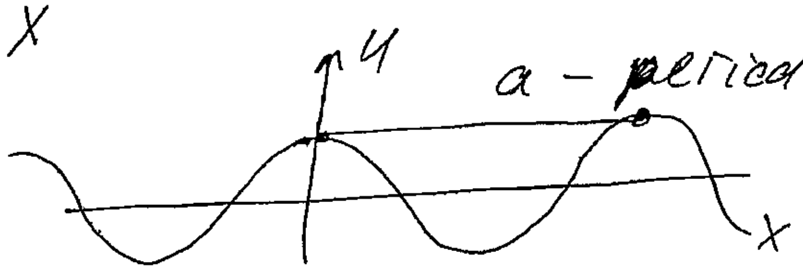
Electron in a periodic potential
Band structure, 1D example
Quazimomentum
Surface states

Electron in a periodic potential. Band structure and quasimomentum.

A simple one-dimensional (1D) model: electron in a weak periodic potential.

$U(x) = 2W \cos gx$



$g = 2\pi/a$ — vector of the reciprocal lattice

electron with momentum k is moving in the potential.
We use perturbation theory to find the electron wave function and the electron energy.
Let L be the total length of the crystal, $L \gg a$

In zero approximation

$$|k\rangle = \psi = \frac{1}{\sqrt{L}} e^{ikx} \quad , \quad \varepsilon_k^{(0)} = \frac{k^2}{2m}$$

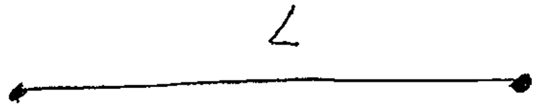
according to perturbation theory

$$\varepsilon_k = \varepsilon_k^{(0)} + \langle k|U|k\rangle + \sum_{k' \neq k} \frac{|\langle k'|U|k\rangle|^2}{\varepsilon_k^{(0)} - \varepsilon_{k'}^{(0)}} + \dots$$

$$\psi_k = |k\rangle + \sum_{k' \neq k} \frac{\langle k'|U|k\rangle}{\varepsilon_k^{(0)} - \varepsilon_{k'}^{(0)}} |k'\rangle + \dots$$

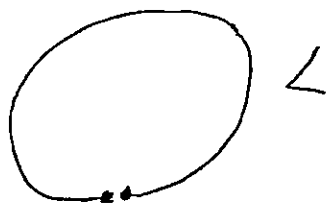
$$\langle k|U|k\rangle = \int_0^L \frac{1}{\sqrt{L}} e^{-ikx} 2W \cos gx \frac{1}{\sqrt{L}} e^{ikx} dx = 0$$

What is the meaning of $\sum_k$?



– crystal.

Let us bend it to the ring of length L



In this case we have to impose the periodic boundary condition

$$\psi(x=0)=\psi(x=0)$$

$$e^{ik\cdot 0}=e^{ikL} \Longrightarrow \boxed{e^{ikL}=1}$$

Hence k takes discrete values

$$k=\frac{2\pi}{L}\cdot \ell \,, \quad \ell \text{ - is an integer number}$$

$$\ell = 0, \pm 1, \pm 2, \ldots$$

Thus, the summation over k, $\sum_k$, is equivalent to the summation over ℓ, $\sum_\ell$.

Offdiagonal matrix element of the potential

$$\langle k'|U|k\rangle = \int_0^L \frac{e^{-ik'x}}{\sqrt{L}}\, 2W\cos gx\, \frac{e^{ikx}}{\sqrt{L}}\, dx =$$

$$= \frac{2W}{L}\int_0^L e^{i(k-k')x}\,\frac{1}{2}\left(e^{igx}+e^{-igx}\right)dx$$

