Valley Spin Sum Rule for Dirac Fermions: Topological Argument

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We consider a two-dimensional lattice system with two sites in its unit cell. In such a system, the Bloch band spectrum can have some valley points, around which Dirac fermions appear as low-energy excitations. The Dirac fermion has at

the $2 \times 2$ unit matrix, and $d_k$ is a three-dimensional vector in the sublattice spin space. The real spin is not

In such a model, there can be some valley points in the energy spectrum. Around the $i$-th valley point $k_i$, the expansion of $d_k$ is given by $d_{k_i} (|k_i|) = d_{k_i} \pm \delta k_{i,x} \partial_{k_{i,x}} d_{k_i} + \delta k_{i,y} \partial_{k_{i,y}} d_{k_i} + O(\delta k^2)$, where $d_{k_i} \cdot \partial_{k_{i,x}} d_{k_i} = d_{k_i} \cdot \partial_{k_{i,y}} d_{k_i} = 0$.

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\begin{align}
|u_k^{(\pm)}\rangle &= \frac{1}{N_k^{\pm}} \left( d_{1k} \pm d_{2k} \right), \\
\text{where } N_k^{\pm} &\text{ is the normalization. We note the fact that we may choose the other expression } |u_k^{(\pm)}\rangle \propto (-d_{1k} + id_{2k}, d_{3k} \mp |d_k|)^T.
\end{align}
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In a general case, we use the following expression for the eigenstate:

In the system, there are two valley points, around which Dirac fermions appear as low-energy excitations. The Dirac fermion has a valley spin $\alpha$ associated with the Pauli matrices $\sigma$. In our argument, we do not introduce any assumptions on these symmetries. Namely, we can show the sum rule generally. We also discuss some similarity to the Nielsen-Ninomiya no-go theorem for lattice fermions in odd-spatial dimensions.

We show a procedure for obtaining the “canonical form” of $d_k$, which leads to the Dirac equation directly. The argument presented here basically relies on that given by Oshikawa.7) We consider the rotation $d_k \rightarrow \sum_l d_{kl} R^m_{kl}$, where $l, m = 1, 2, 3$ denote the coordinates in the sublattice spin space. We see that the Hamiltonian is transformed to $H_k \rightarrow U_k H_k U_k^{-1}$, where $U_k$ is a SU(2) lattice, respectively. These numbers are equivalent, and this fact leads to a sum rule that states that the total sum of the valley spins is absent even in a system without time-reversal and parity symmetries. We can see some similarity between the valley spin and chirality in the Nielsen-Ninomiya no-go theorem in odd-spatial dimensions.

KEYWORDS: valley spin, sum rule, Chern Integer and vortex, Dirac fermion and meron, parity anomaly, graphene, zero-gap organic conductor, topological insulator, Nielsen-Ninomiya no-go theorem

The Bloch band spectrum in some lattice systems have valley points, around which Dirac fermions appear as low-energy excitations. The Dirac fermion has a valley spin $\alpha$ associated with the Pauli matrices $\sigma$, and the Bloch Hamiltonian can be written as $H_k = \epsilon_k \sigma_0 + d_k \cdot \sigma$, where $k$ is the two-dimensional crystal momentum, $\sigma_0$ is

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\begin{align}
\sum_{lm} t_{lm} c_{l} \sigma_0 c_{m}, \text{ where } c_{l} \text{ (} c_{l} \text{)} \text{ is the creation (annihilation)} \text{ operator of an electron at the } l\text{-th site, and } t_{lm} \text{ is the hopping parameter between the } l\text{-th and } m\text{-th sites. In this system, we can introduce the sublattice spins } A \text{ and } B \text{ with the associated Pauli matrices } \sigma, \text{ and the Bloch Hamiltonian can be written as } H_k = \epsilon_k \sigma_0 + d_k \cdot \sigma, \text{ where } k \text{ is the two-dimensional crystal momentum, } \sigma_0 \text{ is}
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We consider a two-dimensional lattice system with two sites in its unit cell. In such a system, the Bloch band spectrum can have some valley points, around which Dirac fermions appear as low-energy excitations. Each valley point has a valley spin $\pm 1$. In the system, there are two topological numbers counting vortices and merons in the Brillouin zone, respectively. These numbers are equivalent, and this fact leads to a sum rule that states that the total sum of the valley spins is absent even in a system without time-reversal and parity symmetries. We can see some similarity between the valley spin and chirality in the Nielsen-Ninomiya no-go theorem in odd-spatial dimensions.

