Electron Tunneling and Energy Bands

a) An electron of energy E coming from the left of the simple barrier $v(x)$ can be represented by a wave

$$\psi_L(x) = \begin{cases} e^{ikx} + r_L e^{-ikx} & x \leq -a/2 \\ t_L e^{ikx} & x \geq a/2 \end{cases}$$

k being given by the relation $E = \frac{\hbar^2 k^2}{2m}$. An electron coming from the right can be represented by a wave

$$\psi_R(x) = \begin{cases} e^{-ikx} + r_R e^{ikx} & x \geq a/2 \\ t_R e^{-ikx} & x \leq -a/2 \end{cases}$$

If $v(x)$ is not symmetrical to an axes, the reflection and transmission coefficients r, t for the two cases are different. The general wave function for these regions is a linear combination of $\psi_L(x)$ and $\psi_R(x)$:

$$\psi(x) = A\psi_L(x) + B\psi_R(x)$$

A and B being real constants.

Within the barrier $-\frac{a}{2} \leq x \leq \frac{a}{2}$, the wave function

satisfies the one-dimensional Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi(x) = E\,\psi(x)$$

b) for the total periodic potential of the crystal, $V(x)$, the Hamiltonian within the region $-\frac{a}{2} \leq x \leq \frac{a}{2}$ is identical with that for a simple barrier so we can make use of the Bloch theorem to find the general solution of the Schrödinger equation

$$\psi(x+a) = e^{ika}\,\psi(x)$$

with

$$\psi(x) = A\,\psi_L(x) + B\,\psi_R(x)$$

On differentiation with respect to x

$$\frac{d}{dx}\psi(x+a) = e^{ika}\,\frac{d}{dx}\psi(x).$$

At $x = -a/2$

$$A\,\psi_L\left(\frac{a}{2}\right) + B\,\psi_R\left(\frac{a}{2}\right) = e^{ika}\left[A\,\psi_L\left(-\frac{a}{2}\right) + B\,\psi_R\left(-\frac{a}{2}\right)\right]$$

$$A\,\psi_L'\left(\frac{a}{2}\right) + B\,\psi_R'\left(\frac{a}{2}\right) = e^{ika}\left[A\,\psi_L'\left(-\frac{a}{2}\right) + B\,\psi_R'\left(-\frac{a}{2}\right)\right]$$

or

$$A\left[t_L\beta - \alpha(1+r_L\beta)\right] + B\left(1 + r_R\beta - t_R\alpha\beta\right) = 0$$

$$A\left[t_L\beta - \alpha(1-r_L\beta)\right] + B\left(-1 + r_R\beta + t_R\alpha\beta\right) = 0$$

with

$$\alpha \equiv e^{ika} \quad ; \quad \beta \equiv e^{ika}.$$

Taking the sum and difference of the last two equations

$$(t_L\beta - \alpha)A + r_R\beta B = 0$$

$$-r_L\alpha\beta A + (1 - t_R\alpha\beta)B = 0$$

For nontrivial solutions of A, B, the determinant must vanish

$$(t_L t_R - r_L r_R)e^{ika} + e^{-ika} = t_L e^{-ika} + t_R e^{ika}.$$

This gives the relation between the kinetic energy of the electron $E - V = \frac{\hbar^2 k^2}{2m}$, and the wave vector k.

When the crystal is symmetric $\left(v(x) = v(-x)\right)$, which is usually the case,

$$r_L = r_R = r \quad ; \quad t_L = t_R = t$$

the above relation becomes

$$2t\cos(ka) = (t^2 - r^2)e^{ika} + e^{-ika}$$

For $v=0 \Rightarrow \begin{cases} \tau = 0 \\ \epsilon = 1 \end{cases}$ and we have

$$\cos(\kappa a) = \cos(\ell \kappa a)$$

that is $\kappa = \ell \kappa$

EXAMPLES OF CRYSTAL POTENTIAL

The crystal potential $V(x)$ can be written

$$V(x) = 2V_1 \left[1 - \cos G_1 x \right] \qquad G_1 \equiv 2\pi/a$$

$$= -V_1 e^{-iG_1 x} + 2V_1 - V_1 e^{iG_1 x} ,$$

which directly gives the fourier series of our periodic potential.

$$V_{-G_1} = -V_1 \quad ; \quad V_0 = 2V_1 \quad ; \quad V_{+G_1} = -V_1$$

In general,

$$V(x) = \sum_G V_G \, e^{iGx}$$

where the fourier coefficients V_G are related to $V(x)$ by the formula (see Ashcroft/Mermin eq. 8.32)

$$V_G = \frac{1}{2\pi/a} \int_{-a/2}^{+a/2} dx \, e^{-iGx} \, V(x)$$

The general central equation is

$$(\lambda_q - E) c_q + \sum_{G'} V_{G'} c_{q-G'} = 0 \quad ; \quad \lambda_q \equiv \frac{\hbar^2 q^2}{2m}$$

where q is the wave vector of the free electrons and the value extends in the whole k-space $-\infty < q < +\infty$.

