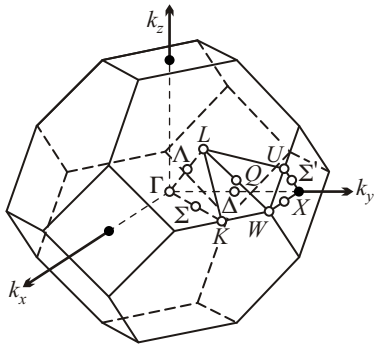
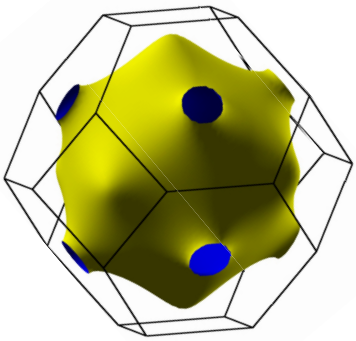
The Bychkov-Rashba effect

1 Surface states



The Brillouin zone of an fcc lattice.



The Fermi surface of Au.

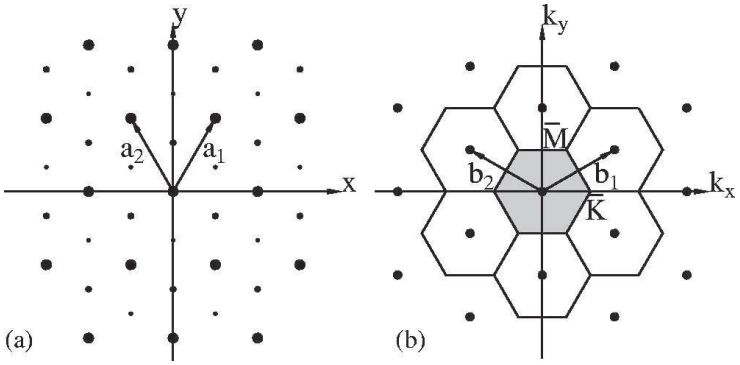


FIG. 1. The Au(111) surface. (a) Top view of the first three surface layers (first, second, and third layer: large, medium-sized, and small filled circles, respectively). $\vec{a}_1$ and $\vec{a}_2$ are the basis vectors of the direct lattice. The z axis points towards the bulk. (b) Two-dimensional reciprocal lattice with basis vectors $\vec{b}_1$ and $\vec{b}_2$. The first Brillouin zone is marked gray. The two representative symmetry points $\overline{\mathrm{K}}$ and $\overline{\mathrm{M}}$ mark a corner $[\vec{k}_{\parallel}(\overline{\mathrm{K}}) = (\vec{b}_1 - \vec{b}_2)/2]$ and a center $[\vec{k}_{\parallel}(\overline{\mathrm{M}}) = (\vec{b}_1 + \vec{b}_2)/2]$ of the Brillouin-zone boundary, respectively.

(From J. Henk, A. Ernst, and P. Bruno, Phys. Rev. B **68**, 165416 (2003).)

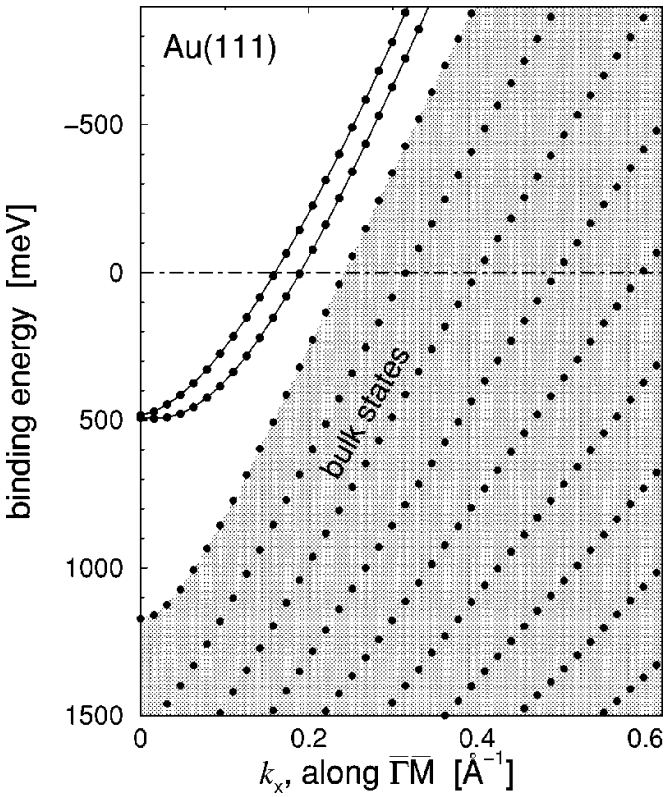


FIG. 1. Results of the band-structure calculation along the $\overline{\Gamma}\overline{M}$ direction for a 23-layer slab of Au(111). The shaded area represents the projected bulk states, and the solid lines give the surface state dispersion. The Fermi level has been adjusted to the experimental position.

(From G. Nicolay *et al.*, Phys. Rev. B **65**, 033407 (2001).)

