Comment - For free electrons the energy eigenstates are specified ~~for~~ by a wave vector $\vec{k}$ that can take a value anywhere in k-space. For an electron in a periodic potential, we said eigenstates should be specified by a discrete band index n and a crystal momentum $\vec{q}$ that must lie only in the 1st BZ. But if we take the problem of the periodic potential and let $U \to 0$, we recover the free electron case. So how can these two ways of labeling eigenstates both be valid?

Answer: We can represent even free electron states using the band index n and $\vec{q}$ in 1st BZ as quantum numbers. For any $\vec{k}$, anywhere in k-space, we can always write $\vec{k} = \vec{q} + \vec{K}$ where $\vec{K}$ is a unique R.L. vector closest to $\vec{k}$ and $\vec{q}$ therefore must be in the 1st B.Z. This follows from the equivalence of all points in the R.L. (since it is a Bravais lattice) and from the definition of the 1st BZ as the set of wave vectors closer to the origin than to any other $\vec{K}$ in the R.L.

Then for any $\vec{k} = \vec{q} + \vec{K}$ in the n^{th} Brillouin Zone

write $E^0(\vec{k}) = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2(\vec{q}+\vec{K})}{2m} = E_n(\vec{q})$

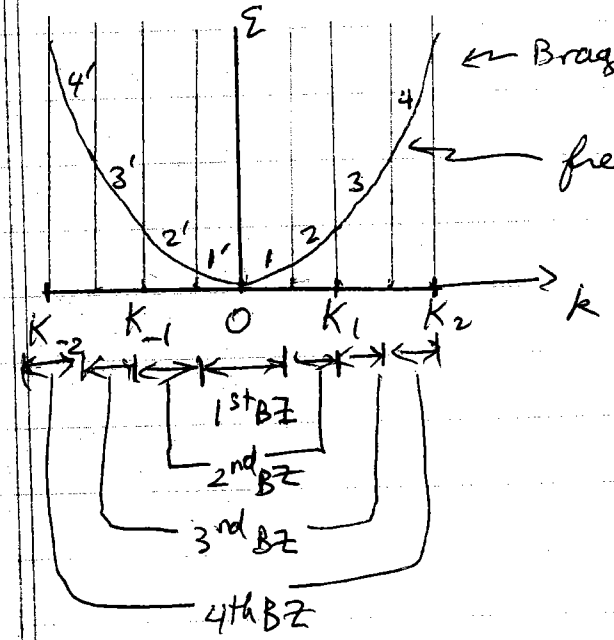
↑ energy at crystal momentum $\vec{q}$ in band index "n"

Thus the band index gives the B.Z. in which the corresponding free electron wavevector $\vec{k}$ lies.

Ex: in a 1D B.L. of lattice constant a

R.L. vectors are $K_n = \left(\frac{2\pi}{a}\right) n$, $n = 0, \pm 1, \pm 2, \ldots$

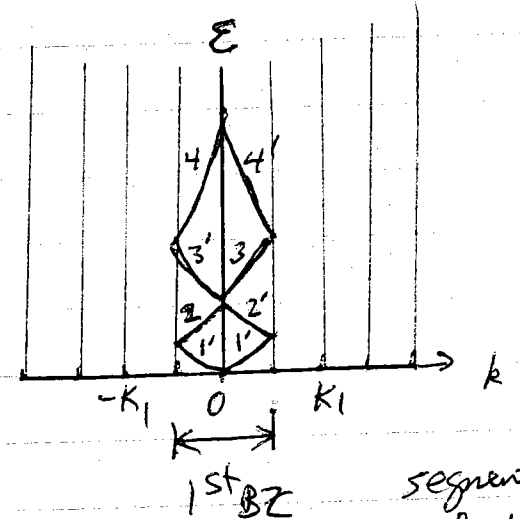
Bragg planes at $k = \frac{K_n}{2} = \left(\frac{\pi}{a}\right) n$



← Bragg planes

← free electron $E^0(k)$

can translate the section of curve in n^{th} BZ back into 1st BZ by subtracting appropriate K from $\vec{k}$



representing free electron states by $\vec{q}$ in 1st BZ.

