Electrons in a Weak Periodic Potential

One can gain substantial insight into the structure imposed on the electronic energy levels by a periodic potential, if that potential is very weak. This approach might once have been regarded as an instructive, but academic, exercise. We now know, however, that in many cases this apparently unrealistic assumption gives results surprisingly close to the mark. Modern theoretical and experimental studies of the metals found in groups I, II, III, and IV of the periodic table (i.e., metals whose atomic structure consists of *s* and *p* electrons outside of a closed-shell noble gas configuration) indicate that the conduction electrons can be described as moving in what amounts to an almost constant potential. These elements are often referred to as "nearly free electron" metals, because the starting point for their description is the Sommerfeld free electron gas, modified by the presence of a *weak* periodic potential. In this chapter we shall examine some of the broad general features of band structure from the almost free electron point of view. Applications to particular metals will be examined in Chapter 15.

It is by no means obvious why the conduction bands of these metals should be so free-electron-like. There are two fundamental reasons why the strong interactions of the conduction electrons with each other and with the positive ions can have the net effect of a very weak potential.

1. The electron-ion interaction is strongest at small separations, but the conduction electrons are forbidden (by the Pauli principle) from entering the immediate neighborhood of the ions because this region is already occupied by the core electrons.
2. In the region in which the conduction electrons are allowed, their mobility further diminishes the net potential any single electron experiences, for they can *screen* the fields of positively charged ions, diminishing the total effective potential.

These remarks offer only the barest indication of why the following discussion has extensive practical application. We shall return later to the problem of justifying the nearly free electron approach, taking up point 1 in Chapter 11 and point 2 in Chapter 17.

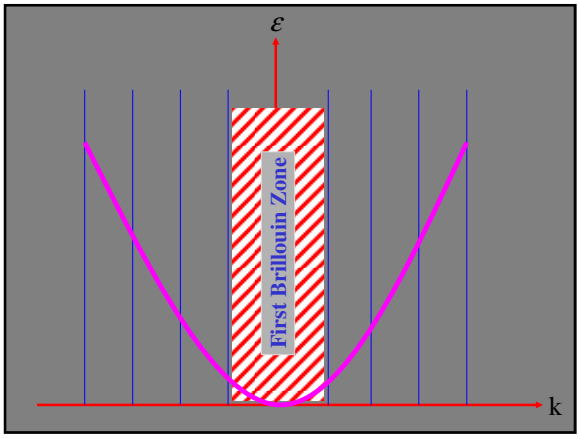
EMPTY LATTICE APPROXIMATION

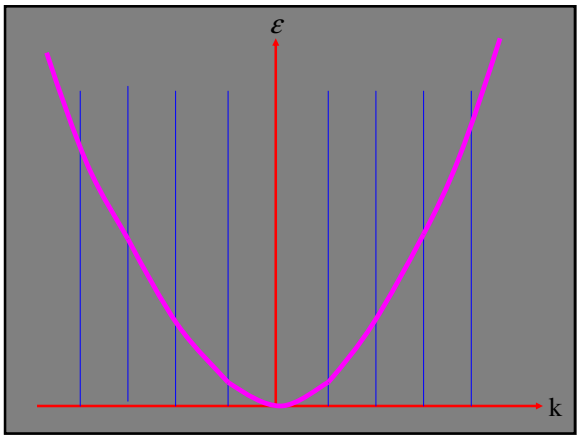
$$V = 0$$

$$\frac{-\hbar^2}{2M}\frac{\partial^2 \Psi_{0k}(x)}{\partial x^2} = \varepsilon_{0k}\Psi_{0k}(x)$$

$$\Psi_{0k}(x) = \frac{1}{\sqrt{L}}e^{ikx}$$

$$\varepsilon_{0k} = \frac{\hbar^2 k^2}{2m}$$





NEARLY FREE ELECTRON (NFE) APPROXIMATION

Now we consider the weak periodic potential

$H \rightarrow H + v$

v is a weak potential

Weak v means that the kinetic energy is much larger than the potential energy

$$E_1(k) = E_1^0(k) + \left\langle \Psi_{1,k}^{(0)} \middle| v \middle| \Psi_{1,k}^{(0)} \right\rangle + \sum_{k',n} \frac{\left| \left\langle \Psi_{n,k'}^{(0)} \middle| v \middle| \Psi_{1,k}^{(0)} \right\rangle \right|^2}{E_1^0(k) - E_n^0(k')}$$

$$\left\langle n,k' \middle| v \middle| 1,k \right\rangle \equiv \left\langle \Psi_{n,k'}^{(0)} \middle| v \middle| \Psi_{1,k}^{(0)} \right\rangle = \int \Psi_{n,k'}^{(0)*} v \Psi_{1,k}^{(0)} dx$$

$$\left\langle 1,k \middle| v \middle| 1,k \right\rangle \equiv \left\langle \Psi_{1,k}^{(0)} \middle| v \middle| \Psi_{1,k}^{(0)} \right\rangle = \frac{1}{L}\int e^{-ikx} v(x) e^{ikx} dx = \frac{1}{L}\int_0^L v dx$$

Which is independent of k

$$E_l(k) = E_l^0(k) + \left\langle \Psi_{l,k}^{(0)} \middle| v \middle| \Psi_{l,k}^{(0)} \right\rangle + \sum_{k',n} \frac{\left| \left\langle \Psi_{n,k'}^{(0)} \middle| v \middle| \Psi_{l,k}^{(0)} \right\rangle \right|^2}{E_l^0(k) - E_n^0(k')}$$

Thus this term does not depend on k

$$E_l(k) = E_l^0(k) + \sum_{k',n} \frac{\left| \left\langle \Psi_{n,k'}^{(0)} \middle| v \middle| \Psi_{l,k}^{(0)} \right\rangle \right|^2}{E_l^0(k) - E_n^0(k')}$$

The potential is periodic $\Rightarrow$ $v(x+R) = v(x)$

$$v(x) = \sum_g v_g e^{igx}$$

$$E_l(k) = E_l^0(k) + \left\langle \Psi_{l,k}^{(0)} \middle| v \middle| \Psi_{l,k}^{(0)} \right\rangle + \sum_{k',n} \frac{\left| \left\langle \Psi_{n,k'}^{(0)} \middle| v \middle| \Psi_{l,k}^{(0)} \right\rangle \right|^2}{E_l^0(k) - E_n^0(k')}$$

Now let us go through the third term

$$v(x) = \sum_g v_g e^{igx}$$

$$\langle n,k'|v|l,k\rangle \equiv \left\langle \Psi_{n,k'}^{(0)} \middle| v \middle| \Psi_{l,k}^{(0)} \right\rangle = \int \Psi_{n,k'}^{(0)*} v \Psi_{l,k}^{(0)} dx =$$

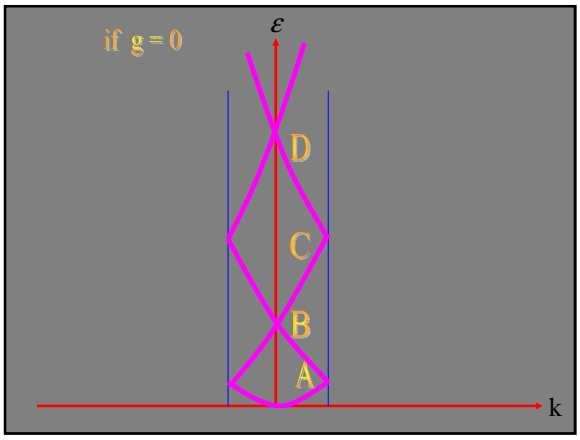
$$= \frac{1}{L} \sum_g v_g \int_0^L e^{-ik'x} e^{igx} e^{ikx} dx = \frac{1}{L} \sum_g v_g \int_0^L e^{-ik'x} e^{i(k+g)x} dx$$

$$k = \frac{2\pi}{L} n, \quad k' = \frac{2\pi}{L} n' \qquad \frac{1}{L} \int_0^L e^{-ik'x} e^{i(k+g)x} dx = \delta_{k',k+g}$$