The low-energy electronic features of graphene\(^9\) and the zero-gap organic conductor \((\text{BEDT-TTF})_2\text{I}_3\)\(^10,11\) can be well described by gapless Dirac fermions.

In this study, we consider a two-dimensional lattice system with two sites in its unit cell and discuss valley points. Each valley point has a valley spin $\pm 1$, which is well-defined as long as the intervalley mixing can be neglected, i.e., in the long-wavelength limit. We focus on the relation among the valley spin and two kinds of topological numbers counting vortices\(^3,12,13\) and merons\(^4,14,15\) in the Brillouin zone, respectively. It has been shown generally that these numbers are equivalent on a two-torus.\(^16\) Using long-wavelength formalism, we show that this equivalence leads to the fact that the total sum of the valley spins is absent. This sum rule is obvious when the system preserves time-reversal or parity symmetry, since a valley spin flips under these symmetry transformations. In our argument, we do not introduce any assumptions on these symmetries. Namely, we can show the sum rule more generally. We also discuss some similarity to the Nielsen-Ninomiya no-go theorem for lattice fermions in odd-spatial dimensions.\(^17\) We use the natural unit $\hbar = c = 1$.

We start from a tight-binding model on a two-dimensional lattice system with two sites in the unit cell:

\begin{math}
H = \sum_{lm} t_{lm} c_{l} \sigma_0 c_{m}, \text{ where } c_{l} \text{ (} c_{l} \text{)} \text{ is the creation (annihilation)} \text{ operator of an electron at the } l\text{-th site, and } t_{lm} \text{ is the hopping parameter between the } l\text{-th and } m\text{-th sites. In this system, we can introduce the sublattice spins } A \text{ and } B \text{ with the associated Pauli matrices } \sigma, \text{ and the Bloch Hamiltonian can be written as } H_k = \epsilon_k \sigma_0 + d_k \cdot \sigma, \text{ where } k \text{ is the two-dimensional crystal momentum, } \sigma_0 \text{ is}
\end{math}

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such an ambiguity can be removed as follows. First, we let $d_k \rightarrow |d_k|e_3$. We focus on the lower energy state (the discussion for the upper energy one is completely parallel), and $(A)$ if $|u_{k_i}^{(-)}| \rightarrow (0, 0, \exp[i \tan^{-1}(d_{2k_i}/d_{1k_i})])^T$, it is consistent with the behavior of expression (1) we have chosen. However, $(B)$ if $|u_{k_i}^{(-)}| \rightarrow (0, 1)^T$, it is inconsistent. This behavior coincides with that of the other expressions for $|u_{k_i}^{(-)}|$. Thus, we flip $d_{k_i} \rightarrow -|d_{k_i}|e_3$ [i.e., rotate $\pi$ around the $e_2$ axes] and then $|u_{k_i}^{(-)}| \rightarrow (-1, 0)^T$, which is consistent with eq. (1). After performing an appropriate transformation, we introduce the mass parameter $m_1 = d_{3k_i}$, which is positive in case $(A)$, and negative in case $(B)$. Obviously, $|m_i|$ gives the band gap at $k_i$.

Now, the vectors $\partial_{k_i} d_{k_i}$ and $\partial_{k_i} d_{k_i}$ are in the plane perpendicular to $e_3$ [see, eq. (2)]. These two are not orthogonal, in general. Let us define the rank-2 tensor $A_{\mu \nu} = \partial_{k_i} d_{k_i} \cdot \partial_{k_i} d_{k_i}$, where $\mu, \nu = x, y$. This is a symmetric tensor. This tensor would be regular at a relative sign between the coefficients of $k_x, k_y$, which is consistent with the behavior of expression (1). After performing an appropriate transformation, we introduce the mass parameter $m_1 = d_{3k_i}$, which is positive in case $(A)$, and negative in case $(B)$. Obviously, $|m_i|$ gives the band gap at $k_i$.

The canonical form eq. (3) leads to the Dirac equation, and the excitation near $k_i$ is described by the Dirac fermion and becomes dominant when the band gap given by $2|m_i|$ is sufficiently small compared with the bandwidth. The Dirac cone arises in the limit $|m_i| \rightarrow 0$. We also note that the vector eq. (3) takes the configuration of a meron.\(^{14,15}\)

In the limit of $\delta k \rightarrow 0$,

$$|u_{k_i}^{(-)}| \rightarrow \begin{cases} 0 & (m_i > 0), \\ \tau_i e^{i \theta_i} & (m_i < 0), \end{cases}$$

where $\theta_i = \tan^{-1}(v_{ix} k_y/v_{iy} k_x)$.