2 Isotropic Bychkov-Rashba effect

Consider planewave-like surface states in a non-magnetic host,

$$\varphi_{\mathbf{k}s}\left(\mathbf{r}\right)=\frac{1}{\sqrt{N}}\chi_{s}\,e^{i\mathbf{k}\mathbf{r}}f\left(z\right)\ , \tag{1}$$

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 and $f\left(z\right)$ describes the exponentional decay of the wavefunction along the direction normal to the surface. Let us suppose that these states are eigenfunctions of the Hamiltonian, H_0, in absence of spin-orbit coupling,

$$H_{0}\varphi_{\mathbf{k}s}=\left(E_{0}+\frac{\hbar^{2}\mathbf{k}^{2}}{2m^{*}}\right)\varphi_{\mathbf{k}s}\ . \tag{2}$$

The spin-orbit coupling (SOC),

$$H_{SOC}=\frac{\hbar}{4m^{2}c^{2}}(\boldsymbol{\nabla}V\times\mathbf{p})\boldsymbol{\sigma}=-\frac{\hbar}{4m^{2}c^{2}}(\boldsymbol{\nabla}V\times\boldsymbol{\sigma})\,\mathbf{p} \tag{3}$$

acts on these states as

$$H_{SOC}\,\varphi_{\mathbf{k}s}\left(\mathbf{r}\right)=-\frac{\hbar^{2}}{4m^{2}c^{2}\sqrt{N}}(\boldsymbol{\nabla}V\left(\mathbf{r}\right)\times\boldsymbol{\sigma}\,\chi_{s})\,e^{i\mathbf{k}\mathbf{r}}\left(f\left(z\right)\,\mathbf{k}\,+\frac{df\left(z\right)}{idz}\mathbf{e}_{z}\right)\ , \tag{4}$$

where $\mathbf{e}_z$ is the unitvector normal to the surface.

By making use of the periodicity parallel to the surface, the matrixelements of SOC can be expressed as

$$\langle\mathbf{k}'s'|H_{SOC}|\mathbf{k}s\rangle=\delta_{\mathbf{k}\mathbf{k}'}\left[(\boldsymbol{\alpha}\times\boldsymbol{\sigma}_{s's})\,\mathbf{k}+(\boldsymbol{\beta}\times\boldsymbol{\sigma}_{s's})\,\mathbf{e}_{z}\right] \tag{5}$$

with

$$\boldsymbol{\alpha}=-\frac{\hbar^{2}}{4m^{2}c^{2}}\int_{V_{0}}d^{3}r\,\boldsymbol{\nabla}V\left(\mathbf{r}\right)\,f^{2}\left(z\right)\ , \tag{6}$$

and

$$\boldsymbol{\beta}=\frac{i\hbar^{2}}{4m^{2}c^{2}}\int_{V_{0}}d^{3}r\,\boldsymbol{\nabla}V\left(\mathbf{r}\right)\,f\left(z\right)\frac{df\left(z\right)}{dz}\,, \tag{7}$$

where V_0 is the two-dimensional unit cell of the surface, which, in principle, extends for $-\infty<z<\infty$.

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

$$\nabla V\left(\mathbf{r}\right)\simeq\mathbf{e}_{z}\frac{\partial V\left(\mathbf{r}\right)}{\partial z} \tag{8}$$

which implies

$$\boldsymbol{\alpha}=\alpha\mathbf{e}_{z}\,,\,\boldsymbol{\beta}=\beta\mathbf{e}_{z}\,, \tag{9}$$

$$\alpha=-\frac{\hbar^{2}}{4m^{2}c^{2}}\int_{V_{0}}d^{3}r\frac{\partial V\left(\mathbf{r}\right)}{\partial z}f^{2}\left(z\right)\ , \tag{10}$$

$$\beta=\frac{i\hbar^{2}}{4m^{2}c^{2}}\int_{V_{0}}d^{3}r\,\frac{\partial V\left(\mathbf{r}\right)}{\partial z}\,f\left(z\right)\frac{df\left(z\right)}{dz}\,. \tag{11}$$

Obviously, the term containing $\boldsymbol{\beta}$ vanishes in Eq. (5), consequently,

$$H_{SOC}\left(\mathbf{k}\right)=\alpha(\mathbf{e}_z\times\boldsymbol{\sigma})\,\mathbf{k}=\alpha\left(\sigma_x k_y-\sigma_y k_x\right)\,. \tag{12}$$

The eigenfunctions of the Hamilton operator $H=H_0+H_{SOC}$ are linear combinations of $\varphi_{\mathbf{k}s}\left(\mathbf{r}\right)$,

$$H\psi_{\mathbf{k}}\left(\mathbf{r}\right)=E_{\mathbf{k}}\psi_{\mathbf{k}}\left(\mathbf{r}\right)$$

$$\psi_{\mathbf{k}}\left(\mathbf{r}\right)=\sum_{s=\pm1}c_{\mathbf{k}s}\varphi_{\mathbf{k}s}\left(\mathbf{r}\right)\,,$$

which leads to the equation,

$$\left[E_0+\frac{\hbar^2\mathbf{k}^2}{2m^*}+\alpha\left(\sigma_x k_y-\sigma_y k_x\right)\right]c_{\mathbf{k}}=E_{\mathbf{k}}c_{\mathbf{k}}\,, \tag{13}$$