$$\langle n,k'|v|l,k\rangle = v_g \qquad \text{if} \quad k' = k + g$$

$$E_l(k) = E_l^0(k) + \left\langle \Psi_{l,k}^{(0)} \middle| v \middle| \Psi_{l,k}^{(0)} \right\rangle + \sum_{k',n} \frac{\left| \left\langle \Psi_{n,k'}^{(0)} \middle| v \middle| \Psi_{l,k}^{(0)} \right\rangle \right|^2}{E_l^0(k) - E_n^0(k')}$$

$$E_l(k) = E_l^0(k) + \sum_{g,n} \frac{v_g^2}{E_l^0(k) - E_n^0(k+g)}$$



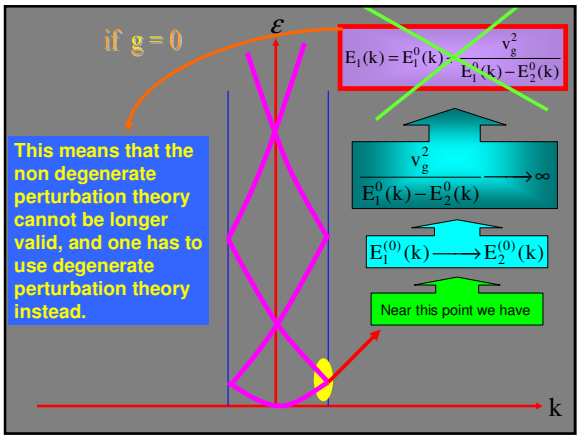
$$E_l(k) = E_l^0(k) + \sum_{g,n} \frac{v_g^2}{E_l^0(k) - E_n^0(k+g)}$$

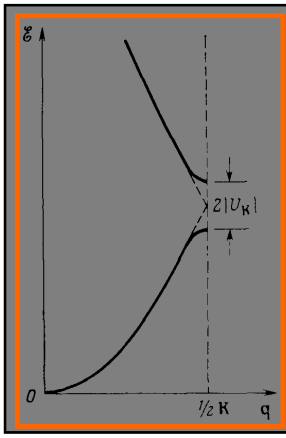
if g = 0

$$E_l(k) = E_l^0(k) + \sum_n \frac{v_g^2}{E_l^0(k) - E_n^0(k)}$$

We can using a good approximation ignore the interactions of C and D and … bands with the A band. If we only consider the nearest B band, then:

$$E_l(k) = E_l^0(k) + \frac{v_g^2}{E_l^0(k) - E_2^0(k)}$$





$$E_1(k) = E_1^0(k) + \frac{v_g^2}{E_1^0(k) - E_2^0(k)}$$

if $|k| < \frac{\pi}{a} \longrightarrow E_2^{(0)}(k+g) > E_1^{(0)}(k)$

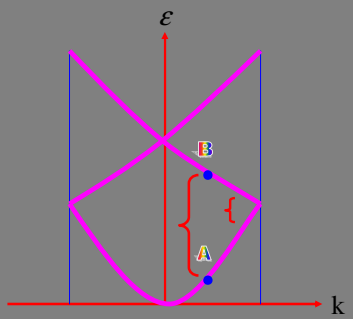
$\longrightarrow E_1(k) < E_1^{(0)}(k)$

if $|k| > \frac{\pi}{a} \longrightarrow E_1^{(0)}(k) > E_2^{(0)}(k+g)$

$\longrightarrow E_1(k) > E_1^{(0)}(k)$

Electrons in the weak periodic potential

NEARLY FREE ELECTRON (NFE) APPROXIMATION



non degenerate perturbation theory cannot be longer valid!

$$H\psi = \varepsilon\psi$$

$$-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r})$$

$$U(\mathbf{r}+\mathbf{R}) = U(\mathbf{r})$$

Translation Lattice Vector

Now suppose we are dealing with one dimensional problem

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U(x)\psi = \varepsilon\psi$$

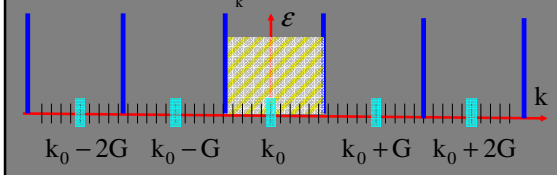
$$n(\mathbf{r}+\mathbf{R}) = n(\mathbf{r})$$

$$U(x) = \sum_G U_G e^{iGx}$$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \sum_G U_G e^{iGx}\right)\psi = \varepsilon\psi$$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \sum_G U_G e^{iGx}\right)\psi = \varepsilon\psi$$

$$\psi(x) = \sum_k C(k)e^{ikx}$$



$$\psi(x) = \sum_k C(k)e^{ikx} = \sum_G C(k_0+G)e^{i(k_0+G)x} = \sum_G C(k_0-G)e^{i(k_0-G)x}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\sum_k C(k)e^{ikx} = \frac{\hbar^2}{2m}\sum_k C(k)k^2e^{ikx}$$

$$U(x)\psi(x) = \sum_G U_G e^{iGx}\sum_k C(k)e^{ikx} = \sum_{k,G} U_G C(k)e^{i(k+G)x}$$

$$k \longrightarrow k-G$$

$$U(x)\psi(x) = \sum_{k,G} U_G C(k-G)e^{ikx}$$

$$\frac{\hbar^2}{2m}\sum_k C(k)k^2e^{ikx} + \sum_{k,G} U_G C(k-G)e^{ikx} = \varepsilon\sum_k C(k)e^{ikx}$$

$$\frac{\hbar^2}{2m}\sum_k C(k)k^2e^{ikx} + \sum_{k,G} U_G C(k)e^{ikx} = \varepsilon\sum_k C(k)e^{ikx}$$

Now we multiply both sides of the above equation by $e^{ik'x}$ and then take integrals of both sides

$$\frac{1}{L}\int_0^L dx e^{-ik'x}e^{ikx} = \delta_{kk'}$$

$$\frac{1}{L}\int_0^L dx e^{-ik'x}e^{ikx} = \frac{1}{L}\begin{cases}\frac{1}{i(k-k')}\left(e^{i(k-k')x}-1\right) & k \neq k' \\ L & k=k'\end{cases} = \delta_{kk'}$$

$$k = \frac{2\pi}{L}n, \quad k' = \frac{2\pi}{L}n'$$

$$e^{i(k-k')x} = e^{i\left(\frac{2\pi}{L}n - \frac{2\pi}{L}n'\right)L} = e^{i2\pi(n-n')} = 1$$

$$\frac{\hbar^2}{2m}C(k')k'^2+\sum_G U_G C(k'-G)=\varepsilon C(k')$$

$k' \longrightarrow k$

$$\frac{\hbar^2}{2m}C(k)k^2+\sum_G U_G C(k-G)=\varepsilon C(k)$$

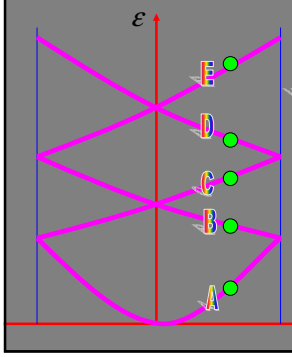
$$\left(\frac{\hbar^2}{2m}k^2-\varepsilon\right)C(k)+\sum_G U_G C(k-G)=0$$

$$\frac{\hbar^2}{2m}k^2=\lambda_k$$

$$(\lambda_k-\varepsilon)C(k)+\sum_G U_G C(k-G)=0$$

Electrons in the weak periodic potential

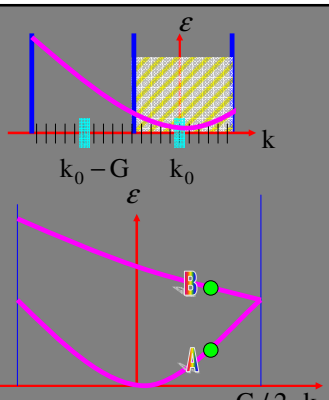
NEARLY FREE ELECTRON (NFE) APPROXIMATION



I(A, B)>I(A, C)>I(A,D)>...