Integers label corresponding sections of the curves in the two equivalent representations

segments of curve labeled n or n came from the n BZ of free electron

Comments:

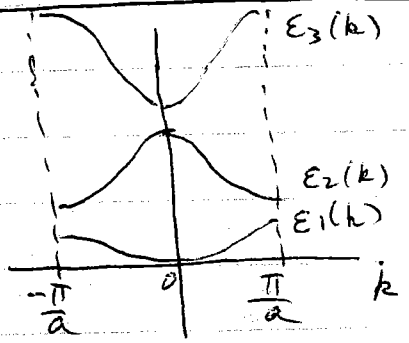
① Because $\vec{k}$ enters the matrix equation as a parameter via the terms $\varepsilon^{\circ}_{\vec{k}+\vec{K}}$, we expect that the eigenvalues $\varepsilon_n(\vec{k})$ are smooth continuous functions of $\vec{k}$.

② Because $\varepsilon_n(\vec{k})$ is periodic in $\vec{k}$, $\varepsilon_n(\vec{k}+\vec{K}) = \varepsilon_n(\vec{k})$, we must have that $\varepsilon_n(\vec{k})$ has a maximum and a minimum and varies continuously between them. This is why $\varepsilon_n(\vec{k})$ is refered to as an energy band

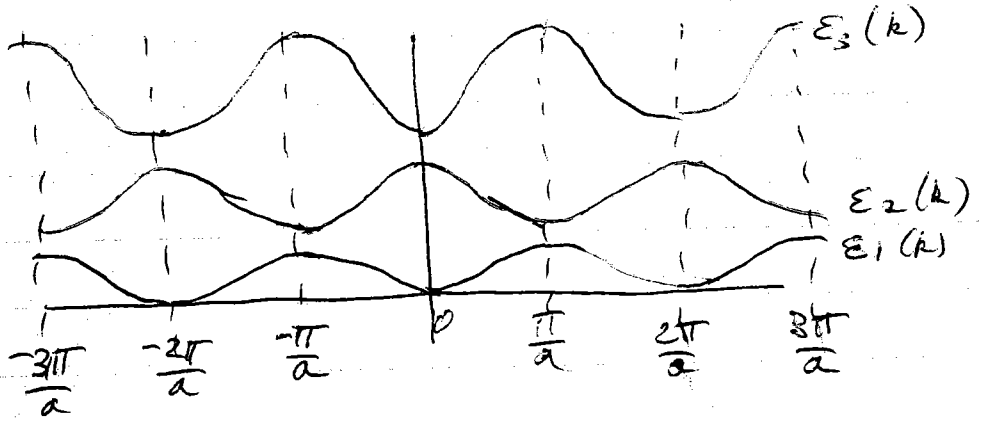
③ Since $\psi_{\vec{k}n}(\vec{r}) = \sum_{\vec{K}} e^{i(\vec{k}-\vec{K})\cdot\vec{r}} c_{\vec{k}-\vec{K}}$ is no longer a pure plane wave, $\psi_{\vec{k}n}$ is NOT an eigenstate of momentum. This is reasonable since with the periodic potential turned on the system no longer has translational invariance. However the system does have invariance in translations by B.L. vectors $\vec{R}$. This is why $\psi_{\vec{k}n}$ mixes only wavevectors related to $\vec{k}$ by $\vec{k}' = \vec{k} - \vec{K}$ for $\vec{K}$ in R.L. Because of this difference, $\vec{k}$ is called the "crystal momentum" — it is not the true momentum. In collisions, the true momentum of an electron is only "conserved" modulus a R.L. vector $\vec{K}$.

④ Because $\psi_{kn}(\vec{r})$ and $\varepsilon_n(\vec{k})$ are periodic in k-space, the states $\vec{k}$ and $\vec{k}+\vec{K}$ are not physically different. Nevertheless it is sometimes convenient to represent states by a $\vec{k}$ that is not in the 1st BZ. This is most often done when one wants to make closer analogy to free electrons. One therefore has three commonly used schemes for representing band structure. We illustrate these in 1D

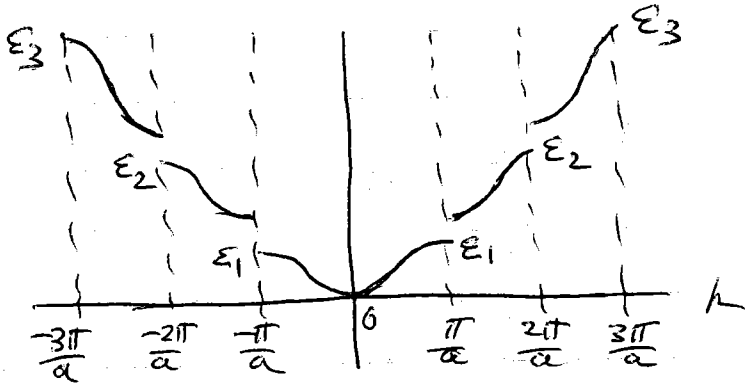
Reduced zone scheme : restrict $\vec{k}$ to 1st BZ for all energy bands ∩



Repeated zone scheme : show all values of $\vec{k}$, with $\varepsilon_n(\vec{k})$ periodic in $\vec{k}$



Extended Zone scheme : show energy band n using $\vec{k}$ vectors in n^{th} BZ.



