# Online Supplemental Material: Anomalous Electron Trajectory in Topological Insulators

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## DIAGRAM TECHNIQUE IN THE ABSENCE OF EXTERNAL FIELD

We consider a single-particle Hamiltonian of electron in a general form

$$\begin{aligned} H &= \epsilon\left(k\right)+\sum_i d_i\left(k\right)\sigma^i \\ &= \epsilon\left(k\right)+D\left(k\right) \end{aligned} \tag{1}$$

where $\epsilon\left(k\right)$ denotes the kinetic energy and the second term describes the spin-orbit interactions or interband coupling.

In the Heisenberg picture, the position operator of electron $y_H(t)$ evolving with time $t$ can be obtained by

$$\begin{aligned} y_H(t) &= e^{iHt/\hbar}ye^{-iHt/\hbar}, \\ &= y(0)+(it/\hbar)[H,y]+\frac{(it/\hbar)^2}{2!}[H,[H,y]]+\cdots, \\ &= y(0)+(it/\hbar)\epsilon^y+\sum_{n=1}\frac{(it/\hbar)^n}{n!}T_n, \end{aligned} \tag{2}$$

where we show the notions explicitly:

$$\begin{aligned} \epsilon^y &= [\epsilon,y]=-i\partial_{k_y}\epsilon, \\ T_1 &= [H,y]=[D,y], \\ T_2 &= [H,T_1]=[D,T_1], \\ &\vdots \\ T_n &= [D,T_{n-1}]. \end{aligned} \tag{3}$$

The above equation involves the infinite summation of the commutators $T_n$ and therefore it is not easy to obtain the analytical expression of the position operator $y_H(t)$. In order to calculate the commutation in arbitrary order and the summation, we develop a diagram technique as follow which makes the lengthy calculation of the commutation much easier. Utilizing the similarity between the commutation relationship $[\sigma_i,\sigma_j]=2i\varepsilon_{ijk}\sigma_k$ and the vector cross production $\boldsymbol{A}\times\boldsymbol{B}=\varepsilon_{ijk}A_iB_j\boldsymbol{e}_k$, we obtain the following relationship

$$\begin{aligned} D\left(k\right)=d_1\sigma^1+d_2\sigma^2+d_3\sigma^3 &\rightarrow \boldsymbol{D}=\left(d_1,d_2,d_3\right), \\ T_1=[H,y]=t_0+t_1\sigma^1+t_2\sigma^2+t_3\sigma^3 &\rightarrow \boldsymbol{T}_1=\left(t_1,t_2,t_3\right), \\ T_2=[H,T_1]=[D,T_1] &\rightarrow 2i\left(\boldsymbol{D}\times\boldsymbol{T}_1\right), \\ &\cdots \\ T_{n+1}=[H,T_n]=[D,T_n] &\rightarrow 2i\left(\boldsymbol{D}\times\boldsymbol{T}_n\right). \end{aligned} \tag{4}$$

These relationships can be illustrated in Fig. 1. From this figure, one can see that the vectors $\boldsymbol{T}_{2n+1}$ and $\boldsymbol{T}_{2n}$ $(n=1,2,3\cdots)$ point along the two perpendicular axes, respectively, but the magnitudes (or lengths) of the vectors $\boldsymbol{T}_{2n+1}$ and $\boldsymbol{T}_{2n}$ are both geometrical series. This character allows us to get the analytical expression of the infinite summation.

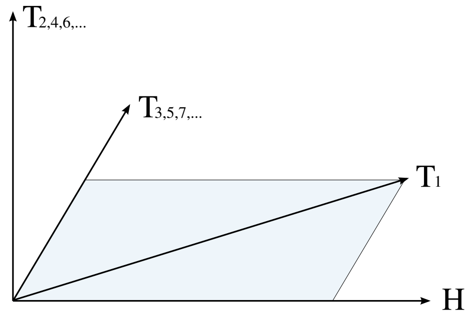


FIG. 1: Illustrating figure showing how to calculate $T_n$ using the vector cross times (see Eq.[4]).

Summing up all the terms, we get an analytical expression for the position operator of electron

$$y_H(t) = y(0) + \frac{it}{\hbar}\left(\epsilon^y + T_1\right) + \frac{T_2}{2|D|^2}\left[\cos\left(2|D|t/\hbar\right) - 1\right] + \frac{iT_3}{2|D|^3}\left[\sin\left(2|D|t/\hbar\right) - \left(2|D|t/\hbar\right)\right], \tag{5}$$

where $|D| = \sqrt{d_1^2 + d_2^2 + d_3^2}$.

