Supplemental material to the article "Aharonov–Bohm oscillations caused by non-topological surface states in Dirac nanowires"

1. Derivation of anisotropic Dirac Hamiltonian and symmetry restrictions for boundary conditions in bismuth antimony alloys. Here we derive the $\mathbf{k}\cdot\mathbf{p}$-Hamiltonian for electrons in L-valley of bismuth antimony which is of the form of the anisotropic Dirac Hamiltonian. In addition we calculate spectra of surface states for this Hamiltonian. The small group of the L-point is C_{2h}[1]. The Cartesian system is chosen as follows: x axis is perpendicular to the mirror $\Gamma - T - L$ plane, z coincides with $\Gamma - T$ direction. It is well known that in pure bismuth two-band approximation gives adequate picture of band dispersion in L-valleys [2]. These bands are transformed according to $L_a = (L_7, L_8)$ and $L_s = (L_6, L_5)$ irreducible representations of the C_{2h} point group. L_s is symmetric and L_a changes the sign under the inversion. We will use the invariant method [3] to derive the $\mathbf{k}\cdot\mathbf{p}$-Hamiltonian from the symmetry consideration. To further proceed we explicitly write down the matrices of $L_{s,a}$ double group representations of the C_{2h} elements: $D_{s,a}(E) = \sigma_0$, $D_s(I) = -D_a(I) = \sigma_0$, $D_s(C_2(x)) = -D_a(C_2(x)) = -i\sigma_z$, $D_{s,a}(M_x) = -i\sigma_z$; $D_{s,a}(g) = -D_{s,a}(\overline{g})$, where g is an element of C_{2h}. The invariant method requires that for any element g of the point group the Hamiltonian should satisfy the following condition $H(\mathbf{k}) = D(g)H(g^{-1}\mathbf{k})D^{-1}(g)$. In the band subspace the Hamiltonian is of the form:

$$H(\mathbf{k}) = \begin{pmatrix} H_{ss}(\mathbf{k}) & H_{sa}(\mathbf{k}) \\ H_{as}(\mathbf{k}) & H_{aa}(\mathbf{k}) \end{pmatrix}. \tag{1}$$

The most interesting in Eq. (1) is the non-diagonal terms that represents $\mathbf{k}\cdot\mathbf{p}$-interaction between L_s and L_a bands. The upper right term should satisfy the condition $H_{sa}(\mathbf{k}) = D_s(g)H_{sa}(g^{-1}\mathbf{k})D_a^{-1}(g)$. Direct product of $L_s \times L_a^* = 2L_3 + 2L_4$, where L_3 transforms as x and L_4 as y or z. Using representation matrices mentioned above we obtain that σ_0 and σ_z transform as y or z, σ_x, σ_y transforms as x. Therefore the $\mathbf{k}\cdot\mathbf{p}$-interaction term explicitly reads as follows

$$H_{sa}(\mathbf{k}) = (t_1\sigma_x + t_2\sigma_y)k_x + (u_{11}\sigma_z - iu_{12}\sigma_0)k_y + (u_{12}\sigma_z - iu_{22}\sigma_0)k_z. \tag{2}$$

From time-reversal symmetry follows that $t_{1,2}, u_{11,12,21,22}$ are real parameters. Hermiticity of the Hamiltonian (1) leads to identity: $H_{as} = H_{sa}^{+}$. In zero order in momentum for diagonal terms of the Hamiltonian (1) we retain only constant terms $H_{ss} = -H_{aa} = m\sigma_0$, where $2m$ plays the role of the band gap. Finally, we get the following form of the two-band $\mathbf{k}\cdot\mathbf{p}$-Hamiltonian:

$$H = \begin{pmatrix} m & 0 & u_1k_y + u_2k_z & tk_x \\ 0 & m & t^*k_x & -u_1^*k_y - u_2^*k_z \\ u_1^*k_y + u_2^*k_z & tk_x & -m & 0 \\ t^*k_x & -u_1k_y - u_2k_z & 0 & -m \end{pmatrix}, \tag{3}$$

