -1, 0, 1$

$\ldots + V_{-1}e^{-i\left(\frac{2\pi}{a}\right)x} + V_0 e^0 + V_1 e^{i2\pi/a x} + \ldots$

FEM

NFEM

$V_{-1} = V_1 \Rightarrow V(x) = V_1\cos\left(\frac{2\pi}{a}x\right)$

$\int_0^L \phi_1^{0*}\left(V_{-p}e^{-i\frac{2\pi}{a}px} + V_p e^{i\frac{2\pi}{a}px}\right)\phi_2^0$

$\neq 0$ om $k_1 = k_2 \pm \frac{2\pi}{a}\cdot p$ URVALSREGEL $k_2 = k_1 \pm \frac{2\pi}{a}p$.

$= 0$ annars.

$2\pi/a$: 1:a BZ.

(Fig. 5.13 s 123)

Ansats: $\phi = c_1\phi_1 + c_2\phi_2 + \ldots c_5\phi_5 \Rightarrow E_1 \ldots E_5$.

Räkna t.o.m. 23.