## ANALYTICAL EXPRESSION FOR ELECTRON TRAJECTORY: ADIABATIC APPROXIMATION

The Hamiltonian for a two-dimensional topological insulator, a HgTe quantum well with an inverted band structure described by the BHZ model, under a uniform electric filed is

$$H(k)_{\uparrow\downarrow} = H_0(k)_{\uparrow\downarrow} + V(x_i),$$

where $H_0(k)_{\uparrow\downarrow} = C - Dk^2 \pm Ak_x\sigma^x + Ak_y\sigma^y + (M - Bk^2)\sigma^z$, $V(\mathbf{x}) = -e\mathbf{E}\cdot\mathbf{r}\sigma^z$. After the proper unitary transformation $U(k)_{\uparrow\downarrow}$ which can diagonalize the $H_0(k)$, i. e., $\tilde{H}_0 = U(k)_{\uparrow\downarrow}H_0(k)_{\uparrow\downarrow}U^\dagger(k)_{\uparrow\downarrow}$, then $H^{\rm eff}_{\uparrow\downarrow} = \tilde{H}_0(k) - e\sum_{i=x,y}E_iD_{i,\uparrow\downarrow}$, where

$$\tilde{H}_0(k) = C - Dk^2 + \begin{pmatrix} -\sqrt{A^2k^2 + (M - Bk^2)^2} & 0 \\ 0 & \sqrt{A^2k^2 + (M - Bk^2)^2} \end{pmatrix},$$

$$U(k)_{\uparrow\downarrow} = \begin{pmatrix} \frac{\mp[-Bk^2 + M - \sqrt{A^2k^2 + (M-Bk^2)^2}]}{A(k_x \pm ik_y)\sqrt{1 + \frac{(Bk^2 - M + \sqrt{A^2k^2+(M-Bk^2)^2})}{A^2k^2}}} & \frac{-Bk^2 + M + \sqrt{A^2k^2+(M-Bk^2)^2}}{A(k_x \pm ik_y)\sqrt{1 + \frac{(Bk^2 + M + \sqrt{A^2k^2+(M-Bk^2)^2})}{A^2k^2}}} \\ \frac{1}{\sqrt{1 + \frac{(Bk^2 - M + \sqrt{A^2k^2+(M-Bk^2)^2})}{A^2k^2}}} & \frac{1}{\sqrt{1 + \frac{(-Bk^2 + M + \sqrt{A^2k^2+(M-Bk^2)^2})}{A^2k^2}}} \end{pmatrix},$$

and

$$\tilde{A}_i(k)_{\uparrow\downarrow} = -i\cdot U(k)_{\uparrow\downarrow}\partial_{k_i}U^\dagger(k)_{\uparrow\downarrow}\cdot U(k)_{\uparrow\downarrow}\sigma^z U^\dagger(k)_{\uparrow\downarrow}.$$

The analytical expression is too *lengthy* to be omitted here. Adopting the adiabatic approximation, we neglect the interband transitions, i.e., neglecting the off-diagonal matrix elements of $\tilde{A}$,

$$F_{xy}(k)_{\uparrow\downarrow} = i[D_i, D_j] = \begin{pmatrix} \pm\frac{A^2(M^2 - B^2k^4)}{2[A^2k^2 + (M-Bk^2)^2]^2} & 0 \\ 0 & \pm\frac{A^2(M^2 - B^2k^4)}{2[A^2k^2 + (M-Bk^2)^2]^2} \end{pmatrix}.$$

The equation of motion for the spin-up/down $(\uparrow\downarrow)$ negative/positive branch ($\lambda = \pm1$) can be written as:

$$k_i = k_{i0} + \lambda\frac{eE_i}{\hbar}t,$$

$$\frac{dx_{\uparrow\downarrow}}{dt} = -\frac{2D}{\hbar}k_x + \lambda\frac{2B(M-Bk^2)-A^2}{\hbar\sqrt{A^2k^2+(M-Bk^2)^2}}k_x \pm \frac{eE_y}{\hbar}\frac{A^2(M^2-B^2k^4)}{2[A^2k^2+(M-Bk^2)^2]^2},$$
$$\frac{dy_{\uparrow\downarrow}}{dt} = -\frac{2D}{\hbar}k_y + \lambda\frac{2B(M-Bk^2)-A^2}{\hbar\sqrt{A^2k^2+(M-Bk^2)^2}}k_y \mp \frac{eE_x}{\hbar}\frac{A^2(M^2-B^2k^4)}{2[A^2k^2+(M-Bk^2)^2]^2}.$$

