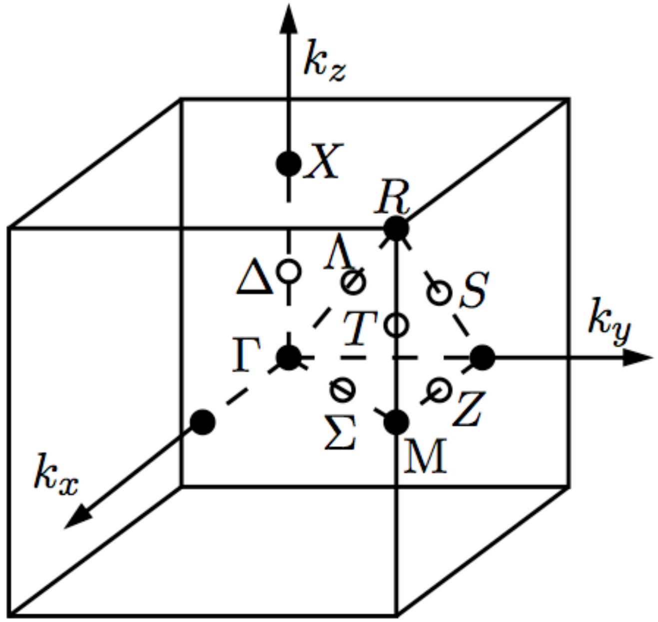
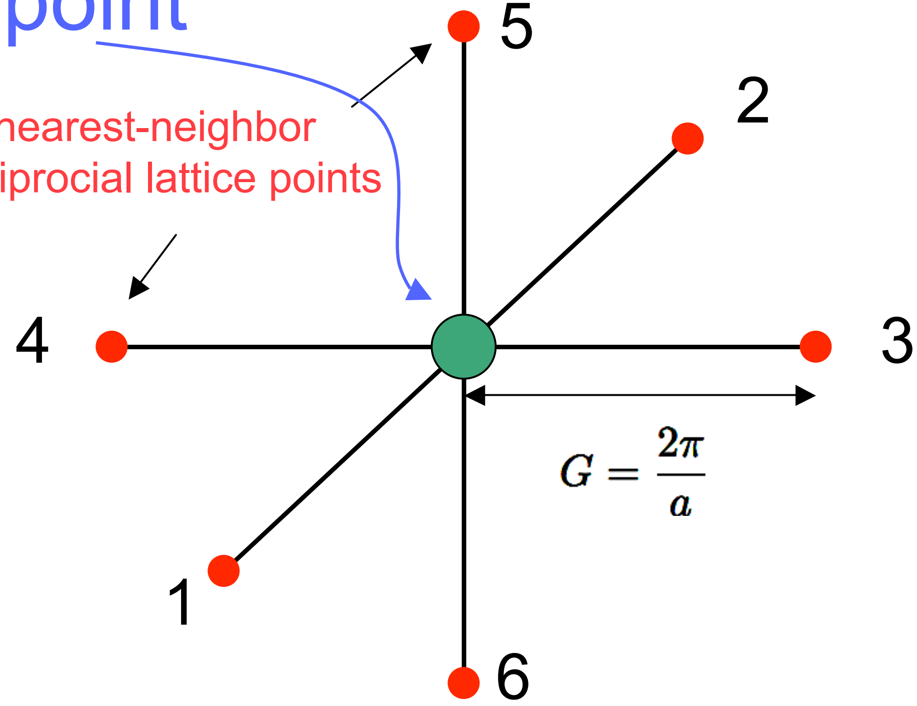
Nearly free electron approximation - simple cubic lattice

Brillouin zone



Γ-point



$$\vec{G}_1 = \frac{2\pi}{a}(1,0,0), \quad \vec{G}_2 = \frac{2\pi}{a}(-1,0,0),$$
$$\vec{G}_3 = \frac{2\pi}{a}(0,1,0), \quad \vec{G}_4 = \frac{2\pi}{a}(0,-1,0),$$
$$\vec{G}_5 = \frac{2\pi}{a}(0,0,1), \quad \vec{G}_6 = \frac{2\pi}{a}(0,0,-1).$$

