Counting Pseudo Landau Levels in Spatially Modulated Dirac Systems

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In a system with Dirac cones, spatial modulation in material parameters induces a pseudo magnetic field, which acts like an external magnetic field. Here, we derive a concise formula to count the pseudo Landau levels in the simplest setup for having a pseudo magnetic field. The formula is so concise that it is helpful in seeing the essence of the phenomenon, and in considering the experimental design for the pseudo magnetic field. Furthermore, it is revealed that anisotropic Dirac cones are advantageous in pseudo Landau level formation in general. The proposed setup is relatively easy to be realized by spatial modulation in the chemical composition, and we perform an estimation of the pseudo magnetic field in an existing material (an antiperovskite material), by following the composition dependence with the help of the ab-initio method.

The external magnetic field is not the only source of the Landau levels. For instance, a certain strain on graphene leads to the so-called pseudo magnetic field and the resultant Landau level structures [1][4]. This phenomenon is tied to the most intriguing property of graphene, i.e., the emergent relativistic electron, or the existence of Dirac cone in the band structure [5]. Having a Dirac cone, the key toward the finite pseudo magnetic field is the resemblance between the shift of the Dirac cone in the Brillouin zone and the minimal coupling in the U(1) gauge theory. Since the essence is simply the Dirac cone shift, the idea is not limited to graphene, but is applicable to any system with emergent linear dispersion, such as three-dimensional Dirac/Weyl semimetals [6][15].

The study of the pseudo magnetic field has several important aspects. Obviously, it is conceptually interesting to observe magnetic phenomena like chiral magnetic effect [12] or quantum oscillations [13] without actually applying magnetic field. Furthermore, the field strength can possibly exceed the maximum available strength for the real magnetic field. As an extreme case, even for a system inert to the real magnetic field (e.g., neutral particle systems, photonic or phononic crystals [16][17]), the pseudo magnetic field can be influential as far as there are Dirac cones. Typically, Dirac cones come with pairs, resulting in multiple Dirac nodes in the Brillouin zone, and the direction of the pseudo magnetic field depends on the nodes. (So, a pseudo magnetic field is regarded as an axial magnetic field.) Then, if the real and pseudo magnetic field coexist, they enhance or cancel with each other depending on the nodes, which induces the valley imbalance [13][18][20]. In that sense, the study of the pseudo magnetic field also has potential importance in valleytronics as next functionalization of materials.

As we have noted, the essence of the pseudo magnetic field is the similarity between the Dirac/Weyl node shift and the minimal coupling. The shift of Dirac/Weyl nodes can be induced in many ways [21][22], and the strain has been frequently used in the context of the pseudo magnetic field in the literature. However, the strain is not the only choice: the spatial dependence of the magnetic moment [6][24], or the spatially modulating chemical composition should be equally sufficient. In this paper, we consider a simple setup for the pseudo magnetic field generation, which is expected to be relatively easy to realize with the spatial modulation of the chemical composition. We first give a notably concise formula [Eq. (8)] for the number of observable pseudo Landau levels. The formula requires only two dimensionless parameters $N$ and $R$, where $N$ characterizes the length scale of the spatial modulation, while $R$ characterizes the size of the Dirac/Weyl node shift. The conciseness of the formula makes the essence of the pseudo magnetic field transparent, and helps to consider experimental designs. Furthermore, inspired by the simple formula, it is pointed out that anisotropic Dirac cones are better than the isotropic ones to appreciate the pseudo Landau level structure. In the latter half of this paper, we perform semi ab-initio estimation of $R$ in a real material, antiperovskite $\text{A}_3\text{SnO}_3$ (A=Ca,Sr) [25][28], to make a quantitative argument on the pseudo magnetic field generation.