When $E_y = k_y = 0$, the integration of the topological term [1], $\mp\frac{eE_x}{\hbar}\frac{A^2(M^2-B^2k^4)}{2[A^2k^2+(M-Bk^2)^2]^2}$, represents the electron's orbital motion in the $y$ axis brought by the effective field strength $F_{xy}$,

$$y^{\rm orb}_{\uparrow\downarrow} = \int dk\frac{A^2(M^2-B^2k^4)}{2[A^2k^2+(M-Bk^2)^2]^2}.$$

To the second order of $k$,

$$y^{\rm orb}_{\uparrow\downarrow} = \mp\frac{A^2}{2M^2}k + O(k)^3,$$

and for the $k\to\infty$ limit,

$$y^{\rm orb}_{\uparrow\downarrow} \to \mp\frac{iA\pi\left(\sqrt{\frac{B^2}{A^2-2BM-iA\sqrt{-A^2+4BM}}} - \sqrt{\frac{B^2}{A^2-2BM+iA\sqrt{-A^2+4BM}}}\right)}{4\sqrt{-2A^2+8BM}},$$

which is about 14.31nm adopting the parameters in Ref. [2]. We can see that this topological shift have a upper limit during a single ballistic motion.

Next, we derive the analytical expression for the trembling motion, i.e., the *Zitterbewegung* [3]. We assume the wave function has the form of $|\psi(x,t)\rangle = \exp(-ie\mathbf{E}\cdot\mathbf{r}\sigma_z t/\hbar)|u(x,t)\rangle$, and substitute $|\psi(x,t)\rangle$ into the Schrödinger equation

$$i\hbar\partial_t|\psi(x,t)\rangle = [H_0(k)_{\uparrow\downarrow} + e\mathbf{E}\cdot\mathbf{r}\sigma_z]|\psi(x,t)\rangle,$$

where $H_0(k)_{\uparrow\downarrow} = C - Dk^2 \pm Ak_x\sigma^x + Ak_y\sigma^y + (M-Bk^2)\sigma^z$, because

$$i\hbar\partial_t|\psi(x,t)\rangle = [e\mathbf{E}\cdot\mathbf{r}\sigma_z]|\psi(x,t)\rangle + \exp(-ie\mathbf{E}\cdot\mathbf{r}\sigma_z t/\hbar)[i\hbar\partial_t|u(x,t)\rangle],$$

we get a time-dependent Schrödinger equation

$$i\hbar\partial_t|u(x,t)\rangle = H_0(k,t)|u(x,t)\rangle,$$

where $k_i(t) = k_{i0} + \lambda\frac{eE_i}{\hbar}t$. We assume that $|u(x,t)\rangle = \sum_\lambda C_\lambda(t)\exp(-i\alpha_\lambda)U^\dagger(k)|\lambda\rangle$, where $|\lambda\rangle$ represents any eigenstate of $S_z$, that is $S_z|\lambda\rangle = \lambda|\lambda\rangle$, so $U^\dagger(k)_{\uparrow\downarrow}|\lambda\rangle$ is the instant eigenstate of $H_0(k)_{\uparrow\downarrow}$, $H_0(k)_{\uparrow\downarrow}U^\dagger(k)_{\uparrow\downarrow}|\lambda\rangle = \epsilon_\lambda(t)U^\dagger(k)_{\uparrow\downarrow}|\lambda\rangle$, where $\epsilon_{\frac{1}{2}/\frac{3}{2}}(t) = C - Dk^2 \mp \sqrt{A^2k^2+(M-Bk^2)^2}$. $\alpha_\lambda = (1/\hbar)\int_0^t\epsilon_\lambda(t')dt'$. Because

$$\begin{aligned} i\hbar\partial_t|u(x,t)\rangle &= i\hbar\textstyle\sum_\lambda[\partial_t C_\lambda(t)]\exp(-i\alpha_\lambda)U^\dagger(k)_{\uparrow\downarrow}|\lambda\rangle \\ &+ \textstyle\sum_\lambda C_\lambda(t)[\epsilon_\lambda(t)\exp(-i\alpha_\lambda)]U^\dagger(k)_{\uparrow\downarrow}|\lambda\rangle \\ &+ i\hbar\textstyle\sum_\lambda C_\lambda(t)\exp(-i\alpha_\lambda)[\partial_t U^\dagger(k)_{\uparrow\downarrow}]|\lambda\rangle, \end{aligned}$$

and

$$H_0|u(x,t)\rangle = \textstyle\sum_\lambda C_\lambda(t)[\epsilon_\lambda(t)\exp(-i\alpha_\lambda)]U^\dagger(k)_{\uparrow\downarrow}|\lambda\rangle$$

thus

$$\textstyle\sum_\lambda[\partial_t C_\lambda(t)]\exp(-i\alpha_\lambda)U^\dagger(k)_{\uparrow\downarrow}|\lambda\rangle + \sum_\lambda C_\lambda(t)\exp(-i\alpha_\lambda)[\partial_t U^\dagger(k)_{\uparrow\downarrow}]|\lambda\rangle = 0.$$