where $u_1 = u_{11} - iu_{12}$, $u_2 = u_{21} - iu_{22}$, $t = t_1 - it_2$. Next step to the Dirac Hamiltonian is to perform unitary transformation $\widetilde{\Psi} = U\Psi$ with $U = \exp\left(-i\beta\tau_0 \otimes \sigma_z - i\gamma\tau_z \otimes \sigma_z\right)$ together with rotation in yz

plane on some angle α (5). After an appropriate choice of β, γ, and α to make $u_{1,2}$ and t real positive parameters, we arrive to the diagonal in spin and momentum form of H (3):

$$\widetilde{H}_{\pm} = m\tau_z \otimes \sigma_0 \pm v_2 k'_y \tau_x \otimes \sigma_z - v_3 k'_z \tau_y \otimes \sigma_0 + v_1 k_x \tau_x \otimes \sigma_x, \tag{4}$$

where

$$v_1 = |t|$$

,

$$v_2 = \sqrt{|u_1|^2 \cos^2\alpha + \Re(u_1 u_2^*) \sin 2\alpha + |u_2|^2 \sin^2\alpha}$$

,

$$v_3 = \sqrt{|u_2|^2 \cos^2\alpha - \Re(u_1 u_2^*) \sin 2\alpha + |u_1|^2 \sin^2\alpha}.$$

Primes under k_y, k_z mean that they are determined in the rotated Cartesian system. The rotation angle α has the following value

$$\alpha = \frac{1}{2}\arctan\left(\frac{2\Re(u_1 u_2^*)}{|u_1|^2 - |u_2|^2}\right). \tag{5}$$

$\widetilde{H}_{\pm}$ is determined up to the sign of the second term. This sign has no impact on the energy dispersion. However it distinguishes two topologically distinct classes of the Hamiltonian (4) and is known as a 'mirror chirality' [4].

Finally we perform unitary transformation $U_{\pm}$ that reduces the Hamiltonian (4) to the standard (but anisotropic) form of the Dirac Hamiltonian [5]:

$$H_D = U_{\pm}\widetilde{H}_{\pm}U_{\pm}^{+} = m\tau_z \otimes \sigma_0 + v_1 k_x \tau_x \otimes \sigma_x + v_2 k'_y \tau_x \otimes \sigma_y + v_3 k'_z \tau_x \otimes \sigma_z. \tag{6}$$

$U_{\pm}$ matrices read as follows

$$U_{\pm} = \frac{e^{i\frac{\pi}{4}}}{\sqrt{2}} \begin{pmatrix} -i & \pm 1 & 0 & 0 \\ \pm i & 1 & 0 & 0 \\ 0 & 0 & 1 & \pm i \\ 0 & 0 & \pm 1 & -i \end{pmatrix} \tag{7}$$

Boundary condition for the four-component wave function $\Psi = (\Psi_c, \Psi_v)$ that obeys the 3D Dirac equation $H_D\Psi = E\Psi$ can be obtain from Hermiticity of H_D (6) in the restricted region and time-reversal symmetry [6]. It is of the following form:

$$\left[\sigma_0 \Psi_v - i a_0 \left(n_x \sigma_x + n_y \frac{v_2}{v_1}\sigma_y + n_z \frac{v_3}{v_1}\sigma_z\right)\Psi_c\right]_S = 0, \tag{8}$$

where n_x, n_y, n_z are coordinates of an inner normal to a surface S in the rotated Cartesian system. For surfaces with $n_x = 0$ we may additionally force the BC (8) to be invariant under the mirror symmetry M_x, if there is no surface reconstruction. For the basis of the Hamiltonian H_D the mirror symmetry operator is expressed by $D(M_x) = i\tau_0 \otimes \sigma_y$. Invariance of the BC (8) under the mirror reflection imposes the following restriction on the BC operator $\hat{\Gamma}$: $\hat{\Gamma} = D(M_x)\hat{\Gamma}D^{-1}(M_x) = e^{i\delta}\hat{\Gamma}$, where

$$\hat{\Gamma} = \begin{pmatrix} -ia_0\left(n_x\sigma_x + n_y\frac{v_2}{v_1}\sigma_y + n_z\frac{v_3}{v_1}\sigma_z\right) & 1 \\ 0 & 0 \end{pmatrix}, \tag{9}$$

$e^{i\delta}$ is an arbitrary phase. This results in restriction $a_0 = 0$ if $n_z \neq 0$. In case of $n_z = 0$ there is no limitation for a_0. It should be noted that the reflection plane is its own for the every L-valley. Therefore if $a_0 = 0$ due to the mirror symmetry for one L-valley, it is not necessarily the case for the other L-valleys. The non-reconstructed (111) surface is the only surface for which the all three inequivalent L-valleys have mirror planes.

