Theory of Semiconductor Devices
(반도체 소자 이론)

Lecture 6

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Energy Bands

Empty Lattice Model

- Substantial amount of information can be obtained about the wavevector of a Bloch electron ***without*** reference to the specific nature of the ***effective*** one-electron potential energy, $U(\mathbf{r})$.
-We can also obtain the general form and degeneracy (states at the same energy) of Bloch electron energy bands by solving the one-electron Schrodinger equation (2 .3) for $U(\mathbf{r}) = 0$.
- The solutions, of course, are ***identical to*** those obtained for ***free electrons*** (2.4) and consist of plane waves with wavevectors, **k**, which are continuous throughout the reciprocal lattice. For this reason, the resulting energy values (2 .5) , given by

$$\mathscr{E}(k) = \frac{\hbar^2}{2m}\mathbf{k}^2 \qquad (2.33)$$

are referred to as *free-electron* or ***empty lattice*** energy bands. The relationship between $\mathscr{E}$ and **k** in (2 .33) is referred to as a ***parabolic*** energy band.

- To determine the *general* form of the energy bands for Bloch electrons, we wish to ***reduce*** the free-electron wavevector, **k**, ***to the first Brillouin zone***.
- As we saw in Fig. 2.2 this can be done for any wavevector (including a free electron wavevector) by a *suitable* choice of reciprocal lattice vector,

$$\mathbf{k} = \mathbf{k}' + \mathbf{K} \qquad (2.34)$$

Empty Lattice Model

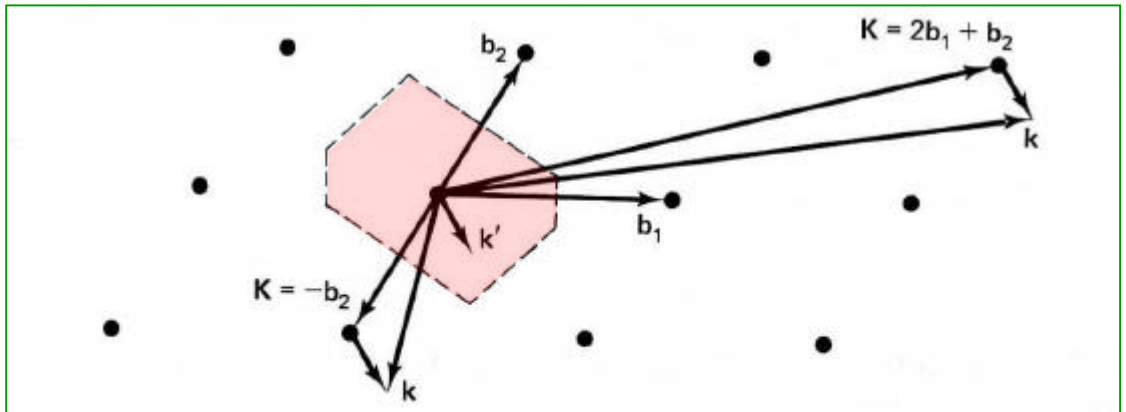

Figure 2.2 A two-dimensional reciprocal lattice indicating that any wavevector **k** in a higher Brillouin zone can be reduced to a value **k′** in the first Brillouin zone by choosing the appropriate reciprocal lattice vector **K**.

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Empty Lattice Model

- The wavefunction (2.4) is then

$$\psi_k(\mathbf{r}) = A \exp\left[i(\mathbf{k}' + \mathbf{K})\cdot\mathbf{r}\right] \tag{2.35}$$

which is a Bloch wavefunction (2 .10) with

$$u_k(\mathbf{r}) = A \exp\left(i\mathbf{K}\cdot\mathbf{r}\right) \tag{2.36}$$

- From (2.34) and (2 .33) the empty lattice energy bands are

$$\mathscr{E}(\mathbf{k}) = \frac{\hbar^2}{2m}(\mathbf{k}' + \mathbf{K})^2 \tag{2.37}$$

where K is given by (1.17) as

$$\mathbf{K} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3 \tag{2.38}$$

and *h*, *k*, *l* are integers .

