1 One-dimensional lattice

1.1 Gap formation in the nearly free electron model

Periodic potential

$$V(x) = \sum_{n=-\infty}^{\infty} V_n \, e^{i(2\pi n/a)x} \tag{1}$$

Bloch function

$$\psi_k(x) = e^{ika} u_k(x) \tag{2}$$

$$u_k(x) = \sum_{n=-\infty}^{\infty} c_{nk} \, e^{i(2\pi n/a)x} \tag{3}$$

Schrödinger equation

$$\left[\frac{1}{2m}\left(k + \frac{\hbar}{i}\frac{d}{dx}\right)^2 + \sum_{n'=-\infty}^{\infty} V_{n'} \, e^{i(2\pi n'/a)x}\right]\left(\sum_{n=-\infty}^{\infty} c_{nk} \, e^{i(2\pi n/a)x}\right) = E \sum_{n=-\infty}^{\infty} c_{nk} \, e^{i(2\pi n/a)x} \tag{4}$$

$$\Downarrow$$

$$\sum_{n=-\infty}^{\infty} c_{nk}\varepsilon_{nk} e^{i(2\pi n/a)x} + \sum_{n,n'=-\infty}^{\infty} c_{nk} V_{n'} \, e^{i(2\pi (n+n')/a)x} = E \sum_{n=-\infty}^{\infty} c_{nk} \, e^{i(2\pi n/a)x} \tag{5}$$

$$\varepsilon_{nk} = \frac{\hbar^2 \left(k + \frac{2\pi n}{a}\right)^2}{2m} \tag{6}$$

$$\Downarrow$$

$$c_{nk}(\varepsilon_{nk} - E) + \sum_{n'=-\infty}^{\infty} V_{n-n'} c_{n'k} = 0 \tag{7}$$

For simplicity, let's choose

$$V(x) = V\left(e^{i(2\pi/a)x} + e^{-i(2\pi/a)x}\right) \tag{8}$$

$$\Downarrow$$

$$c_{nk}(\varepsilon_{nk} - E) + V c_{n-1,k} + V c_{n+1,k} = 0 \tag{9}$$

$$\Downarrow$$

$$c_{0k}(\varepsilon_{0k} - E) + V c_{-1,k} + V c_{1,k} = 0 \tag{10}$$

$$c_{1k}(\varepsilon_{1k} - E) + V c_{0,k} + V c_{2,k} = 0 \tag{11}$$

$$\vdots$$

$$c_{-1,k}(\varepsilon_{-1,k} - E) + V c_{-2,k} + V c_{0,k} = 0 \tag{12}$$

$$c_{-2,k}(\varepsilon_{-2,k} - E) + V c_{-3,k} + V c_{-1,k} = 0 \tag{13}$$

$$\vdots$$

$$\Downarrow$$

$$c_{0k}\left(\varepsilon_{0k}-E\right)+Vc_{-1,k}+\frac{V^2}{E-\varepsilon_{1k}}\left(c_{0,k}+c_{2,k}\right)+\ldots=0 \tag{14}$$

$$c_{-1,k}\left(\varepsilon_{-1,k}-E\right)+Vc_{0,k}+\frac{V^2}{E-\varepsilon_{-2,k}}\left(c_{-3,k}+c_{-1,k}\right)+\ldots=0 \tag{15}$$

Thus, for weak potential V and for

$$\varepsilon_{0k}\approx\varepsilon_{-1,k}\Longrightarrow k\simeq\frac{\pi}{a} \tag{16}$$

the first order approach

$$c_{0k}\left(\varepsilon_{0k}-E\right)+Vc_{-1,k}=0 \tag{17}$$

$$c_{-1,k}\left(\varepsilon_{-1,k}-E\right)+Vc_{0,k}=0 \tag{18}$$

can be used, whereas the wavefunction can be expressed as

$$\psi_k\left(x\right)=\frac{c_{0k}}{\sqrt{Na}}\left[e^{ikx}+\frac{V}{E-\frac{\hbar^2(k-2\pi/a)^2}{2m}}e^{i(k-2\pi/a)x}\right] \tag{19}$$

Secular equation

$$\det\begin{pmatrix}\varepsilon_{0k}-E & V\\ V & \left(\varepsilon_{-1,k}-E\right)\end{pmatrix}=0 \tag{20}$$

$$\left(\varepsilon_{0k}-E\right)\left(\varepsilon_{-1,k}-E\right)-V^2=0 \tag{21}$$

$$E^2-\left[\varepsilon_{0k}+\varepsilon_{-1,k}\right]E+\varepsilon_{0k}\varepsilon_{-1,k}-V^2=0 \tag{22}$$