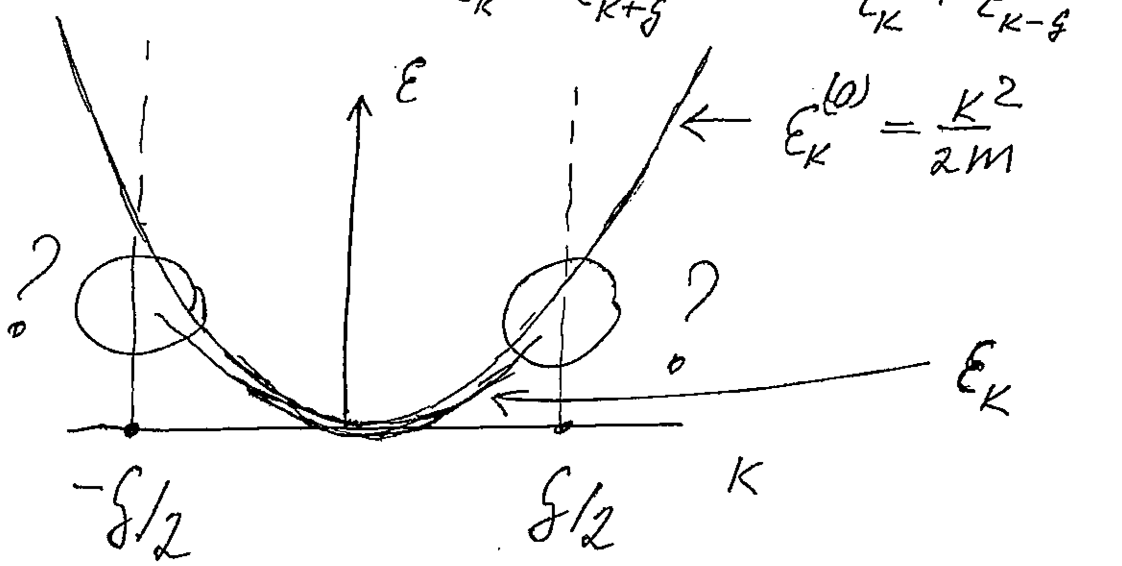
Hence

$$\langle k'|U|k\rangle = \begin{cases} W & \text{if } k'-k = \pm g \\ 0 & \text{if } k'-k \neq \pm g \end{cases}$$

Come back to the energy

$$\varepsilon_k = \varepsilon_k^{(0)} + \sum_{k' \neq k} \frac{|\langle k'|U|k\rangle|^2}{\varepsilon_k^{(0)} - \varepsilon_{k'}^{(0)}} = \varepsilon_k^{(0)} + \sum_{\pm} \frac{\langle k \pm g|U|k\rangle^2}{\varepsilon_k^{(0)} - \varepsilon_{k\pm g}^{(0)}} =$$

$$= \varepsilon_k^{(0)} + \frac{W^2}{\varepsilon_k^{(0)} - \varepsilon_{k+g}^{(0)}} + \frac{W^2}{\varepsilon_k^{(0)} + \varepsilon_{k-g}^{(0)}}$$



Brillouin zone (BZ)

Non degenerate perturbation theory fails near boundaries of BZ, $\varepsilon_{g/2}^{(0)} = \varepsilon_{\frac{g}{2}-g}^{(0)}$

In the degenerate perturbation theory one considers $|k\rangle$ and $|k-g\rangle$ at equal footing.

$$\psi = \alpha|k\rangle + \beta|k-g\rangle$$

$$H = \frac{p^2}{2m} + U$$

matrix elements of the Hamiltonian

$$\langle k|H|k\rangle = \varepsilon_k^{(0)}$$

$$\langle k-g|H|k-g\rangle = \varepsilon_{k-g}^{(0)}$$

$$\langle k-g|H|k\rangle = \langle k|H|k-g\rangle = W$$

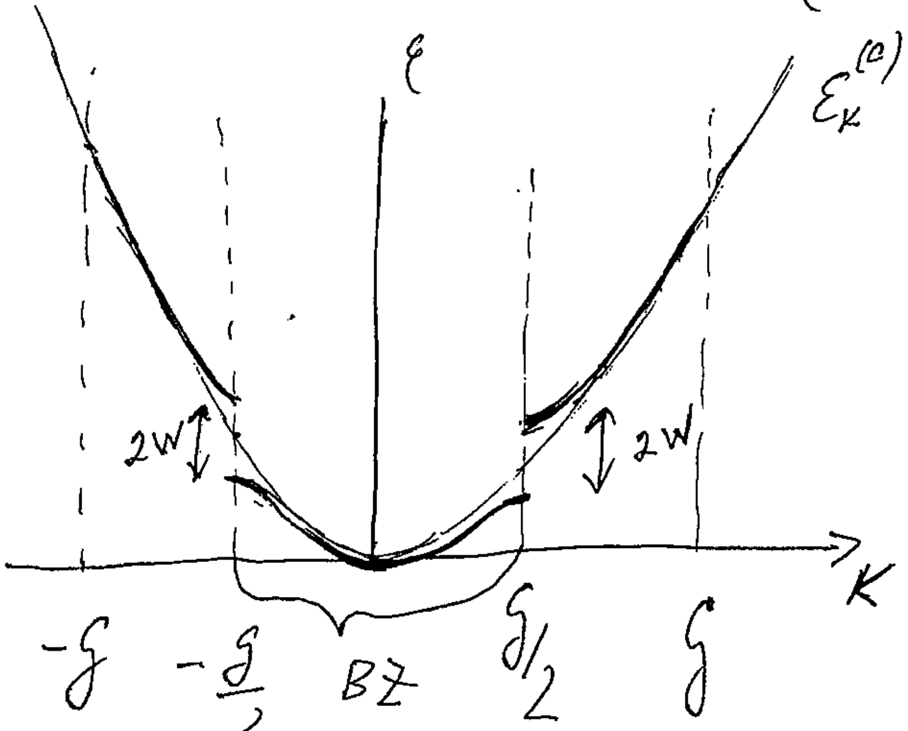
Hence the Hamiltonian can be represented as 2×2 matrix.