$$\Downarrow$$

$$\left[\begin{array}{cc}E_0+\frac{\hbar^2\mathbf{k}^2}{2m^*} & \alpha\left(k_y+ik_x\right)\\ \alpha\left(k_y-ik_x\right) & E_0+\frac{\hbar^2\mathbf{k}^2}{2m^*}\end{array}\right]\left[\begin{array}{c}c_{\mathbf{k}+}\\ c_{\mathbf{k}-}\end{array}\right]=E_{\mathbf{k}}\left[\begin{array}{c}c_{\mathbf{k}+}\\ c_{\mathbf{k}-}\end{array}\right] \tag{14}$$

$$\Downarrow$$

$$\left(E_0+\frac{\hbar^2\mathbf{k}^2}{2m^*}-E_{\mathbf{k}}\right)^2-\alpha^2\left(k_x^2+k_y^2\right)=0 \tag{15}$$

$$\Downarrow$$

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

2.1 Alternative representation

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

$$E_k^{\pm}=\begin{cases}E_0+\frac{\hbar^2k^2}{2m^*}\pm\alpha k & \text{if}\quad k>0\\ \\ E_0+\frac{\hbar^2k^2}{2m^*}\mp\alpha k & \text{if}\quad k<0\end{cases}\,. \tag{16}$$

Defining

$$E_k^{\rightarrow}=E_k^{-}\Theta\left(k\right)+E_k^{+}\left[1-\Theta\left(k\right)\right] \tag{17}$$

$$=\frac{\hbar^2k^2}{2m^*}-\alpha k=E_0+E_R+\frac{\hbar^2\left(k-\Delta k/2\right)^2}{2m^*}\,, \tag{18}$$

and

$$E_k^{\leftarrow}=E_k^{+}\Theta\left(k\right)+E_k^{-}\left[1-\Theta\left(k\right)\right] \tag{19}$$

$$=\frac{\hbar^2k^2}{2m^*}+\alpha k=E_0+E_R+\frac{\hbar^2\left(k+\Delta k/2\right)^2}{2m^*}\,, \tag{20}$$

with

$$\frac{\hbar^2 \Delta k}{2m^*} = \alpha \Longrightarrow \Delta k = \frac{2m^* \alpha}{\hbar^2} \,, \tag{21}$$

and the Rashba energy,

$$E_R = -\frac{\hbar^2 \left(\Delta k\right)^2}{8m^*} = -\frac{m^* \alpha^2}{2\hbar^2} \,, \tag{22}$$

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

3 Spin-polarization in k-space

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

$$H_{\mathbf{k}} = \begin{bmatrix} E_0 + \frac{\hbar^2 k^2}{2m^*} & i\alpha k e^{-i\varphi} \\ -i\alpha k e^{i\varphi} & E_0 + \frac{\hbar^2 k^2}{2m^*} \end{bmatrix} \tag{23}$$

and the eigenvectors are solutions of the equation

$$\begin{bmatrix} \mp\alpha k & i\alpha k e^{-i\varphi} \\ -i\alpha k e^{i\varphi} & \mp\alpha k \end{bmatrix} \begin{bmatrix} c^{\pm}_{\mathbf{k}+} \\ c^{\pm}_{\mathbf{k}-} \end{bmatrix} = 0 \tag{24}$$

$$\Downarrow$$

$$\begin{bmatrix} \mp 1 & i e^{-i\varphi} \\ -i e^{i\varphi} & \mp 1 \end{bmatrix} \begin{bmatrix} c^{\pm}_{\mathbf{k}+} \\ c^{\pm}_{\mathbf{k}-} \end{bmatrix} = 0 \tag{25}$$

$$\Downarrow$$

$$\begin{bmatrix} c^{\pm}_{\mathbf{k}+} \\ c^{\pm}_{\mathbf{k}-} \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \mp 1 \\ i e^{i\varphi} \end{pmatrix} \,. \tag{26}$$

By taking into account that the wavefunctions $\varphi_{\mathbf{k}s}$ are normalized, the expectation value of the Pauli matrices related to the eigenstates is defined by

$$\boldsymbol{P}^{\pm}_{\mathbf{k}} = \langle \psi^{\pm}_{\mathbf{k}} | \boldsymbol{\sigma} | \psi^{\pm}_{\mathbf{k}} \rangle = \langle c^{\pm}_{\mathbf{k}} | \boldsymbol{\sigma} | c^{\pm}_{\mathbf{k}} \rangle \,, \tag{27}$$

which is referred to as the spin-polarization vector in the reciprocal space. Straightforward calculations yield

$$P^{\pm}_x = \frac{1}{2} \begin{pmatrix} \mp 1 & -i e^{-i\varphi} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \mp 1 \\ i e^{i\varphi} \end{pmatrix} = \pm \sin\varphi \tag{28}$$

$$P^{\pm}_y = \frac{1}{2} \begin{pmatrix} \mp 1 & -i e^{-i\varphi} \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} \mp 1 \\ i e^{i\varphi} \end{pmatrix} = \mp \cos\varphi \tag{29}$$

$$P^{\pm}_z = \frac{1}{2} \begin{pmatrix} \mp 1 & -i e^{-i\varphi} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \mp 1 \\ i e^{i\varphi} \end{pmatrix} = 0 \tag{30}$$

i.e.,

$$\boldsymbol{P}_{\mathbf{k}}^{\pm} = \begin{pmatrix} \pm\sin(\varphi) \\ \mp\cos(\varphi) \\ 0 \end{pmatrix} = \frac{1}{k} \begin{pmatrix} \pm k_y \\ \mp k_x \\ 0 \end{pmatrix} \tag{31}$$