- Thus it can be seen that **K** serves as an index for the different energy bands.
- Since there are an ***infinite*** number of *h*, *k*, *l*, there are an ***infinite*** number of energy bands.

Empty Lattice Model

- We can demonstrate these free-electron energy bands most simply by looking at values of **k** in the direction of **K** ***without*** reference to a specific crystal structure. This gives the one-dimensional energy bands shown in Fig. 2.4.

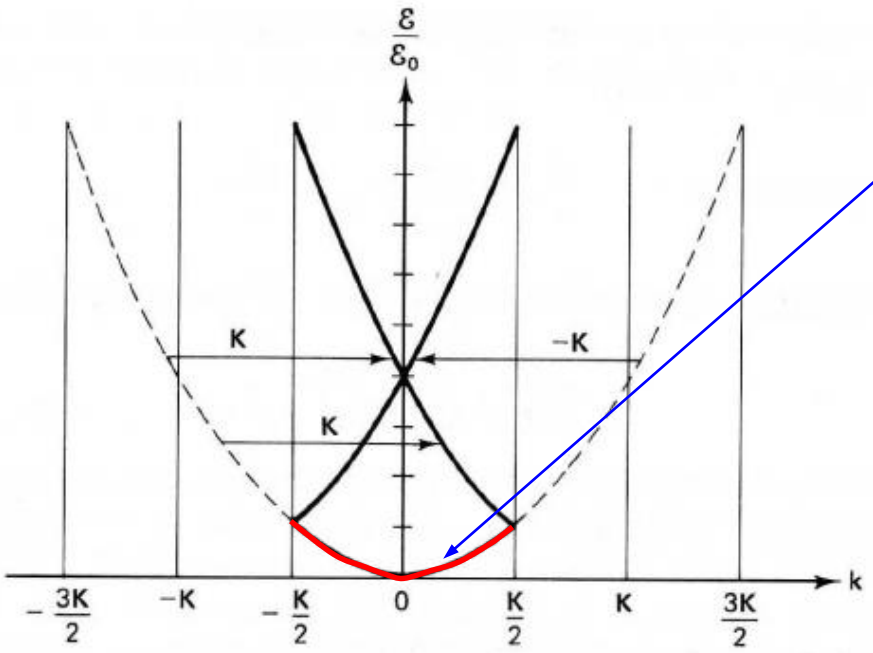
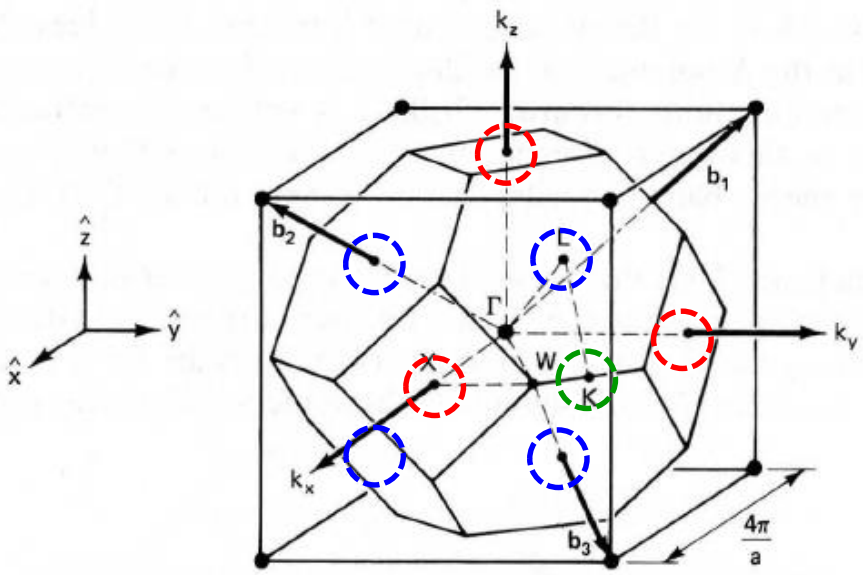


Figure 2.4 Empty lattice energy bands for **k** in the direction of **K**. The dashed line shows the parabolic free-electron description. $\mathscr{E}_0 = (\hbar^2/2m)(\frac{1}{2}\,\mathbf{K})^2$ is the energy at $\pm\frac{1}{2}\,\mathbf{K}$, the boundaries of the first Brillouin zone.