$$H = \begin{pmatrix} \varepsilon_k^{(0)} & W \\ W & \varepsilon_{k-g}^{(0)} \end{pmatrix}, \quad H\psi = \varepsilon\psi$$

$$\psi = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

$$\begin{vmatrix} \varepsilon_K^{(0)} - \varepsilon & W \\ W & \varepsilon_{K-g}^{(0)} - \varepsilon \end{vmatrix} = 0$$

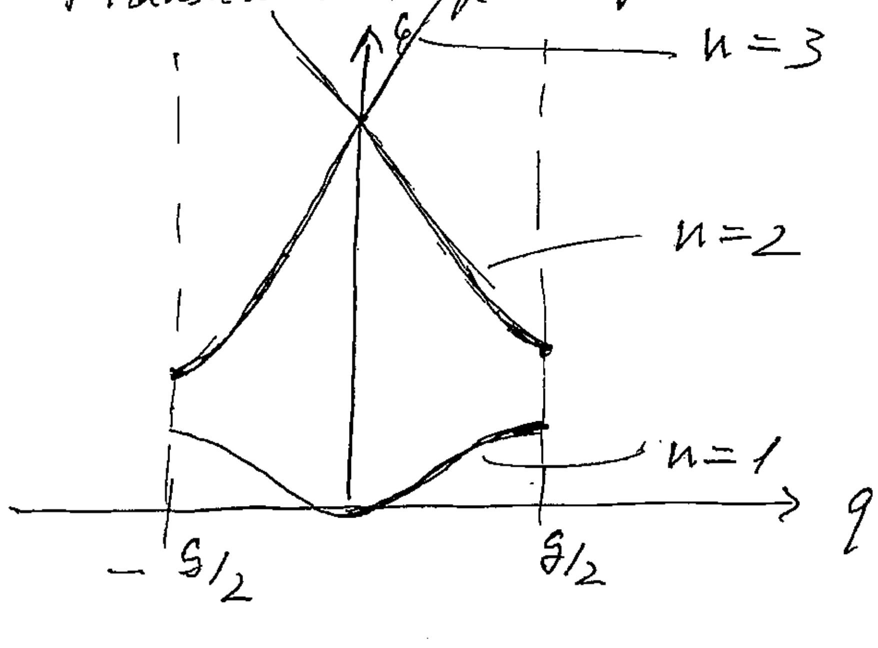
$$\varepsilon = \frac{1}{2}\left(\varepsilon_K^{(0)} + \varepsilon_{K-g}^{(0)}\right) \pm \sqrt{\left(\frac{\varepsilon_K^{(0)} - \varepsilon_{K-g}^{(0)}}{2}\right)^2 + W^2}$$



momentum

$-\infty < K < \infty$

Translation of dispersion to the BZ

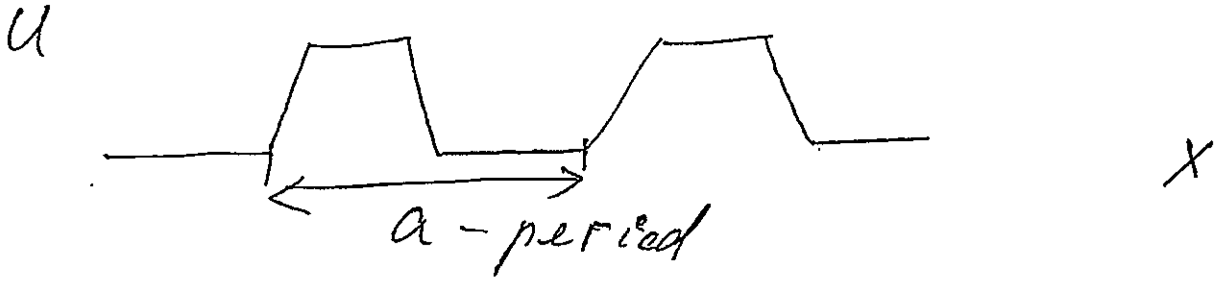


quasimomentum

$-\frac{g}{2} < q < \frac{g}{2}$

We considered a ~~perfect~~ $2W\cos gx$ potential.