Further we study the spectra of surface states for the anisotropic 3D Dirac equation $H_D\Psi = E\Psi$ with the BC (8) on plane surface with $\mathbf{n} = (0,0,1)$. For this surface k_x, k_y are good quantum numbers. After some algebra we arrive to the following energy spectra of surface states:

$$\begin{aligned} &E = s\tfrac{2\tilde{a}_0}{1+\tilde{a}_0^2}\sqrt{v_1^2k_x^2 + v_2^2k_y^2} + m\tfrac{1-\tilde{a}_0^2}{1+\tilde{a}_0^2}, \\ &2m\tilde{a}_0 - s(1-\tilde{a}_0^2)\sqrt{v_1^2k_x^2 + v_2^2k_y^2} \geq 0, \end{aligned} \tag{10}$$

where $\tilde{a}_0 = a_0v_3/v_1$, $s = \pm$. Eq.(10) is an anisotropic version of surface state dispersion that are displayed in Fig. 1 of the main text. As it was noted above the mirror symmetry forces a_0 to zero. In this case we have flat band surface state spectrum $E = m$.

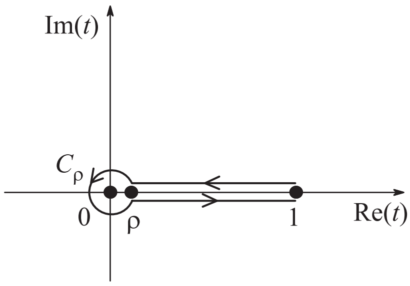

Figure 1: Integration loop that is used for evaluation of $M(a,b,z)$ in (23)

2. Derivation of anisotropic Dirac Hamiltonian and symmetry restrictions for boundary conditions in lead tin chalcogenides. Here we derive the standard 3D Dirac Hamiltonian [5] for L-valley of lead tin chalcogenides and analyze what constrictions if any the mirror symmetry imposes on the BC (8). In the face-centric cubic lattice the small group of L-point is D_{3d}. It is considered that the two relevant spin degenerate bands transform according to L_6^+ and L_6^- representations of double group [7]. We will derive the $\mathbf{k}{\cdot}\mathbf{p}$-Hamiltonian for L-valley on the [111] edge of the Brillouin zone. Therefore it is convenient to work in a coordinate system with $z||[111]$, $y||[1\bar{1}0]$, $x||[\bar{1}\bar{1}2]$ [8]. The basis functions of L_6^+ can be chosen as $|\uparrow\rangle, |\downarrow\rangle$ and $|z\uparrow\rangle, |z\downarrow\rangle$ for L_6^-. Following the similar procedure that was described for bismuth antimony in the previous section we obtain the following Hamiltonian:

$$H = m\tau_z \otimes \sigma_0 + v_1(k_x\tau_x \otimes \sigma_y - k_y\tau_x \otimes \sigma_x) + v_2k_z\tau_y \otimes \sigma_0 \tag{11}$$

where as usual $2m$ plays the role of the band gap, v_1, v_2 are real parameters. The order of the bands determines only the sign of m. The operator of symmetry reflection in $\Gamma - T - L$ plane for this representation is expressed by the matrix $D(M_y) = i\tau_0 \otimes \sigma_y$. Finally the unitary transformation

$$U_1 = \begin{pmatrix} \sigma_z & 0 \\ 0 & -i\sigma_0 \end{pmatrix} \tag{12}$$

reduces the Hamiltonian (11) to the standard Dirac one:

$$H_D = m\tau_z \otimes \sigma_0 + v_1(k_x\tau_x \otimes \sigma_x + k_y\tau_x \otimes \sigma_y) + v_2 k_z \tau_x \otimes \sigma_z. \tag{13}$$