Eigenvalues:

$$E_{\pm}\left(k\right)=\frac{1}{2}\left[\varepsilon_{0k}+\varepsilon_{-1,k}\right]\pm\frac{1}{2}\left(\left[\varepsilon_{0k}-\varepsilon_{-1,k}\right]^2+4V^2\right)^{1/2} \tag{23}$$

In case of $k=\pi/a$

$$E_{\pm}\left(k=\frac{\pi}{a}\right)=\frac{\hbar^2\pi^2}{2ma^2}\pm|V| \tag{24}$$

with the wavefunctions

$$\psi_{\pm}\left(x\right)=\frac{1}{\sqrt{Na}}\left[e^{i\pi x/a}\pm\left(\mathrm{sign}\,V\right)e^{-i\pi x/a}\right] \tag{25}$$

E	ψ	
	$V>0$	$V<0$
$\frac{\hbar^2\pi^2}{2ma^2}+\lvert V\rvert$	$\cos(\pi x/a)$	$\sin(\pi x/a)$
$\frac{\hbar^2\pi^2}{2ma^2}-\lvert V\rvert$	$\sin(\pi x/a)$	$\cos(\pi x/a)$
	indirect gap	direct gap

Table 1: Eigenfunctions at $k=\frac{\pi}{a}$ for the lowest two bands of a one-dimensional simple lattice.

1.2 Surface state

Surface potential:

$$V(x)=\begin{cases} 2V\cos\left(\frac{\pi}{a}x\right) & x<0 \\ V_0\left(>\frac{\hbar^2\pi^2}{2ma^2}+|V|\right) & x>0 \end{cases} \tag{26}$$

We look for a solution of the Schrödinger equation in the gap, i.e.,

$$\frac{\hbar^2\pi^2}{2ma^2}-|V|<E<\frac{\hbar^2\pi^2}{2ma^2}+|V| \tag{27}$$

Wavefunction in the vacuum region, $x>0$,

$$\underline{\psi(x)=\alpha e^{-k_0 x}} \tag{28}$$

$$\underline{k_0=\sqrt{V_0-E}} \tag{29}$$

We know that for $x<0$ the Schrödinger equation has no propagating solutions with energy lying in the gap. For large x the wavefunction should, however, be a solution of the Schrödinger equation for the bulk. This problem can be handled as in the previous section, but with a complex wavenumber, $k-i\mu$ $(\mu>0)$. This ensures that the wavefunction exponentially decays in the bulk region. According to Eq. (19) the wavefunction can be written as

$$\psi(x)=Be^{\mu x}\left[e^{ikx}+\frac{V}{E-\frac{\hbar^2(k-2\pi/a-i\mu)^2}{2m}}e^{i(k-2\pi/a)x}\right] \tag{30}$$

Regarding the scattering problem, we have to note that the current density for $x>0$ is zero, since the wavefunction is real. The current density for the incoming wave is

$$j_{in}=\frac{\hbar}{m}\,\mathrm{Im}\left(e^{-i(k-i\mu)x}\frac{d}{dx}e^{i(k-i\mu)x}\right)=\frac{\hbar k}{m} \tag{31}$$

while for the reflected wave,

$$j_{refl} = \frac{\hbar\,(k - 2\pi/a)}{m} \left| \frac{V}{E - \frac{\hbar^2(\pi/a - i\mu)^2}{2m}} \right|^2 \quad . \tag{32}$$

Note that these values are modified by the normalization of the wavefunctions. We are now interested in the reflection coefficient that must be unity (no transmission),

$$R = \frac{|j_{refl}|}{|j_{in}|} = \left| \frac{k - 2\pi/a}{k} \right| \left| \frac{V}{E - \frac{\hbar^2(k - 2\pi/a - i\mu)^2}{2m}} \right|^2 = 1 \tag{33}$$

which yields a complicated relationship between E, k and μ.