Note: However one represents the band structure, each band contains only N distinct allowed values of $\vec{k}$ consistent with the Born-von Karman boundary conditions. ⇒ each band can contain 2N electron states (2 for spin ↑ or ↓)

N = # primitive cells in crystal (= # ions if we have a simple BL and not a lattice with a basis)

(5) If one computes the expectation of velocity in a Bloch electron state, one finds

$$\vec{v}_n(\vec{k}) = \langle \psi_{nk} | \frac{\hbar}{i}\vec{\nabla} | \psi_{nk} \rangle = \int d^3r\, \psi^*_{nk}(\vec{r}) \frac{\hbar}{i}\vec{\nabla} \psi_{nk}(\vec{r})$$

$$= \frac{1}{\hbar}\vec{\nabla}_k \varepsilon_n(\vec{k})$$

← looks just like group velocity, but is exact result for expectation value of $\vec{v}$ in eigenstate

↑ gradient with respect to $\vec{k}$

proof follows

Main point is that the eigenstates of an electron in a periodic potential, although they are not eigenstates of momentum, nevertheless have a

well defined, generally finite, value for their average velocity. Therefore, in spite of the interaction of the electron with the periodic potential, the electron in its eigenstate moves with a steady velocity even if no net force (for example from an electric field) is applied to it. This is contrast to Drude's classical picture in which collisions between the electron ad the ions served to randomize any initial electron velocity on the collision time scale τ. The reason Drude's picture does not hold is because of the wave nature of the electron and its phase coherent scattering off the ions.

A nonperturbative proof for $\boxed{\vec{v}_{\vec{k}} = \frac{1}{\hbar}\frac{\partial \varepsilon_{\vec{k}}}{\partial \vec{k}}}$

The Bloch function is known to be of the form [ignore band index]

$$\psi_{\vec{k}}(\vec{x}) = e^{i\vec{k}\cdot\vec{x}}\, u_{\vec{k}}(\vec{x})$$

where $u_{\vec{k}}(\vec{x})$ is periodic in the Bravais lattice and satisfies

$$H_{\vec{k}}\, u_{\vec{k}} = \varepsilon_{\vec{k}}\, u_{\vec{k}} \qquad (1)$$

where

$$H_{\vec{k}} = \frac{\hbar^2}{2m}\left(\frac{1}{i}\nabla + \vec{k}\right)^2 + U(\vec{x}) \qquad (2)$$

Note that $H_{\vec{k}}$ is Hermitian for any $\vec{k}$.

Suppose $u_{\vec{k}}(\vec{x})$ is normalized as

$$\int_{\Omega} |u_{\vec{k}}|^2 d^3\vec{x} = 1 \qquad (3)$$

where Ω is a primitive cell

From (2) we have

$$\frac{\partial u^*_{\vec{k}}}{\partial \vec{k}}\, H_{\vec{k}}\, u_{\vec{k}} = \varepsilon_{\vec{k}}\, \frac{\partial u^*_{\vec{k}}}{\partial \vec{k}}\, u_{\vec{k}} \qquad (4)$$

Taking complex conjugate of eq. (4) yields [using $H^*_{\vec{k}} = H_{-\vec{k}}$]

$$\frac{\partial u_{\vec{k}}}{\partial \vec{k}}\, H_{-\vec{k}}\, u^*_{\vec{k}} = \varepsilon_{\vec{k}}\, \frac{\partial u_{\vec{k}}}{\partial \vec{k}}\, u^*_{\vec{k}} \qquad (5)$$

Adding (4) and (5) and integrating over the primitive cell Ω we get

$$\varepsilon_{\vec{k}}\, \frac{\partial}{\partial \vec{k}} \int_{\Omega} |u_{\vec{k}}|^2 d^3\vec{x} = \int_{\Omega} \left[\frac{\partial u^*_{\vec{k}}}{\partial \vec{k}}\, H_{\vec{k}}\, u_{\vec{k}} + \frac{\partial u_{\vec{k}}}{\partial \vec{k}}\, H_{-\vec{k}}\, u^*_{\vec{k}}\right] d^3\vec{x}$$

