$$\psi(\vec{r}) = \sum_{\vec{k}} C(\vec{k})\, e^{i\vec{k}\cdot\vec{r}}$$

$$U(\vec{r}) = \sum_{\vec{G}} \phi_{\vec{G}}\, e^{i\vec{G}\cdot\vec{r}}$$

Innsatt i Schrödinger ligningen: (husk $\nabla^2 \to (ik)^2 = -k^2$)

$$\sum_{\vec{k}} \left(\frac{\hbar^2}{2m}k^2 - E\right) C(\vec{k})\, e^{i\vec{k}\cdot\vec{r}} + \sum_{\vec{k}'}\sum_{\vec{G}} \phi_{\vec{G}}\, C(k')\, e^{i\overbrace{(\vec{G}+\vec{k}')}^{\vec{k}}\cdot\vec{r}} = 0$$

$$\Rightarrow \boxed{\left(\frac{\hbar^2 k^2}{2m} - E\right) C(\vec{k}) + \sum_{\vec{G}} \phi_{\vec{G}}\, C(\vec{k}-\vec{G}) = 0}$$ for alle tillatte $\vec{k}$.

$\vec{G}$ resiprok gittervektor.

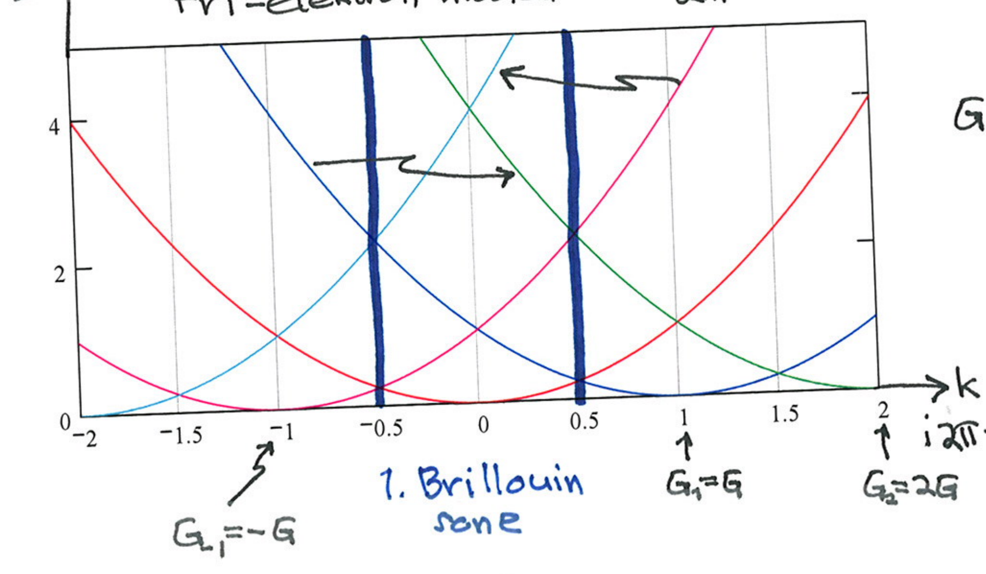
<u>I en dimensjon:</u> la G være minste resiproke gittervektor

$$G = \frac{2\pi}{a}.$$

Ligningen kobler <u>bare</u> sammen de ukjente

$$\ldots\; C(k-2G),\; C(k-G),\; C(k),\; C(k+G),\; C(k+2G),\; \ldots$$

Fri-elektron modell $E = \frac{\hbar^2}{2m}(k-G_n)^2$



i 2π-enheter (=G)

$G = \frac{2\pi}{a} = 2\pi$ for $a=1$.

For valgt $\vec{k}_0$: $E(\vec{k}_0+\vec{G}) = E(\vec{k}_0)$

Alle energinivåer finnes innen 1. Brillouin sone

$\rightarrow$ holder å se på 1. sone.

Enkel modell:

periodisk U: $U(x) = 2U\cos(\frac{2\pi}{a}x) = Ue^{i\frac{2\pi}{a}x} + Ue^{-\frac{2\pi}{a}x}$

har generelt $U(x) = \sum_G \phi_G e^{iGx}$ med $G = \frac{2\pi}{a}$.

$$= \ldots + \phi_{-2G}e^{-i2Gx} + \phi_{-G}e^{-iGx} + \phi_0 e^0 + \phi_G e^{iGx} + \phi_{2G}e^{i2Gx} + \ldots$$

$$\Rightarrow \boxed{\phi_{-G} = U \text{ og } \phi_G = U}$$

Antår stående elektronbølger for $k = \pm\frac{1}{2}G = \pm\frac{\pi}{a}$:

$$\psi^{\pm}(x) = e^{i\frac{\pi}{a}x} \pm e^{-i\frac{\pi}{a}x} = \underbrace{C(\tfrac{1}{2}G)}_{=1}e^{i\frac{1}{2}G\cdot x} + \underbrace{C(-\tfrac{1}{2}G)}_{=1}e^{-i\frac{1}{2}G\cdot x}$$

Altså $\boxed{C(\tfrac{1}{2}G) \text{ og } C(-\tfrac{1}{2}G) \text{ eneste Fourierkomponenter}}$

$\frac{\hbar^2}{2m}(\frac{1}{2}G)^2 = \frac{\hbar^2}{2m}(-\frac{1}{2}G)^2 \equiv \lambda$. (kinetisk energi)

Får ligningsett for å finne energien E:

$$\boxed{\begin{aligned}(\lambda - E)\,C(\tfrac{1}{2}G) + U\,C(-\tfrac{1}{2}G) &= 0\\ (\lambda - E)\,C(-\tfrac{1}{2}G) + U\,C(\tfrac{1}{2}G) &= 0\end{aligned}}$$

Løsning kun mulig hvis determinanten $= 0$.

$$\begin{vmatrix} \lambda - E & U \\ U & \lambda - E \end{vmatrix} = 0$$

$$\Rightarrow \boxed{E = \lambda \pm U = \frac{\hbar^2}{2m}(\tfrac{1}{2}G)^2 \pm U}$$

Altså energigap $E_g = 2U$ for $k = \frac{1}{2}G = \pm\frac{\pi}{a}$.

Sonegrense 1. Brillouinsone