If we restrict the k-space to the 1st Brillouin zone through the transformation

$$q = k - G ,$$

the central equation becomes

$$(\lambda_{k-G} - E)\, c_{k-G} + \sum_{G'} V_{G'-G}\, c_{k-G'}$$

For our specific potential the 5×5 block of the determinant of the coefficients is given by the five equations for $G = \pm 2G_1, \pm G_1, 0$.

For $G = -2G_1$ the central equation is

$$(\lambda_{k+2G_1} - E)\, c_{k+2G_1} + V_{-3G_1+2G_1}\, c_{k+3G_1} + V_{-2G_1+2G_1}\, c_{k+2G_1} + V_{-G_1+2G_1}\, c_{k+G_1}$$

For $G = -G_1$

$$(\lambda_{k+G_1} - E)\, c_{k+G_1} + V_{-2G_1+G_1}\, c_{k+2G_1} + V_{-G_1+G_1}\, c_{k+G_1} + V_{G_1}\, c_k$$

For $G = 0$

$$(\lambda_k - E)\, c_k + V_{-G_1}\, c_{k+G_1} + V_0\, c_k + V_{G_1}\, c_{k-G_1}$$

And similar for $G = G_1, 2G_1$

The 5×5 matrix is (with $-\varepsilon \equiv -E + 2V_1$)

$$\begin{pmatrix}
(\lambda_{u-2G_1} - \varepsilon) & -V_1 & 0 & 0 & 0 \\
-V_1 & \lambda_{u-G_1} - \varepsilon & -V_1 & 0 & 0 \\
0 & -V_1 & \lambda_u - \varepsilon & -V_1 & 0 \\
0 & 0 & -V_1 & \lambda_{u+G_1} - \varepsilon & -V_1 \\
0 & 0 & 0 & -V_1 & \lambda_{u+2G_1} - \varepsilon
\end{pmatrix}$$

b) for $u = 0$

$$\lambda_{u-2G_1} = \lambda_{u+2G_1} = \frac{\hbar^2}{2m}(2G_1)^2$$

$$\lambda_{u-G_1} = \lambda_{u+G_1} = \frac{\hbar^2}{2m}(G_1)^2$$

$$\lambda_u = 0$$

Terms $\pm G$ are degenerate. Applying perturbation theory between the second ($n=2$) and the third band ($n=3$) we can neglect all off-diagonal elements and there is

no splitting. As a matter of fact,

$$\left| \lambda_{k-2G_1} - \lambda_{k-G_1} \right| \ll V_1$$

We can see this result also by writing $\langle \psi_1 | V(x) | \psi_2 \rangle$ for $k=0$

$$\psi_1 = \frac{1}{\sqrt{L}} e^{-iG_1 x} \quad ; \quad \psi_2 = \frac{1}{\sqrt{L}} e^{iG_1 x}$$

$$E_{12}(k=0) = \frac{1}{L} \int_0^L V(x) e^{-i2G_1 x} dx = 0$$

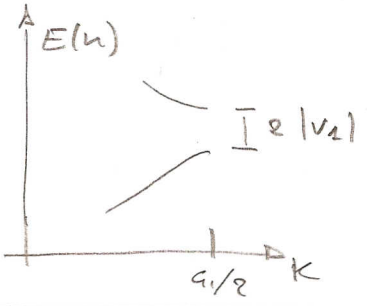
The integral is the fourier transform of the potential, which does not have components for $G = 2G_1$

$(V_{2G_1} = 0)$

- For $k = \pi/a$

$\psi_{k=-G_1/2}$ and $\psi_{k=+G_1/2}$ are degenerate. Therefore,

$$\begin{vmatrix} \lambda_{k-G_1} - \varepsilon & -V_1 \\ -V_1 & \lambda_k - \varepsilon \end{vmatrix} = 0 \quad \Rightarrow \quad \varepsilon_\pm = \varepsilon_0 \pm |V_1|$$



GENERAL PROPERTIES OF THE BLOCH ELECTRONS

a) $$\psi_{\vec{k}}(\vec{r}) = \sum_{G'} c_{k-G'}\, e^{i(k-G')x}$$

$$\psi_{\vec{k}+\vec{G}}(\vec{r}) = \sum_{G'} c_{k+G-G'}\, e^{i(k+G-G')x} = \left(\sum_{G''} c_{k-G''}\, e^{-iG''x}\right) e^{ikx}$$