(6)

Since $H_{-\vec{k}}$ is Hermitian,

$$\int_{\Omega} \frac{\partial u_{\vec{k}}}{\partial \vec{k}} H_{-\vec{k}} u_{\vec{k}}^{*} \, d^3\vec{x} = \left[\int_{\Omega} u_{\vec{k}} H_{-\vec{k}} \frac{\partial u_{\vec{k}}^{*}}{\partial \vec{k}} \, d^3\vec{x} \right]^{*}$$

$$= \int_{\Omega} u_{\vec{k}}^{*} H_{\vec{k}} \frac{\partial u_{\vec{k}}}{\partial \vec{k}} \, d^3\vec{x} \qquad (7)$$

Thus, (3), (6) and (7) together imply

$$\int_{\Omega} \left[\frac{\partial u_{\vec{k}}^{*}}{\partial \vec{k}} H_{\vec{k}} u_{\vec{k}} + u_{\vec{k}}^{*} H_{\vec{k}} \frac{\partial u_{\vec{k}}}{\partial \vec{k}} \right] d^3\vec{x} = 0 \qquad (8)$$

However, (1) and (3) directly imply

$$\mathcal{E}_{\vec{k}} = \int_{\Omega} u_{\vec{k}}^{*} H_{\vec{k}} u_{\vec{k}} \, d^3\vec{x} \qquad (9)$$

Differentiate eq. (7) with respect to $\vec{k}$ and exploit (8) we have

$$\frac{\partial \mathcal{E}_{\vec{k}}}{\partial \vec{k}} = \int_{\Omega} u_{\vec{k}}^{*} \frac{\partial H_{\vec{k}}}{\partial \vec{k}} u_{\vec{k}} \, d^3\vec{x}$$

$$= \frac{\hbar^2}{m} \int_{\Omega} u_{\vec{k}}^{*} \left(\frac{1}{i} \nabla + \vec{k} \right) u_{\vec{k}} \, d^3\vec{x}$$

or

$$\frac{1}{\hbar} \frac{\partial \mathcal{E}_{\vec{k}}}{\partial \vec{k}} = \frac{1}{m} \int_{\Omega} \psi_{\vec{k}}^{*} \left(\frac{\hbar}{i} \nabla \right) \psi_{\vec{k}} \, d^3\vec{x} = \vec{V}_{\vec{k}}$$

Energy gaps in the Weak Potential Approximation

If U is a weak perturbation

(1) Consider $\vec{k}$, not necessarily in 1st BZ, such that $\vec{k}$ is NOT near any Bragg planes on the energy scale U

i.e. $|\varepsilon_k^0 - \varepsilon_{k+K}^0| \gg U$ for any K in R.L.

Then $c_k \sim o(1)$ while $c_{k-K} \sim o(U)$
and $|\varepsilon_k - \varepsilon_k^0| \sim o(U^2)$

From Schrodinger Eqn in k-space

$$(*) \quad (\varepsilon - \varepsilon_k^0)\, c_k = \sum_{K \neq 0} U_K\, c_{k-K}$$

$$c_k = \sum_{K \neq 0} \frac{U_K\, c_{k-K}}{(\varepsilon - \varepsilon_k^0)} \sim o(1) \text{ if } c_{k-K} \sim o(U) \text{ and } (\varepsilon - \varepsilon_k^0) \sim o(U)$$

$$c_{k-K} = \sum_{K' \neq K} \frac{U_{K'-K}\, c_{k-K'}}{\varepsilon - \varepsilon_{k-K}^0}$$

$$(**) \quad \sim \frac{U_{-K}\, c_k}{\varepsilon - \varepsilon_{k-K}^0} \sim o(U) \text{ if } c_k \sim o(1) \text{ and } (\varepsilon - \varepsilon_{k-K}^0) \sim o(1)$$

↑ true since $\varepsilon \sim \varepsilon_k^0$ and $|\varepsilon_k^0 - \varepsilon_{k-K}^0| \gg U$

substitute (**) into (*) to get shift in energy

$$(\varepsilon - \varepsilon_k^0)\, c_k = \sum_{K \neq 0} \frac{U_K\, U_{-K}\, c_k}{\varepsilon - \varepsilon_{k-K}^0}$$

$$(\varepsilon - \varepsilon_k^0) = \sum_{K \neq 0} |U_K|^2 / (\varepsilon_k^0 - \varepsilon_{k-K}^0) + o(U^3)$$