The BC for the Hamiltonian (13) is of the form Eq.(8) with $v_2 = v_1$. It should be noted that the mirror operator for the representation of the Hamiltonian (13) is $\widetilde{D}(M_y) = U_1^+ D(M_y) U_1 = -i\tau_z \otimes \sigma_y$. The mirror symmetry does not impose any restrictions on the BC for surfaces that are of the mirror symmetry (in our case they are determined by $n_y = 0$ with n_x, n_z are arbitrary) as we have

$$M_y \hat{\Gamma}\Psi\Big|_S = \widetilde{D}(M_y)\hat{\Gamma}\widetilde{D}^{-1}(M_y)\widetilde{D}(M_y)\Psi\Big|_S = -\hat{\Gamma}\widetilde{\Psi}\Big|_S = 0, \tag{14}$$

where the BC operator is expressed by

$$\hat{\Gamma} = \begin{pmatrix} -ia_0\left(n_x\sigma_x + n_z\frac{v_2}{v_1}\sigma_z\right) & 1 \\ 0 & 0 \end{pmatrix}. \tag{15}$$

In the isotropic case the Eq. (15) transforms to the formula (4) of the main text.

3. Derivation of dispersion equation in magnetic field. The Dirac equation $H_D\Psi = E\Psi$ and BC $\Gamma\Psi = 0$ can be reduced to the problem only for ψ_c spinor. In nanowire with longitudinal magnetic field the spinor components $\psi_{c1,c2}$ obey equations

$$\left(-\frac{\partial^2}{\partial r^2} - \frac{\partial}{r\partial r} + \frac{(j \mp 1/2)^2}{r^2} + \frac{j \pm 1/2}{\lambda^2} + \frac{r^2}{4\lambda^4}\right)\psi_{c1,c2} = (E^2 - m^2 - k_z^2)\psi_{c1,c2}, \tag{16}$$

and BC:

$$\begin{pmatrix} ik_z & \left[\partial_r + \frac{j+1/2}{R} + \frac{R}{2\lambda^2} + a_0(E+m)\right] \\ \left[\partial_r - \frac{j-1/2}{R} - \frac{R}{2\lambda^2} + a_0(E+m)\right] & -ik_z \end{pmatrix} \begin{pmatrix} \psi_c^{(1)}(r) \\ \psi_c^{(2)}(r) \end{pmatrix}\Bigg|_{r=R} = 0. \tag{17}$$

where we take into account conservation of longitudinal quasi-momentum k_z and total angular momentum projection j. After substitution

$$\psi_c^{(1,2)} = \xi^{|j\mp 1/2|/2}\exp(-\xi/2)w_{1,2}(\xi), \tag{18}$$

where $\xi = r^2/2\lambda^2$ functions $w_{1,2}(\xi)$ satisfy the degenerate hypergeometric equation:

$$\xi w_{1,2}'' + (|j \mp 1/2| + 1 - \xi)w_{1,2}' + \left(\Delta - \frac{|j \mp 1/2| + (j \pm 1/2) + 1/2}{2}\right)w_{1,2} = 0, \tag{19}$$

where $\Delta = \lambda^2\left(E^2 - m^2 - \hbar^2 v^2 k_z^2\right)/2\hbar^2 v^2$. Therefore normalizable solution in the limit $r \to 0$ is expressed via Kummer's function $M(\alpha, \beta, \xi)$:

$$\psi_c^{(1,2)}(r) = C_{1,2}\left(\frac{r}{\sqrt{2}\lambda}\right)^{|j\mp1/2|} e^{-\frac{r^2}{4\lambda^2}} M\left(-\Delta + \frac{|j\mp1/2|+(j\pm1/2)+1}{2}, |j\mp1/2|+1, \frac{r^2}{2\lambda^2}\right). \tag{20}$$

We are interested in spectra for $j \leq -1/2$. Substitution of the wave function (20) in the BC (17) allow us obtain the dispersion equation:

$$\left[2j - 1 - a_0 R(E+m)\widetilde{M}\right] \cdot \left[\frac{R^2 k^2}{2\left(j - \frac{1}{2}\right)} + \frac{a_0 R(E+m)}{\widetilde{M}}\right] + k_z^2 R^2 = 0, \tag{21}$$

where

$$\widetilde{M} = \frac{M(1-\Delta, -j+3/2, R^2/2\lambda^2)}{M(-\Delta, -j+1/2, R^2/2\lambda^2)}. \tag{22}$$