- The lowest-lying band in the first Brillouin zone is obtained by setting **K** = 0 in (2.37) and letting **k** range from $-\frac{1}{2}$K to $+\frac{1}{2}$K.
- Continuing this procedure, an *infinite* number of energy bands are generated in the first Brillouin zone, each indexed with a separate reciprocal lattice vector.
- These free-electron energy bands , however, are of ***most*** interest in three dimensions, where they illustrate the form and ***degeneracy*** of electron states for a specific lattice.

Empty Lattice Model for fcc

- As an example , we consider the general form and degeneracies of the empty lattice energy bands for the face-centered cubic lattice .
- The reciprocal space for this lattice is shown in Fig. 2.5. Values of wavevector, k , for some of the high-symmetry points in the Brillouin zone are:



Γ-point: $\mathbf{k} = 0$

X-points: $\mathbf{k} = \pm\frac{2\pi}{a}\hat{x}, \quad \pm\frac{2\pi}{a}\hat{y}, \quad \pm\frac{2\pi}{a}\hat{z}$

L-points: $\mathbf{k} = \pm\frac{\pi}{a}(\hat{x}+\hat{y}+\hat{z}), \quad \pm\frac{\pi}{a}(-\hat{x}+\hat{y}+\hat{z}),$

$\pm\frac{\pi}{a}(\hat{x}-\hat{y}+\hat{z}), \quad \pm\frac{\pi}{a}(\hat{x}+\hat{y}-\hat{z})$

K-points: $\mathbf{k} = \pm\frac{3}{2}\frac{\pi}{a}(\hat{x}+\hat{y})$, etc.

W-points: $\mathbf{k} = \pm\frac{\pi}{a}(2\hat{x}+\hat{y})$, etc.

Figure 2.5 Reciprocal lattice points, primitive vectors, first Brillouin zone, and several high symmetry points for the face-centered cubic direct lattice. This is reciprocal space for crystals with the diamond, sphalerite, and sodium chloride structures.

Empty Lattice Model for fcc

- In the discussion to follow it is convenient to express the reciprocal lattice vectors (points) in terms of their components along orthogonal unit vectors .

Using (1.23) in (2.38), we obtain

$$\mathbf{b}_1 = \frac{2\pi}{a}(-\hat{x} + \hat{y} + \hat{z}), \quad \mathbf{b}_2 = \frac{2\pi}{a}(\hat{x} - \hat{y} + \hat{z}), \quad \mathbf{b}_3 = \frac{2\pi}{a}(\hat{x} + \hat{y} - \hat{z})$$

$$\mathbf{K} = \frac{2\pi}{a}[(-h + k + l)\hat{x} + (h - k + l)\hat{y} + (h + k - l)\hat{z}] \quad (2.40)$$

$$\mathbf{K} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$$

- Let us first consider the lowest-lying energy band given by (2.37).

→ This is given by $h = k = l = 0$ or $\mathbf{K} = 0$.
The minimum of the band is $\mathscr{E} = 0$ at $\mathbf{k} = 0$ or at the Γ-point. The energy of this band increases ***parabolically*** with increasing **k** in the Brillouin zone until it reaches the values, $\mathscr{E} = (\hbar^2/2m)(2\pi/a)^2$ at the X-points, $\mathscr{E} = (\hbar^2/2m)(\sqrt{3}\,\pi/a)^2$ at the L-points, and so on in different directions.

-From (2.35) there is ***only one*** wavefunction that corresponds to this range of energies up to the zone boundaries, so this lowest-lying energy band is nondegenerate (except for the two fold spin degeneracy).

- We see from (2.37) that there are an infinite number of energy values for **k** = 0, corresponding to the infinite number of reciprocal lattice points.