(2) Now consider $\vec{k}$ that lies near to a Bragg plane on the energy scale U. If the Bragg plane bisects $\vec{K}_0$, then

$$|\varepsilon_k^0 - \varepsilon_{k-K_0}^0| \lesssim U$$

Now $$(\varepsilon - \varepsilon_k^0) c_k = U_{K_0} c_{k-K_0} + \sum_{k \neq 0, K_0} U_k c_{k-K}$$

$$(\varepsilon - \varepsilon_{k-K_0}^0) c_{k-K_0} = U_{-K_0} c_k + \sum_{K' \neq 0, K_0} U_{K'-K_0} c_{k-K'}$$

$$(\varepsilon - \varepsilon_{k-K}^0) c_{k-K} = U_{-K} c_k + U_{K-K_0} c_{k-K_0} + \sum_{K' \neq 0, K_0} U_{K'-K} c_{k-K'}$$

Above is consistent with $c_k, c_{k-K_0} \sim O(\frac{1}{\varepsilon})$, $c_{k-K} \sim O(U)$

$(\varepsilon - \varepsilon_k^0), (\varepsilon - \varepsilon_{k-K_0}^0) \sim O(U)$

To lowest order the above reduces to the pair of equations

$$\begin{pmatrix} \varepsilon - \varepsilon_k^0 & -U_{K_0} \\ -U_{-K_0} & \varepsilon - \varepsilon_{k-K_0}^0 \end{pmatrix} \begin{pmatrix} c_k \\ c_{k-K_0} \end{pmatrix} = 0$$

will have a non trivial solution only when the determinant of the matrix vanishes

$$\Rightarrow \quad (\varepsilon - \varepsilon_k^0)(\varepsilon - \varepsilon_{k-K_0}^0) = |U_{K_0}|^2$$

$$\varepsilon^2 - \varepsilon(\varepsilon_k^0 + \varepsilon_{k-K_0}^0) + \varepsilon_k^0 \varepsilon_{k-K_0}^0 - |U_{K_0}|^2 = 0$$

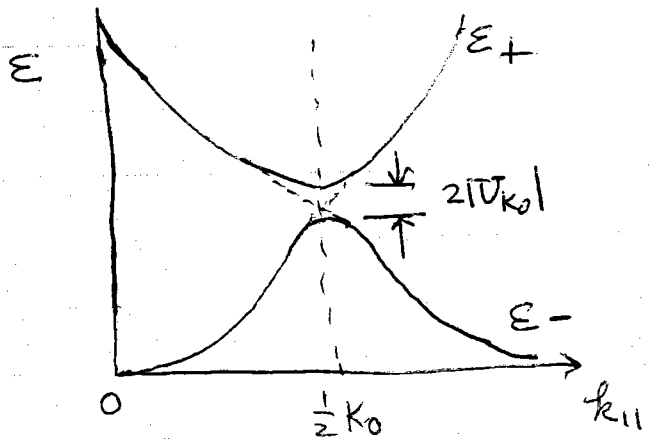
$$\varepsilon_\pm = \frac{\varepsilon_k^0 + \varepsilon_{k-K_0}^0}{2} \pm \sqrt{\frac{(\varepsilon_k^0 + \varepsilon_{k-K_0}^0)^2}{4} - \varepsilon_k^0 \varepsilon_{k-K_0}^0 + |U_K|^2}$$

$$(*) \quad \varepsilon_\pm = \frac{\varepsilon_k^0 + \varepsilon_{k-K_0}^0}{2} \pm \sqrt{\left(\frac{\varepsilon_k^0 - \varepsilon_{k-K_0}^0}{2}\right)^2 + |U_{K_0}|^2}$$

when $\vec{k}$ is exactly on a Bragg plane, $\varepsilon_k^0 = \varepsilon_{k-K_0}^0$

$$\varepsilon_\pm = \varepsilon_k^0 \pm |U_{K_0}|$$

gives gap $\Delta\varepsilon = \varepsilon_+ - \varepsilon_- = 2|U_{K_0}|$ at Bragg plane



energy dispersion relation from (*)

$$k_\parallel = \vec{k} \cdot \hat{K}_0$$

From (*) one can show that $\vec{v}_k = \frac{1}{\hbar}\frac{\partial \varepsilon}{\partial \vec{k}}$ has a vanishing component in the direction of $\vec{K}_0$ when ~~$\vec{k}$~~ $\vec{k}$ lies exactly on the Bragg plane - reasonable as $\vec{k}$ on Bragg plane $\Rightarrow$ we have a standing wave in $\hat{K}_0$ direction.