Obviously,

$$\left|\boldsymbol{P}_{\mathbf{k}}^{\pm}\right| = 1 \tag{32}$$

$$\boldsymbol{P}_{\mathbf{k}}^{\pm} \cdot \mathbf{k} = 0 \tag{33}$$

and

$$\boldsymbol{P}_{\mathbf{k}}^{-} = -\boldsymbol{P}_{\mathbf{k}}^{+} \ . \tag{34}$$

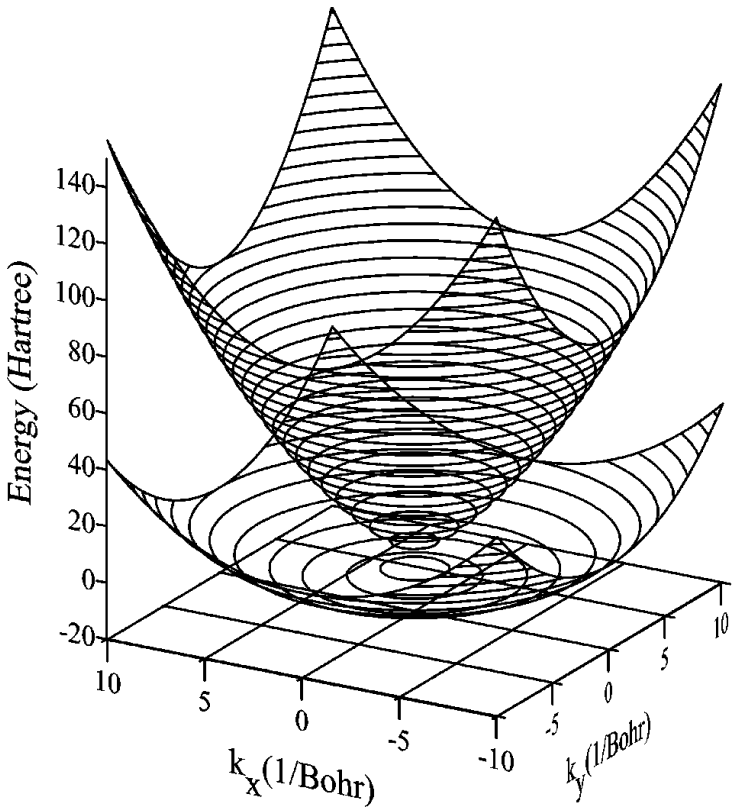


FIG. 2. Rashba spin-orbit interaction in a two-dimensional electron gas. The dispersions $E_{\pm}(\vec{k}_{\parallel})$ of free electrons are shown for γ_{so}=4/Bohr, $\vec{k}_{\parallel}=(k_x,k_y)$. The "inner" state ["+" in Eq. (6)] shows strong dispersion, the "outer" weak dispersion ["−" in Eq. (6)]. 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).

(From J. Henk, A. Ernst, and P. Bruno, Phys. Rev. B **68**, 165416 (2003).)

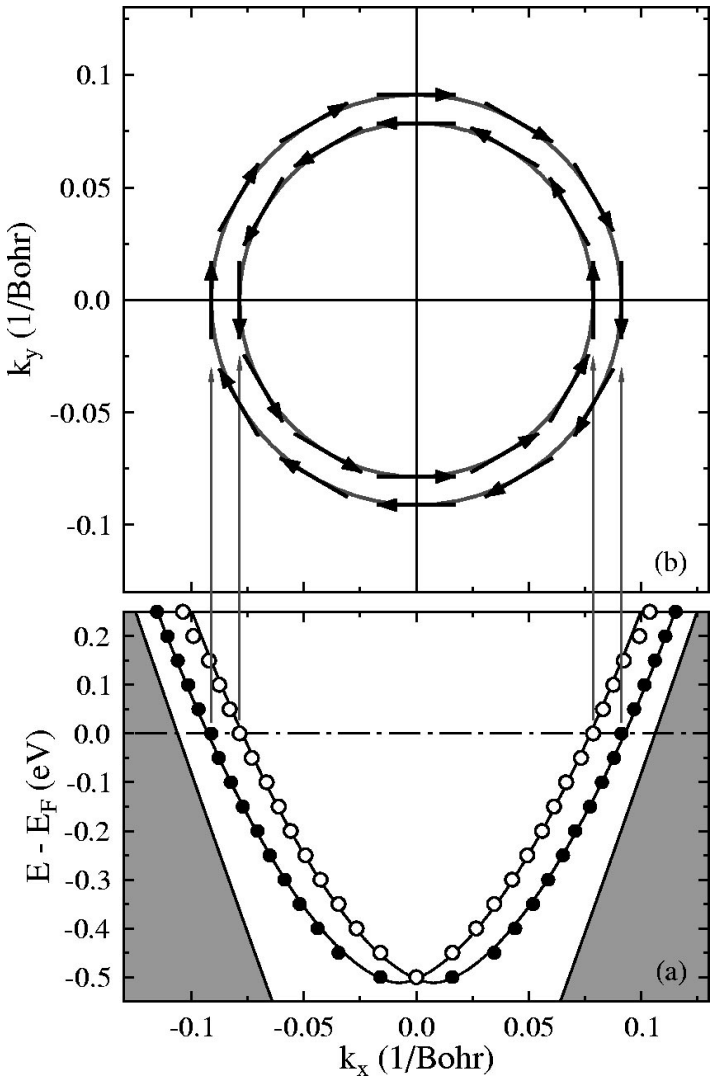
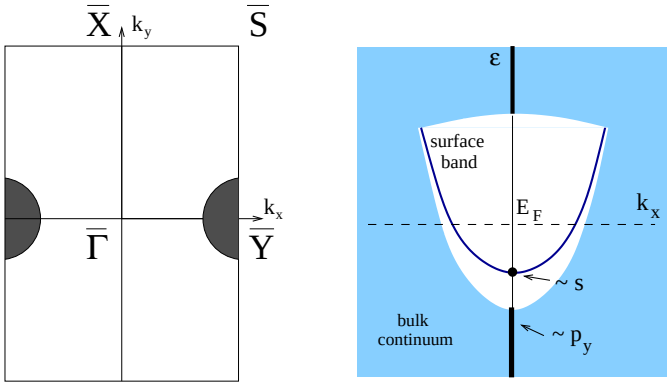


