Condensed Matter Physics

PHY 5111

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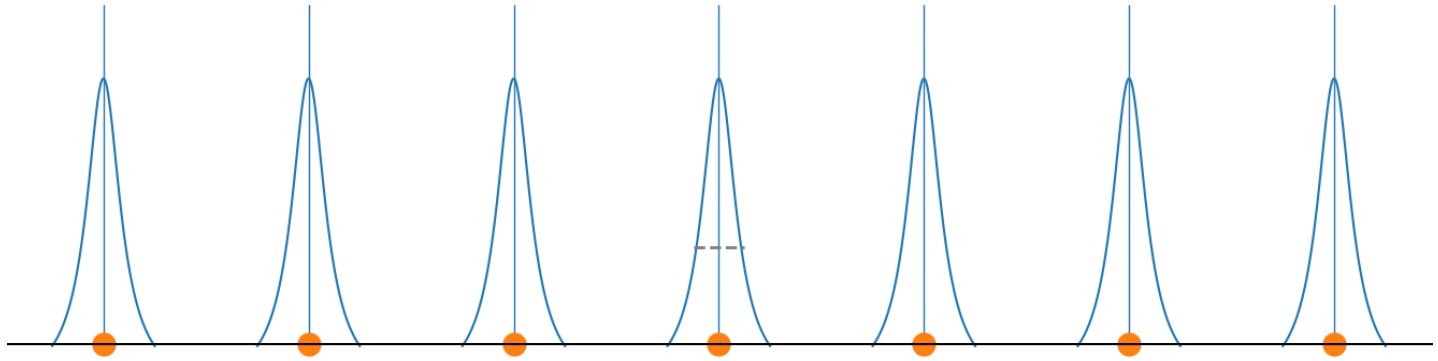
Nearly Free and Tightly Bound Electrons