$\uparrow$ $G'' \equiv G' - G$

$$= u_{\vec{k}}(\vec{r})\, e^{i\vec{k}\vec{r}}$$

$$= \psi_{\vec{k}}(\vec{r})$$

$$\Rightarrow \boxed{\psi_{\vec{k}+\vec{G}}(\vec{r}) = \psi_{\vec{k}}(\vec{r})}$$

Thus

$$H\psi_{k+G} = E_{k+G}\psi_{k+G} = E_{k+G}\psi_k$$

$$H\psi_{k+G} = H\psi_k = E_k\psi_k$$

$$\Rightarrow \boxed{E_{n,k+G} = E_{n,k}}$$

b) If we apply the translation operator $T_{\vec{R}}$ to the complex conjugate of the Bloch function,

$$T_{\vec{R}}\,\psi^*_{n,\vec{k}}(\vec{r}) = \psi^*_{n,\vec{k}}(\vec{r}+\vec{R}) = \left(e^{i\vec{k}\cdot\vec{R}}\,\psi_{n,\vec{k}}(r)\right)^*$$

$$= e^{-i\vec{k}\vec{R}}\,\psi^*_{n,\vec{k}}(\vec{r})$$

i.e., it is an eigenstate of $T_{\vec{R}}$ with eigenvalue $e^{-ik\cdot R}$

$$\Rightarrow \boxed{\psi^*_{n,\vec{k}}(\vec{r}) = \psi_{n,-\vec{k}}(\vec{r})}$$

This, in turn, implies

$$E_{m,-\vec{\kappa}} = \langle \psi_{m,-\kappa} | H | \psi_{\nu,-\kappa} \rangle$$

$$= \int d^3\tau \; \psi^*_{m,-\vec{\kappa}}(\vec{\tau}) \, H \, \psi_{\nu,-\vec{\kappa}}(\vec{\tau}) =$$

$$= \int d^3\tau \; \psi_{m,\kappa}(\vec{\tau}) \, H \, \psi^*_{m,\kappa}(\vec{\tau})$$

$$= \langle \psi_{m,\vec{\kappa}} | H | \psi_{\nu,\vec{\kappa}} \rangle^*$$

which, since H is Hermitian ($\langle \beta | H | \alpha \rangle = \langle \alpha | H | \beta \rangle^*$), implies

$$\boxed{E_{m,-\vec{\kappa}} = E_{m,\vec{\kappa}}}$$

c) We take the first derivative of $E_m(\vec{\kappa})$ at $\vec{\kappa} = \vec{G}/2$ in the direction of $\vec{G}$

$$\frac{\partial}{\partial \kappa} E_{m,\kappa}\Big|_{\vec{\kappa}=\vec{G}/2} = \lim_{\Delta\kappa \to 0} \left(\frac{1}{2\Delta\kappa}\right)\left(\langle \psi_{m,\frac{G}{2}+\Delta\kappa} | H | \psi_{m,\frac{G}{2}+\Delta\kappa} \rangle - \langle \psi_{m,\frac{G}{2}-\Delta\kappa} | H | \psi_{m,\frac{G}{2}-\Delta\kappa} \rangle \right)$$

but

$$\langle \psi_{m,\frac{G}{2}-\Delta\kappa} | H | \psi_{m,\frac{G}{2}-\Delta\kappa} \rangle = \langle \psi_{m,\frac{G}{2}-\Delta\kappa-G} | H | \psi_{m,\frac{G}{2}-\Delta\kappa-G} \rangle =$$

$$= \langle \psi_{m,-\frac{G}{2}-\Delta\kappa} | H | \psi_{\nu,-\frac{G}{2}-\Delta\kappa} \rangle = \langle \psi_{m,\frac{G}{2}+\Delta\kappa} | H | \psi_{m,\frac{G}{2}+\Delta\kappa} \rangle$$

where we used that $\psi_{m,\kappa+G} = \psi_{m,\kappa}$. Thus assuming the $E_{m,\kappa}$ is continuous

$$\boxed{\frac{\partial}{\partial \kappa} E_{m,\kappa}\Big|_{\vec{\kappa}=\vec{G}/2} = 0}$$

The electron bands at the zone boundaries have either a maximum or a minimum in the direction normal to the boundary.

The same is true at the zone center but for every direction

$$\frac{\partial}{\partial k} E_n(k)\Big|_{\vec{k}=0} = \lim_{\Delta\vec{k}\to 0} \left(\frac{1}{2\Delta\vec{k}}\right)\left[\langle\psi_{n,\Delta\vec{k}}|H|\psi_{n,\Delta\vec{k}}\rangle - \langle\psi_{n,-\Delta\vec{k}}|H|\psi_{n,-\Delta\vec{k}}\rangle\right]$$

$$= 0$$

by using $E_{n,-\vec{k}} = E_{n,\vec{k}}$

$$\boxed{\nabla_{\vec{k}} E_{n,\vec{k}}\Big|_{\vec{k}=0} = 0}$$