The preceding arguments, a bit more systematically:

Consider the effect of the periodic potential on the free electron state with wavevector $\vec{k}$ and energy ε_k^0. The potential will mix in plane wave states with $\vec{k}-\vec{K}$, $\vec{K}$ in R.L., and shift the energy eigenvalue from ε_k^0 to a new ε. For weak $U(\vec{r})$, ε is close to ε_k^0. Schrodinger's equation for the Fourier coefficients is

$$(*) \quad (\varepsilon - \varepsilon^0_{k-K})\, c_{k-K} = \sum_{K' \neq K} U_{K'-K}\, c_{k-K'}$$

The right hand side can be no bigger than $O(U)$ (since by normalization we will assume all $|c_{k-K}| \leq 1$)
$\Rightarrow$ the left hand side can be no bigger than $O(U)$.

(1) If $\vec{k}$ is not near any Bragg plane on energy scale of $O(U)$, ie $|\varepsilon^0_k - \varepsilon^0_{k-K}| \gg U$ for all $\vec{K} \neq 0$ in R.L. then it is only $(\varepsilon - \varepsilon^0_k)$ that can be small; $(\varepsilon - \varepsilon^0_{k-K})$ will be bigger than $O(U)$ for all $\vec{K} \neq 0$.
$\Rightarrow$ we must have $c_{k-K} \sim O(U)$ for all $\vec{K} \neq 0$.
Since we start with the free electron state at $\vec{k}$, then $c_k \sim O(1)$.

From above eqn (*) setting $\vec{K} = 0$

$$(\varepsilon - \varepsilon^0_k)\, c_k = \sum_{K' \neq 0} U_{K'}\, c_{k-K'}$$

If $c_{k-K'} \sim O(U)$ and $c_k \sim O(1)$ $\Rightarrow (\varepsilon - \varepsilon^0_k) \sim O(U^2)$

so (1) when $\vec{k}$ is not near any Bragg plane
then $c_k \sim O(1)$, $c_{k-K} \sim O(U)$, $(\varepsilon - \varepsilon_k^0) \sim O(U^2)$

periodic potential has relatively little effect on the free electron state.

(2) Now suppose $\vec{k}$ is near the Bragg plane that bisects the reciprocal lattice vector $\vec{K}_0$, but $\vec{k}$ is not near any of the Bragg planes, i.e.

$$|\varepsilon_k^0 - \varepsilon_{k-K_0}^0| \lesssim U \quad \text{but} \quad |\varepsilon_k^0 - \varepsilon_{k-K}^0| \gg U \text{ for all } \vec{K} \neq 0, \vec{K}_0.$$

From (*) we can write

$$(1)\quad (\varepsilon - \varepsilon_k^0)\, c_k = U_{K_0}\, c_{k-K_0} + \sum_{K' \neq 0, K_0} U_{K'}\, c_{k-K'}$$

$$(2)\quad (\varepsilon - \varepsilon_{k-K_0}^0)\, c_{k-K_0} = U_{-K_0}\, c_k + \sum_{K' \neq 0, K_0} U_{K'-K_0}\, c_{k-K'}$$

$\vec{K} \neq 0, \vec{K}_0$ (3)
$$(\varepsilon - \varepsilon_{k-K}^0)\, c_{k-K} = U_{-K_0}\, c_k + U_{K_0-K}\, c_{k-K_0} + \sum_{K' \neq 0, K_0} U_{K'-K}\, c_{k-K'}$$

Now we can say that $(\varepsilon - \varepsilon_{k-K}^0)$ must be greater than $O(U)$ for $\vec{K} \neq 0, K_0$, so (3) $\Rightarrow$ c_{k-K} must be no bigger than $O(U)$. So the last term on the right in all three equations above is no bigger than $O(U^2)$. Next, $c_k \sim O(1)$ since we start with free electron of wave vector $\vec{k}$, so from (2)

we must ~~can't~~ conclude that $(\varepsilon - \varepsilon^0_{k-K_0})\, c_{k-K_0} \sim O(U)$,

But $(\varepsilon - \varepsilon^0_{k-K_0})$ should not be bigger than $O(U)$ (since the difference is due to the potential U) and c_{k-K_0} ~~should not~~ cannot be bigger than $O(1)$.

$\Rightarrow$ only possibility is $c_{k-K_0} \sim O(1)$ and $(\varepsilon - \varepsilon^0_{k-K_0}) \sim O(U)$. $\Rightarrow (\varepsilon - \varepsilon^0_k) \sim O(U)$ also.