Act $U(k)_{\uparrow\downarrow}$ and $\langle\lambda'|$ to the left side,

$$[\partial_t C_{\lambda'}(t)]\exp(-i\alpha_{\lambda'}) + \textstyle\sum_\lambda C_\lambda(t)\exp(-i\alpha_\lambda)\langle\lambda'|U(k)_{\uparrow\downarrow}\partial_t U^\dagger(k)_{\uparrow\downarrow}|\lambda\rangle = 0.$$

For the helicity state, $|1/2\rangle = (1,0)^T$, $|3/2\rangle = (0,1)^T$, we set the initial state $C_{1/2}(0) = 1$, $C_{3/2}(0) = 0$. The adiabatic approximation assumes that $0 \simeq C_{3/2}(t) \ll C_{1/2}(t)$ is always satisfied, which leads to

$$\begin{aligned}\partial_t C_{1/2}(t) &\simeq -C_{1/2}(t)\,\langle 1/2|\,U(k)_{\uparrow\downarrow}\partial_t U^\dagger(k)_{\uparrow\downarrow}\,|1/2\rangle\,,\\ \partial_t C_{3/2}(t) &\simeq -C_{1/2}(t)\exp(i\Delta\alpha)\,\langle 3/2|\,U(k)_{\uparrow\downarrow}\partial_t U^\dagger(k)_{\uparrow\downarrow}\,|1/2\rangle\,,\\ \Delta\alpha &= \alpha_{3/2}-\alpha_{1/2} = (1/\hbar)\textstyle\int_0^t \Delta\epsilon(t')dt'.\end{aligned}$$

Because $y^{\rm ZB}_{\uparrow\downarrow} = C^*_{3/2}C_{1/2}e^{-i\Delta\alpha}\,\langle 3/2|\,iU(k)_{\uparrow\downarrow}\partial_{k_y}U^\dagger(k)_{\uparrow\downarrow}\,|1/2\rangle$ +h.c., Then we can calculate the $U(k)_{\uparrow\downarrow}\partial_t U^\dagger(k)_{\uparrow\downarrow}$ and $U(k)_{\uparrow\downarrow}\partial_{k_y}U^\dagger(k)_{\uparrow\downarrow}$. When $E_y = \partial k_y/\partial t = 0$,

$$U(k)_{\uparrow\downarrow}\partial_t U^\dagger(k)_{\uparrow\downarrow} = U(k)_{\uparrow\downarrow}\frac{\partial}{\partial k_x}U^\dagger(k)_{\uparrow\downarrow}\cdot\frac{\partial k_x}{\partial t},$$

at small $k$,

$$\begin{aligned}U(k)_{\uparrow\downarrow}\frac{\partial}{\partial k_x}U^\dagger(k)_{\uparrow\downarrow}\Big|_{k=0} &= \begin{bmatrix} 0 & \pm\frac{A}{2M}\\ \mp\frac{A}{2M} & 0\end{bmatrix} + O(k^2),\\ U(k)_{\uparrow\downarrow}\frac{\partial}{\partial k_y}U^\dagger(k)_{\uparrow\downarrow}\Big|_{k=0} &= \begin{bmatrix} 0 & -\frac{iA}{2M}\\ -\frac{iA}{2M} & 0\end{bmatrix} + O(k^2),\end{aligned}$$

Notice that the $U(k)_{\uparrow\downarrow}\partial_{k_y}U^\dagger(k)_{\uparrow\downarrow}$ and $\langle 3/2|\,iU(k)_{\uparrow\downarrow}\partial_{k_y}U^\dagger(k)_{\uparrow\downarrow}\,|1/2\rangle$ is only finite for the diagonal and off-diagonal matrix elements, respectively. Therefore

$$\begin{aligned}\partial_t C_{1/2}(t)_{\uparrow\downarrow} &= 0,\\ \partial_t C_{3/2}(t)_{\uparrow\downarrow} &= \mp\frac{A}{2M}\frac{eE_x}{\hbar}\exp(i\Delta\alpha).\end{aligned}$$

Adopting the adiabatic approximation, $\epsilon_\lambda(t)$ are slowly varying functions of the time $t$,

$$C_{3/2}(t)_{\uparrow\downarrow} = \mp\frac{A}{2M}\frac{eE_x}{\Delta\epsilon(t)}\exp(i\Delta\alpha).$$