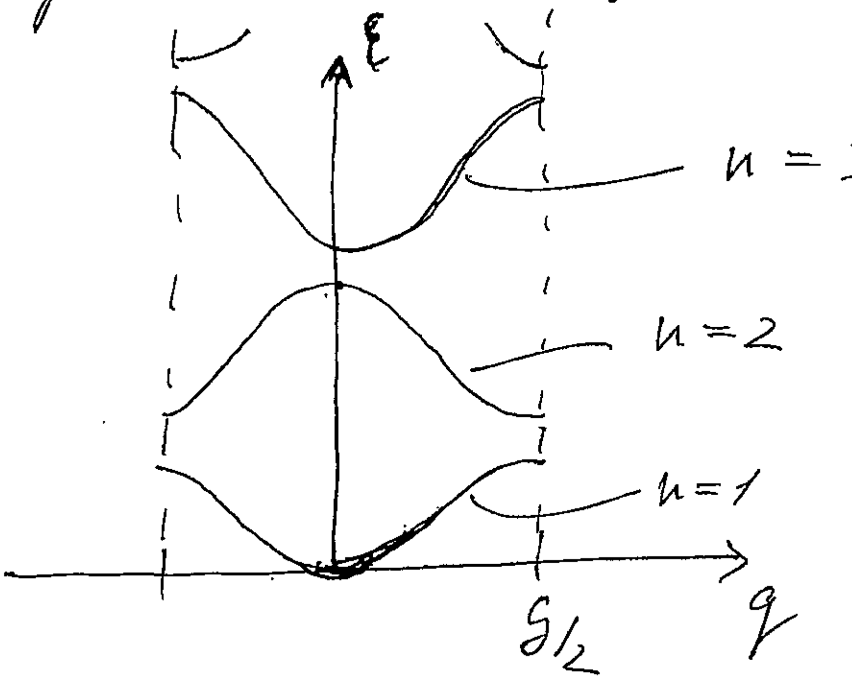
For a general periodic potential



all harmonics are nonzero

$$U(x) = 2W_1 \cos gx + 2W_2 \cos 2gx + 2W_3 \cos 3gx + \ldots$$

Therefore gaps are opened at all dispersion crossings.



$-\frac{g}{2} < q < g/2$

Lessons we learn from this example.

1. There are allowed and forbidden energy bands: band structure

2. Instead of momentum we get quasimomentum $-\frac{g}{2} < q < \frac{g}{2}$, and we also get integer index n, enumerating the band

$\psi_1(x)$ – 1st BZ

$\psi_2(x)$ – 2nd BZ

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3. $$\psi_1(x) = \alpha_q e^{iqx} + \beta_q e^{i(q-g)x} =$$

$$= e^{iqx} \underbrace{\left[\alpha_q + \beta_q e^{-igx}\right]}_{\text{periodic function of } x}$$

$$\psi_1(x+a) = e^{iq(x+a)}\left[\alpha_q + \beta_q e^{-igx}\right]$$

$$\boxed{\psi_1(x+a) = e^{iqa}\psi_1(x)}$$ Bloch theorem

Surface (edge) state

Consider electron moving in a weak 1D periodic potential

$$U(x) = 2W \cos gx \quad , \quad g = \frac{2\pi}{a}$$

The system is described by matrix Hamiltonian, see lecture notes

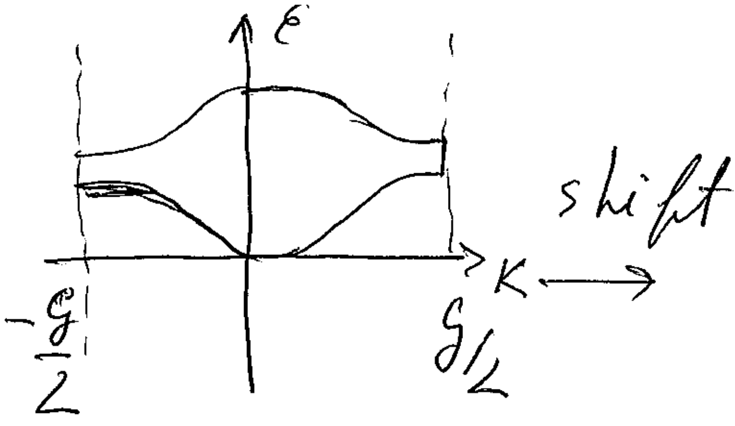
$$H = \begin{pmatrix} \varepsilon_k^{(0)} & W \\ W & \varepsilon_{k-g}^{(0)} \end{pmatrix} \quad , \text{ set } \hbar = 1$$