FIG. 3. *L*-gap surface states on Au(111). (a) Dispersion of the spin-orbit split surface states along $\overline{\mathrm{K}}$-$\overline{\Gamma}$-$\overline{\mathrm{K}}$ [i.e., $\vec{k}_{\parallel}=(k_x,0)$]. Open (closed) symbols belong to the inner (outer) surface state. Gray arrows point from the 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)].

(From J. Henk, A. Ernst, and P. Bruno, Phys. Rev. B **68**, 165416 (2003).)

4 Anisotropic Bychkov-Rashba effect

We will consider surface states around a high-symmetry point of the 2D BZ (or SBZ), denoted by $\mathbf{Q}$. In case, of the L-gap surface states of noble metals this is the center of the SBZ, i.e. the $\overline{\Gamma}$ point, but similar surface states exist around the $\overline{\mathrm{Y}}$ point of the SBZ of the Au(110) surface as demonstrated below.



Left: Sketch of the fcc(110) Surface Brillouin Zone. The dark area denotes the projection of the L-gap of bulk Au. Right: Structure of the surface energy spectrum in the absence of SO interaction, along the line $\mathbf{k} = (k_x, 0)$. Surface states in the relative gap with $\mathbf{k} \neq 0$ can be built up from states indicated by the thick black lines and the black circle at $\mathbf{k} = 0$. Note that $\mathbf{k} = 0$ corresponds to the $\overline{\mathrm{Y}}$ point of the Brillouin zone. (From E. Simon *et al.*, Physical Review B **81**, 235438 (2010).

A Bloch state corresponding to $\mathbf{k} + \mathbf{Q}$ is given by

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i(\mathbf{k}+\mathbf{Q})\mathbf{r}} u_{\mathbf{k}+\mathbf{Q}}(\mathbf{r}) \ , \tag{35}$$

where the $u_{\mathbf{k}+\mathbf{Q}}$ is periodic on the real lattice,

$$u_{\mathbf{k}+\mathbf{Q}}(\mathbf{r}+\mathbf{R}) = u_{\mathbf{k}+\mathbf{Q}}(\mathbf{r}) \ . \tag{36}$$

Next we write the Bloch function in the from

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\mathbf{r}} \varphi_{\mathbf{k}}(\mathbf{r}) \ , \tag{37}$$

where the function $\varphi_{\mathbf{k}}(\mathbf{r})$ defined as

$$\varphi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{Q}\mathbf{r}} u_{\mathbf{k}+\mathbf{Q}}(\mathbf{r}) \tag{38}$$

satisfies the boundary condition,

$$\varphi_{\mathbf{k}}(\mathbf{r}+\mathbf{R}) = e^{i\mathbf{Q}\mathbf{R}} \varphi_{\mathbf{k}}(\mathbf{r}) \ , \tag{39}$$

and it is the eigenfunction of $H(\mathbf{k}, \mathbf{r}) = e^{-i\mathbf{k}\mathbf{r}} H(\mathbf{r}) e^{i\mathbf{k}\mathbf{r}}$ .The Hamilton operator $H(\mathbf{k}, \mathbf{r})$ can be written as

$$H(\mathbf{k}, \mathbf{r}) = H^0(\mathbf{k}, \mathbf{r}) \ I_2 + H_{SOC}(\mathbf{k}, \mathbf{r}) \tag{40}$$

with

$$H^0(\mathbf{k},\mathbf{r}) = \frac{(\mathbf{p}+\hbar\mathbf{k})^2}{2m} + V(\mathbf{r}) - \frac{(\mathbf{p}+\hbar\mathbf{k})^4}{8m^3c^2} + \frac{\hbar^2}{8m^2c^2}\Delta V(\mathbf{r}) \tag{41}$$

and

$$H_{SOC}(\mathbf{k},\mathbf{r}) = \mathbf{L}(\mathbf{k},\mathbf{r})\,\sigma \tag{42}$$

$$\mathbf{L}(\mathbf{k},\mathbf{r}) = \frac{\hbar}{4m^2c^2}\left(\boldsymbol{\nabla}V(\mathbf{r}) \times (\mathbf{p}+\hbar\mathbf{k})\right). \tag{43}$$