NFE

Let be only I(A,B)<>0



$$(\lambda_k-\varepsilon)C(k)+\sum_G U_G C(k-G)=0$$

$$\begin{cases}(\lambda_k-\varepsilon)C(k)+U_G C(k-G)=0 & k=k\\ (\lambda_{k-G}-\varepsilon)C(k-G)+U_{-G}C(k)=0 & k=k-G\end{cases}$$

$$U_G=U_{-G}=U$$

$$\begin{cases}(\lambda_k-\varepsilon)C(k)+UC(k-G)=0 & k=k\\ (\lambda_{k-G}-\varepsilon)C(k-G)+UC(k)=0 & k=k-G\end{cases}$$

$$\begin{vmatrix}\lambda_k-\varepsilon & U\\ U & \lambda_{k-G}-\varepsilon\end{vmatrix}=0$$

$$\begin{vmatrix}\lambda_k-\varepsilon & U\\ U & \lambda_{k-G}-\varepsilon\end{vmatrix}=0$$

$$\varepsilon=\frac{\lambda_k+\lambda_{k-G}}{2}\pm\sqrt{\left(\frac{\lambda_k+\lambda_{k-G}}{2}\right)^2+U^2}$$

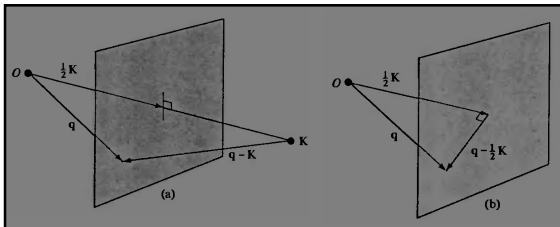
At the edge of the 1BZ:

K=G/2

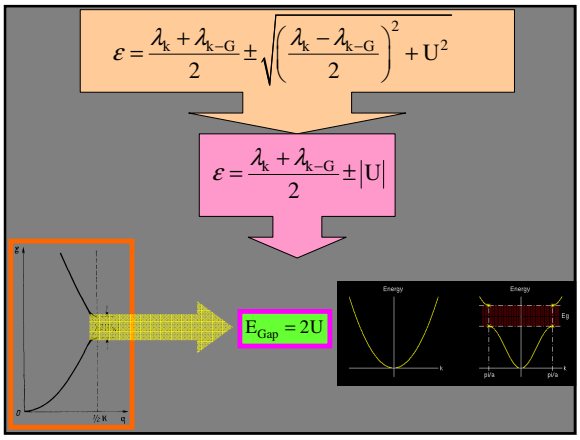
$\lambda_k=\lambda_{k-G}$

$$\lambda_k=\frac{\hbar^2k^2}{2m}=\frac{\hbar^2}{2m}(G/2)^2$$

$$\lambda_{k-G}=\frac{\hbar^2(G/2-G)^2}{2m}=\frac{\hbar^2}{2m}(-G/2)^2=\frac{\hbar^2}{2m}(G/2)^2$$



(a) If $|\mathbf{q}| = |\mathbf{q} - \mathbf{K}|$, then the point $\mathbf{q}$ must lie in the Bragg plane determined by $\mathbf{K}$. (b) If the point $\mathbf{q}$ lies in the Bragg plane, then the vector $\mathbf{q} - \frac{1}{2}\mathbf{K}$ is parallel to the plane.



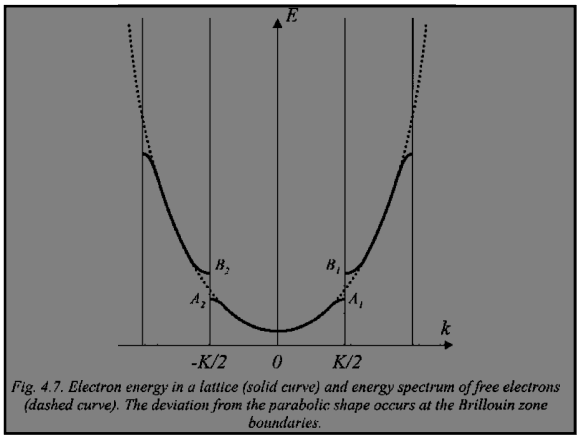


Fig. 4.7. Electron energy in a lattice (solid curve) and energy spectrum of free electrons (dashed curve). The deviation from the parabolic shape occurs at the Brillouin zone boundaries.

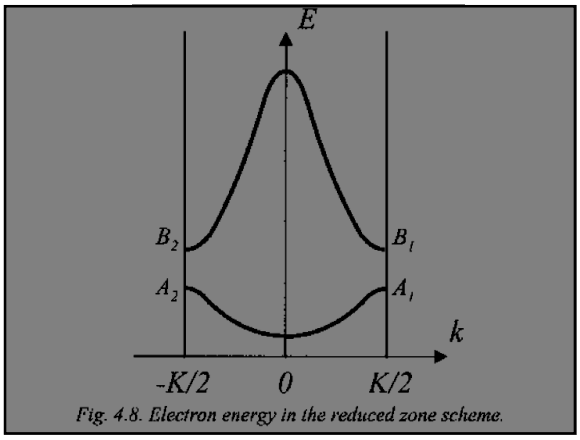
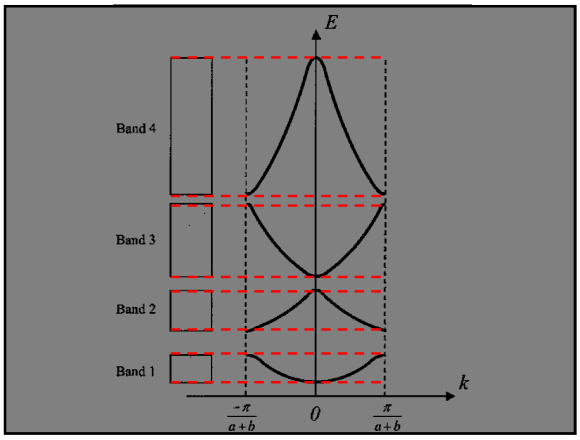


Fig. 4.8. Electron energy in the reduced zone scheme.



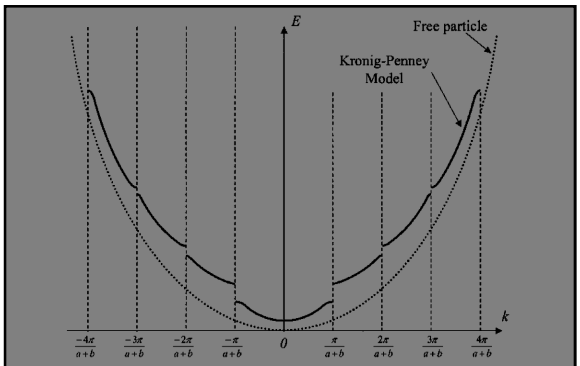


Fig. 4.6. One-dimensional E-k relationship in the extended-zone representation in the Kronig-Penney model. The parabolic relation for the free particle is shown in dotted lines for comparison. The deviation from a parabolic shape occurs mainly at the Brillouin zone boundaries.

ENERGY BANDS IN ONE DIMENSION

We can illustrate these general conclusions in one dimension, where twofold degeneracy is the most that can ever occur. In the absence of any interaction the electronic energy levels are just a parabola in k (Figure 9.4a). To leading order in the weak one-dimensional periodic potential this curve remains correct except near Bragg "planes" (which are points in one dimension). When q is near a Bragg "plane" corresponding to the reciprocal lattice vector K (i.e., the point $\frac{1}{2}K$) the corrected energy levels are determined by drawing another free electron parabola centered around K (Figure 9.4b), noting that the degeneracy at the point of intersection is split by $2|U_K|$ in such a way that both curves have zero slope at that point, and redrawing Figure 9.4b to get Figure 9.4c. The original free electron curve is therefore modified as in Figure 9.4d. When all Bragg planes and their associated Fourier components are included, we end up with a set of curves such as those shown in Figure 9.4e. This particular way of depicting the energy levels is known as the *extended-zone scheme*.