Empty Lattice Model for fcc

- The next energy value above zero at the Γ-point occurs for $h = \pm 1$, or $k = \pm 1$, or $l = \pm 1$ in (2.38). From (2.40) these reciprocal lattice vectors are given by

$$\mathbf{K} = \frac{2\pi}{a}(-\hat{x} + \hat{y} + \hat{z}) \qquad (2.41)$$

for $h = \pm 1$, and so on. Since the magnitude of all these **K** vectors is the same, $(2\pi/a)\sqrt{3}$, the energy level is

$$\mathscr{E}(0) = \frac{\hbar^2}{2m}\left(\frac{2\sqrt{3}\,\pi}{a}\right)^2 \qquad (2.42)$$

- From. (2.35) there are eight wavefunctions that have this energy at k = 0, so this point is ***eightfold degenerate***.

- The next highest level above (2.42) occurs for $h = k = 1$, $l = 0$ and so on, or for

$$\mathbf{K} = \frac{2\pi}{a}(2\hat{z}) \qquad (2.43)$$

and so on. The energy of this point ***is sixfold degenerate*** and has the value

$$\mathscr{E}(0) = \frac{\hbar^2}{2m}\left(\frac{4\pi}{a}\right)^2 \qquad (2.44)$$

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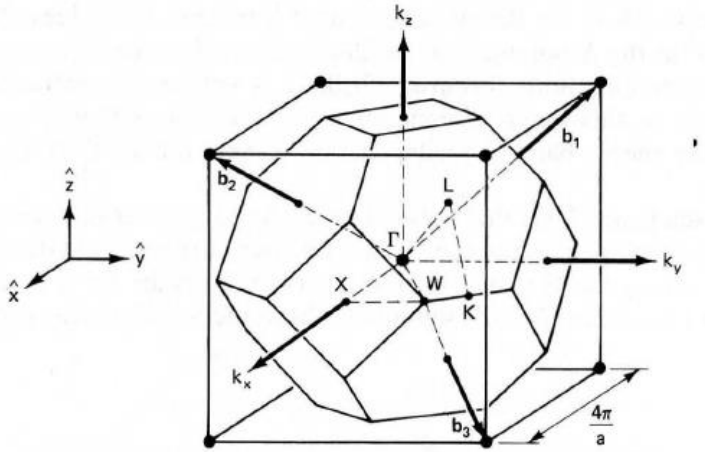

Figure 2.5 Reciprocal lattice points, primitive vectors, first Brillouin zone, and several high symmetry points for the face-centered cubic direct lattice. This is reciprocal space for crystals with the diamond, sphalerite, and sodium chloride structures.

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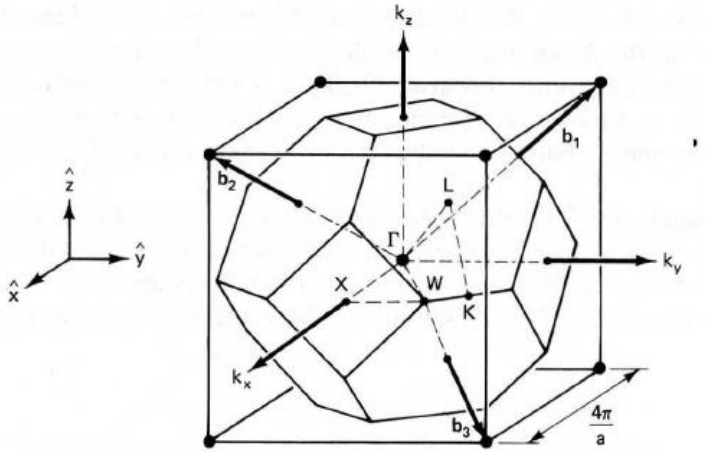

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Empty Lattice Model for fcc

- By generating a sufficient number of energy levels at the Γ-point and following them out to the desired high-symmetry points on the zone boundary with (2.37), we obtain the empty lattice energy bands for the face-centered cubic lattice shown in Fig. 2.6.