Instead of the solving exactly the eigenvalue equation of $H(\mathbf{k},\mathbf{r})$, we consider surface states that are nondegenerate eigenstates of $H^0(\mathbf{k},\mathbf{r})$,

$$H^0(\mathbf{k},\mathbf{r})\,\varphi_{\mathbf{k}}(\mathbf{r}) = \varepsilon^0(\mathbf{k})\,\varphi_{\mathbf{k}}(\mathbf{r}), \tag{44}$$

and use first order perturbation theory in the space of the two spinor functions, $\varphi_{\mathbf{k}s}(\mathbf{r}) = \varphi_{\mathbf{k}}(\mathbf{r})\,\chi_s$, by diagonalizing the matrix of spin-orbit interaction, called the Bychkov-Rashba Hamiltonian,

$$H_{\mathrm{BR}}(\mathbf{k}) = \gamma(\mathbf{k})\,\sigma, \tag{45}$$

with

$$\gamma(\mathbf{k}) = \langle\varphi_{\mathbf{k}}|\,\mathbf{L}(\mathbf{k})\,|\varphi_{\mathbf{k}}\rangle. \tag{46}$$

We are looking for possible forms of $\gamma(\mathbf{k})$ by making use of time reversal invariance and point-group symmetry.

Time reversal transformation acts as

$$T^{-1}H^0(\mathbf{k},\mathbf{r})\,T = CH^0(\mathbf{k},\mathbf{r})\,C = H^0(-\mathbf{k},\mathbf{r}) \tag{47}$$

$$T^{-1}\mathbf{L}(\mathbf{k},\mathbf{r})\,T = C\mathbf{L}(\mathbf{k},\mathbf{r})\,C = -\mathbf{L}_{-\mathbf{k}}(\mathbf{r}) \tag{48}$$

$$T^{-1}\sigma T = -\sigma \tag{49}$$

and, consequently,

$$T^{-1}H(\mathbf{k},\mathbf{r})\,T = H(-\mathbf{k},\mathbf{r}). \tag{50}$$

implying

$$\varepsilon^0(-\mathbf{k}) = \varepsilon^0(\mathbf{k}) \tag{51}$$

and

$$\varphi_{-\mathbf{k}}(\mathbf{r}) = e^{i\theta}C\varphi_{\mathbf{k}}(\mathbf{r}) = e^{i\theta}\varphi_{\mathbf{k}}(\mathbf{r})^*, \tag{52}$$

where $\theta \in \mathbb{R}$ is an arbitrary phase. Let's check the boundary condition for $\varphi_{-\mathbf{k}}(\mathbf{r})$:

$$\varphi_{-\mathbf{k}}(\mathbf{r}+\mathbf{R}) = \varphi_{\mathbf{k}}(\mathbf{r}+\mathbf{R})^* = e^{-i\mathbf{Q}\mathbf{R}}\varphi_{\mathbf{k}}(\mathbf{r})^* = e^{-i\mathbf{Q}\mathbf{R}}\varphi_{-\mathbf{k}}(\mathbf{r}), \tag{53}$$

which is equivalent with the condition (39) for

$$-\mathbf{Q} = \begin{cases} \mathbf{Q} \\ \mathbf{Q}+\mathbf{K} \end{cases}. \tag{54}$$

This is obviously satisfied for the $\overline{\Gamma}$ point of any SBZ, but also for the $\overline{\mathrm{Y}}$ point of the fcc(110) SBZ, since $2\mathbf{Q} = \frac{2\pi}{b}(1,0,0)$ is a reciprocal lattice vector, where $b = \frac{\sqrt{2}}{2}a$, with a being the cubic lattice constant.

Furthermore,

$$\begin{aligned}\gamma\left(-\mathbf{k}\right) &= \left\langle\varphi_{-\mathbf{k}}\right|\mathbf{L}\left(-\mathbf{k}\right)\left|\varphi_{-\mathbf{k}}\right\rangle = -\left\langle C\varphi_{\mathbf{k}}\right|C\mathbf{L}\left(\mathbf{k}\right)\varphi_{\mathbf{k}}\rangle = -\left\langle\varphi_{\mathbf{k}}\right|\mathbf{L}\left(\mathbf{k}\right)\varphi_{\mathbf{k}}\rangle^{*} \\ &= -\left\langle\varphi_{\mathbf{k}}\right|\mathbf{L}\left(\mathbf{k}\right)\varphi_{\mathbf{k}}\rangle = -\gamma\left(\mathbf{k}\right) \ . \end{aligned} \tag{55}$$