If we insist on specifying all the levels by a wave vector k in the first Brillouin zone, then we must translate the pieces of Figure 9.4e, through reciprocal lattice vectors, into the first Brillouin zone. The result is shown in Figure 9.4f. The representation is that of the *reduced-zone scheme* (see page 142).

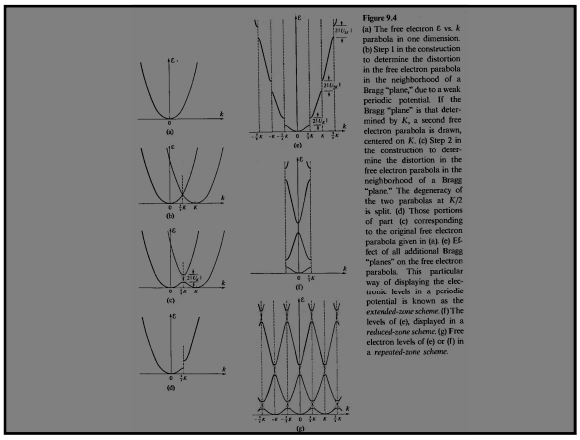


Figure 9.4
(a) The free electron $\mathcal{E}$ vs. k parabola in one dimension. (b) Step 1 in the construction to determine the distortion in the free electron parabola in the neighborhood of a Bragg "plane," due to a weak periodic potential. If the Bragg "plane" is that determined by K, a second free electron parabola is drawn, centered on K. (c) Step 2 in the construction to determine the distortion in the free electron parabola in the neighborhood of a Bragg "plane." The degeneracy of the two parabolas at $K/2$ is split. (d) Those portions of part (c) corresponding to the original free electron parabola given in (a). (e) Effect of all additional Bragg "planes" on the free electron parabola. This particular way of displaying the electronic levels in a periodic potential is known as the *extended-zone scheme*. (f) The levels of (e), displayed in a *reduced-zone scheme*. (g) Free electron levels of (e) or (f) in a *repeated-zone scheme*.

$$\psi(x)=\sum_k C(k)e^{ikx}$$

IF we again keep only two terms due to the NFE approximation, then:

$$\psi(x)=C(k)e^{ikx}+C(k-G)e^{i(k-G)x}$$

We now prove that C(k) = + C(k-G) or - C(k-G) at the edge of the 1BZ:

$$(\lambda_k-\varepsilon)C(k)+UC(k-G)=0$$

$$\frac{C(k-G)}{C(k)}=\frac{\varepsilon-\lambda_k}{U}=\frac{\lambda_k\pm U-\lambda_k}{U}=\pm 1$$

We had shown that

$$\varepsilon=\frac{\lambda_k+\lambda_{k-G}}{2}\pm|U|$$

$\lambda_k=\lambda_{k-G}$

$$\varepsilon=\lambda_k\pm|U|$$

$$\psi(x)=C(k)e^{ikx}+C(k-G)e^{i(k-G)x}$$

$$=C(k)\left(e^{ikx}\pm e^{-ikx}\right)=C(k)\left(e^{iG/2x}\pm e^{-iG/2x}\right)$$

$$\psi(x)\propto\begin{cases}\cos(G/2x)\\ \sin(G/2x)\end{cases}\qquad G=\frac{2\pi}{a}$$

$$\psi(x)\propto\begin{cases}\cos(\pi/Lx)\longrightarrow\psi^+\\ \sin(\pi/Lx)\longrightarrow\psi^-\end{cases}$$

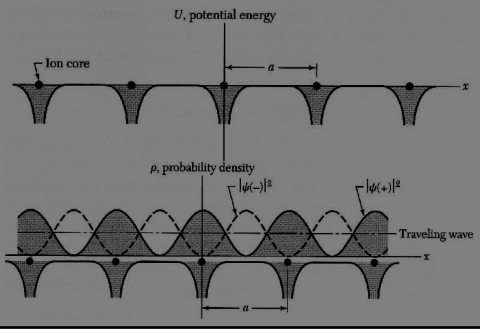
Since these two coefficients are the dominant ones in the plane-wave expansion (9.1), it follows that if $U_K > 0$, then

$$|\psi(\mathbf{r})|^2\propto(\cos\tfrac{1}{2}\mathbf{K}\cdot\mathbf{r})^2,\quad \varepsilon=\varepsilon_q^0+|U_K|,$$
$$|\psi(\mathbf{r})|^2\propto(\sin\tfrac{1}{2}\mathbf{K}\cdot\mathbf{r})^2,\quad \varepsilon=\varepsilon_q^0-|U_K|,$$

while if $U_K < 0$, then

$$|\psi(\mathbf{r})|^2\propto(\sin\tfrac{1}{2}\mathbf{K}\cdot\mathbf{r})^2,\quad \varepsilon=\varepsilon_q^0+|U_K|,$$
$$|\psi(\mathbf{r})|^2\propto(\cos\tfrac{1}{2}\mathbf{K}\cdot\mathbf{r})^2,\quad \varepsilon=\varepsilon_q^0-|U_K|.$$

Sometimes the two types of linear combination are called "*p*-like" ($|\psi|^2 \sim \sin^2 \frac{1}{2}\mathbf{K}\cdot\mathbf{r}$) and "*s*-like" ($|\psi|^2 \sim \cos^2 \frac{1}{2}\mathbf{K}\cdot\mathbf{r}$) because of their position dependence near lattice points. The *s*-like combination, like an atomic *s*-level, does not vanish at the ion; in the *p*-like combination the charge density vanishes as the square of the distance from the ion for small distances, which is also a characteristic of atomic *p*-levels.

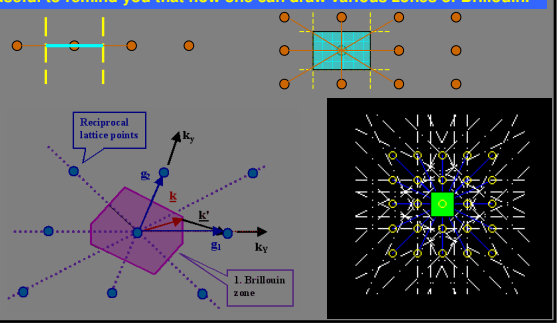


Okay. In the NFE model we find that the band structure behaves similar to the free electron approximation far from the edge of the Brillouin zone. Indeed the band structure of the NFE approximation deviates from free electron model only in the adjacent of the edge of the Brillouin zone.

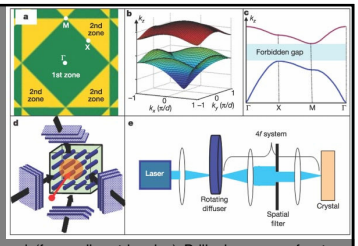
Therefore, it is important to learn how one can plot the band structure of an empty thee dimensional lattice.

Band Structure plotting of empty 3 dimensional lattices

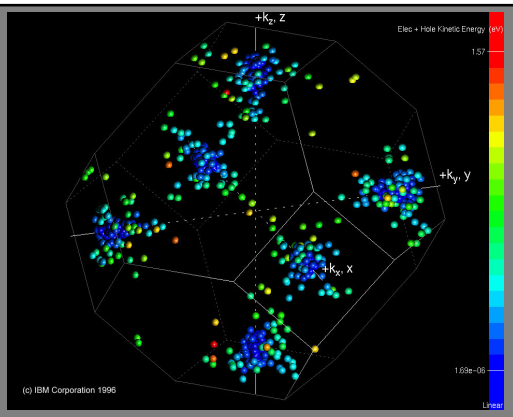
Before learning how to plot band structure in an empty space, it is useful to remind you that how one can draw various zones of Brillouin.