➡

$$u_{\vec{k}=0}(\vec{r}) = \sum_{n=1}^{6} c_n e^{i\vec{r}\cdot\vec{G}_n}$$

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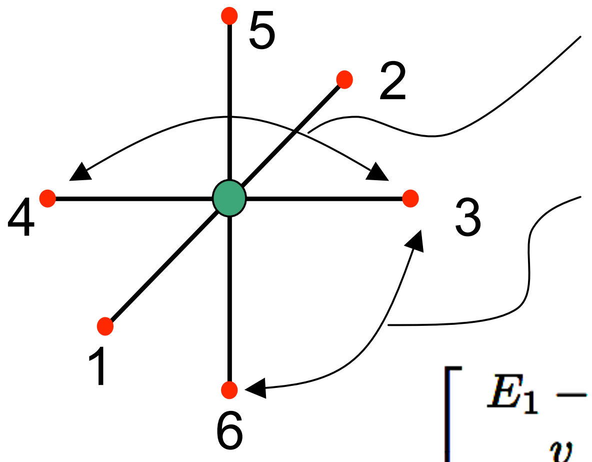

$$v = V_{2\vec{G}_n}$$

$$u = V_{\vec{G}_n + \vec{G}_{n'}}$$

$$E_1 = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2$$

$$\det \begin{bmatrix} E_1 - E & v & u & u & u & u \\ v & E_1 - E & u & u & u & u \\ u & u & E_1 - E & v & u & u \\ u & u & v & E_1 - E & u & u \\ u & u & u & u & E_1 - E & v \\ u & u & u & u & v & E_1 - E \end{bmatrix} = 0$$

$$\vec{G}_1 = \tfrac{2\pi}{a}(1,0,0), \quad \vec{G}_2 = \tfrac{2\pi}{a}(-1,0,0),$$
$$\vec{G}_3 = \tfrac{2\pi}{a}(0,1,0), \quad \vec{G}_4 = \tfrac{2\pi}{a}(0,-1,0),$$
$$\vec{G}_5 = \tfrac{2\pi}{a}(0,0,1), \quad \vec{G}_6 = \tfrac{2\pi}{a}(0,0,-1).$$

$\Rightarrow$

$$u_{\vec{k}=0}(\vec{r}) = \sum_{n=1}^{6} c_n e^{i\vec{r}\cdot\vec{G}_n}$$

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$$u_{\vec{k}=0}(\vec{r}) = \sum_{n=1}^{6} c_n e^{i\vec{r}\cdot\vec{G}_n}$$

$$G = \frac{2\pi}{a}$$

Γ	$E = \epsilon_{n\boldsymbol{k}=\boldsymbol{G}_1}$	$(c_1, c_2, c_3, c_4, c_5, c_6)$	$u_{\boldsymbol{k}=0}(\boldsymbol{r})$	d_Γ
Γ_1^+	$E_1 + v + 4u$	$(1,1,1,1,1,1)/\sqrt{(6)}$	$\phi_0 = \cos Gx + \cos Gy + \cos Gz$	1
Γ_3^+	$E_1 + v - 2u$	$(-1,-1,-1,-1,2,2)/2\sqrt{3}$ $(1,1,-1,-1,0,0)/2$	$\phi_{3z^2-r^2} = 2\cos Gz - \cos Gx - \cos Gy$, $\phi_{\sqrt{3}(x^2-y^2)} = \sqrt{3}(\cos Gx - \cos Gy)$	2
Γ_4^-	$E_1 - v$	$(1,-1,0,0,0,0)/\sqrt{2}$ $(0,0,1,-1,0,0)/\sqrt{2}$ $(0,0,0,0,1,-1)/\sqrt{2}$	$\phi_x = \sin Gx$ $\phi_y = \sin Gy$ $\phi_z = \sin Gz$	3

even	basis function	odd	basis function
Γ_1^+	$1, x^2+y^2+z^2$	Γ_1^-	$xyz(x^2-y^2)(y^2-z^2)(z^2-x^2)$
Γ_2^+	$(x^2-y^2)(y^2-z^2)(z^2-x^2)$	Γ_2^-	xyz
Γ_3^+	$\{2z^2-x^2-y^2, \sqrt{3}(x^2-y^2)\}$	Γ_3^-	$xyz\{2z^2-x^2-y^2, \sqrt{3}(x^2-y^2)\}$
Γ_4^+	$\{s_x, s_y, s_x\}$	Γ_4^-	$\{x, y, z\}$
Γ_5^+	$\{yz, zx, xy\}$	Γ_5^-	$xyz(x^2-y^2)(y^2-z^2)(z^2-x^2)\{yz, zx, xy\}$