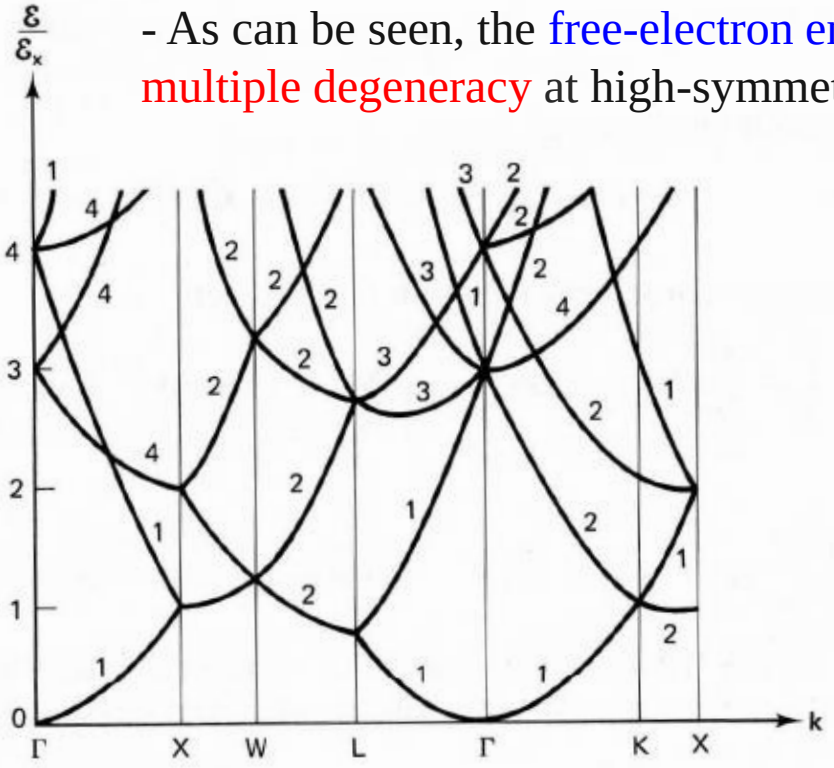

Figure 2.6 Empty lattice energy bands for the face-centered cubic direct lattice. The numbers indicate the degeneracy of each band. $\mathscr{E}_x = (\hbar^2/2m)(2\pi/a)^2$ is the energy at the X-points. [After F. Herman in *An Atomistic Approach to the Nature and Properties of Materials*, ed. J. A. Pask (New York: Wiley, 1967).]

- As can be seen, the free-electron energy bands are fairly complicated , with multiple degeneracy at high-symmetry points, and the electrons can range through ***all*** energy values.

- When we apply a ***periodic*** potential to the one-electron Schrodinger equation, however, some of the degeneracy at the zone boundaries will be removed and the electrons will be constrained to certain energy values.

- These effects are demonstrated in the nearly free electron model.

Empty Lattice Model for fcc

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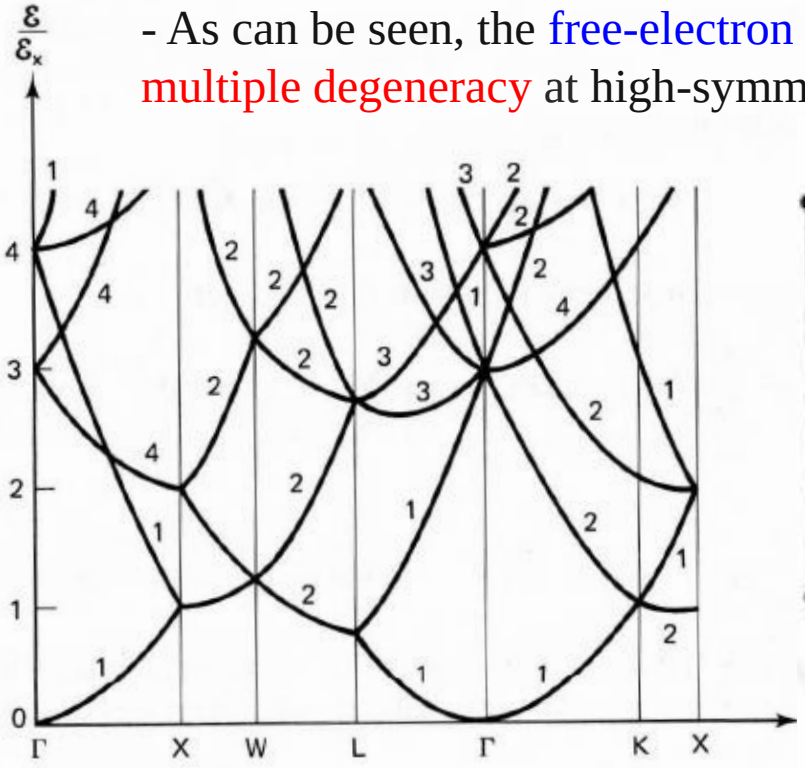