4. Surface states spectra in strong magnetic field. In this section we derive approximate spectra of surface states in strong magnetic field limit. For that we use an integral representation of Kummer's function $M(a, b, z)$ [9] (for the case $\mathrm{Re}(b-a) > 0$):

$$M(a, b, z) = -\frac{1}{2\pi i}\frac{\Gamma(b)\Gamma(1-a)}{\Gamma(b-a)}\int_1^{(0+)} e^{zt}(-t)^{a-1}(1-t)^{b-a-1}dt \tag{23}$$

where integration is performed in a closed loop in the complex t-plane starting from the point $t = 1$ and going-round zero in positive direction. For evaluation of $M(...)$ we choose the loop shown on Fig. 1. Therefore the integral in Eq. (23) can be expressed as follows:

$$\int_1^{(0+)} = \int_1^{\rho} + \int_{C_\rho} + \int_{\rho}^{1} = \int_{C_\rho} + \left(e^{i2\pi a} - 1\right)\int_{\rho}^{1}, \tag{24}$$

here circle of radius ρ should be chosen so that integral in C_ρ would be much smaller than integral from ρ to 1 (and a does not equal to integers that is the case for surface states). We show that this condition can be satisfied in the limit $z \gg b, z \gg a$. For parameters of $M(...)$ in dispersion Eq. (21) this limit is:

$$\begin{cases} \frac{\Phi}{\Phi_0} \gg |j - 1/2| \\ \frac{\Phi}{\Phi_0} \gg \lambda^2(E^2 - m^2 - k_z^2)/2 \\ |j - 1/2| > \lambda^2(E^2 - m^2 - k_z^2)/2. \end{cases} \tag{25}$$

Now we calculate the second integral (after the second equality) in Eq. (24) by the Laplace method. This integral we represent as follows:

$$\int_\rho^1 e^{zt} t^{a-1}(1-t)^{b-a-1}dt = \int_\rho^1 e^{zt+(a-1)\ln t+(b-a-1)\ln(1-t)} \equiv \int_\rho^1 e^{g(a,b,z;t)}, \tag{26}$$

where the last equality should be considered as definition of a function $g(a, b, z; t)$. In the case under consideration (25) the function $g(a, b, z; t)$ in the above Eq. (26) has an abrupt maximum t_0 in the interval $(\rho, 1)$:

$$t_0 = \frac{z - b + 2}{z} - \frac{1 - a}{z - b + 2}. \tag{27}$$

Therefore we evaluate integral as follows

$$\int_\rho^1 e^{g(a,b,z;t)} \approx \sqrt{\frac{2\pi}{|g''(a,b,z;t_0)|}}e^{g(a,b,z;t_0)} = \sqrt{\frac{2\pi(b-2)}{z^2}}e^{z-b+2-\frac{z(1-a)}{z-b+2}}\left(\frac{z-b+2}{z}-\frac{(1-a)}{z-b+2}\right)^{a-1}\left(1-\frac{z-b+2}{z}+\frac{1-a}{z-b+2}\right)^{b-a-1}. \tag{28}$$

The value ρ is chosen so that the integral over circle C_ρ would be much smaller than the integral over interval $(\rho;1)$:

$$\int_{C_\rho} e^{g(a,b,z;t)} \approx e^{\rho z}\rho^{a-1} \ll (e^{i2\pi a}-1)\int_\rho^1 e^{g(a,b,z;t)} \approx e^{z-b+2}\sqrt{\frac{2\pi(b-2)}{z^2}}. \tag{29}$$

The condition (29) can always be fulfilled for surface states ($a \neq 0; -1; -2; -3; \dots$) in the limit under consideration (25). After substitution of approximation (28) in (21) and retaining leading terms, we obtain the spectrum of surface subbands in the strong magnetic field limit (25):

$$E_{k_z js} = sv\hbar\sqrt{k_z^2 + \frac{(j+\Phi-1/2)^2}{R^2}} + E_0, \tag{30}$$

where $\Phi = \pi eBR^2/hc$ is the number of the magnetic flux quanta through the wire cross section, $v = 2ac/(1+a^2)$, $E_0 = mc^2(1-a_0^2)/(1+a_0^2)$. This spectrum holds true under conditions (25).