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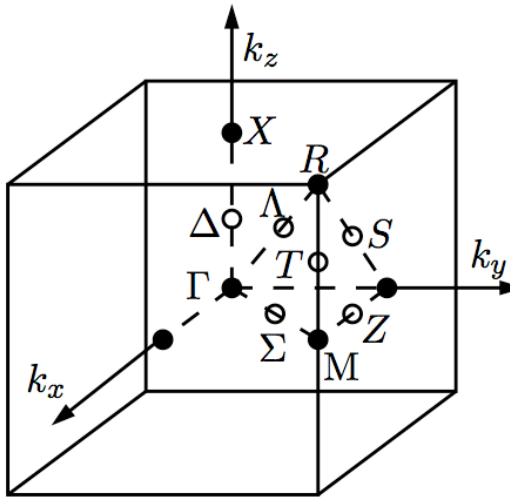

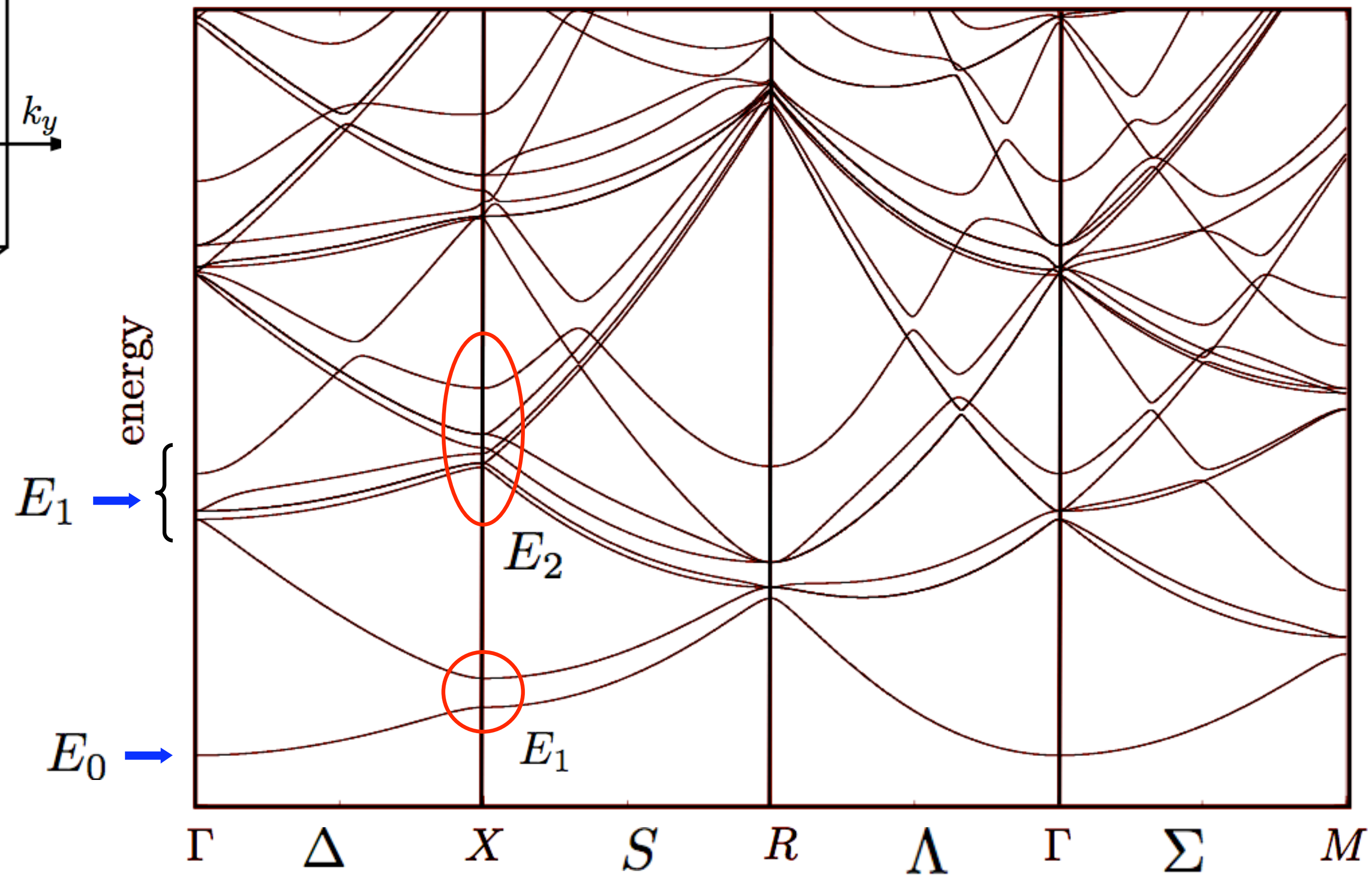

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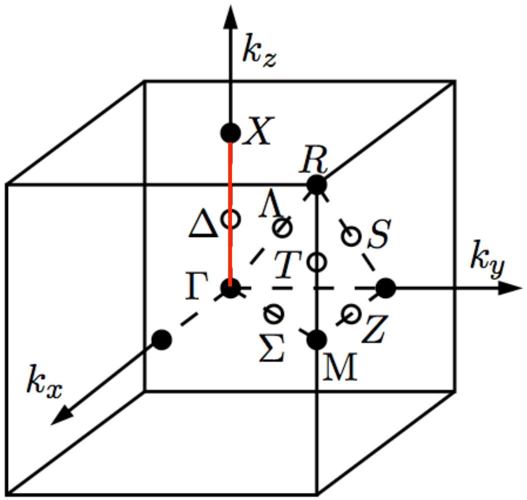

Δ-line

O_h	C_{4v}	
Γ_1^+	Δ_1	1
Γ_3^+	$\Delta_1 \oplus \Delta_3$	1+1
Γ_4^-	$\Delta_1 \oplus \Delta_5$	1+2

representation	base function
Δ_1	$1, z$
Δ_2	$xy(x^2 - y^2)$
Δ_3	$x^2 - y^2$
Δ_4	xy
Δ_5	$\{x, y\}$

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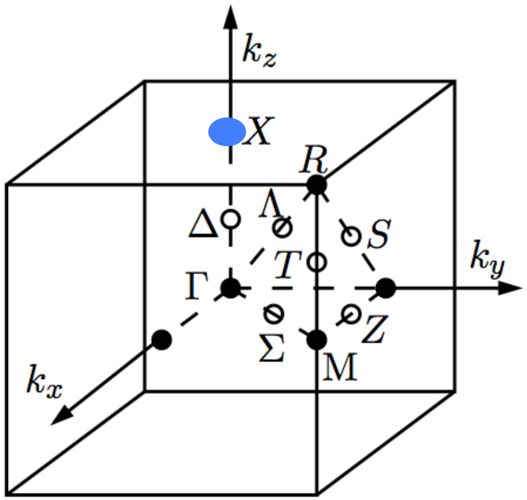

X-point

$$E_0 = \frac{\hbar^2}{2m}\left(\frac{G}{2}\right)^2$$

parabolas around

$$\vec{G}_1 = \vec{0} \qquad \vec{G}_2 = \frac{2\pi}{a}(0,0,1)$$

$$X_1^+: \quad E = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 - |V_{\vec{G}_2}|, \quad e^{iG_2 z/2}\cos\left(\frac{G_2 z}{2}\right),$$

$$X_2^-: \quad E = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 + |V_{\vec{G}_2}|, \quad e^{iG_2 z/2}\sin\left(\frac{G_2 z}{2}\right).$$

