Supplementary materials for "Quantum anomalous semimetals"

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One-dimensional time-dependent model We present an exact solution of a two-level problem to demonstrate the non-Abelian topological properties of 1D massless Wilson fermions. For simplicity, we consider a two-level system,

$$H_{1D}(t) = \frac{\hbar\omega_0}{2}\sin\omega t\sigma_x + \hbar\omega_0 \sin^2\frac{\omega t}{2}\sigma_y. \tag{1}$$

The Hamiltonian is periodic with a time T, $H_{1D}(t+T) = H_{1D}(t)$. The instantaneous energy eigenvalues are $E_\chi = \chi\hbar\omega_0 \sin\frac{\omega t}{2}$ with $\chi = \pm 1$. The two bands cross at time $\omega t = 0$ or $\omega T = 2\pi$. The model possesses the glide mirror symmetry, $\mathcal{G}(\omega t) = \begin{pmatrix} 0 & e^{-i\omega t} \\ 1 & 0 \end{pmatrix}$ such that $\mathcal{G}(\omega t)H_{1D}(t)\mathcal{G}^{-1}(\omega t) = H_{1D}(t)$. The symmetry operator has the relation $\mathcal{G}^2(\omega t) = e^{-i\omega t}$, and its eigenvalues are $\chi e^{-i\omega t/2}$. The two eigen states of $G(\omega t)$ are $\phi_\chi(t) = \frac{1}{\sqrt{2}}\begin{pmatrix} \chi e^{-i\omega t/2} \\ 1 \end{pmatrix}$, which are also the energy eigenstates of $H(t)$. Using the instantaneous states as the basis, we can write the time-dependent state as

$$\Psi(t) = \sum_\chi c_\chi(t)\exp[-i\int_0^t E_\chi(t')dt'/\hbar]\phi_\chi(t). \tag{2}$$

Substituting the state into the time-dependent Schrodinger equation, one obtains

$$\partial_t c_\chi = i\sum_{\chi'}\frac{\omega}{4}\chi\chi'\exp[i(\chi-\chi')\frac{\alpha}{2}\sin^2\frac{\omega t}{4}]c_{\chi'} \tag{3}$$

with $\alpha = 8\omega_0/\omega$. Here we have used $\phi_\chi^\dagger(t)i\partial_t\phi_{\chi'}(t) = \frac{\omega}{4}\chi\chi'$ and the dynamic phase $\int_0^t dt'\chi\omega_0\sin\frac{\omega t'}{2} = \chi\frac{4\omega_0}{\omega}\sin^2\frac{\omega t}{4}$. Transforming into the form of integral equation,

$$c_\chi(t) = e^{i\frac{\omega t}{4}}\left[c_\chi(0) - i\frac{\omega}{4}\int_0^t dt'\exp[i\alpha\sin^2\frac{\omega t'}{4}]c_{-\chi}(t')\right]. \tag{4}$$

For a large value of α, i.e., the system varies very slowly compared to the energy scale $\hbar\omega_0$, and the phase factor oscillates rapidly with time in the integral; thus, the integral part tends to approach zero as $\alpha \to +\infty$. At $t = T$, we may utilize the integral

$$\int_0^{\pi/2} dx\exp[i\alpha\sin^2 x] = \frac{\pi}{2}e^{i\frac{\alpha}{2}}J_0(\frac{\alpha}{2}) \tag{5}$$

where the zero-order Bessel function $J_0(\frac{\alpha}{2}) \to \frac{2}{\sqrt{\alpha\pi}}\cos[\frac{\alpha}{2}-\frac{\pi}{4}]$ for a large α. Thus in the adiabatic condition, $c_\chi(t) \to e^{i\frac{\omega t}{4}}c_\chi(t=0)$. Assume the initial state $\Psi(t=0) = \sum_\chi c_\chi(t=0)\phi_\chi(t=0)$. Note that $\phi_\chi(t+T) = \phi_{-\chi}(t)$. At $t = T$, one obtains

$$\Psi(T) = e^{i\frac{\pi}{2}}\sum_\chi e^{-i\chi\frac{\alpha}{2}}\phi_{-\chi}(0)\phi_\chi^\dagger(0)\Psi(0) = -i\sigma_z e^{-i\frac{\alpha}{2}\sigma_x}\Psi(0). \tag{6}$$

At $t = 2T$, $\Psi(2T) = e^{i\pi}\Psi(0)$. The state evolves back to the initial state and gains a π Berry phase after two periods of time.

Furthermore, with the help of numerical calculation, the consequence can be extended to a general case in one dimension.