Condensed Matter Physics – Michael P. Marder

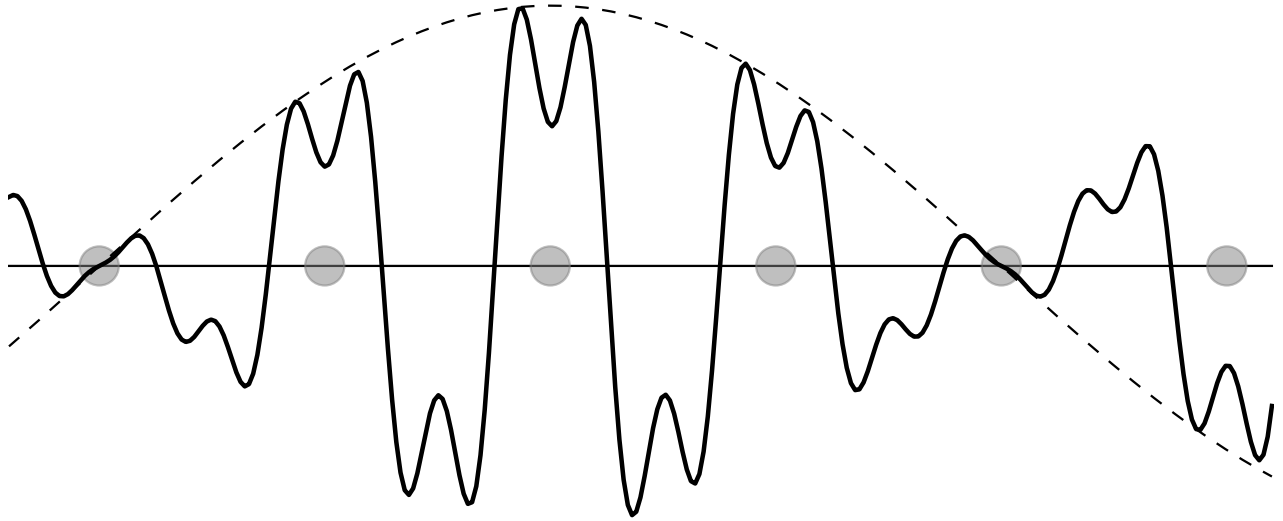
Chapter 8

Bloch's Theorem

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

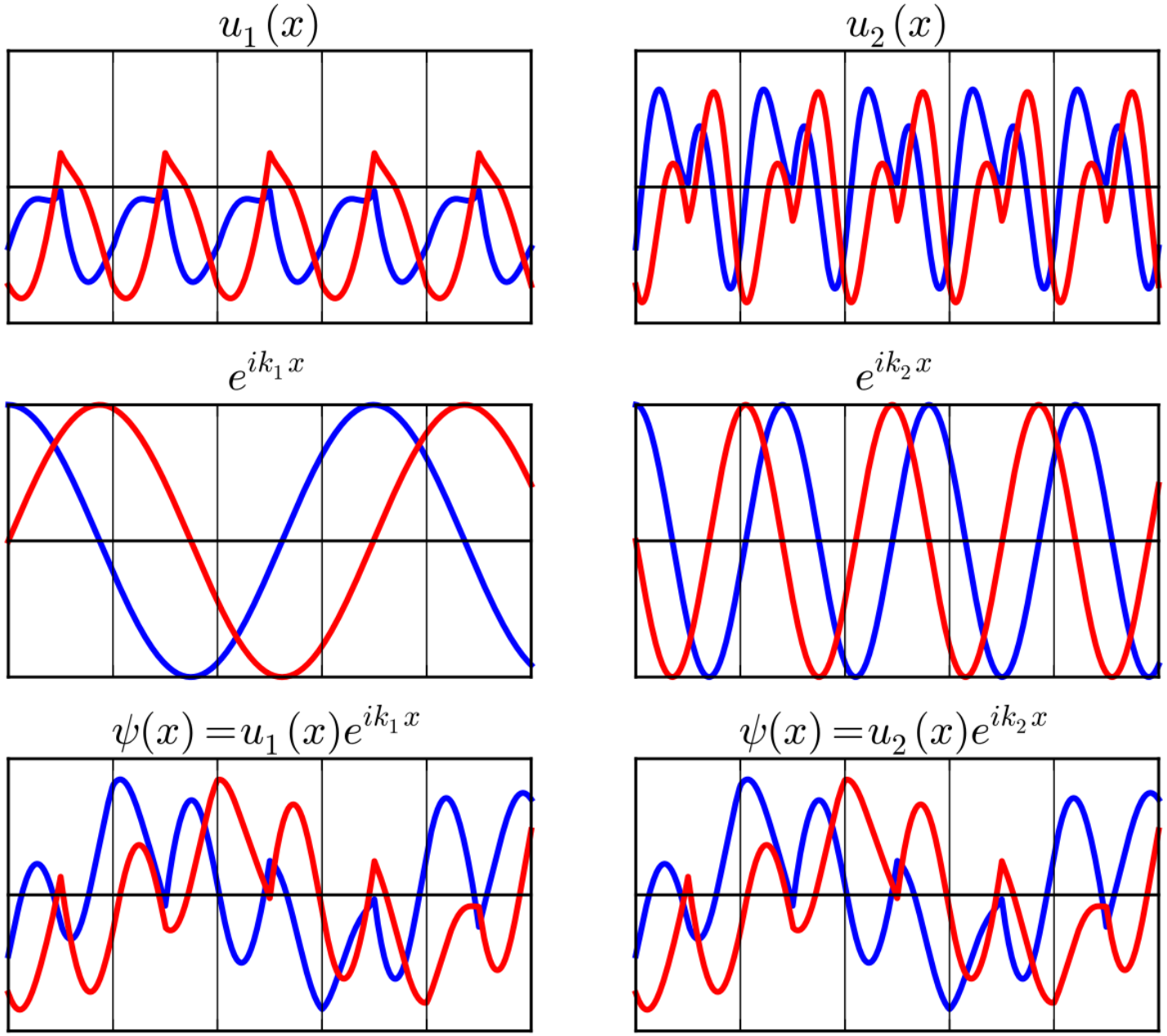


$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u(\mathbf{r})$$

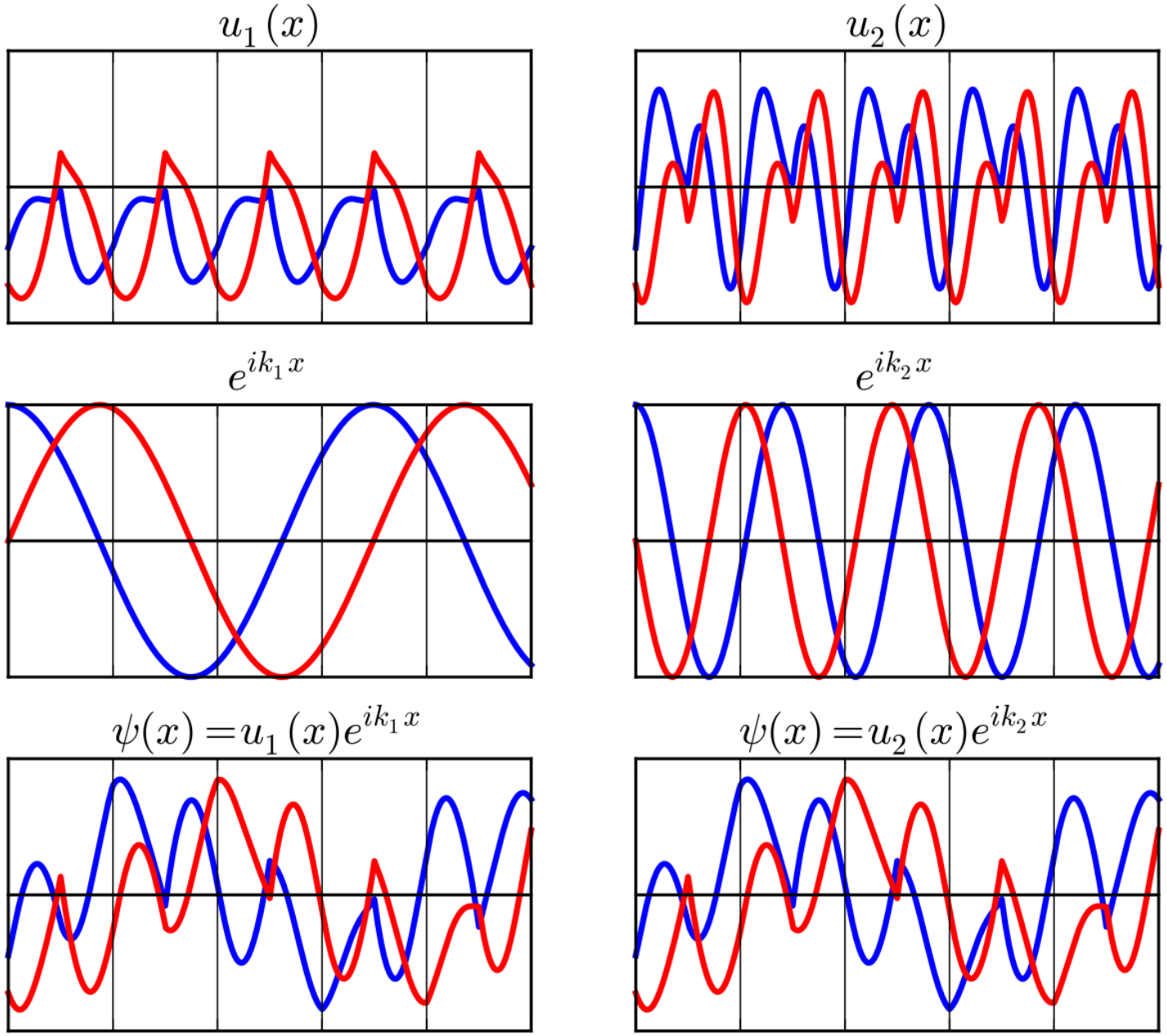


Bloch wave function

$$\psi(\mathbf{r}) = \mathrm{e}^{\mathbf{ik}\cdot\mathbf{r}}\, u(\mathbf{r})$$



A Bloch wave function (bottom) can be broken up into the product of a periodic function (top) and a plane-wave (center). The left side and right side represent the same Bloch state broken up in two different ways, involving the wave vector k_1 (left) or k_2 (right). The difference (k_1−k_2) is a reciprocal lattice vector. In all plots, blue is real part and red is imaginary part.



How strong is the interaction?

Nearly Free Electrons

$$(\mathcal{E}^0_{\vec{q}} - \mathcal{E})\psi\ (\vec{q}) + \sum_{\vec{K}} U_{\vec{K}}\psi(\vec{q} - \vec{K}) = 0.$$

A formal means to treat the potential U as small is to define

$$U_{\vec{K}} = \Delta\ w_{\vec{K}}$$

Δ is the small parameter in terms of which perturbation theory will expand.