Let $g \in G$ the point-group of the surface,

$$V\left(g^{-1}\mathbf{r}\right) = V\left(\mathbf{r}\right) \ . \tag{56}$$

We have learned already that

$$H^{0}\left(\mathbf{k}, g^{-1}\mathbf{r}\right) = H^{0}\left(g\mathbf{k}, \mathbf{r}\right) \ , \tag{57}$$

while

$$\begin{aligned}\mathbf{L}\left(\mathbf{k}, g^{-1}\mathbf{r}\right) &= \frac{\hbar}{4m^{2}c^{2}}\left(\boldsymbol{\nabla}V\left(g^{-1}\mathbf{r}\right)\times\left(g^{-1}\mathbf{p}+\hbar\mathbf{k}\right)\right) = \frac{\hbar}{4m^{2}c^{2}}\left(g^{-1}\boldsymbol{\nabla}V\left(\mathbf{r}\right)\times\left(g^{-1}\mathbf{p}+\hbar\mathbf{k}\right)\right) \\ &= \frac{\hbar}{4m^{2}c^{2}}\det\left(g\right)\ g^{-1}\left(\boldsymbol{\nabla}V\left(\mathbf{r}\right)\times\left(\mathbf{p}+\hbar g\mathbf{k}\right)\right) = \det\left(g\right)\ g^{-1}\mathbf{L}\left(g\mathbf{k}, \mathbf{r}\right) \ , \end{aligned} \tag{58}$$

where $\det\left(g\right) = 1$ for proper rotations and $\det\left(g\right) = -1$ for inproper rotations. If $U_{g} \in SU\left(2\right)$ is the 2×2 unitary matrix representation of g,

$$U_{g}\sigma U_{g}^{-1} = \det\left(g\right)\ g^{-1}\sigma \tag{59}$$

the Hamilton operator remains invariant against the symmetry transformation g,

$$U_{g}\, H\left(\mathbf{k}, g^{-1}\mathbf{r}\right) U_{g}^{-1} = H\left(g\mathbf{k}, \mathbf{r}\right) \ . \tag{60}$$

The point-group symmetry implies

$$H^{0}\left(\mathbf{k}, g^{-1}\mathbf{r}\right)\varphi_{\mathbf{k}}\left(g^{-1}\mathbf{r}\right) = H^{0}\left(g\mathbf{k}, \mathbf{r}\right)\varphi_{\mathbf{k}}\left(g^{-1}\mathbf{r}\right) = \varepsilon^{0}\left(\mathbf{k}\right)\varphi_{\mathbf{k}}\left(g^{-1}\mathbf{r}\right) \ , \tag{61}$$

thus

$$\varepsilon^{0}\left(g\mathbf{k}\right) = \varepsilon^{0}\left(\mathbf{k}\right) \tag{62}$$

and

$$\varphi_{\mathbf{k}}\left(g^{-1}\mathbf{r}\right) = e^{i\tau}\varphi_{g\mathbf{k}}\left(\mathbf{r}\right) \tag{63}$$

for $\tau \in \mathbb{R}$. Inspecting the boundary condition for $\varphi_{g\mathbf{k}}\left(\mathbf{r}\right)$,

$$\begin{aligned}\varphi_{g\mathbf{k}}\left(\mathbf{r}+\mathbf{R}\right) &= e^{i\tau}\varphi_{\mathbf{k}}\left(g^{-1}\mathbf{r}+g^{-1}\mathbf{R}\right) = e^{i\mathbf{Q}\left(g^{-1}\mathbf{R}\right)}\varphi_{\mathbf{k}}\left(g^{-1}\mathbf{r}\right) = e^{i(g\mathbf{Q})\mathbf{R}}\varphi_{\mathbf{k}}\left(g^{-1}\mathbf{r}\right) \\ &= e^{i(g\mathbf{Q})\mathbf{R}}\varphi_{g\mathbf{k}}\left(\mathbf{r}\right) \ , \end{aligned} \tag{64}$$

Eq. (39) is satisfied if

$$g\mathbf{Q} = \left\{ \begin{array}{c} \mathbf{Q} \\ \mathbf{Q}+\mathbf{K} \end{array} \right. \ , \tag{65}$$

i.e. we should restrict g to the little group of $\mathbf{Q}$! From Eqs. (58) and (63) we can then deduce

$$\gamma\left(g\mathbf{k}\right) = \left\langle\varphi_{g\mathbf{k}}\right|\mathbf{L}\left(g\mathbf{k}\right)\left|\varphi_{g\mathbf{k}}\right\rangle = \left\langle\varphi_{\mathbf{k}}\right|\det\left(g\right)\ g\mathbf{L}\left(\mathbf{k}\right)\left|\varphi_{\mathbf{k}}\right\rangle = \det\left(g\right)\ g\,\gamma\left(\mathbf{k}\right) \ . \tag{66}$$