Solutions of the domain-wall bound state The method used in this section can be found in Refs. [1, 2]. We start with the 1D modified Dirac equation,

$$(-i\hbar v\partial_x\sigma_1 + b(x)\partial_x^2\sigma_3)\psi(x) = E\psi(x) \tag{7}$$

where $b = b_0\mathrm{sgn}(x)$, the sign of b changes at $x = 0$. To find the solution of the zero-energy bound state, we take $E = 0$ and multiply σ_1 from the left-hand side, it follows that the solution has the form $\psi(x) = \chi_y\phi(x)$ where χ_y is the eigenspinor of σ_y with the eigenvalue η: $\sigma_2\chi_y = \eta\chi_y$. Then, the equation is reduced to

$$(\hbar v + \eta b(x)\partial_x)\partial_x\phi(x) = 0. \tag{8}$$

The general solution is $\partial_x\phi(x) = c\exp[-\int \frac{\hbar v}{\eta b(x)}dx]$ and η is determined by the boundary condition $\phi \to 0$ when $x \to \pm\infty$. Thus $\varphi(x) = \chi_y\sqrt{|\frac{\hbar v}{b_0}|}\exp\left(-|\hbar v x/b_0|\right)$ with $\eta = \mathrm{sgn}(b_0)$.

For a 2D domain wall, we take the periodic boundary condition along the y direction, and the momentum $p_y = \hbar k_y$ is a good quantum number. The equation reads

$$\left[\hbar v(-i\partial_x\sigma_1 + k_y\sigma_2) - b(x)(-\partial_x^2 + k_y^2)\sigma_3\right]\psi(x, y) = E\psi(x, y). \tag{9}$$

Except for the solutions for the bulk states there always exists the bound state solution near the the domain wall

$$\psi_{2D}(x, y) = \frac{1}{\sqrt{2\pi}}\chi_y\sqrt{\lambda_2(k_y)}\exp\left(-\lambda_2(k_y)|x| + ik_y y\right) \tag{10}$$

with $\lambda_2(k_y) = \frac{\hbar v}{2|b_0|} + \sqrt{\left(\frac{\hbar v}{2b_0}\right)^2 + k_y^2}$, and the energy dispersion is $E = \mathrm{sgn}(b_0)v\hbar k_y$. The effective velocity $v_{eff} = \partial E/\partial\hbar k_y = \mathrm{sgn}(b_0)v$, in which the sign of b determines the flowing direction of particles in the chiral bound states.

For a 3D domain wall, we take the periodic boundary condition along the y and z direction. The Hamiltonian is reduced to

$$H_{3D}(x, k_y, k_z) = \hbar v(-i\partial_x\alpha_1 + k_y\alpha_2 + k_z\alpha_3) - b(x)(-\partial_x^2 + k_y^2 + k_z^2)\beta. \tag{11}$$

To solve the equation, we rewrite $H_{3D}(x, k_y, k_z) = H_{1D}(x, k_y, k_z) + \hbar v(k_y\alpha_2 + k_z\alpha_3)$. Two solutions of the zero energy for H_{1D} are

$$\psi_\pm(x, k_y, k_z) = \frac{1}{2\pi}\chi_\pm\sqrt{\lambda_3(k_y, k_z)}\exp\left(-\lambda_3(k_y, k_z)|x| + ik_y y + ik_z z\right) \tag{12}$$

with $\lambda_3(k_y, k_z) = \frac{\hbar v}{2|b_0|} + \sqrt{\left(\frac{\hbar v}{2b_0}\right)^2 + k_y^2 + k_z^2}$ and $\chi_+ = \frac{1}{2}(1, -\mathrm{sgn}(b_0), i, -i\mathrm{sgn}(b_0))^T$, $\chi_- = \frac{1}{2}(1, \mathrm{sgn}(b_0), -i, -i\mathrm{sgn}(b_0))^T$. Using the two states as the basis, we obtain the effective Hamiltonian for the bound states at the interface,

$$H_{eff}(k_y, k_z) = \mathrm{sgn}(b_0)(k_x\sigma_1 - k_y\sigma_2), \tag{13}$$

which describes a gapless Dirac cone located at the interface of the domain wall.

Symmetry enforced band crossing Generally, the symmetry-enforced band crossings can be movable at some high symmetry line [3, 4, 5, 6, 7, 8, 9, 10, 11] or pinned at a particular high-symmetry point in the Brillouin zone [12, 13, 14, 15, 16].