Let us examine the sum rule

$$\sigma_i = 0,$$  \hspace{1cm} (5)

where the summation is taken for all of the valley points in the band. This rule is obvious when the system preserves time-reversal and/or parity symmetry, since the valley spin is odd under time-reversal and parity transformations. Actually, this rule is satisfied in symmetric systems like graphene\(^9\) and the zero-gap organic conductor $\alpha$-BEDT-TTF\(^{21,10,11}\).

We show the sum rule in a more general manner. We do not introduce any assumptions on time-reversal and parity symmetries. We consider two topological numbers for the lower energy band:

$$N_{\text{vor}} = \int_{BZ} \frac{d^2 k}{2\pi i} \nabla_k \times A_k,$$  \hspace{1cm} (6)

$$N_{\text{mer}} = \int_{BZ} \frac{d^2 k}{4\pi} d_k \cdot (\partial_{k_x} d_{k_x} \times \partial_{k_y} d_{k_y}),$$  \hspace{1cm} (7)

where $A_k = (u_{k_i}^{(-)} \nabla_k u_{k_i}^{(-)}, d_k = d_k/|d_k|$, and $\int_{BZ} d^2 k$ denotes the integral over the entire Brillouin zone. These two numbers characterize the topological structure of the lower band.\(^{20}\) Generally, we can show that\(^{16}\)

$$N_{\text{vor}} = N_{\text{mer}}.$$

Let us estimate these numbers using the long-wavelength formations eqs. (3) and (4). $N_{\text{vor}}$ is the Chern number that counts the total vorticity of the lower-band state,\(^{12,13}\) i.e.,

$$\int_{BZ} \frac{d^2 k}{2\pi i} \nabla_k \times A_k = \sum_i \oint_{\text{around } k_i} d_k \cdot A_k,$$  \hspace{1cm} (9)

$$= \sum_i \tau_i \theta(m_i) = 0, \pm 1, \pm 2, \cdots,$$

where $\theta(x)$ is the step function. We can show it as follows: We may write $A_k = A_k^{\text{vor}} + A_k^{\text{mer}}$. The first part $A_k^{\text{vor}}$ is defined to pick up the vortex singularity of the lower-band state eq. (4). Namely,

$$A_k^{\text{vor}} = i \nabla_k \left\{ \sum_i \tau_i \theta(m_i) \tan^{-1}(v_{iy}(k_y - k_{iy})/v_{ix}(k_x - k_{ix})) \right\},$$

which gives the bottom line of eq. (9).\(^{13}\) The remaining part $A_k^{\text{mer}}$ is, therefore, regular and does not contribute to $N_{\text{vor}}$, since the integral is defined on the entire Brillouin zone (two-torus).\(^{13}\) Then, we obtain eq. (9).

On the other hand, $N_{\text{mer}}$ is related to merons in the Brillouin zone.\(^{14,15}\) First, we vary all of the mass parameters $\{m_i| i = 1, 2, \cdots\}$ to be infinitesimal without closing the gaps, i.e., without sign changes. This deformation does not change $N_{\text{mer}}$ because of its topological nature. From the configuration of a meron shown in eq. (3), we see that the integrand around $k_i$ is

$$d_k \cdot (\partial_{k_x} d_k \times \partial_{k_y} d_k) = \frac{m_i \tau_i v_{ix} v_{iy}}{(v_{ix}^2 \delta k_x^2 + v_{iy}^2 \delta k_y^2 + m_i^2)^{3/2}},$$

which is valid for a small $\delta k$. To estimate its contribution to $N_{\text{mer}}$, we should introduce the appropriate momentum
cutoff $\Lambda_k$ around $k_i$, which is comparable to the bandwidth on the energy scale. On the other hand, the integrand eq. (11) is localized strongly around $k_i$ since its extension is characterized by an infinitesimally small $|m_i|$. Therefore, the contribution around $k_i$ can be obtained from the integration of eq. (11) without a momentum cut off, which gives a half-quantized number, $\sgn(m_i)\tau_i/2$. This is the so-called “parity anomaly”.1–7,14,15) Then, $N_{\text{mer}}$ is given by the sum of contributions from all valley points, i.e.,

$$\int_{BZ} \frac{d^2k}{4\pi} \left( \partial_{k_x} \hat{d}_k \times \partial_{k_y} \hat{d}_k \right) = \sum_i \frac{1}{2} \sgn(m_i)\tau_i. \quad (12)$$