$$\psi(\vec{q}) = \psi^{(0)}\ (\vec{q}) + \psi^{(1)}\ (\vec{q})\ \Delta + \ldots; \quad \mathcal{E} = \mathcal{E}^{(0)} + \Delta\ \mathcal{E}^{(1)} + \ldots.$$

Nearly Free Electrons

Zeroth Order:

$$\psi^{(0)}(\vec{q})\left[\mathcal{E}^{0}_{\vec{q}}-\mathcal{E}^{(0)}\right]=0.$$

Extended zone scheme:

$$\psi^{(0)}_{\vec{k}}(\vec{q})=\delta_{\vec{k},\vec{q}}$$

$$\Rightarrow \psi^{(0)}_{\vec{k}}(\vec{r})=e^{i\vec{k}\cdot\vec{r}}$$

$$\Rightarrow \mathcal{E}^{(0)}=\mathcal{E}^{0}_{\vec{k}}$$

Reduced zone scheme:

$$\psi^{(0)}_{n\vec{k}}(\vec{q})=\delta_{\vec{K}_n+\vec{k},\vec{q}}$$

$$\Rightarrow \psi^{(0)}_{n\vec{k}}(\vec{r})=e^{i(\vec{k}+\vec{K}_n)\cdot\vec{r}}$$

$$\Rightarrow \mathcal{E}^{(0)}_{nk}=\mathcal{E}^{0}_{\vec{k}+\vec{K}_n}.$$

Nearly Free Electrons

First Order:

$$[\mathcal{E}^0_{\vec{q}} - \mathcal{E}^0_{\vec{k}}]\psi^{(1)}_{\vec{k}}(\vec{q}) + \sum_{\vec{K}} w_{\vec{K}}\psi^{(0)}_{\vec{k}}(\vec{q}-\vec{K}) - \mathcal{E}^{(1)}\psi^{(0)}_{\vec{k}}(\vec{q}) = 0.$$

Taking $\psi^{(0)}_{\vec{k}}$ from previous solution and evaluation at $\vec{q} = \vec{k}$ gives $\mathcal{E}^{(1)} = w_0$.