In 1D, the fermion doubling problem can be evaded by considering the nonsymmorphic symmetry which is a combination of a fractional lattice translation and a spatial operation. In this situation, the degenerate point is movable according to the model parameters. Consider a one-dimensional bipartite chain where the

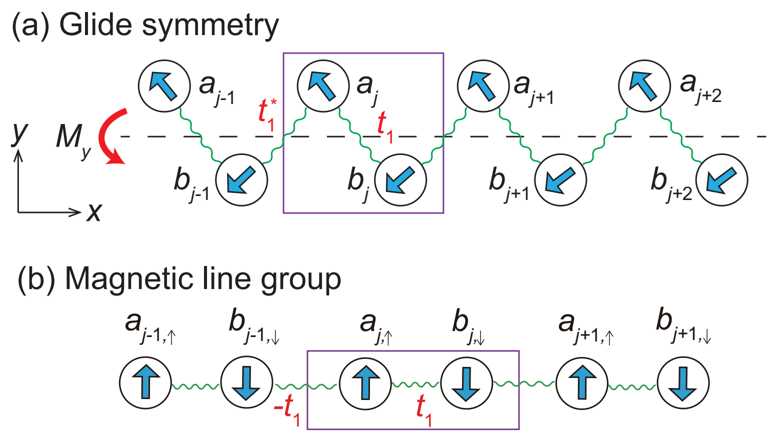

Figure 1: Illustration of (a) the glide symmetry and (b) the magnetic line group in one dimensional lattice.

two sites can be equivalently represented by a local up or down vector object as shown in Fig. 1(a). Under a transformation $\bar{M}_y = M_y \mathbf{t}_{1/2}$ that is a combination of the mirror operator M_y and a spatial translation of half of the lattice spacing $\mathbf{t}_{1/2}$, the system is invariant. $\bar{M}_y$ transforms the annihilation operators for the two sublattices as $\bar{M}_y a_j \bar{M}_y^{-1} = b_j$ and $\bar{M}_y b_j \bar{M}_y^{-1} = a_{j+1}$, where a_j and b_j are the annihilation operators for the sublattices A and B in site j, respectively. A tight-binding model can be constructed as

$$H = \sum_j \left(t_1 a_j^\dagger b_j + t_2 a_j^\dagger b_{j-1} + \text{H.c.} \right), \tag{14}$$

where H.c. denotes the Hermitian conjugation, t_1 and t_2 are the intracell and intercell hopping strength, respectively. The glide mirror symmetry of H (i.e., $\bar{M}_y H \bar{M}_y^{-1} = H$) requires $t_1 = t_2^*$. In the basis of $\psi_k = [a_k, b_k]^T$, the Hamiltonian can be represented as

$$H = \sum_k \psi_k^\dagger \mathcal{H}_k \psi_k = \sum_k \psi_k^\dagger \begin{bmatrix} 0 & t_1 + t_1^* e^{ik} \\ t_1^* + t_1 e^{-ik} & 0 \end{bmatrix} \psi_k, \tag{15}$$

and the glide mirror operator is explicitly expressed as

$$\bar{M}_y = \begin{bmatrix} 0 & 1 \\ e^{-ik} & 0 \end{bmatrix}, \tag{16}$$

which is a function of k, a necessary condition for glide symmetry. As $\bar{M}_y^2 = M_y^2 \mathbf{t}_{1/2}^2 = e^{-ik}$ is a translation for one unit cell, and $[\bar{M}_y, \mathcal{H}_k] = 0$ thus the energy eigenstates can be labeled by the eigenvalues of $\bar{M}_y$ which are $\pm e^{-ik/2}$. Upon shifting one reciprocal lattice vector G, $k \to k + G$, the eigenvalues of $\bar{M}_y$ switch places $\pm e^{-i(k+G)/2} = \mp e^{-ik/2}$, which requires that the two energy branches must have odd times of crossing in one Brillouin zone. The bulk spectrum for this model can be obtained as $E_k = \pm\sqrt{2|t_1|^2 + t_1^{*2} e^{ik} + t_1^2 e^{-ik}}$ and there is a single band crossing point at $k_c = \pi + \operatorname{Im} \ln (t_1/t_1^*)$. The low energy Hamiltonian H_{eff} can be obtained by expanding the full Hamiltonian (15) around the degenerate point. To the linear order δk, we have $H_{eff} = v_f \begin{pmatrix} 0 & e^{ik_c/2} \\ e^{-ik_c/2} & 0 \end{pmatrix} \delta k$ with $v_f = Im(t_1 e^{-ik_c/2})$. There exists a unitary matrix $\mathcal{C} = \begin{pmatrix} 0 & e^{ik_c/2} \\ e^{-ik_c/2} & 0 \end{pmatrix}$ commuting with H_{eff} which defines the chiral symmetry of the system in low energy limit. From Eq. (15), the off-diagonal element for Q matrix is $q(k) = \frac{t_1 + t_1^* e^{ik}}{|t_1 + t_1^* e^{ik}|}$. The winding number density $iq^{-1}(k)\partial_k q(k) = -\frac{1}{2}$ is a constant for this special case which yields $w_{1D} = -\frac{1}{2}$.