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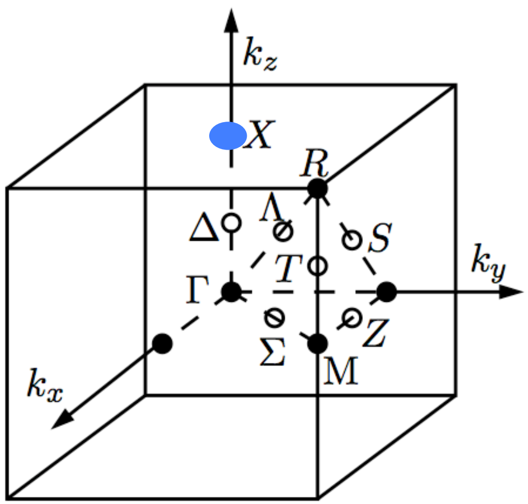
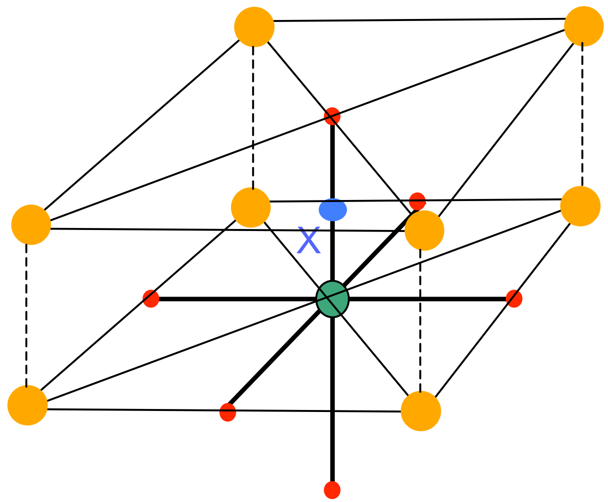


X-point

$$E_2 = \frac{\hbar^2}{2m}\left(\frac{\sqrt{5}\pi}{a}\right)^2$$



parabolas around

$$\vec{G}_1 = \frac{2\pi}{a}(1,0,0), \quad \vec{G}_2 = \frac{2\pi}{a}(1,0,1), \quad \vec{G}_3 = \frac{2\pi}{a}(-1,0,0), \quad \vec{G}_4 = \frac{2\pi}{a}(-1,0,1),$$

$$\vec{G}_5 = \frac{2\pi}{a}(0,1,0), \quad \vec{G}_6 = \frac{2\pi}{a}(0,1,1), \quad \vec{G}_7 = \frac{2\pi}{a}(0,-1,0), \quad \vec{G}_8 = \frac{2\pi}{a}(0,-1,1).$$

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X-point

$$E_2 = \frac{\hbar^2}{2m}\left(\frac{\sqrt{5}\pi}{a}\right)^2$$

representation	$u_{\boldsymbol{k}=\pi(0,0,1)/a}(\boldsymbol{r})$	degeneracy
X_1^+	$(\cos(Gx)+\cos(Gy))e^{iGz/2}\cos(Gz/2)$	1
X_3^+	$(\cos(Gx)-\cos(Gy))e^{iGz/2}\cos(Gz/2)$	1
X_5^+	$\{\sin(Gx)e^{-iGz/2}\sin(Gz/2), \sin(Gy)e^{iGz/2}\sin(Gz/2)\}$	2
X_2^-	$(\cos(Gx)+\cos(Gy))e^{iGz/2}\sin(Gz/2)$	1
X_4^-	$(\cos(Gx)-\cos(Gy))e^{iGz/2}\sin(Gz/2)$	1
X_5^-	$\{\sin(Gx)e^{iGz/2}\cos(Gz/2), \sin(Gy)e^{iGz/2}\cos(Gz/2)\}$	2

even	base function	odd	base function
X_1^+	1	X_1^-	$xyz(x^2-y^2)$
X_2^+	$xy(x^2-y^2)$	X_2^-	z
X_3^+	x^2-y^2	X_3^-	xyz
X_4^+	xy	X_4^-	$z(x^2-y^2)$
X_5^+	$\{zx, zy\}$	X_5^-	$\{x, y\}$