$$\psi^{(1)}_{\vec{k}}(\vec{q}) = \left\{ \sum_{\vec{K}\neq 0} w_{\vec{K}} \frac{\delta_{\vec{k},\vec{q}-\vec{K}}}{\mathcal{E}^0_{\vec{k}} - \mathcal{E}^0_{\vec{K}+\vec{k}}} \right\}$$

$$\psi_{\vec{k}}(\vec{q}) \approx \delta_{\vec{q}\vec{k}} + \left\{ \sum_{\vec{K}\neq 0} U_{\vec{K}} \frac{\delta_{\vec{k},\vec{q}-\vec{K}}}{\mathcal{E}^0_{\vec{k}} - \mathcal{E}^0_{\vec{K}+\vec{k}}} \right\}$$

$$\mathcal{E}^0_{\vec{k}} = \mathcal{E}^0_{\vec{K}+\vec{k}}$$

Degenerate Perturbation Theory

One way to obtain a resolution of this problem is to recast Schrödinger's equation in variational form, as discussed in Appendix B. Solving the Schrödinger's equation is equivalent to finding extrema of the functional

$$\langle\psi|(\hat{\mathcal{H}}-\mathcal{E})|\psi\rangle.$$

$$|\psi\rangle=\sum_{i=1}^{l}C_i|\psi_i\rangle.$$

$$\sum_j\langle\psi_i|(\hat{\mathcal{H}}-\mathcal{E})|\psi_j\rangle C_j=0,$$

$$\hat{\mathcal{H}}_{ij}^{\text{eff}}=\langle\psi_i|(\hat{\mathcal{H}}-\mathcal{E})|\psi_j\rangle$$

Bloch's Theorem in Three Dimensions

$$(\mathcal{E}^0_{\vec{q}} - \mathcal{E})\psi(\vec{q}) + \sum_{\vec{K}} U_{\vec{K}}\psi(\vec{q} - \vec{K}) = 0.$$

$$\hat{\mathcal{H}} = \sum_{\vec{q}'} |\vec{q}'\rangle \mathcal{E}^0_{\vec{q}'} \langle \vec{q}'| + \sum_{\vec{q}'\vec{K}'} |\vec{q}'\rangle U_{\vec{K}'} \langle \vec{q}' - \vec{K}'|.$$

$$\langle \vec{q}|\hat{\mathcal{H}} - \mathcal{E}|\psi\rangle$$

Degenerate Perturbation Theory

In the present case, the plan is to restrict all attention to wave functions that are linear combinations of the two vectors $|\psi_1\rangle = |\vec{k}\rangle$ and $|\psi_2\rangle = |\vec{k}+\vec{K}\rangle$, but otherwise solve the Hamiltonian exactly.

$$\begin{vmatrix} \mathcal{E}^0_{\vec{k}} + U_0 - \mathcal{E} & U_{-\vec{K}} \\ U_{\vec{K}} & \mathcal{E}^0_{\vec{k}+\vec{K}} + U_0 - \mathcal{E} \end{vmatrix}$$

$$\mathcal{E} = U_0 + \frac{\mathcal{E}^0_{\vec{k}} + \mathcal{E}^0_{\vec{k}+\vec{K}}}{2} \pm \sqrt{\frac{[\mathcal{E}^0_{\vec{k}} - \mathcal{E}^0_{\vec{k}+\vec{K}}]^2}{4} + |U_{\vec{K}}|^2}.$$

Because $U(\vec{r})$ is real, $U_{-\vec{K}} = U^*_{\vec{K}}$.

Degenerate Perturbation Theory

At the point where $\mathcal{E}^0_{\vec{k}+\vec{K}} = \mathcal{E}^0_{\vec{k}}$ is exactly satisfied, one obtains

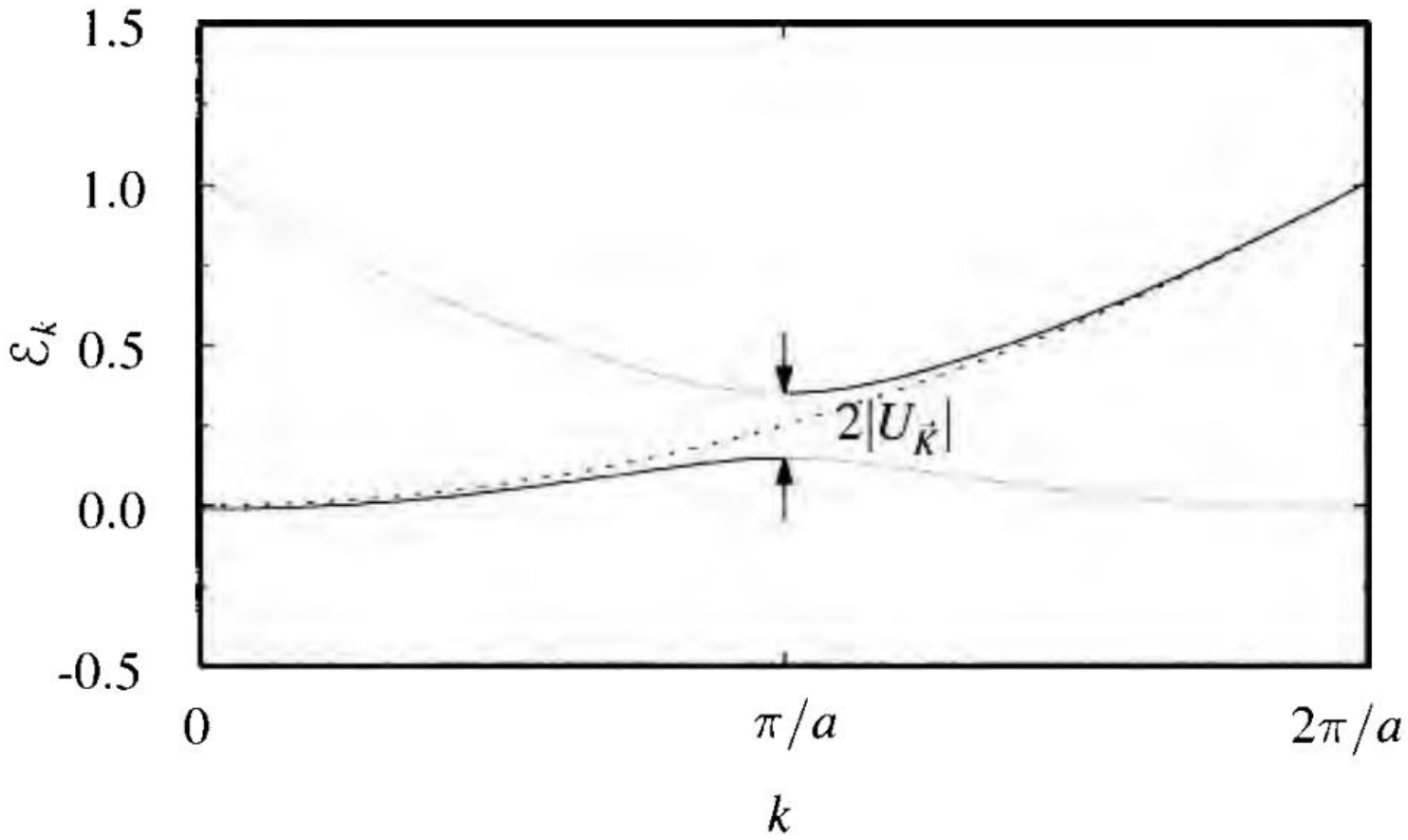
$$\mathcal{E} = \mathcal{E}^0_{\vec{k}} + U_0 \pm |U_{\vec{K}}|.$$