In order to simplify matter, let us confine to the case of $k = \frac{\pi}{a}$,

$$\underline{\psi\,(x) = Be^{\mu x} \left[e^{i\pi x/a} + \frac{V}{E - \frac{\hbar^2(\pi/a - i\mu)^2}{2m}} e^{-i\pi x/a} \right]} \tag{34}$$

and

$$\left| \frac{V}{E - \frac{\hbar^2(\pi/a - i\mu)^2}{2m}} \right| = 1\,. \tag{35}$$

$$\Downarrow$$

$$V^2 = \left(E - \frac{\hbar^2\,(\pi/a + i\mu)^2}{2m} \right) \left(E - \frac{\hbar^2\,(\pi/a - i\mu)^2}{2m} \right) \tag{36}$$

$$= E^2 + E\frac{\hbar^2}{m} \left(\mu^2 - \frac{\pi^2}{a^2} \right) + \left(\frac{\hbar^2}{2m} \right)^2 \left(\frac{\pi^2}{a^2} + \mu^2 \right)^2 \tag{37}$$

$$= E^2 - E\frac{2\hbar^2}{m}\frac{\pi^2}{a^2} + E\frac{\hbar^2}{m} \left(\mu^2 + \frac{\pi^2}{a^2} \right) + \left(\frac{\hbar^2}{2m} \right)^2 \left(\frac{\pi^2}{a^2} + \mu^2 \right)^2 \tag{38}$$

$$\Downarrow$$

$$\left(\frac{\pi^2}{a^2} + \mu^2 \right)^2 + \frac{4m}{\hbar^2} E \left(\frac{\pi^2}{a^2} + \mu^2 \right) + \frac{4m^2}{\hbar^4} E^2 - E\frac{8m}{\hbar^2}\frac{\pi^2}{a^2} - \frac{4m^2}{\hbar^4} V^2 = 0 \tag{39}$$

$$\Downarrow$$

$$\frac{\hbar^2\mu^2}{2m} = -\left(E + \frac{\hbar^2\pi^2}{2ma^2} \right) + \left(4\frac{\hbar^2\pi^2}{2ma^2} E + V^2 \right)^{1/2} \quad . \tag{40}$$

The right-hand side of the above equation is positive, since

$$\left| E + \frac{\hbar^2\pi^2}{2ma^2} \right| < \left(4\frac{\hbar^2\pi^2}{2ma^2} E + V^2 \right)^{1/2} \tag{41}$$

$$\Updownarrow$$

$$E^2 + \left(\frac{\hbar^2\pi^2}{2ma^2}\right)^2 + 2\frac{\hbar^2\pi^2}{2ma^2}E < 4\frac{\hbar^2\pi^2}{2ma^2}E + V^2 \tag{42}$$

$$\Updownarrow$$

$$\left|E - \frac{\hbar^2\pi^2}{2ma^2}\right| < |V| \tag{43}$$

which is indeed satisfied, since the energy of the surface state lies in the gap.

Because of (35) we can introduce a phaseshift δ $(-\pi < \delta < \pi)$ via the relationship,

$$e^{-2i\delta} = \frac{V}{E - \frac{\hbar^2(\pi/a - i\mu)^2}{2m}} \tag{44}$$

and express the wavefunction for $x < 0$ as

$$\underline{\psi(x) = \beta e^{\mu x}\cos\left(\frac{\pi x}{a} + \delta\right).} \tag{45}$$

We are now left with matching the wavefunctions (28) and (45) at a given point $x = x_0$,

$$\alpha e^{-k_0 x_0} = \beta e^{\mu x_0}\cos\left(\frac{\pi x_0}{a} + \delta\right) \tag{46}$$

$$-\alpha k_0 e^{-k_0 x_0} = \beta\mu e^{\mu x_0}\cos\left(\frac{\pi x_0}{a} + \delta\right) - \frac{\beta\pi}{a}e^{\mu x_0}\sin\left(\frac{\pi x_0}{a} + \delta\right) \tag{47}$$

$$\Downarrow$$

$$\alpha\left(k_0 + \mu\right)e^{-k_0 x_0} = \frac{\beta\pi}{a}e^{\mu x_0}\sin\left(\frac{\pi x_0}{a} + \delta\right) \tag{48}$$

$$\Downarrow$$

$$\frac{\pi}{a}\tan\left(\frac{\pi x_0}{a} + \delta\right) = k_0 + \mu \tag{49}$$

Matching at $\underline{x_0 = 0}$ implies

$$\underline{\frac{\pi}{a}\tan(\delta) = k_0 + \mu} \tag{50}$$

that means for any (positive) value of k_0 and μ one can find a δ $(0 < \delta < \pi/2)$ that satisfies the above equation, i.e., a surface state will be formed. Since

$$e^{2i\delta} = \frac{V}{E - \frac{\hbar^2(\pi/a + i\mu)^2}{2m}} = \frac{1}{V}\left(E - \frac{\hbar^2(\pi/a - i\mu)^2}{2m}\right) \tag{51}$$