Oren Cohen, Guy Bartal, Hrvoje Buljan, Tal Carmon, Jason W. Fleischer, Mordechai Segev and Demetrios N. Christodoulides
Nature 433, 500-503(3 February 2005)

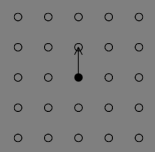


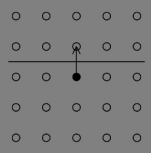
a, First (green square) and second (four yellow triangles) Brillouin zones of a two-dimensional square lattice with the high-symmetry points (, X, and M) marked with white dots. **b**, Transmission spectrum of the first two bands of a two-dimensional square lattice with a lattice period *d*. **c**, Dispersion curves between the symmetry points of the first two bands. Negative curvature in these curves corresponds to normal diffraction regions. **d**, Diagram of the optical induction technique used to obtain the two-dimensional, square photonic lattice. The blue planes with heavy black arrows indicate the plane waves used to optically induce the lattice. The red arrow indicates the direction of a probe beam entering the lattice. The orange circle indicates the width of the probe beam. **e**, Diagram of our set-up for obtaining a spatially incoherent (quasi-thermal), quasi-monochromatic beam.



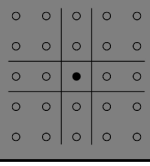
http://www.doitpoms.ac.uk/tlplib/brillouin_zones/zone_construction.php

Draw a line connecting this origin point to one of its nearest neighbors. This line is a reciprocal lattice vector as it connects two points in the reciprocal lattice.



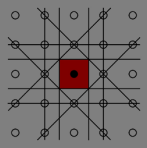


Then draw on a perpendicular bisector to the first line. This perpendicular bisector is a Bragg Plane.

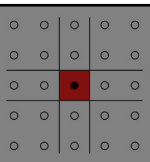


Add the Bragg Planes corresponding to the other nearest neighbours.

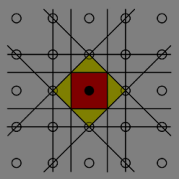
The locus of points in reciprocal space that have no Bragg Planes between them and the origin defines the first Brillouin Zone. It is equivalent to the Wigner-Seitz unit cell of the reciprocal lattice. In the picture below the first Zone is shaded red.



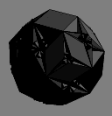
The second Brillouin Zone is the region of reciprocal space in which a point has one Bragg Plane between it and the origin. This area is shaded yellow in the picture below. Note that the areas of the first and second Brillouin Zones are the same.



Now draw on the Bragg Planes corresponding to the next nearest neighbours.

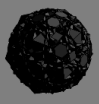


The first twenty Brillouin zones of a 2D hexagonal lattice.



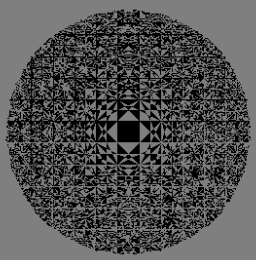
The (outside of) 15th Brillouin zone for the simple cubic.

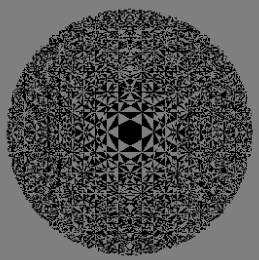
The (outside of) 18th Brillouin zone for the face-centered cubic



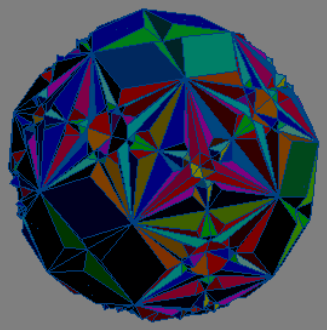
The (outside of) 10th Brillouin zone for the body-centered cubic lattice.

Two dimensional Brillouin zone

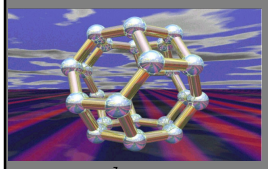


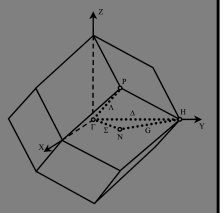


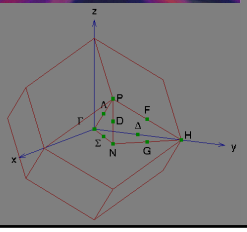
Three dimensional Brillouin zone

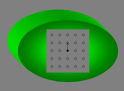


First Brillouin Zone BCC

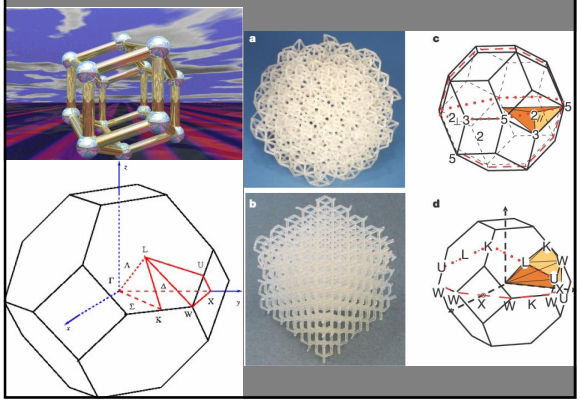


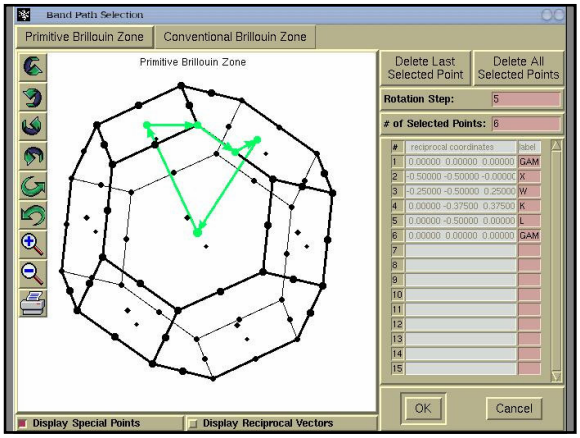




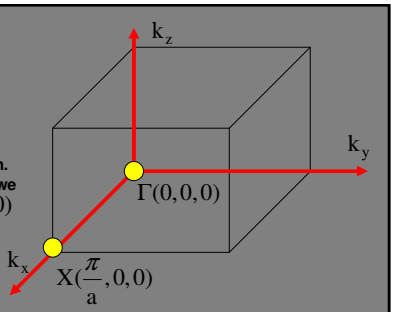


First Brillouin Zone FCC





Band structure of a simple cubic lattice along Γ to X direction. Along this direction we have: $\mathbf{k} = (k_x, 0, 0)$