Thus the *energy gap* $\mathcal{E}_g$ between bands is

$$\mathcal{E}_g = 2|U_{\vec{K}}|.$$

Degenerate Perturbation Theory (1D)

$$\mathcal{E}_g = 2|U_{\vec{K}}|$$



Brillouin Zones

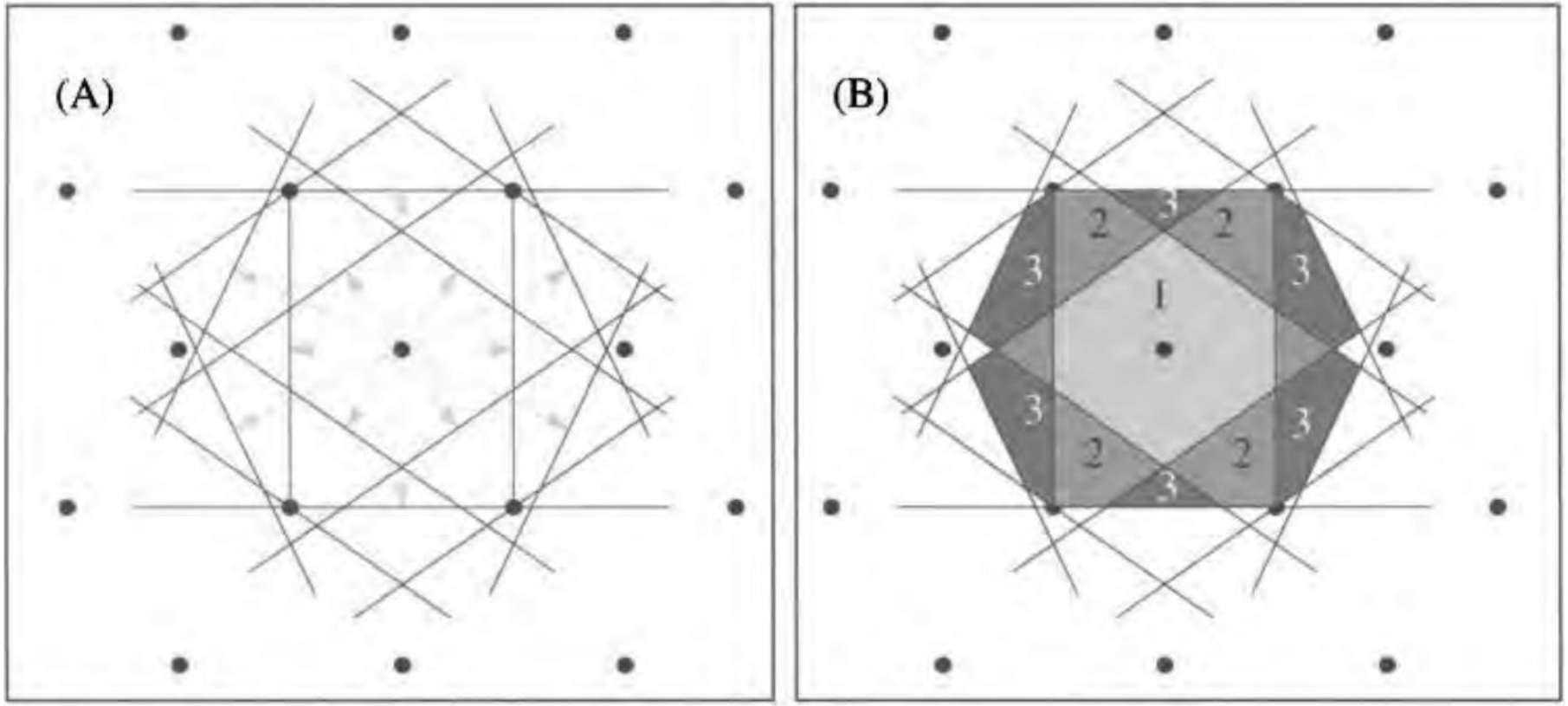


Figure 8.2. Construction of Brillouin zones. (A) Perpendicular bisectors are drawn between the origin and all nearby reciprocal lattice points. These are the zone boundaries. (B) The first, second, and third Brillouin zones are shaded