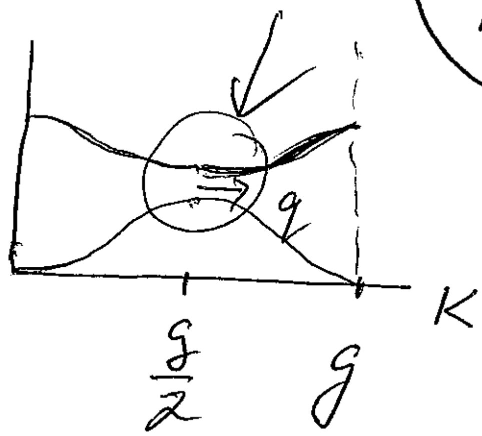
Near boundary of BZ

$$k = \frac{g}{2} + q, \quad q \ll g$$

$$\varepsilon_k^{(0)} = \frac{1}{2m}\left(\frac{g}{2} + q\right)^2 \approx \frac{g^2}{8m} + \frac{gq}{2m}$$

$$\varepsilon_{k-g}^{(0)} = \frac{1}{2m}\left(-\frac{g}{2} + q\right)^2 \approx \frac{g^2}{8m} - \frac{gq}{2m}$$





$$K = \frac{g}{2} + q$$

The Hamiltonian is transformed to

$$H \approx \frac{g^2}{2m} + \begin{pmatrix} vq & w \\ w & -vq \end{pmatrix} = \frac{g^2}{2m} + vq\sigma_z + w\sigma_x$$

$$v = \frac{g}{2m}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} -$$

- Pauli matrixes corresponding to pseudospin 1/2

Eigenenergies are

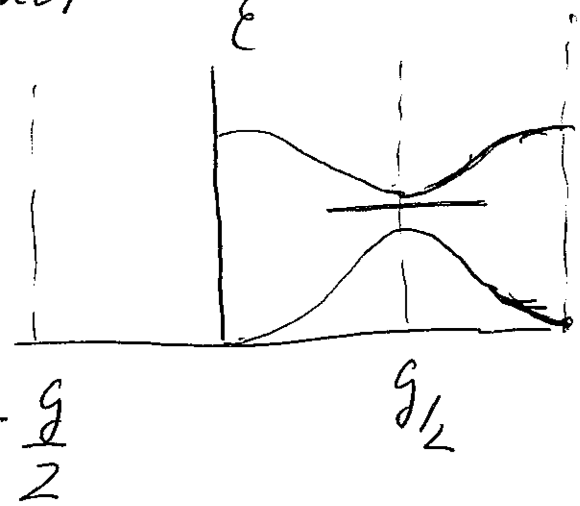
$$\varepsilon_q^{(\pm)} = \frac{g^2}{2m} \pm \sqrt{v^2q^2 + w^2}$$

They describe upper and lower branches of the dispersion, see Fig.

Consider crystal with edge

$$U(x) = \begin{cases} \infty, & x < 0 \\ 2w\cos gx, & x > 0 \end{cases}$$

We look for a surface state inside the forbidden band



$$\boxed{q = k - \frac{g}{2} \to -i\frac{\partial}{\partial x}}$$

$$h = H - \frac{g^2}{2m} = \begin{pmatrix} -iv\frac{\partial}{\partial x} & w \\ w & iv\frac{\partial}{\partial x} \end{pmatrix}$$

$$\psi = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} e^{-\lambda x}$$

$$h\psi = E\psi$$

$$\begin{pmatrix} iv\lambda - E & w \\ w & -iv\lambda - E \end{pmatrix}\begin{pmatrix}\alpha \\ \beta\end{pmatrix} = 0$$

$$E^2 + v^2\lambda^2 - w^2 = 0 \Rightarrow E = \pm\sqrt{w^2 - v^2\lambda^2}$$

parametrization in terms of φ

$$\begin{cases} E = w\sin\varphi \\ v\lambda = w\cos\varphi > 0 \end{cases} \qquad -\frac{\pi}{2} < \varphi < \frac{\pi}{2}$$

$$\begin{pmatrix} ie^{i\varphi} & 1 \\ 1 & -ie^{i\varphi} \end{pmatrix}\begin{pmatrix}\alpha \\ \beta\end{pmatrix} = 0 \Rightarrow \boxed{\beta = -ie^{i\varphi}\alpha}$$