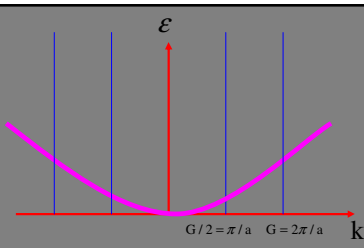


$$\Gamma(0,0,0) \Rightarrow X(\frac{\pi}{a},0,0)$$

$\mathbf{K} = \mathbf{k} + \mathbf{G}$

Outside of the 1BZ

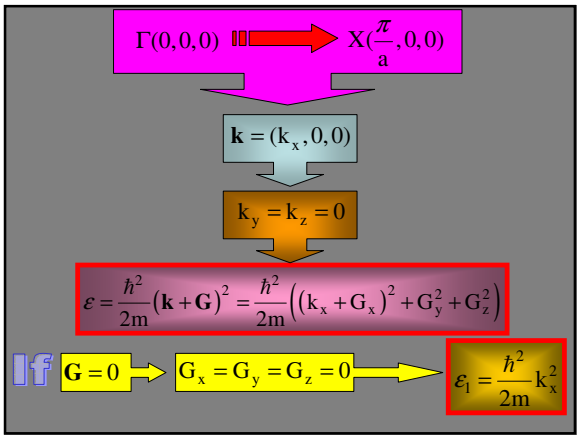
Inside of the 1BZ

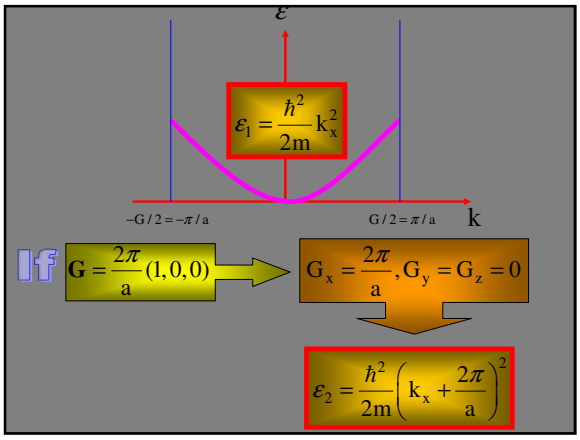


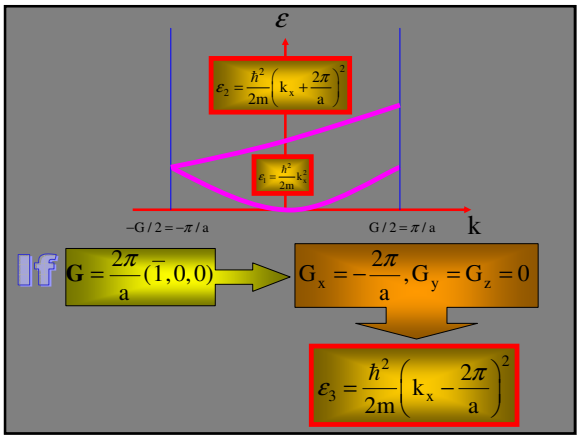
$$\varepsilon = \frac{\hbar^2}{2m}(\mathbf{k}+\mathbf{G})^2 = \frac{\hbar^2}{2m}\left((k_x+G_x)^2+(k_y+G_y)^2+(k_z+G_z)^2\right)$$

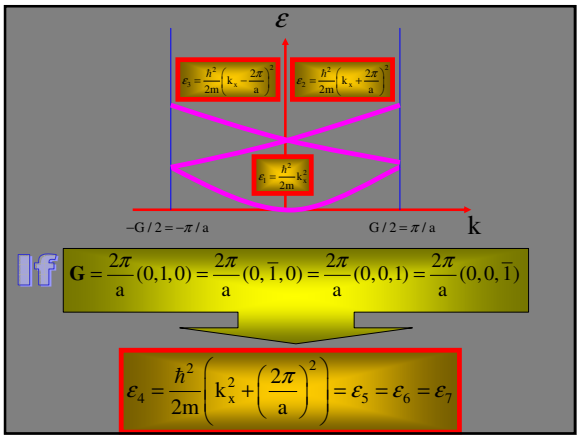
Thus one would take some allowed shortest G vectors and try to plot their corresponded bands

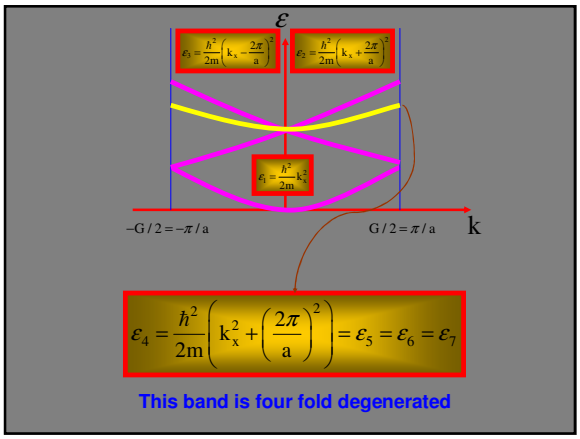
Inside of the 1BZ

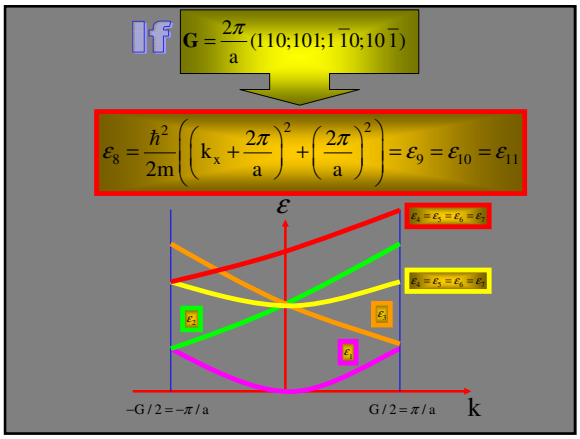

$\Gamma(0,0,0) \rightarrow X(\frac{\pi}{a},0,0)$
$\mathbf{k} = (k_x, 0, 0)$
$k_y = k_z = 0$
$\varepsilon = \frac{\hbar^2}{2m}(\mathbf{k}+\mathbf{G})^2 = \frac{\hbar^2}{2m}\left((k_x+G_x)^2 + G_y^2 + G_z^2\right)$
If $\mathbf{G} = 0 \rightarrow G_x = G_y = G_z = 0 \rightarrow \varepsilon_1 = \frac{\hbar^2}{2m}k_x^2$

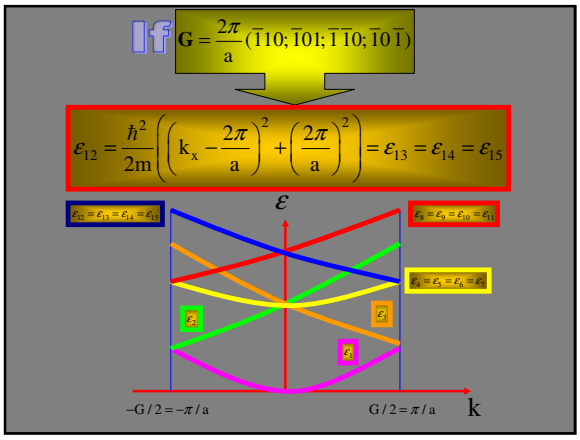

ε
$\varepsilon_1 = \frac{\hbar^2}{2m}k_x^2$
$-G/2 = -\pi/a$
$G/2 = \pi/a$
k
If $\mathbf{G} = \frac{2\pi}{a}(1,0,0) \rightarrow G_x = \frac{2\pi}{a}, G_y = G_z = 0$
$\varepsilon_2 = \frac{\hbar^2}{2m}\left(k_x + \frac{2\pi}{a}\right)^2$

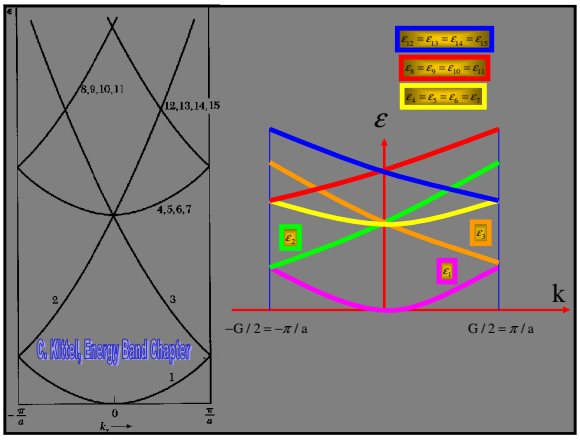

ε
$\varepsilon_2 = \frac{\hbar^2}{2m}\left(k_x + \frac{2\pi}{a}\right)^2$
$\varepsilon_1 = \frac{\hbar^2}{2m}k_x^2$
$-G/2 = -\pi/a$
$G/2 = \pi/a$
k
If $\mathbf{G} = \frac{2\pi}{a}(\bar{1},0,0) \rightarrow G_x = -\frac{2\pi}{a}, G_y = G_z = 0$
$\varepsilon_3 = \frac{\hbar^2}{2m}\left(k_x - \frac{2\pi}{a}\right)^2$