in different colors. The first zone is the set of points closer to the origin than any other reciprocal lattice point, the second zone is the set of points that one reaches by passing a minimum of one zone boundary, and the third zone is the set of points that one reaches by crossing a minimum of two zone boundaries.

Brillouin Zones

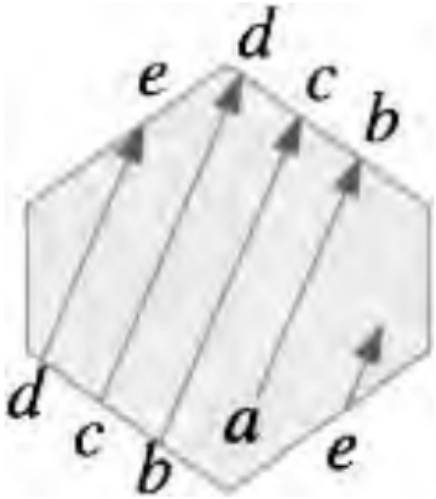
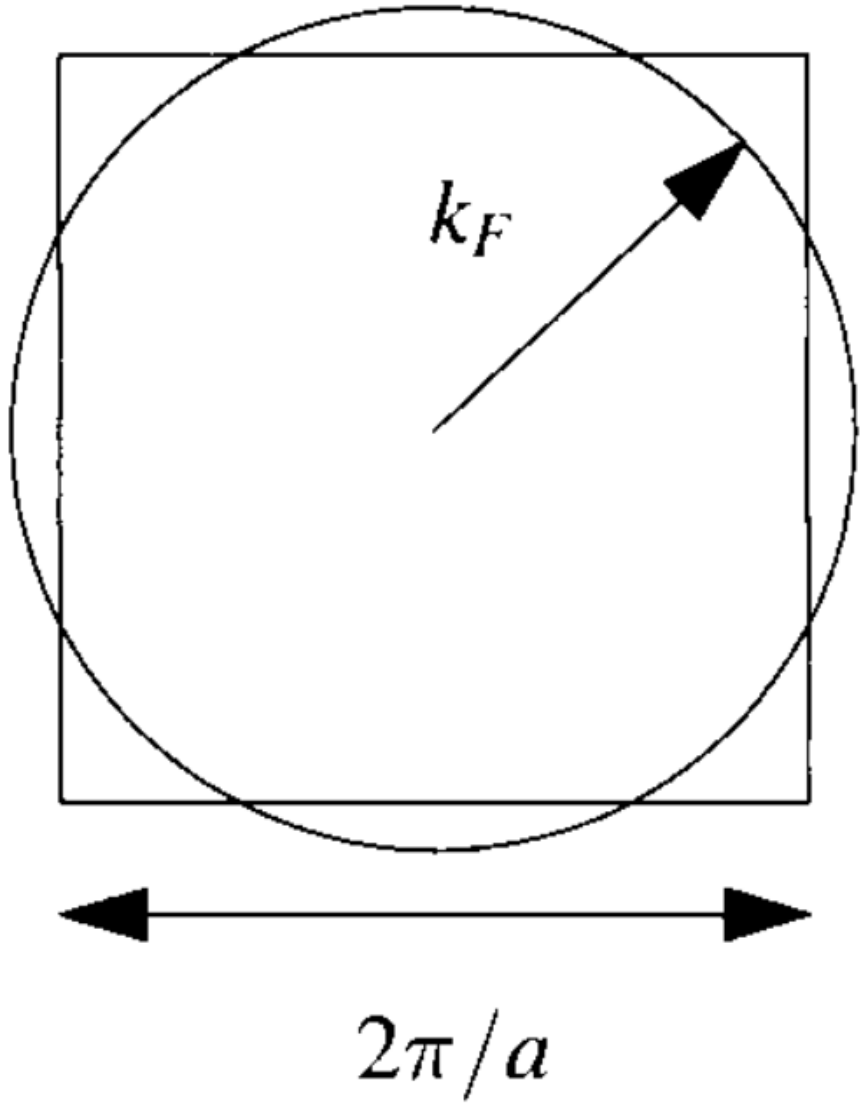
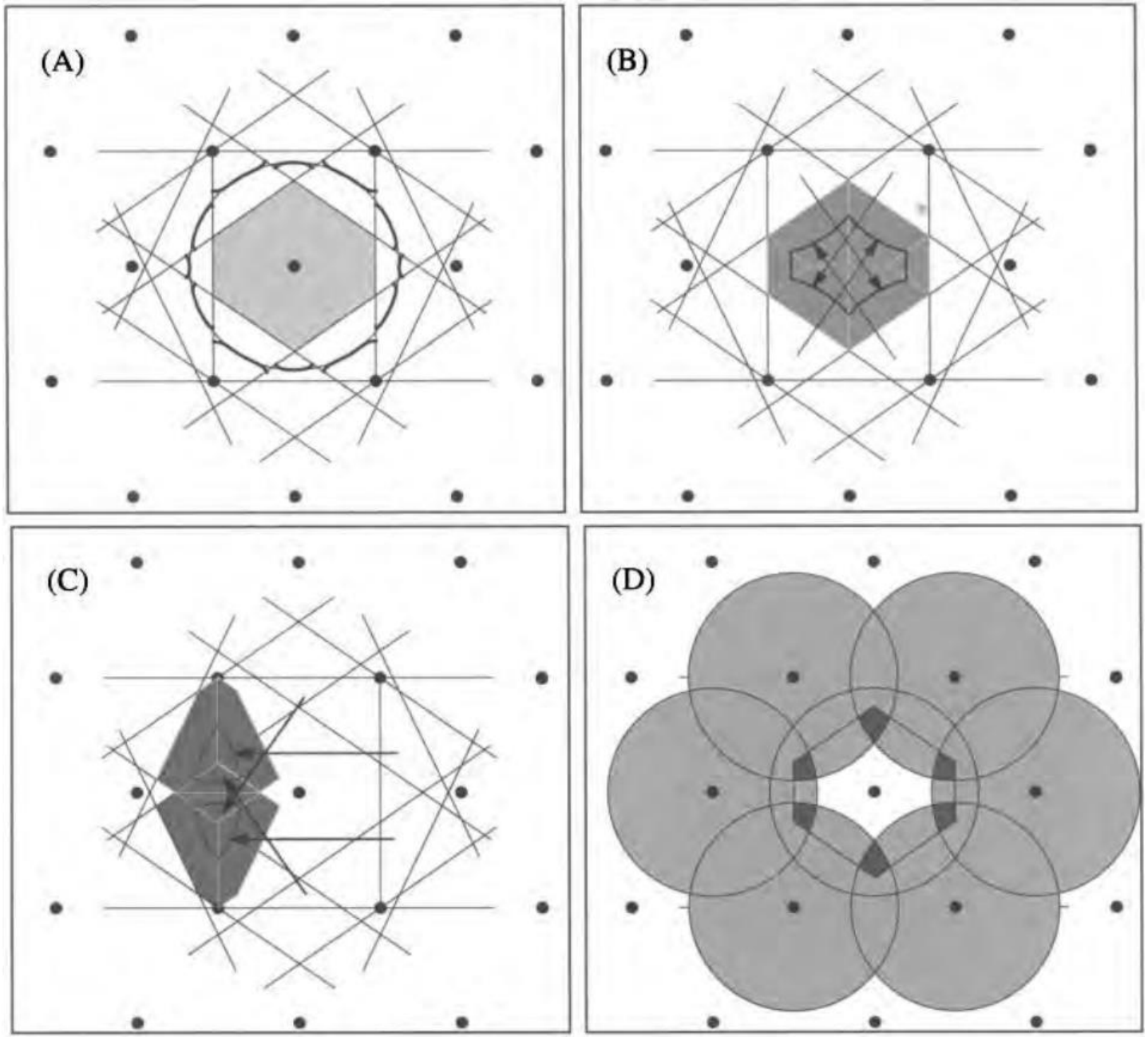