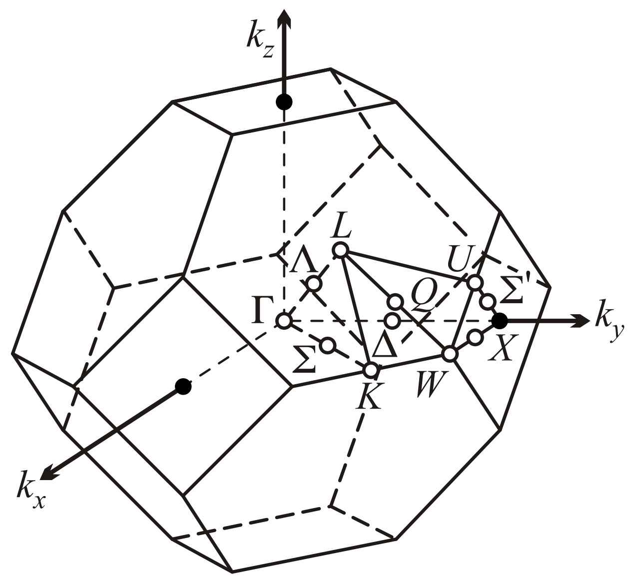
$$= \frac{1}{V}\left(E - \frac{\hbar^2\pi^2}{2ma^2} + \frac{\hbar^2\mu^2}{2m}\right) + i\frac{E\hbar^2\pi\mu}{Vma} \tag{52}$$

a sufficient condition for the existence of the surface state is

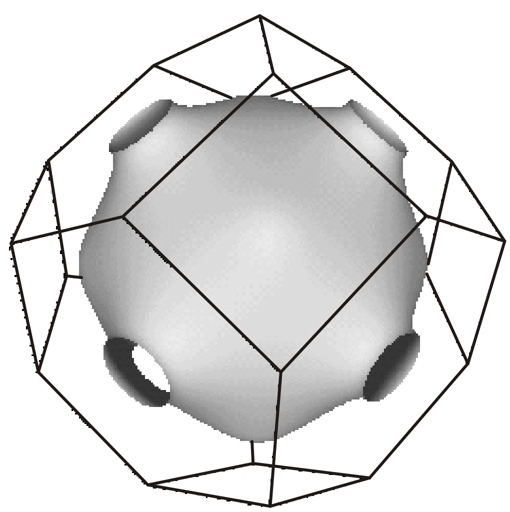
$$\underline{V > 0} \tag{53}$$

This is called a Tamm-state that happens in case of an indirect gap. By matching the wavefunctions at $x_0 = -a/2$, the condition of the surface state is $V > 0$ (Shockley-state, direct gap).