(2) So the above three equations imply

$c_{k-K} \sim O(U)$ for $\bar{K} \neq 0, \bar{K}_0$

$c_{k-K_0} \sim c_k \sim O(1)$

$(\varepsilon - \varepsilon^0_{k-K})$ ~ large when $\bar{K} \neq 0, \bar{K}_0$

$(\varepsilon - \varepsilon^0_k), (\varepsilon - \varepsilon^0_{k-K_0}) \sim O(U)$ ← compare to previous case when not near any Bragg plane – then the energy shift was $O(U^2)$.

To leading order, the above three equations reduce to two equations for c_k and c_{k-K_0}

$$\begin{cases} (\varepsilon - \varepsilon^0_k)\, c_k = U_{K_0}\, c_{k-K_0} \\ (\varepsilon - \varepsilon^0_{k-K_0})\, c_{k-K_0} = U_{-K_0}\, c_k \end{cases}$$

If $\vec{k}$ is near ~~m~~ n Bragg planes, we wind up with $n+1$ equations for c_k, c_{k+K_1}, c_{k+K_2}, ---, c_{k+K_n}.

We can also consider the eigenvectors. ~~Exactly on~~ When $\vec{k}$ is exactly on a Bragg plane and $\varepsilon_\pm = \varepsilon_k^0 \pm |U_{k_0}|$ with $\varepsilon_k^0 = \varepsilon_{k+k_0}^0$ the matrix equation for the two degenerate states is:

$$\begin{pmatrix} \pm|U_{k_0}| & -U_{k_0} \\ -U_{-k_0} & \pm|U_{k_0}| \end{pmatrix} \begin{pmatrix} c_k \\ c_{k-k_0} \end{pmatrix} = 0$$

write $U_{k_0} = |U_{k_0}| e^{i\varphi}$ φ is phase of complex U_{k_0}
Above is then

$$|U_{k_0}| \begin{pmatrix} \pm 1 & -e^{i\varphi} \\ -e^{-i\varphi} & \pm 1 \end{pmatrix} \begin{pmatrix} c_k \\ c_{k-k_0} \end{pmatrix} = 0$$

$$\Rightarrow \quad \pm c_{k-k_0} = e^{-i\varphi} c_k$$
$$c_{k-k_0} = \pm e^{-i\varphi} c_k$$

so the two eigenvectors are $\sim \begin{pmatrix} 1 \\ e^{-i\varphi} \end{pmatrix}$ and $\begin{pmatrix} 1 \\ -e^{-i\varphi} \end{pmatrix} = \begin{pmatrix} c_k \\ c_{k-k_0} \end{pmatrix}$
These are orthonormal as necessary

$$\begin{pmatrix} c_k^* & c_{k-k_0}^* \end{pmatrix} \begin{pmatrix} c_k \\ c_{k-k_0} \end{pmatrix} = 1 - e^{i\varphi} e^{-i\varphi} = 0$$

and correspond to wavefunctions as we saw in our introductory discussion

$$\psi_1 = e^{i\vec{k}\cdot\vec{r}} + e^{-i\varphi} e^{i(\vec{k}-\vec{k}_0)\cdot\vec{r}}$$
$$\psi_2 = e^{i\vec{k}\cdot\vec{r}} - e^{-i\varphi} e^{i(\vec{k}-\vec{k}_0)\cdot\vec{r}}$$

ψ_2 has π phase shift with respect to ψ_1

Velocity and constant energy surface at a Bragg plane

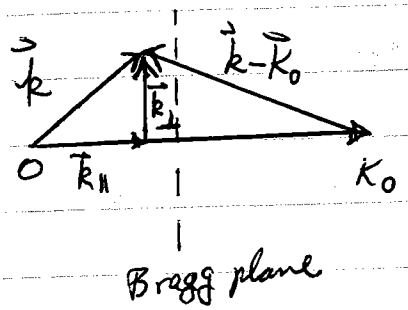
$$\vec{v}_n(\vec{k}) = \frac{1}{\hbar}\frac{\partial \mathcal{E}_n(\vec{k})}{\partial \vec{k}}$$

$\Rightarrow$ normal vector to a constant energy surface, $\mathcal{E}_n(\vec{k}) = \mathcal{E}_0$ constant, points in direction of $\vec{v}_n(\vec{k})$.