ε
$\varepsilon_3 = \frac{\hbar^2}{2m}\left(k_x - \frac{2\pi}{a}\right)^2$
$\varepsilon_2 = \frac{\hbar^2}{2m}\left(k_x + \frac{2\pi}{a}\right)^2$
$\varepsilon_1 = \frac{\hbar^2}{2m}k_x^2$
$-G/2 = -\pi/a$
$G/2 = \pi/a$
k
If $\mathbf{G} = \frac{2\pi}{a}(0,1,0) = \frac{2\pi}{a}(0,\bar{1},0) = \frac{2\pi}{a}(0,0,1) = \frac{2\pi}{a}(0,0,\bar{1})$
$\varepsilon_4 = \frac{\hbar^2}{2m}\left(k_x^2 + \left(\frac{2\pi}{a}\right)^2\right) = \varepsilon_5 = \varepsilon_6 = \varepsilon_7$


ε
$\varepsilon_3 = \frac{\hbar^2}{2m}\left(k_x - \frac{2\pi}{a}\right)^2$
$\varepsilon_2 = \frac{\hbar^2}{2m}\left(k_x + \frac{2\pi}{a}\right)^2$
$\varepsilon_1 = \frac{\hbar^2}{2m}k_x^2$
$-G/2 = -\pi/a$
$G/2 = \pi/a$
k
$\varepsilon_4 = \frac{\hbar^2}{2m}\left(k_x^2 + \left(\frac{2\pi}{a}\right)^2\right) = \varepsilon_5 = \varepsilon_6 = \varepsilon_7$
This band is four fold degenerated


If $\mathbf{G} = \frac{2\pi}{a}(110;101;1\bar{1}0;10\bar{1})$
$\varepsilon_8 = \frac{\hbar^2}{2m}\left(\left(k_x + \frac{2\pi}{a}\right)^2 + \left(\frac{2\pi}{a}\right)^2\right) = \varepsilon_9 = \varepsilon_{10} = \varepsilon_{11}$
ε
$\varepsilon_4 = \varepsilon_5 = \varepsilon_6 = \varepsilon_7$
ε_2
ε_1
ε_3
$-G/2 = -\pi/a$
$G/2 = \pi/a$
k





PRACTICE

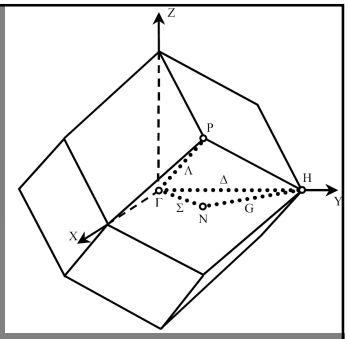
Find the band structure of an empty simple cubic (SC) along (111) direction

Find the band structure of an empty body centered cubic (bcc) along Γ(000) to H(010) for the first four allowed G vectors taking bcc structure factor into account

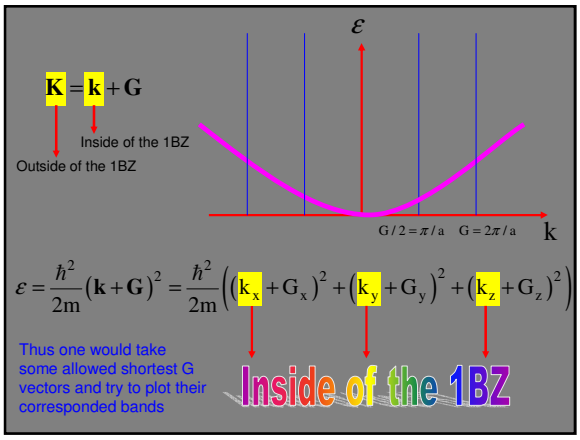
$$S_K = 1 + e^{i\pi(n_1+n_2+n_3)} = 1 + (-1)^{n_1+n_2+n_3} = \begin{cases} 2, & n_1+n_2+n_3 \text{ even,} \\ 0, & n_1+n_2+n_3 \text{ odd.} \end{cases}$$

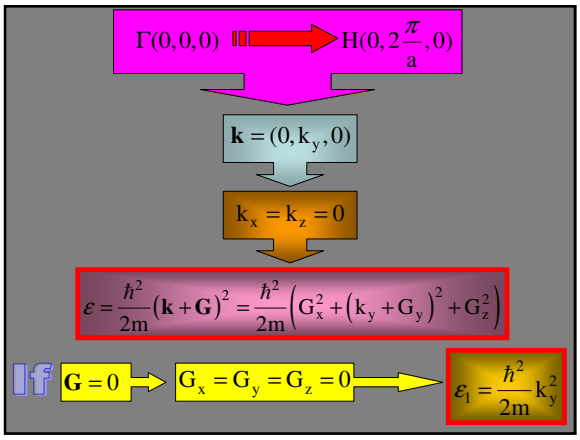
$$\mathbf{G} = \frac{2\pi}{a}\left(n_1\hat{k}_x + n_2\hat{k}_y + n_3\hat{k}_z\right)$$

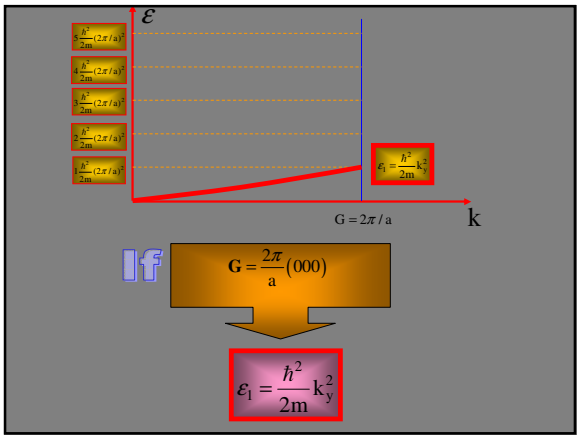
Miller indexes h, k, l

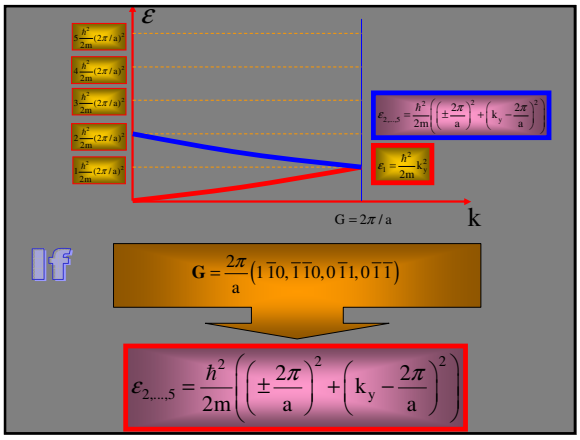


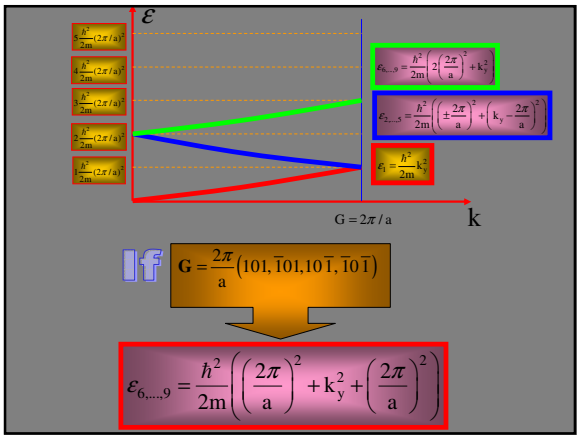
$$\Gamma(0,0,0) \Rightarrow \Delta\left(\frac{\pi}{a}(010)\right) \Rightarrow H\left(\frac{2\pi}{a}(010)\right)$$