Eq. (12) has been verified numerically for arbitrary values of mass parameters using an explicit form of $\hat{d}_k$ on the entire Brillouin zone in a certain tight-binding model.21)

We can see from eqs. (8), (9), and (12) that the number of valley points should be even. We suppose that there are two valley points $k = k_1, k_2$. The extension to a system with $2N$ valley points ($N = 2, 3, 4, \ldots$) is straightforward. We emphasize that time-reversal and parity symmetries are not required here: We do not introduce any restrictions on the locations of valley points or on the values of the mass parameters. Below, we show that eqs. (9) and (12) give the same result and become consistent with eq. (8) when (I) the sum rule (5) is satisfied, but do not when (II) the sum rule is not satisfied.

We examine case (I) first. We can put $\tau_1 = +1$ and $\tau_2 = -1$ without losing generality. From eq. (9), we obtain

$$N_{\text{vor}} = \begin{cases} 
\tau_1 + \tau_2 = 0 & m_1, m_2 > 0, \\
\tau_1 = +1 & m_1 > 0, m_2 < 0, \\
\tau_2 = -1 & m_1 < 0, m_2 > 0, \\
0 & m_1, m_2 < 0.
\end{cases} \quad (13)$$

On the other hand, from eq. (12), we obtain

$$N_{\text{mer}} = \frac{1}{2} \left\{ \frac{m_1}{|m_1|} \tau_1 + \frac{m_2}{|m_2|} \tau_2 \right\}$$

$$= \begin{cases} 
0 & m_1, m_2 > 0, \\
+1 & m_1 > 0, m_2 < 0, \\
-1 & m_1 < 0, m_2 > 0, \\
0 & m_1, m_2 < 0.
\end{cases} \quad (14)$$

Namely, $N_{\text{vor}} = N_{\text{mer}}$. In case (II), we immediately see that $N_{\text{vor}} \neq N_{\text{mer}}$, which is inconsistent with eq. (8).

To sum up, we have shown that two topological numbers shown by eqs. (6) and (7) estimated in the long-wavelength formalism give a result consistent with the general relation eq. (8), when eq. (5) is satisfied.

Let us discuss the configurations of vortices and merons, which are schematically shown in Fig. 1. We note again that the valley spins are fixed at $\tau_1 = +1$ and $\tau_2 = -1$. We note that a vortex with a vorticity equals to $\tau_i$ is located at $k_i$ with $m_i > 0$ [see eq. (4)], on the other hand, a meron with a fractional charge $\sgn(m_i)\tau_i/2$ is located at each $k_i$. Therefore, when (a) $m_1, m_2 > 0$, a vortex and a meron are located at $k_1$, while an antivortex and an antimeron are located at $k_2$. In the case that (b) $m_1 > 0, m_2 < 0$, a vortex is present at $k_1$ but absent from $k_2$, while a meron is located at $k_1$ and $k_2$. In the case that (c) $m_1 < 0, m_2 > 0$, an antivortex is present at $k_2$ but absent from $k_1$, while an antimeron is located at $k_1$ and $k_2$. When (d) $m_1, m_2 < 0$, there are no vortices in the entire Brillouin zone; however, a meron and an antimeron are located at $k_2$ and $k_1$, respectively.

The phases (b) and (c) in Fig. 1 have nonzero topological numbers and break parity and time-reversal symmetries.20) Such phases emerge if some interactions give $m_1$ and $m_2$ with opposite signs. Actually, this mechanism has been proposed by Haldane,6) and its extension to the (time-reversal invariant) quantum spin Hall effect is given by Kane and Mele using a spin activating interaction.22,23) As long as the real spin is not activated, a system with parity and/or time-reversal symmetry is categorized into zero-topological number phase (a) or (d) in Fig. 1. We see that graphene9) and the organic conductor10,11) are the gapless limits of phase (a) or (d).