Let us start with the formulation. The setup in this paper is illustrated in Fig. 1(a). The considered system
consists of three regions, bulk 1, bulk 2, and the buffer region. For having a transparent discussion, we assume that bulk 1 (bulk 2) extends to $y = +\infty$ ($y = -\infty$), which excludes free surfaces from our consideration. Bulk 1 and bulk 2 are similar to each other, having Dirac cones in the band structure, but with slightly different node positions. Namely, the effective model for each region is

$$H_{k}^{(\pm)} = \hbar(v(k \pm k_0)) \cdot \sigma,$$  

(1)

where $k_0$, which denotes the center of Dirac cones, takes different values for the two regions [see Fig. 1(a)]. In the buffer region, we assume that the Dirac cones are smoothly shifted from the position in bulk 1 to the one in bulk 2. For simplicity, our focus is limited to the case that the Dirac cones are shifted in $k_z$ direction. As we can see from Fig. 1(a), the system is periodic in $x$ and $z$ direction, and we have a band structure as a function of $k_x$ and $k_z$. (If a two-dimensional Dirac/Weyl system is our target, we simply neglect any structure along $z$-axis, and omit $k_z$.) Then, the bulk contribution to the band structure typically looks like Fig 1(b) reflecting the shifted node positions. The question is, how about the contribution from the state at the buffer region.

Within the buffer region, the position of the Dirac cones depends on $y$. Then, in a naive treatment, the effective model is assumed to be

$$H^{(\pm)} = \hbar(-i \nabla + k_0(y)) \cdot \sigma,$$  

(2)

which is obtained by replacing $k$ by $-i \nabla$ and taking account of the $y$ dependence of $k_0$. The latter arguments reveal that this naive treatment works well. By comparing Eq. (2) with the standard minimal coupling $(-i \nabla - eA)$, we have

$$A^{(\pm)} = \frac{\hbar}{e} k_0(y).$$  

(3)

Once $A$ is given, the pseudo magnetic field is given by $B = \nabla \times A$. In our setup, the node shift is only in $k_z$ direction, and depends only on $y$, which means that $\frac{\partial A_y}{\partial y}$ is the only relevant component. Assuming that $k_0$ linearly interpolates bulk 1 and bulk 2, the pseudo magnetic field strength $B = |B^{(\pm)}|$ is estimated as

$$B \sim \frac{\hbar \Delta k}{e L},$$  

(4)

where $L$ is the thickness of the buffer region, and $\Delta k$ is the size of the node shift [See Fig. 1(b)].

To make the formulation concise, we introduce two dimensionless parameters $N$ and $R$ respectively as $L = Na$ and $\Delta k = 2\pi R/\alpha$, where $\alpha$ is the lattice constant. (It is implicitly assumed that the lattice constants in $x$ and $y$ are the same, but the extension to anisotropic cases is trivial.) $N$ represents the length scale of the spatial modulation, while $R$ measures the size of the node shift in the unit of the Brillouin zone size. As a rough estimation, using a typical atomic scale $a \approx 5\, \text{Å}$, Eq. (4) leads to

$$B \sim 1.6 \times 10^4 \times \frac{R}{N} \, [\text{T}].$$  

(5)

That is, we potentially have 16 thousand Tesla, and the available strength is reduced by a factor of $R/N$.

The obtained pseudo magnetic field induces the Landau levels. Plugging Eq. (4) into a textbook formula, the energy of $n$th Landau level is

$$E_n = \pm \sqrt{\frac{4\pi e^2 \hbar^2 R|n|}{N\alpha^2}}.$$  

(6)

[For three-dimensional systems, Eq. (6) corresponds to the energy at $k_z = 0$.] However, we should note that not all the Landau levels are observable in the energy spectrum. That is, since we have the bulk regions as well as the buffer region, the Landau levels in the buffer region can be masked by the bulk contribution in the energy spectrum. It turns out that the diamond region with height $\Delta E$ and width $\Delta k$ in Fig. 1(b) is available for the Landau levels (see also the latter arguments on the numerical results in Fig. 2). Since $\Delta E$ is estimated as $\Delta E = \hbar \Delta k$, the condition that the $n$th Landau level falls into this diamond region becomes

$$\sqrt{\frac{4\pi e^2 \hbar^2 R|n|}{N\alpha^2}} < \frac{\hbar \Delta k}{2},$$  

(7)

which leads to a concise expression

$$|n| < \frac{\pi}{4} N R.$$  

(8)

Here we make a short summary: (i) to make the pseudo magnetic field strong, $N$ should be small [Eq. (5)], (ii) to observe the large number of Landau levels, $N$ should be large [Eq. (8)], and (iii) large $R$ is always beneficial.