Figure 8.3. The first Brillouin zone can be viewed as a closed surface whose edges are connected to each other. Therefore a path that appears to be leaving from one edge is actually entering from another, as shown in this representation of straight line motion. This view of the first Brillouin zone is motivated by the fact that physical quantities such as $\mathcal{E}_{\vec{k}}$ are periodic functions over the first Brillouin zone.

Brillouin zone boundary intersection for square lattice in two dimensions



Nearly Free Electron Fermi Surfaces



Brillouin zone	Extended zone scheme	Reduced zone scheme
First	Empty	Empty
Second		
Third		

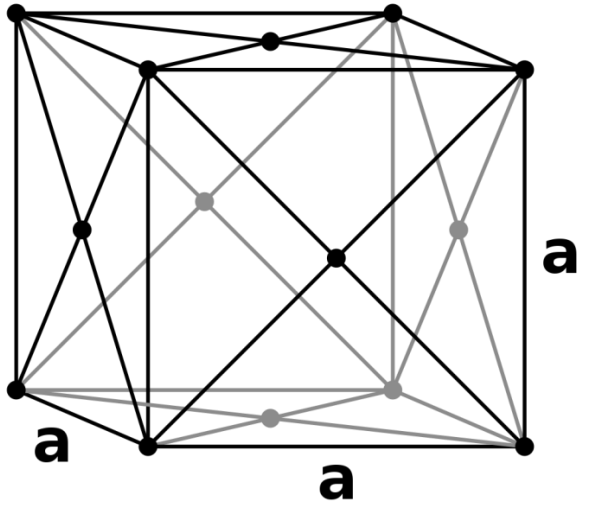
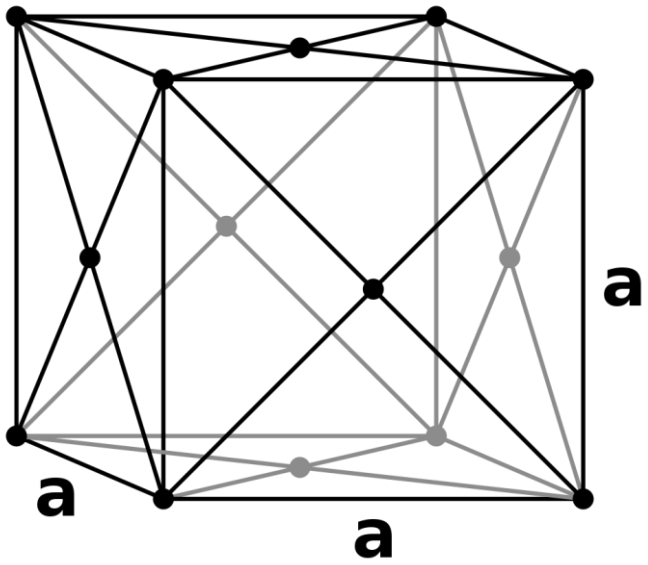