5. Surface states density of states. Here we calculate density of surface states in a quasi-classical limit $|\kappa R/j| \gg \max(|j|, |\Phi|)$ and in the limit of strong magnetic fields (25). For both limits spectra of surface subbands can be represented as follows:

$$E_{k_z js} = sv\hbar\sqrt{k_z^2 + \frac{(j+\Phi-\gamma_B)^2}{R^2}} + E_0, \tag{31}$$

where $\gamma_B = 0$ in quasiclassical limit, and $\gamma_B = 1/2$ in the limit of strong magnetic fields. Therefore for density of surface subbands in the L_z-length nanowire can be represented as follows:

$$\begin{aligned}
D(E) = &\sum_{(k_z,j)\in G} \delta(E - E_{k_z,j}) = \\
&= \int \frac{L_z dk_z}{2\pi}\int dx \sum_j \delta\left(x - \frac{j}{R}\right)\delta(E - s\hbar v\sqrt{k_z^2 + (x + (\Phi-\gamma_B)/R)^2} - E_0) = \\
&= \frac{L_z R}{2\pi}\sum_{n=-\infty}^{\infty}\int dx \int dk_z e^{i2\pi Rnx - i\pi n}\delta(E - s\hbar v\sqrt{k_z^2 + (x+(\Phi-\gamma_B)/R)^2} - E_0) = \\
&= \frac{L_z R}{2\pi}\sum_{n=-\infty}^{\infty}\int dx' \int dk_z e^{i2\pi Rnx' - i2\pi\Phi n + i2\pi\gamma_B n - i\pi n}\delta(E - s\hbar v\sqrt{k_z^2 + x'^2} - E_0) = \\
&= \frac{L_z R}{2\pi}\sum_{n=-\infty}^{\infty}\int_0^{2\pi} d\theta \int k dk e^{i2\pi Rnk\sin\theta - i2\pi\Phi n + i2\pi\gamma_B n - i\pi n}\delta(E - \hbar v k - E_0) = \\
&= \Theta\left[(E-E_0)\,\mathrm{sgn}(a_0(a_0^2-1)) + \hbar v k_e\right]\frac{L_z R\,(E-E_0)}{2\pi(\hbar v)^2}\times \\
&\times \sum_{n=-\infty}^{\infty} e^{-i2\pi\Phi n + i2\pi\gamma_B n - i\pi n}\int_0^{2\pi} d\theta e^{i2\pi Rn((E-E_0)/\hbar v)\sin\theta} =
\end{aligned}$$

$$= \Theta\left[(E-E_0)\,\mathrm{sgn}(a_0(a_0^2-1)) + \hbar v k_e\right] \frac{L_z R\,(E-E_0)}{2\pi(\hbar v)^2} 2\pi \times$$

$$\times \left(1 + 2\sum_{n=1}^{+\infty} J_0\left(\frac{2\pi R(E-E_0)n}{\hbar v}\right)\cos\left(2\pi\Phi n - 2\pi\gamma_B n + \pi n\right)\right) =$$

$$= \Theta\left[(E-E_0)\,\mathrm{sgn}(a_0(a_0^2-1)) + \hbar v k_e\right] \frac{L_z R\,(E-E_0)}{2\pi(\hbar v)^2} 2\pi \times$$

$$\times \left(1 + 2\sqrt{\frac{\hbar v}{\pi^2 R(E-E_0)}} \sum_{n=1}^{+\infty} \frac{\cos\left(\frac{2\pi R(E-E_0)n}{\hbar v}\right)}{\sqrt{n}} \cos\left(2\pi\Phi n - 2\pi\gamma_B n + \pi n\right)\right), \qquad (32)$$

where region for integration in all formulae is $G = \{s\sqrt{k_z^2 + (j+\Phi-\gamma_B)^2/R^2} > k_e\}$, $k_e = 2|a_0|m/c\hbar|1-a_0^2|$, $J_0(x)$ is Bessel function of the first kind. In the last equality in Eq.(32) we use asymptotes of $J_0(x)$ at $x \gg 1$.

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