In the weak potential approximation for $\vec{k}$ near a Bragg plane bisecting R.L. vector $\vec{K}_0$ we had

$$\mathcal{E}_\pm = \frac{\mathcal{E}^0_k + \mathcal{E}^0_{k-K_0}}{2} \pm \sqrt{\left(\frac{\mathcal{E}^0_k - \mathcal{E}^0_{k-K_0}}{2}\right)^2 + |U_{K_0}|^2}$$

Write $\vec{k} = \vec{k}_\parallel + \vec{k}_\perp$ $\rightarrow$ $\vec{k} - \vec{K}_0 = \vec{k}_\parallel - \vec{K}_0 + \vec{k}_\perp$ with $\vec{k}_\parallel$ the component of $\vec{k}$ parallel to $\vec{K}_0$



We can then write $\mathcal{E}_\pm$ as functions of $k_\parallel$ and $k_\perp$

$$\mathcal{E}_\pm = \frac{\hbar^2}{2m}\frac{(k_\parallel^2 + k_\perp^2) + (k_\parallel^2 + K_0^2 - 2k_\parallel K_0 + k_\perp^2)}{2} \pm \sqrt{\left(\frac{\hbar^2}{2m}\right)^2\left(\frac{K_0^2 - 2k_\parallel K_0}{2}\right)^2 + |U_{K_0}|^2}$$

one can then show that

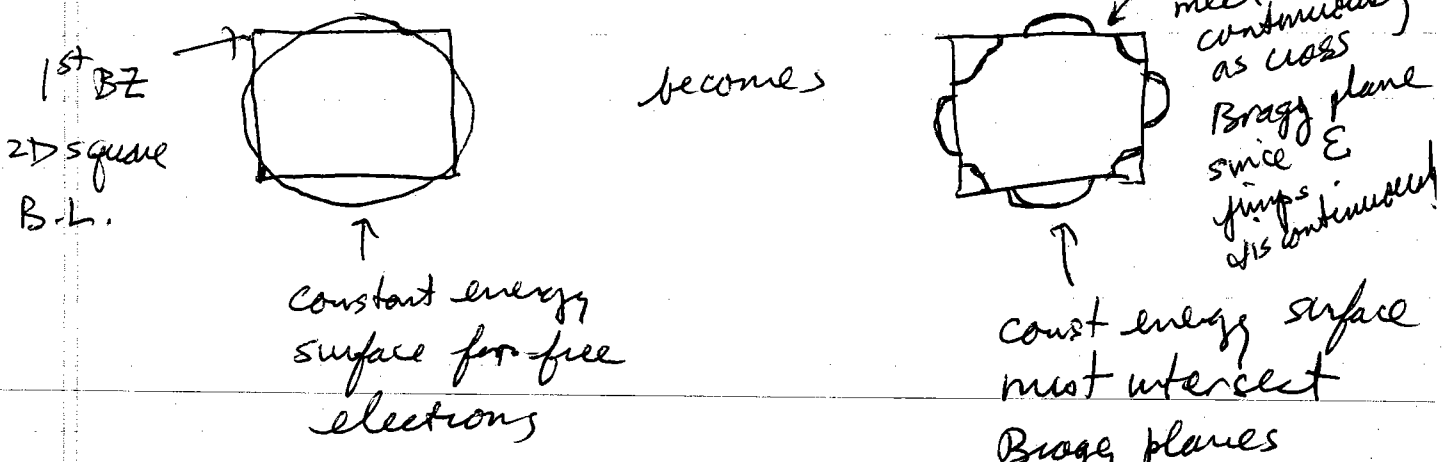
$$\frac{\partial \mathcal{E}_\pm}{\partial k_{11}} \to 0 \quad \text{as} \quad k_{11} \to \frac{K_0}{2}$$, ie when $\vec{k}$ lies exactly on the Bragg plane.

$$\frac{\partial \mathcal{E}_\pm}{\partial k_{11}} = \frac{\hbar^2}{2m}(2k_{11} - K_0) \pm \frac{\frac{1}{2}\left(\frac{\hbar^2}{2m}\right)^2 (K_0^2 - 2k_{11}K_0)(-2k_{11})}{\sqrt{\left(\frac{\hbar^2}{2m}\right)^2 \left(\frac{K_0^2 - 2k_{11}K_0}{2}\right)^2 + |U_{K_0}|^2}}$$

$= 0$ when $k_{11} = \frac{K_0}{2}$

$\Rightarrow$ velocity of electron exactly at Bragg plane is always in a direction lying with the Bragg plane – the component of $\vec{v}_n(k)$ parallel to $\vec{K}_0$, ie: perpendicular to the Bragg plane, vanishes

$\Rightarrow$ constant energy surface must intersect Bragg plane perpendicularly



* these results are only for the weak potential approx