Let us move on to the numerical validation of the derived formula. For this purpose, we introduce a two-dimensional square lattice tight-binding model with mobile Dirac nodes. Specifically, the Hamiltonian is

$$H_k = [1 + \delta + 2(\cos k_x + \cos k_y)] \sigma_z + 2\alpha \sin k_y \sigma_y$$  

(9)

where the lattice constant $a$ is set to 1. By expanding the Hamiltonian with respect to $k_x \equiv k_x - 2\pi/3$ and $k_y$ up to the first order in each of the parameters, we end up with

$$H_k \sim -\sqrt{3}[k_x - \delta k_y \sigma_z + \delta k_y \sigma_y],$$  

(10)

where $\delta = \delta/\sqrt{3}$ and $\tilde{\alpha} = 2\alpha/\sqrt{3}$. That is, $\tilde{\delta}$ behaves as $A_x$, and $\tilde{\alpha}$ is essentially anisotropy of the Fermi velocity, $v_y/v_x$. Therefore, if we assign $\delta/2\pi = 0.05$ for bulk 1, $\delta/2\pi = -0.05$ for bulk 2, and the linearly interpolated
value for the buffer region, $R = 0.1$ is achieved. In the actual calculation, we make the system periodic also in $y$ direction not to have free edges. Namely, the system consists of the repetition of the chunk of bulk 1 – buffer – bulk 2 – buffer.

Figures 2(a)–2(d) summarizes the results for $\tilde{\alpha} = 1$. If there appears some flat sections in the band structure, they can be regarded as the Landau levels. (A flat section gives a peak in the density of state.) For $N = 0$ [Fig. 2(a)], i.e., if the change between bulk 1 and bulk 2 is sharp, only the zeroth Landau level is identified in the band structure. For $N = 1$ [Fig. 2(b)], which results in $\frac{\pi}{4} NR \sim 0.8$, we still only see the zeroth Landau level. If $N$ is further increased to $\frac{\pi}{4} NR \sim 2.4$ [Fig. 2(c)], the $n = 1$ Landau level becomes clearly visible, and we see a small signature of the $n = 2$ Landau level as well. For $N = 50$ leading to $\frac{\pi}{4} NR = 3.9$ [Fig. 2(d)], the clear identification of the Landau levels up to $n = 3$ is possible. All of these observations confirm the formula Eq. (8).

It is worth noting that the expected peak structure in the (local) density of state should be a key to experimental detection of the pseudo Landau levels. Any measurements capable of detecting the density of state, such as STM/STS as a direct measurement or optical conductivity, might be useful.

So far, we have been treating the isotropic Dirac cone. Actually, the anisotropy of the Dirac cone gives significant influence on the observable Landau levels. If the Dirac cone becomes anisotropic, $v^2$ in the left hand side of Eq. (7) is replaced by $v_x v_y$, and $v$ in the right hand side by $v_x$. Consequently, the formula Eq. (8) is rewritten as

$$|n| < \frac{\pi v_x}{4 v_y} NR. \quad (11)$$

This implies that if we have $v_x > v_y$, the number of observable Landau levels increases compared with the isotropic case with the same $NR$. Physically, this is because larger $v_x$ means larger $\Delta E$, and smaller $v_y$ means larger density of states, both of which is advantageous to observe more Landau levels. The formula Eq. (11) is again confirmed using the toy model by modifying $\tilde{\alpha}$. Figures 2(e) and 2(f) shows that for $v_x/v_y \sim 2$ ($\tilde{\alpha} = 2$), the number of the Landau levels is doubled comparing with the isotropic case, while for $v_x/v_y \sim 0.5$ ($\tilde{\alpha} = 0.5$), only the $n = 0$ and $n = 1$ Landau levels are clearly seen. Therefore, if one attempts to observe large number of pseudo Landau levels, it is better to focus on the system with anisotropic Dirac cones.