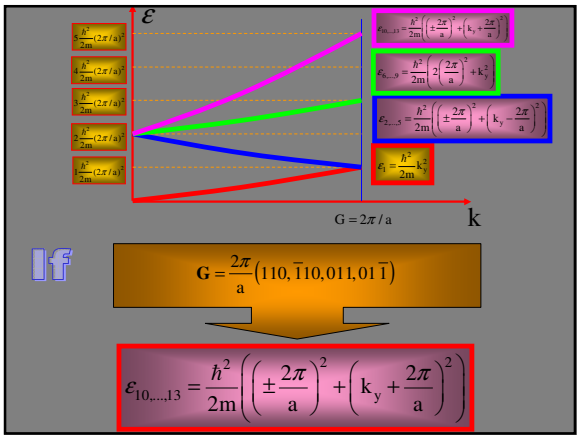


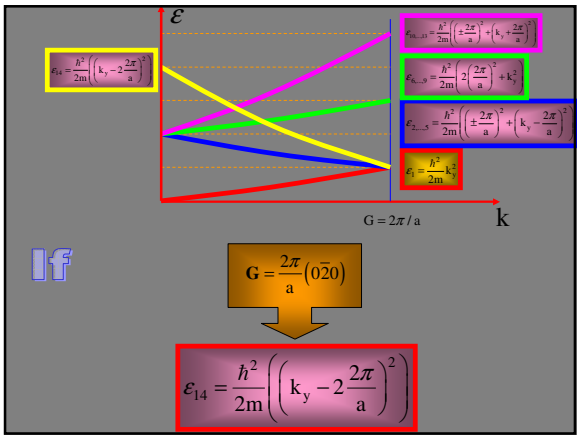


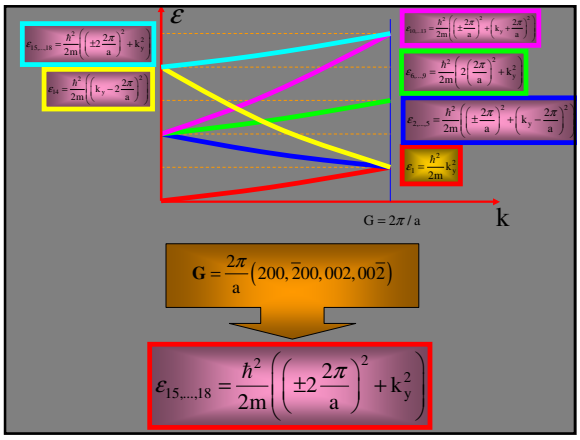

ε
G = 2π / a
k
If
$\mathbf{G} = \frac{2\pi}{a}(000)$
$\varepsilon_1 = \frac{\hbar^2}{2m} k_y^2$

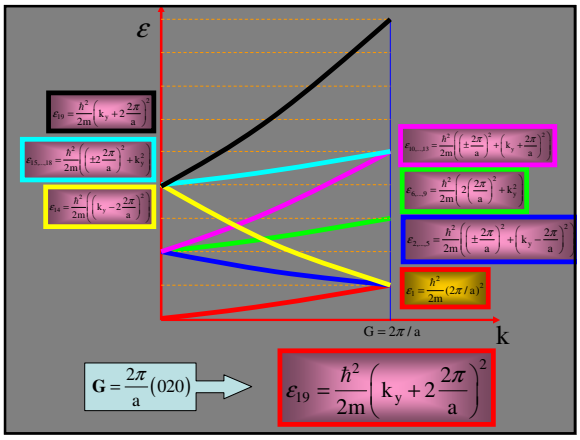

ε
G = 2π / a
k
If
$\mathbf{G} = \frac{2\pi}{a}(1\bar{1}0, \bar{1}10, 0\bar{1}1, \bar{1}\bar{1})$
$\varepsilon_{2,\ldots,5} = \frac{\hbar^2}{2m}\left(\left(\pm\frac{2\pi}{a}\right)^2 + \left(k_y - \frac{2\pi}{a}\right)^2\right)$

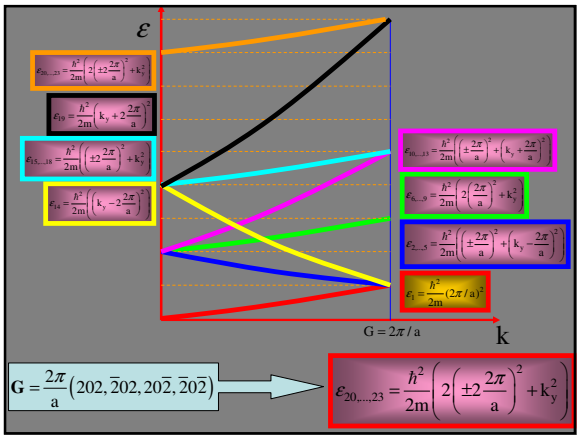

ε
G = 2π / a
k
If
$\mathbf{G} = \frac{2\pi}{a}(101, \bar{1}01, 10\bar{1}, \bar{1}0\bar{1})$
$\varepsilon_{6,\ldots,9} = \frac{\hbar^2}{2m}\left(\left(\frac{2\pi}{a}\right)^2 + k_y^2 + \left(\frac{2\pi}{a}\right)^2\right)$

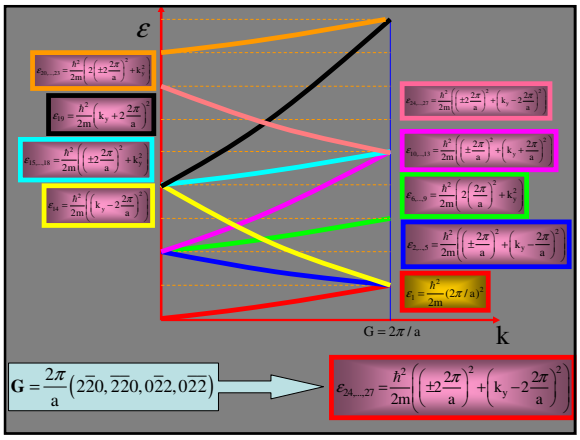

ε
G = 2π / a
k
If
$\mathbf{G} = \frac{2\pi}{a}(110, \bar{1}10, 011, 01\bar{1})$
$\varepsilon_{10,\ldots,13} = \frac{\hbar^2}{2m}\left(\left(\pm\frac{2\pi}{a}\right)^2 + \left(k_y + \frac{2\pi}{a}\right)^2\right)$

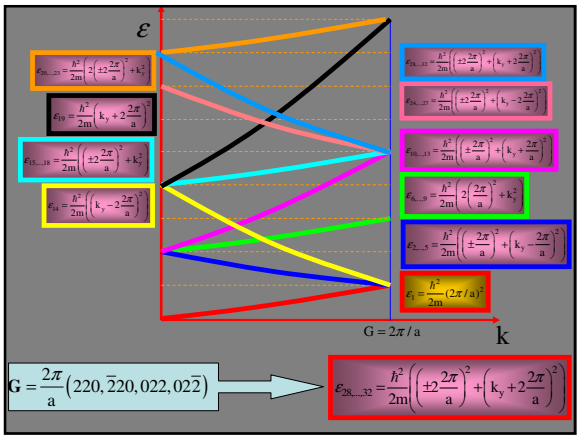

ε
G = 2π / a
k
If
$\mathbf{G} = \frac{2\pi}{a}(0\bar{2}0)$
$\varepsilon_{14} = \frac{\hbar^2}{2m}\left(\left(k_y - 2\frac{2\pi}{a}\right)^2\right)$


ε
G = 2π / a
k
$\mathbf{G} = \frac{2\pi}{a}(200, \bar{2}00, 002, 00\bar{2})$
$\varepsilon_{15,\ldots,18} = \frac{\hbar^2}{2m}\left(\left(\pm 2\frac{2\pi}{a}\right)^2 + k_y^2\right)$









PRACTICE

Find the following empty fcc lattice band structure.
Miller indexes are even or odd.

$X = \left(0, \frac{2\pi}{a}, 0\right)$ $W = \left(\frac{\pi}{a}, \frac{2\pi}{a}, 0\right)$
$L = \left(\frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{a}\right)$ $K = \left(\frac{3\pi}{2a}, \frac{3\pi}{2a}, 0\right)$