The quantum anomalous semimetal in 1D can be also stabilized by the type-IV magnetic double line group generated by $\bar{\mathcal{T}} = \{\mathcal{T}|\frac{1}{2}\}$ which is composed by the time reversal symmetry $\mathcal{T}$ and a fractional lattice translation [16]. The fermion doubling problem is evaded since this time-reversal like symmetry is represented different at $k = 0$ and $G/2$. The degenerate point is pinned at $k = G/2$ where has a 2D irreducible representation. The simplest example of symmetry $\bar{\mathcal{T}}$ is a two-sublattice-site antiferromagnet as shown in Fig. 1(b), where the spins on sites A are the time reverses of the spins on the sites B. To construct a model with symmetry $\bar{\mathcal{T}}$, we consider the system with two sublattice sites of s-orbitals. At each lattice site, there are two spins. We have a total four bands model. The antiferromagnetic potential is assumed to be much stronger than other hopping and energy terms, the system is then effectively split into two two-bands systems. $\bar{\mathcal{T}}$ transforms the annihilation operators of the energetically identical two states as $\bar{\mathcal{T}} a_{j\uparrow} \bar{\mathcal{T}}^{-1} = b_{j\downarrow}$ and $\bar{\mathcal{T}} b_{j\downarrow} \bar{\mathcal{T}}^{-1} = -a_{j+1,\uparrow}$ where $a_{j\uparrow}$ and $b_{j\downarrow}$ are the annihilation operators for spin-up at the sublattices A or spin-down state at the sublattice B in site j. A tight-binding Hamiltonian for this two-band model can be constructed straightforwardly,

$$H = \sum_j \left(t_1 a^\dagger_{j\uparrow} b_{j\downarrow} + t_2 a^\dagger_{j\uparrow} b_{j-1\downarrow} + \text{H.c.} \right) \tag{17}$$

where t_1 and t_2 are the intracell and intercell hopping strength, respectively. The time-reversal like symmetry of H, i.e., $\bar{\mathcal{T}} H \bar{\mathcal{T}}^{-1} = H$, enforces $t_1 = -t_2$ for the hopping strength. We then construct a basis of $\{a_{k\uparrow}, b_{k\downarrow}\}$ by the Fourier transformation $a_{k\uparrow} = \frac{1}{\sqrt{N}} \sum_j e^{-ikR_j} a_{j\uparrow}$ and $b_{k\downarrow} = \frac{1}{\sqrt{N}} \sum_j e^{-ikR_j} b_{j\downarrow}$ where N is the number of unit cells. We have chosen the periodic gauge condition $a_{k+G,\uparrow} = a_{k\uparrow}$ and $b_{k+G\downarrow} = b_{k\downarrow}$. In the basis $\psi_k = [a_{k\uparrow}, b_{k\downarrow}]^T$, the Hamiltonian is represented as $H = \sum_k \psi^\dagger_k \mathcal{H}_k \psi_k$. In terms of the Pauli matrices $\boldsymbol{\sigma}$ acting on the sublattice space, $\mathcal{H}_k$ can be expressed as

$$\mathcal{H}_k = [\text{Re}t_1(1 - \cos k) + \text{Im}t_1 \sin k]\sigma_x + [\text{Re}t_1 \sin k - \text{Im}t_1(1 - \cos k)]\sigma_y. \tag{18}$$

After a basis transformation $\frac{\text{Re}t_1}{|t_1|}\sigma_x - \frac{\text{Im}t_1}{|t_1|}\sigma_y \to \sigma'_x$ and $\frac{\text{Im}t_1}{|t_1|}\sigma_x + \frac{\text{Re}t_1}{|t_1|}\sigma_y \to \sigma'_y$, the Hamiltonian can be rewritten as $\mathcal{H}_k = |t_1|(\sin k\sigma_y + 2\sin^2 \frac{k}{2}\sigma_x)$. The band structure features an unpaired twofold Dirac fermion with the Wilson fermion in Eq. (1) in the main text.

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