Hereafter, we work on the quantitative estimation of the pseudo magnetic field in existing materials. Having formulae Eqs. (7) and (11), the estimation of $R$ is essential, and we derive $R$ in semi ab-initio way. Here, semi ab-initio means that we apply the first-principles density functional theory with a small assumption in the electronic band structure. Since the two-dimensional cases have been studied in graphene extensively, our focus is on the three-dimensional cases – we take the cubic antiperovskite family $A_3\text{SnO}$ ($A =$Ca,Sr), where the three-dimensional Dirac cones are found on $k_x, k_y, k_z$ axes in the first-principles calculation. (Note that the experimental studies on this materials are now in progress.) The great advantage of the antiperovskite family is that we already know the way to tune the electronic structure near the Fermi energy at the qualitative level. Namely, it is natural to expect that the Dirac cone shift is realized by preparing $\text{Ca}_3(3-x)\text{Sn}_3\text{SnO}$ and adjusting $x$. Before we proceed, we would like to point out a minor disadvantage of the antiperovskite family. Strictly speaking, there is a tiny mass gap at the Fermi energy, and therefore, we have to achieve $R$ such that $\Delta E$ is sufficiently larger than the mass gap.

Here, the electronic structure for $0 < x < 1$ is obtained in the following way. Firstly, we apply the first-principles calculation for $x = 0$ and $x = 1$. (The computational details are in parallel with Ref. [35]) Using those results, we construct effective models for $x = 0$ and $x = 1$, and then, the model for arbitrary $x$ is obtained by interpolating the parameters in the effective model. To be quantitative, the construction of the effective model is conducted using the maximally localized Wannier function method implemented in Wannier90 package. In practice, we construct a 12 orbital model where 12 comes from (2 spins) $\times$ (3 $p$-orbitals on Sn atom + $d_{x^2-y^2}/d_{y^2-z^2}/d_{z^2-x^2}$ on $3t$-orbitals of $\text{Sn}$. The model for $x = 0$ has been investigated in Ref. [44]. The two-dimensional case is obtained by taking $k_z$ direction not to have free edges. Namely, the system consists of the repetition of the chunk of bulk 1 – buffer – bulk 2 – buffer.}

FIG. 2. (Color online) The band structure with the pseudo magnetic field for several values of $N$. For (c) and (f), the anisotropy of the Dirac cone is introduced.
Based interpolation, we perform the calculation with a $k$-space folding in the unit cell. The formation of the band structures along the $k_x$ axis for $x = 4/9$ and $x = 5/9$ obtained by the interpolation are shown in Fig. 3. The crossing points at the Fermi energy are the Dirac cones in this system. The inspection of the band structure reveals that the Dirac cone locates at $k_x \approx 0.0075$ for $x = 4/9$, while $k_x \approx 0.1037$ for $x = 5/9$, where the momentum is measured in the unit of $2\pi/a$. At the end, $R$ is estimated to be approximately 0.006.

As a study complementary to the Wannier orbital based interpolation, we perform the calculation with a superstructure, containing Ca and Sr in a ratio $x = 4/9$ and $z = 5/9$. In specific, we consider the superstructure in $z$ direction as shown in the right panels of Fig. 4. Since the unit cell is not enlarged in $x$-$y$ plane, the node shift in $k_x$ direction can be discussed in exactly the same footing as the previous paragraph (no Brillouin zone folding in $k_x$ and $k_y$ direction). Again, assuming that $x = 4/9$ and $z = 5/9$ are sufficiently close to $x = 0.5$, we use the averaged lattice constant. The band structures for $x = 4/9$ and $z = 5/9$ on the $k_z$ axis are shown in Fig. 4. From this result, we extract the node position for $x = 4/9$ as $k_x = 0.109$, while the position for $x = 5/9$ as $k_x = 0.114$, which leads to $R = 0.022$.

To summarize, we derive a compact formula to count the number of the observable Landau levels induced by the pseudo magnetic field. The formula is so simple that the essence of the pseudo magnetic field becomes evident. Having a concise formula is also beneficial in designing experiments on the pseudo Landau levels in real materials. In fact, we show an explicit estimation of the pseudo magnetic field in an antiperovskite Dirac material in an ab-initio manner. For future developments, it is pointed out that anisotropic Dirac cones are more advantageous than isotropic ones in appreciating the pseudo Landau level structure.

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![FIG. 3. (Color online) The band structure of Ca$_{(1-x)}$Sr$_x$SnO obtained with the interpolation using the MLWF method.](image1.png)

![FIG. 4. (Color online) The band structure calculated using the enlarged unit cell with the composition Ca$_{(1-x)}$Sr$_x$SnO. The used crystal structures are shown in the right panels.](image2.png)
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