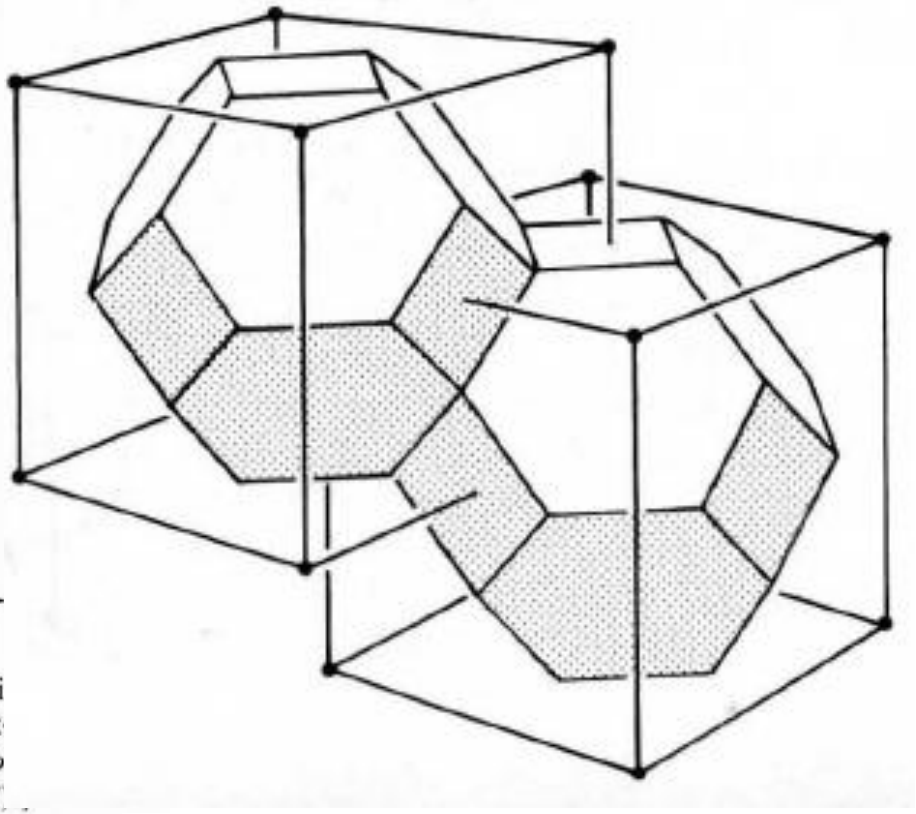

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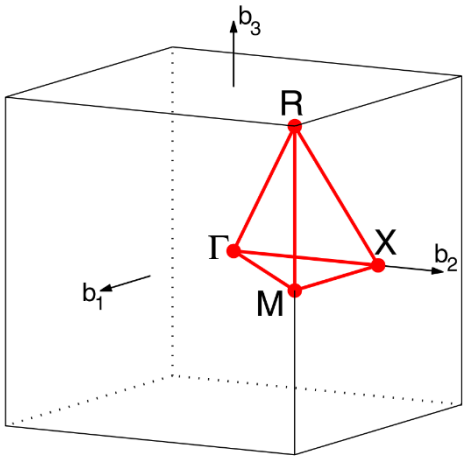