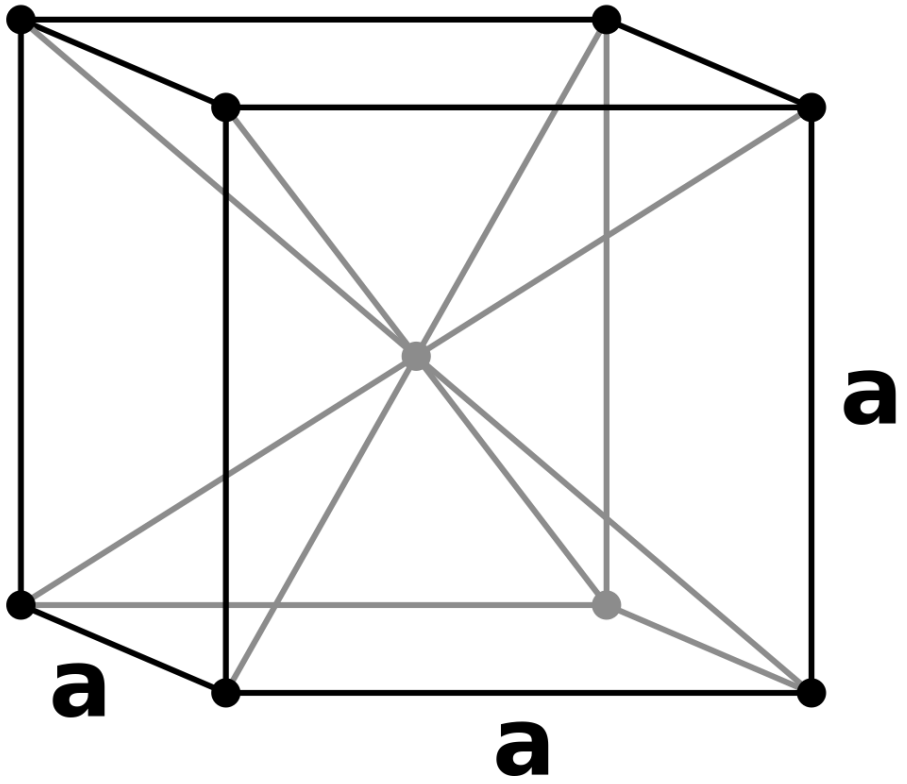
Figure 8.5. Fermi surface for three electrons per site in an fcc crystal. On the left the free-electron Fermi surface is shown in the extended zone scheme, while on the right the same surfaces are projected back into the first Brillouin zone in the reduced zone scheme.



Brillouin zone	1 electron/cell	2 electrons/cell	3 electrons/cell
First			
Second			
Third			

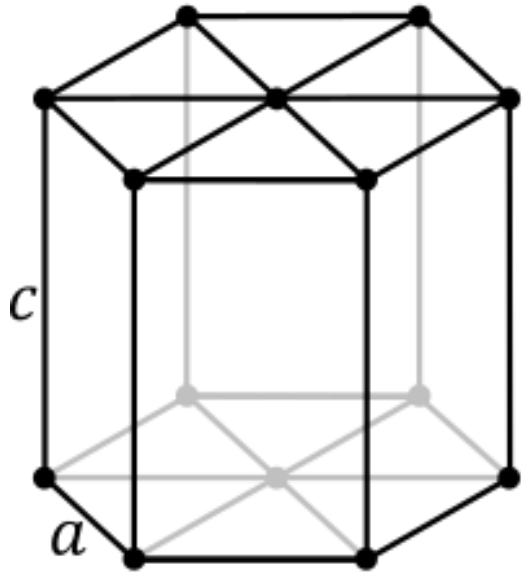
Figure 8.6. Nearly free electron Fermi surfaces for fcc crystals. With three electrons per unit cell the Fermi surface extends slightly into the fourth Brillouin zone, but the pocket is very small and is not shown.

Nearly free electron Fermi surfaces for bcc crystals



Brillouin zone	1 electron/cell	2 electrons/cell	3 electrons/cell
First			
Second			
Third			
Fourth			

Nearly free electron Fermi surfaces for hexagonal crystals



Brillouin zone	2 electrons/cell	4 electrons/cell	4 electrons/cell with hcp extinction
First			
Second			
Third			
Fourth			