Finally we get

$$y^{\rm ZB}_{\uparrow\downarrow} = \pm\frac{A^2}{2M^2}\frac{eE_x}{\Delta\epsilon(t)}\sin(\frac{\Delta\epsilon(t)}{\hbar}t),$$

where $\Delta\epsilon(t) = 2\sqrt{A^2k^2 + (M-Bk^2)^2} = 2\,|M| + O(k^2)$. At small $k$,

$$y^{\rm ZB}_{\uparrow\downarrow} \simeq \pm\frac{A^2}{4M^2}\frac{eE_x}{|M|}\sin(\frac{\Delta\epsilon(t)}{\hbar}t).$$

## THE NUMERICAL CALCULATION OF ELECTRON TRAJECTORY $y(t)$

We assume that the electric field $E = (-E,0,0)$ points along the $-x$ axis without loss of any generality, thus

$$H_{\uparrow\downarrow}(k) = C - Dk^2 + (\pm Ak_x, Ak_y, M-Bk^2)\cdot\sigma - eEx\cdot\sigma_z,$$

or

$$H(k) = C - Dk^2 + Ak_x\cdot s_1 + Ak_y\cdot s_2 + (M-Bk^2)\cdot s_3 - eEx\cdot s_3,$$

where we define

$$s_1 = \begin{bmatrix}\sigma_x & 0\\ 0 & -\sigma_x\end{bmatrix}, s_2 = \begin{bmatrix}\sigma_y & 0\\ 0 & \sigma_y\end{bmatrix}, s_3 = \begin{bmatrix}\sigma_z & 0\\ 0 & \sigma_z\end{bmatrix},$$

$$s_4 = \begin{bmatrix} \sigma_x & 0 \\ 0 & \sigma_x \end{bmatrix}, s_5 = \begin{bmatrix} \sigma_y & 0 \\ 0 & -\sigma_y \end{bmatrix}, s_6 = \begin{bmatrix} \sigma_z & 0 \\ 0 & -\sigma_z \end{bmatrix},$$

then

$$\frac{d\langle k_x\rangle}{dt} = \frac{eE}{\hbar}\langle s_3\rangle,$$
$$\frac{d\langle k_y\rangle}{dt} = 0,$$

$$\frac{d\langle x\rangle}{dt} = -\frac{2D}{\hbar}\langle k_x\rangle + \frac{A}{\hbar}\langle s_1\rangle - \frac{2B}{\hbar}\langle k_x\rangle\langle s_3\rangle,$$
$$\frac{d\langle y\rangle}{dt} = -\frac{2D}{\hbar}\langle k_y\rangle + \frac{A}{\hbar}\langle s_2\rangle - \frac{2B}{\hbar}\langle k_y\rangle\langle s_3\rangle,$$

$$\frac{d\langle s_1\rangle}{dt} = -2\frac{M - B\langle k\rangle^2 - eE\langle x\rangle}{\hbar}\langle s_5\rangle + \frac{2A}{\hbar}\langle k_y\rangle\langle s_6\rangle,$$
$$\frac{d\langle s_2\rangle}{dt} = 2\frac{M - B\langle k\rangle^2 - eE\langle x\rangle}{\hbar}\langle s_4\rangle - \frac{2A}{\hbar}\langle k_x\rangle\langle s_6\rangle,$$
$$\frac{d\langle s_3\rangle}{dt} = -\frac{2A}{\hbar}\langle k_y\rangle\langle s_4\rangle + \frac{2A}{\hbar}\langle k_x\rangle\langle s_5\rangle,$$

$$\frac{d\langle s_4\rangle}{dt} = -2\frac{M - B\langle k\rangle^2 - eE\langle x\rangle}{\hbar}\langle s_2\rangle + \frac{2A}{\hbar}\langle k_y\rangle\langle s_3\rangle,$$
$$\frac{d\langle s_5\rangle}{dt} = 2\frac{M - B\langle k\rangle^2 - eE\langle x\rangle}{\hbar}\langle s_1\rangle - \frac{2A}{\hbar}\langle k_x\rangle\langle s_3\rangle,$$
$$\frac{d\langle s_6\rangle}{dt} = -\frac{2A}{\hbar}\langle k_y\rangle\langle s_1\rangle + \frac{2A}{\hbar}\langle k_x\rangle\langle s_2\rangle.$$

For a given initial state, we can calculate the electron trajectory $\langle y(t)\rangle$ involving with the time $t$ numerically.

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