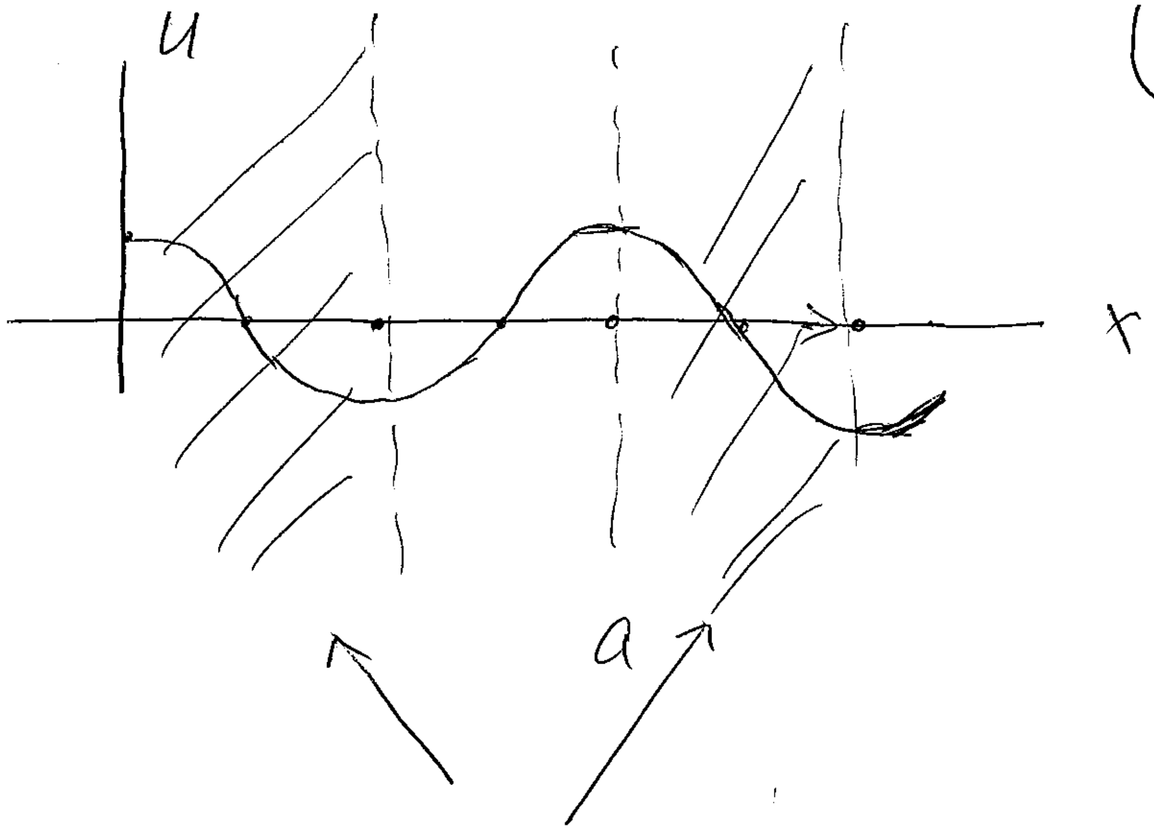
$$\psi(x) = \left(\alpha e^{i\frac{G}{2}x} + \beta e^{-i\frac{G}{2}x}\right)e^{-\lambda x}$$

infinite wall at $x = b \Rightarrow \psi(b) = 0$

$$\psi(b) = \alpha e^{i\frac{G}{2}b}\underbrace{\left[1 - ie^{i\varphi - iGb}\right]}_{=0}e^{-\lambda b} = 0$$

$$\boxed{\varphi = -\frac{\pi}{2} + Gb} = -\frac{\pi}{2} + 2\pi\frac{b}{a}$$

There is a solution only if $\boxed{0 < b < \frac{a}{2}}$



allowed regions to cut the crystal and to get a surface (edge) state

Lessons

1) To get a surface state one needs to cut crystall at a special position

2) The surface state can have spin up or spin down.