The phase transition specified by the jump of the topological numbers occurs when $m_i$ changes its sign.6,7,15) For instance, let us see a transition from phase (d) to phase (b) in Fig. 1, where the jumps of the topological numbers are $\Delta N_{\text{vor}} = \Delta N_{\text{mer}} = 1$. We change $m_1$ continuously from a negative value to a positive value. At the transition point $m_1 = 0$, a Dirac cone appears at $k_1$ in the energy spectrum,6) and a vortex and a meron are created and an antimeron is annihilated. The other Dirac-type spectrum at $k_2$ with an opposite valley spin remains massive and hidden in the higher-energy part of the spectrum when its mass is comparable to the bandwidth.6,24)

Let us discuss some relations to the Nielsen-Ninomiya no-go theorem on the lattice fermion doubling in odd-dimensional.6,17,18,24) When the system possesses
parity symmetry, the sum rule eq. (5) becomes obvious as we mentioned earlier, and the number of valley points should be even. Besides, the energy gap at a point is forbidden by the symmetry, since the mass term \( m_{\alpha} \sigma_i \) comes from the symmetry-breaking staggered potential. (Note that, at a valley point, the parity-invariant mass term \( m_{\alpha} \sigma_i \) is allowed in graphene,\(^{22,23}\) but, we do not consider an interaction that activates the real spin) Therefore, we immediately see the fermion doubling. The role of the valley spin is similar to that of the chirality (the eigenvalue of \( \gamma_5 \) operator that can be defined in odd-dimensional space only) in the no-go theorem. A crucial difference is that the valley spin is still well-defined for a massive Dirac fermion as long as the intervalley scattering can be neglected; on the other hand, chirality is not.

Our discussion would be related to the argument given in ref.\(^{18}\) in which a two-dimensional analog of “chiral symmetry” is introduced artificially; however, the former appaers rather simpler.

The situation becomes somewhat indefinite in parity-symmetry-breaking systems. As we have shown, the sum rule (5) is also satisfied in such systems. Owing to the sum rule (5), if we found a valley point, there should be another point with an opposite valley spin. We assume the following: (A) Band gaps at these paired points \( |m_1| \) and \( |m_2| \) are degenerate, i.e., \( |m_1| = |m_2| \equiv m \). The presence of time-reversal symmetry is a sufficient condition for this degeneracy.\(^{25}\) (B) The gap amplitude \( m \) is sufficiently smaller than the bandwidth. Under these assumptions, we find the statement: A massive Dirac fermion is always excited with its doubling partner that has an opposite valley spin, when the system has particle-hole symmetry (i.e., \( \epsilon_k = 0 \)) and the Fermi level lies in the gap. Assumptions (A) and (B) would be, at least, approximately, satisfied when the symmetry-breaking perturbations are small.

The surface of a three-dimensional time-reversal invariant topological insulator\(^{8,26,27}\) provides an exceptional case for the sum rule (5). In such a system, the topological \( \theta \)-term exists in the bulk region as the hallmark of the \( Z_2 \) topological order, and has a surface term that coincides with the Chern-Simons term with a half-quantized Hall conductivity. This fact indicates that a single Dirac cone without a hidden partner in the higher-energy region exists at a time-reversal invariant point in the Brillouin zone for the surface state, since such a cone gives a half-quantized conductivity owing to parity anomaly\(^{1-7,14,15}\) and matches with the presence of the Chern-Simons term. Thus, the sum rule fails. The topological connection between the bulk and boundary regions, the so-called “bulk-boundary correspondence”\(^{8,26,27}\) causes this unique situation. This is somewhat similar to the fact that the doubling partner mentioned in the no-go theorem\(^{17}\) with opposite chirality is absent in the one-dimensional edge state of the quantized Hall effect where the bulk-boundary correspondence is also at work.\(^{28,29}\)

In summary, we have pointed out that the equivalence of two topological numbers [see eqs. (6), (7), and (8)] leads to the sum rule (5) for the valley spin defined in the long-wavelength formalism. The sum rule is obvious when the system preserves time-reversal and/or parity symmetry, since a valley spin is odd under these symmetry transformations. In this study, the sum rule has been shown independently of the presence or absence of these symmetries. Basically, the valley spin at each valley point is determined by the detailed structure of the lattice tight-binding Hamiltonian. It seems interesting that a rigorous rule comes from a topological argument that is independent of the details of the Hamiltonian. We also emphasize that, to close the valley spin, we can see an analog of the fermion doubling theorem in odd-dimensional space\(^{17,18}\) in a rather simple manner.

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