The Brillouin zone of an fcc lattice



The Fermi surface of Cu



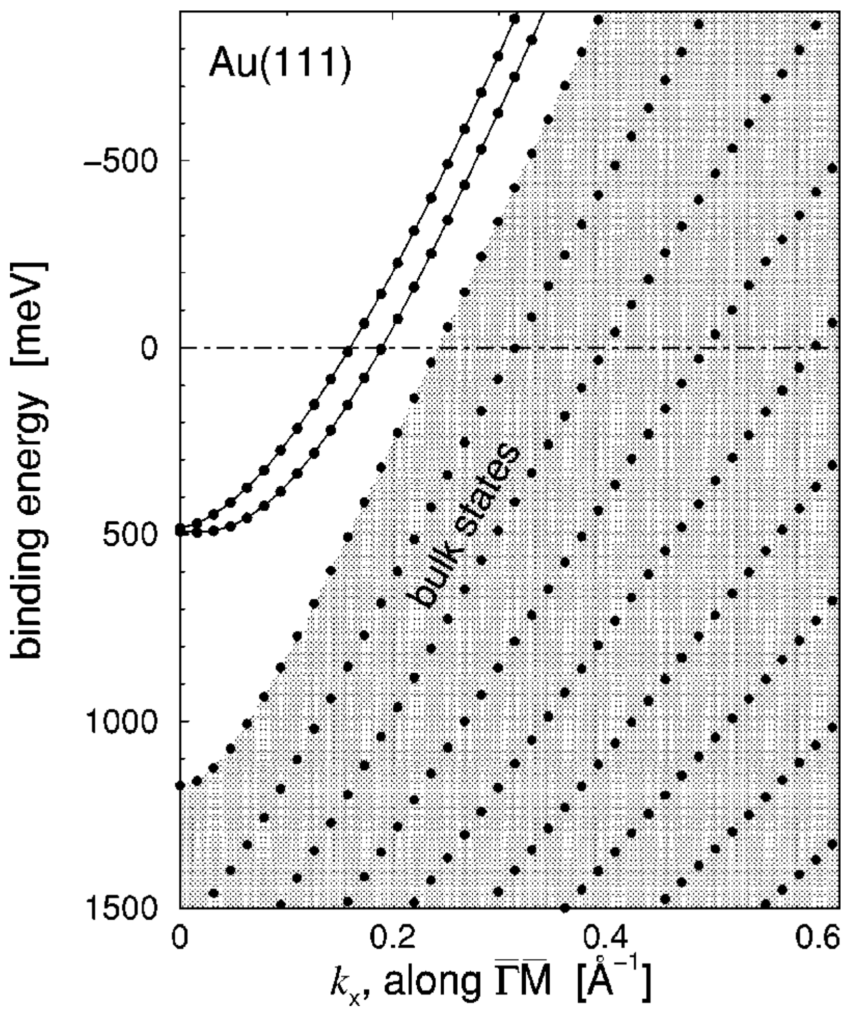


FIG. 1. Results of the band-structure calculation along the $\overline{\Gamma}\overline{M}$ direction for a 23-layer slab of Au(111). The shaded area represents the projected bulk states, and the solid lines give the surface state dispersion. The Fermi level has been adjusted to the experimental position.

2 The Bychkov-Rashba effect

Planewave-like surface state in a non-magnetic host:

$$\varphi_{\mathbf{k}s}(\mathbf{r}) = \frac{1}{\sqrt{N}} \chi_s \, e^{i\mathbf{kr}} \;, \tag{54}$$

where χ_s is a spinor, $\mathbf{k} = (k_x, k_y) \in SBZ$ (Surface Brillouin zone), N is the number of sites on the 2D lattice. These states are eigenfunctions of the Hamiltonian, H_0, in absence of spin-orbit coupling

$$H_0 \varphi_{\mathbf{k}s} = \left(E_0 + \frac{\hbar^2 \mathbf{k}^2}{2m^*} \right) \varphi_{\mathbf{k}s} \; . \tag{55}$$

The spin-orbit coupling (SOC),

$$H_{SOC} = -\frac{\hbar}{4m^2c^2} (\nabla V \times \mathbf{p}) \sigma = \frac{\hbar}{4m^2c^2} (\nabla V \times \sigma) \mathbf{p} \; . \tag{56}$$

acts on these states as

$$H_{SOC} \, \varphi_{\mathbf{k}s}(\mathbf{r}) = \frac{\hbar^2}{4m^2c^2\sqrt{N_{_{\parallel}}}} (\nabla V(\mathbf{r}) \times \sigma \chi_s) \, \mathbf{k} \, e^{i\mathbf{kr}} \; . \tag{57}$$

The matrixelements of SOC can be expressed as

$$\langle \mathbf{k}' s' | H_{SOC} | \mathbf{k} s \rangle = \delta_{\mathbf{k}\mathbf{k}'} (\alpha_{\mathbf{k}} \times \sigma_{s's}) \, \mathbf{k} \tag{58}$$

$$\alpha_{\mathbf{k}} = \frac{\hbar^2}{4m^2c^2} \int_{WS} d^3 r e^{-i\mathbf{kr}} \nabla V(\mathbf{r}) \, e^{i\mathbf{kr}} \tag{59}$$

According to the simplest model of the Rashba-effect only the normal component of $\nabla V(\mathbf{r})$ is taken into account,

$$\nabla V(\mathbf{r}) \simeq \mathbf{e}_z \frac{dV(z)}{dz} \tag{60}$$

which implies

$$\alpha_{\mathbf{k}} = \alpha \mathbf{e}_z \tag{61}$$

$$\alpha = \frac{\hbar^2}{4m^2c^2} \int_{WS} d^3 r \frac{dV(z)}{dz} \tag{62}$$

and, correspondingly,

$$\underline{H_{SOC}(\mathbf{k}) = \alpha (\mathbf{e}_z \times \sigma) \, \mathbf{k} = \alpha \, (\sigma_x k_y - \sigma_y k_x)} \tag{63}$$