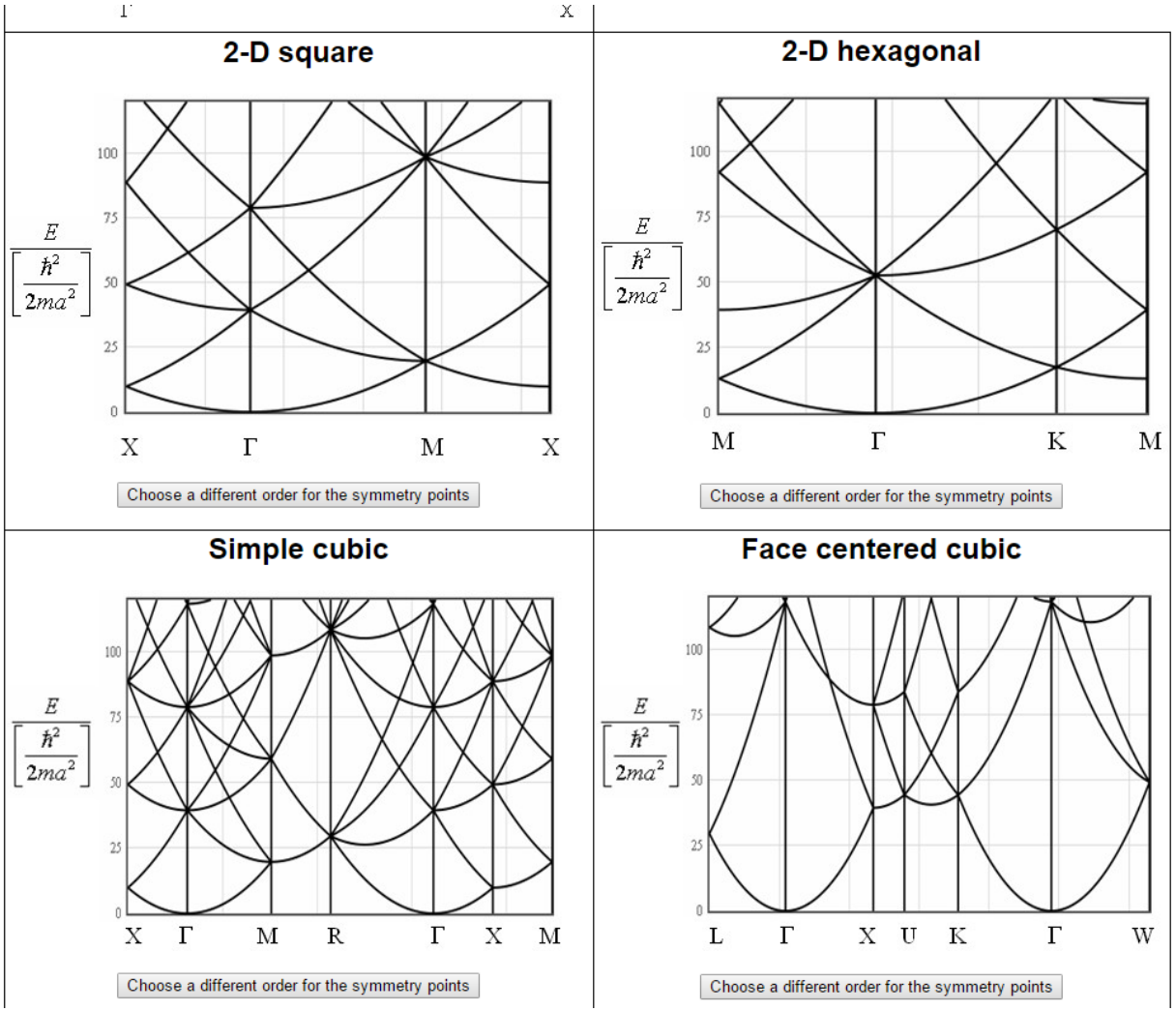

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