Eqs. (51), (55), (62) and (66) are useful to find the parametric forms of $\varepsilon^0(\mathbf{k})$ and $\gamma(\mathbf{k})$. First we note that the Taylor expansion of $\varepsilon^0(\mathbf{k})$ and $\gamma(\mathbf{k})$ contain just even and odd powers of the components of k, respectively. Usually we go up to second power for $\varepsilon^0(\mathbf{k})$,

$$\varepsilon^0(\mathbf{k}) = \varepsilon^0 + b_{20}k_x^2 + b_{11}k_xk_y + b_{02}k_y^2 \tag{67}$$

and third power for $\gamma(\mathbf{k})$,

$$\gamma(\mathbf{k}) = \begin{pmatrix} c_{10}k_x + c_{01}k_y \\ d_{10}k_x + d_{01}k_y \\ e_{10}k_x + e_{01}k_y \end{pmatrix} + \begin{pmatrix} c_{30}k_x^3 + c_{21}k_x^2k_y + c_{12}k_xk_y^2 + c_{03}k_y^3 \\ d_{30}k_x^3 + d_{21}k_x^2k_y + d_{12}k_xk_y^2 + d_{03}k_y^3 \\ e_{30}k_x^3 + e_{21}k_x^2k_y + e_{12}k_xk_y^2 + e_{03}k_y^3 \end{pmatrix}. \tag{68}$$

As an example we consider the case when the little group of $\mathbf{Q}$ is C_{2v} such as for the $\overline{\mathrm{Y}}$ point of the SBZ of the Au(110) surface. All we have to know are the action of the symmetry operations:

	E	C_2	σ_x	σ_y
x	x	$-x$	x	$-x$
y	x	$-y$	$-y$	y
z	z	z	z	z

.

To get the second-order parametric form of $\varepsilon^0(\mathbf{k})$ we apply σ_x or σ_y (C_2 doesn't give any restriction):

$$b_{20}k_x^2 + b_{11}k_xk_y + b_{02}k_y^2 \underset{\sigma_x}{\to} b_{20}k_x^2 - b_{11}k_xk_y + b_{02}k_y^2$$

from which $b_{11} = 0$ follows:

$$\varepsilon^0(\mathbf{k}) = \varepsilon^0 + b_{20}k_x^2 + b_{02}k_y^2$$

The linear terms in $\gamma(\mathbf{k})$ can also be obtained by applying σ_x or/and σ_y:

$$c_{10}k_x + c_{01}k_y \underset{\sigma_x}{\to} c_{10}k_x - c_{01}k_y = -c_{10}k_x - c_{01}k_y \to c_{10} = 0$$
$$c_{10}k_x + c_{01}k_y \underset{\sigma_y}{\to} -c_{10}k_x + c_{01}k_y = c_{10}k_x + c_{01}k_y \to c_{10} = 0$$

$$d_{10}k_x + d_{01}k_y \underset{\sigma_x}{\to} d_{10}k_x - d_{01}k_y = d_{10}k_x + d_{01}k_y \to d_{01} = 0$$

$$e_{10}k_x + e_{01}k_y \underset{\sigma_x}{\to} e_{10}k_x - e_{01}k_y = -e_{10}k_x - e_{01}k_y \to e_{10} = 0$$
$$e_{10}k_x + e_{01}k_y \underset{\sigma_y}{\to} -e_{10}k_x + e_{01}k_y = -e_{10}k_x - e_{01}k_y \to e_{01} = 0$$

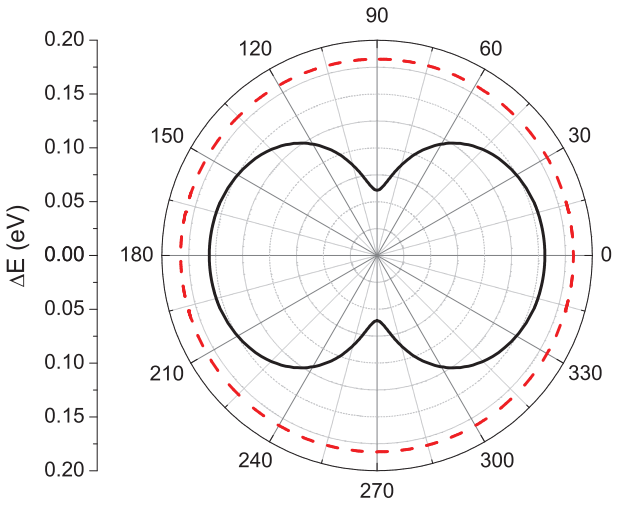
thus, up to first power in k,

$$\gamma^{(1)}(\mathbf{k}) = \begin{pmatrix} c_{01}k_y \\ d_{10}k_x \\ 0 \end{pmatrix},$$

and

$$H_{\mathrm{BR}}^{(1)}(\mathbf{k}) = c_{01}k_y\sigma_x + d_{10}k_x\sigma_y\,,$$

i.e. the dispersion of the BR states is not isotropic, which is the case only if $d_{10} = -c_{01}$.



Energy differences, $\varepsilon^+(\mathbf{k}) - \varepsilon^-(\mathbf{k})$, for the Rashba-split surface state of Au(110) (solid black line) and Au(111) (dashed red line) as a function of the polar angle $\varphi = \arctan \frac{k_y}{k_x}$, shown in units of degree around the graph. The magnitude of $\mathbf{k}$ was fixed to satisfy $\varepsilon^+(\mathbf{k}) = \varepsilon_F$. The energy scale is indicated by the axis on the left. (From E. Simon *et al.*, Physical Review B **81**, 235438 (2010).

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