Neglecting the interaction with the bulk states, one has to solve the following eigenvalue problem,

$$\left[E_0 + \frac{\hbar^2 \mathbf{k}^2}{2m^*} + \alpha \, (\sigma_x k_y - \sigma_y k_x) \right] \psi_{\mathbf{k}} = E_{\mathbf{k}} \psi_{\mathbf{k}} \;, \tag{64}$$

i.e.,

$$\begin{bmatrix} E_0 + \frac{\hbar^2 \mathbf{k}^2}{2m^*} & \alpha \, (k_y + i k_x) \\ \alpha \, (k_y - i k_x) & E_0 + \frac{\hbar^2 \mathbf{k}^2}{2m^*} \end{bmatrix} \psi_{\mathbf{k}} = E_{\mathbf{k}} \psi_{\mathbf{k}} \tag{65}$$

$$\Downarrow$$

$$\left(E_0 + \frac{\hbar^2 \mathbf{k}^2}{2m^*} - E_{\mathbf{k}}\right)^2 - \alpha^2 \left(k_x^2 + k_y^2\right) = 0 \tag{66}$$

$$\Downarrow$$

$$\underline{E_{\mathbf{k}}^{\pm} = E_0 + \frac{\hbar^2 \mathbf{k}^2}{2m^*} \pm \alpha \left|\mathbf{k}\right|} \; .$$

2.1 Alternative representation

Taking any direction in the SBZ, $\mathbf{k} = k\,\widehat{e}$,

$$E_k^{\pm} = \begin{cases} E_0 + \frac{\hbar^2 k^2}{2m^*} \pm \alpha k & \text{if} \quad k > 0 \\ E_0 + \frac{\hbar^2 k^2}{2m^*} \mp \alpha k & \text{if} \quad k < 0 \end{cases} . \tag{67}$$

Defining

$$E_k^{\rightarrow} = E_k^{-}\Theta\left(k\right) + E_k^{+}\left[1 - \Theta\left(k\right)\right] \tag{68}$$

$$= \frac{\hbar^2 k^2}{2m^*} - \alpha k = E_0 + E_R + \frac{\hbar^2 \left(k - \Delta k/2\right)^2}{2m^*} \; , \tag{69}$$

and

$$E_k^{\leftarrow} = E_k^{+}\Theta\left(k\right) + E_k^{-}\left[1 - \Theta\left(k\right)\right] \tag{70}$$

$$= \frac{\hbar^2 k^2}{2m^*} + \alpha k = E_0 + E_R + \frac{\hbar^2 \left(k + \Delta k/2\right)^2}{2m^*} + E_R \; , \tag{71}$$

with

$$\frac{\hbar^2 \Delta k}{2m^*} = \alpha \Longrightarrow \Delta k = \frac{2m^* \alpha}{\hbar^2} \; , \tag{72}$$

and the Rashba energy,

$$E_R = -\frac{\hbar^2 \left(\Delta k\right)^2}{8m^*} = -\frac{m^* \alpha^2}{2\hbar^2} \; , \tag{73}$$

we indeed get two parabolas shifted left and right by $\Delta k/2$ and downwards by E_R.

3 Spin-polarization

By introducing $\mathbf{k} = k\left(\cos\left(\varphi\right), \sin\left(\varphi\right)\right)$, the Hamiltonian can be written as

$$H_{\mathbf{k}} = \begin{bmatrix} E_0 + \frac{\hbar^2 k^2}{2m^*} & i\alpha k e^{-i\varphi} \\ -i\alpha k e^{i\varphi} & E_0 + \frac{\hbar^2 k^2}{2m^*} \end{bmatrix} \tag{74}$$

and the eigenvectors are solutions of the equation

$$\left[\begin{array}{cc} \mp\alpha k & i\alpha k e^{-i\varphi} \\ -i\alpha k e^{i\varphi} & \mp\alpha k \end{array}\right]\psi_{\mathbf{k}}^{\pm}=0 \tag{75}$$

$$\Downarrow$$

$$\left[\begin{array}{cc} \mp 1 & i e^{-i\varphi} \\ -i e^{i\varphi} & \mp 1 \end{array}\right]\psi_{\mathbf{k}}^{\pm}=0 \tag{76}$$

The solutions are

$$\underline{\psi_{\mathbf{k}}^{\pm}=\frac{1}{\sqrt{2}}\left(\begin{array}{c} \mp 1 \\ i e^{i\varphi} \end{array}\right)}\,. \tag{77}$$

The spin-polarization of the eigenstates is defined by

$$\underline{\overrightarrow{P}_{\mathbf{k},\pm}=\langle\psi_{\mathbf{k}}^{\pm}|\overrightarrow{\sigma}|\psi_{\mathbf{k}}^{\pm}\rangle} \tag{78}$$

$$\Downarrow$$

$$P_{\pm}^{x}=\frac{1}{2}\left(\begin{array}{cc} \mp 1 & -i e^{-i\varphi} \end{array}\right)\left(\begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array}\right)\left(\begin{array}{c} \mp 1 \\ i e^{i\varphi} \end{array}\right)=\pm\sin\varphi \tag{79}$$

$$P_{\pm}^{y}=\frac{1}{2}\left(\begin{array}{cc} \mp 1 & -i e^{-i\varphi} \end{array}\right)\left(\begin{array}{cc} 0 & -i \\ i & 0 \end{array}\right)\left(\begin{array}{c} \mp 1 \\ i e^{i\varphi} \end{array}\right)=\mp\cos\varphi \tag{80}$$

$$P_{\pm}^{z}=\frac{1}{2}\left(\begin{array}{cc} \mp 1 & -i e^{-i\varphi} \end{array}\right)\left(\begin{array}{cc} 1 & 0 \\ 0 & -1 \end{array}\right)\left(\begin{array}{c} \mp 1 \\ i e^{i\varphi} \end{array}\right)=0 \tag{81}$$

i.e.,

$$\underline{\overrightarrow{P}_{\mathbf{k},\pm}=\left(\begin{array}{c} \pm\sin(\varphi) \\ \mp\cos(\varphi) \\ 0 \end{array}\right)=\frac{1}{k}\left(\begin{array}{c} \pm k_y \\ \mp k_x \\ 0 \end{array}\right)} \tag{82}$$

Obviously,

$$\left|\overrightarrow{P}_{\mathbf{k},\pm}\right|=1 \tag{83}$$

$$\overrightarrow{P}_{\mathbf{k},\pm}\cdot\mathbf{k}=0 \tag{84}$$

and

$$\overrightarrow{P}_{\mathbf{k},-}=-\overrightarrow{P}_{\mathbf{k},+}\,. \tag{85}$$

One can define the *helicity operator*,

$$\underline{h_{\mathbf{k}}}=\frac{1}{\alpha k}H_{SOC}(\mathbf{k})=\underline{\frac{1}{k}\left(\sigma_x k_y-\sigma_y k_x\right)}=\left(\begin{array}{cc} 0 & i e^{-i\varphi} \\ -i e^{i\varphi} & 0 \end{array}\right) \tag{86}$$

for which

$$[h_{\mathbf{k}},H_{\mathbf{k}}]=0 \tag{87}$$

and

$$h_{\mathbf{k}}^2 = I \tag{88}$$

thus, the eigenvalues of $h_{\mathbf{k}}$ are ± 1.

Since

$$\begin{pmatrix} 0 & ie^{-i\varphi} \\ -ie^{i\varphi} & 0 \end{pmatrix} \begin{pmatrix} \mp 1 \\ ie^{i\varphi} \end{pmatrix} = \pm \begin{pmatrix} -1 \\ ie^{i\varphi} \end{pmatrix} \tag{89}$$

it follows that $\psi_{\mathbf{k}}^{\pm}$ are also the eigenfunctions of $h_{\mathbf{k}}$,

$$\underline{h_{\mathbf{k}} \psi_{\mathbf{k}}^{\pm} = \pm \psi_{\mathbf{k}}^{\pm}} \, . \tag{90}$$

J. Henk, A. Ernst, and P. Bruno, Phys. Rev. B (2003)

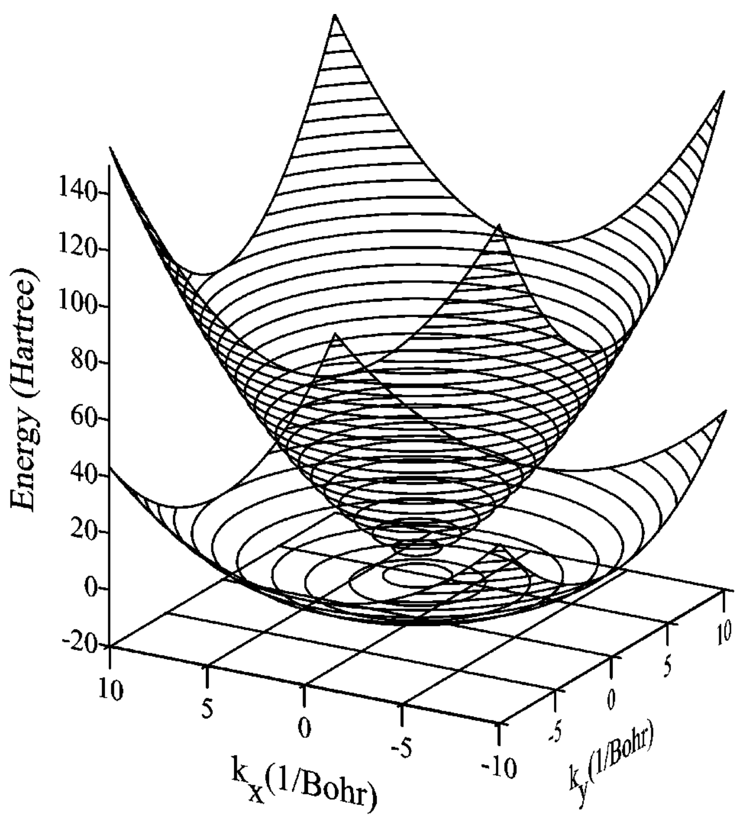


FIG. 2. Rashba spin-orbit interaction in a two-dimensional electron gas. The dispersions $E_{\pm}(\vec{k}_{\parallel})$ of free electrons are shown for $\gamma_{so} = 4$/Bohr, $\vec{k}_{\parallel} = (k_x, k_y)$. The "inner" state ["+" in Eq. (6)] shows strong dispersion, the "outer" weak dispersion ["−" in Eq. (6)]. Both surfaces touch each other at $\vec{k}_{\parallel} = 0$. For a better illustration, the Rashba effect is extremely exaggerated (compared to typical two-dimensional electron gases).

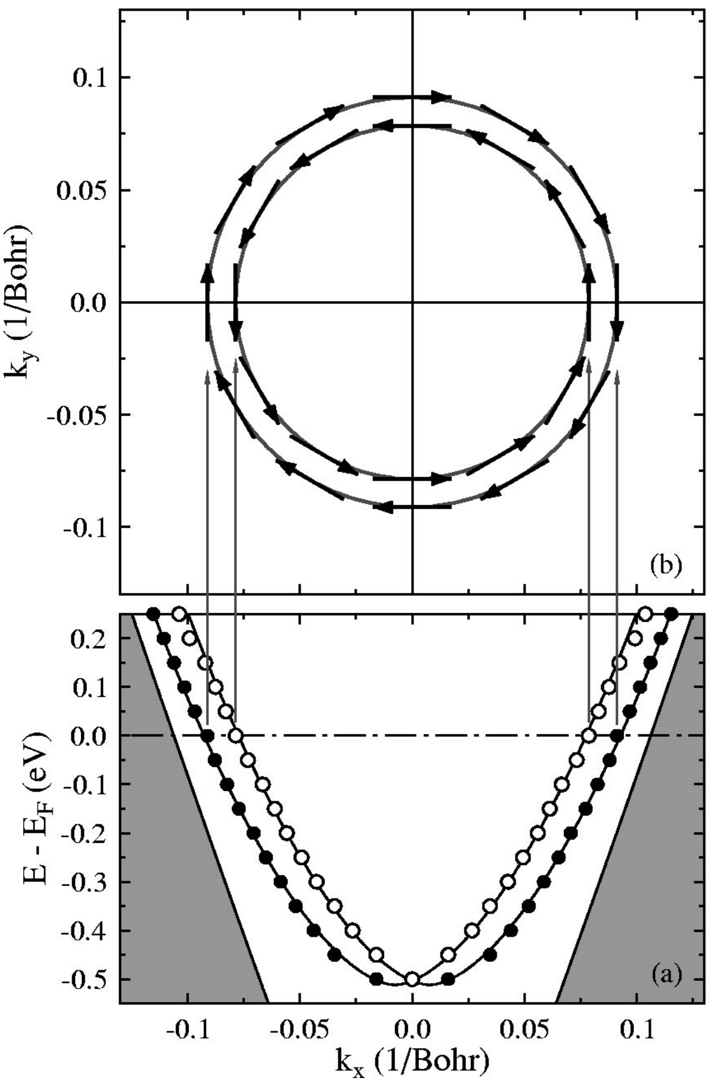


FIG. 3. *L*-gap surface states on Au(111). (a) Dispersion of the spin-orbit split surface states along $\overline{\mathrm{K}}$-$\overline{\Gamma}$-$\overline{\mathrm{K}}$ [i.e., $\vec{k}_{\parallel}=(k_x,0)$]. Open (closed) symbols belong to the inner (outer) surface state. Gray arrows point from the surface states at the Fermi energy E_{F} to the momentum distribution shown in panel b. The region of bulk bands is depicted by gray areas. (b) Momentum distribution at E_{F}. The thick arrows indicate the in-plane spin polarization [P_x and P_y, according to Eq. (9)].