Orbital analogue of quantum anomalous Hall effect in \( p \)-band systems

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We investigate the topological insulating states of the \( p \)-band systems in optical lattices induced by the onsite orbital angular momentum polarization, which exhibit gapless edge modes in the absence of Landau levels. This effect arises from the energy level splitting between the onsite \( p_x + ip_y \) and \( p_x - ip_y \) orbitals by rotating each optical lattice site around its own center. At large rotation angular velocities, this model naturally reduces to two copies of Haldane's quantum Hall model without Landau levels. The distribution of Berry curvature in the momentum space and the quantized Chern numbers are calculated. The experimental realization is also discussed.

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The integer quantum Hall (QH) effect has generate tremendous research interests for several decades. The precise quantization of the Hall conductance is due to the topologically non-trivial band structure characterized by the Thouless-Kohmoto-Nightingale-den Nijs (TKNN) number, or the Chern number \([1,2]\). The origin of the QH effect has also deep connections to the parity anomaly of 2D Dirac fermions \([3,4,8]\). Although breaking time-reversal (TR) symmetry is required, Landau levels (LL) are not necessary for the QH effect. For example, Haldane \([8]\) constructed a QH model with average zero flux per unit cell but with complex-valued hopping integrals. Recently, QH insulators have been generalized to the topological quantum spin Hall (QSH) insulators which keep time-reversal (TR) symmetry and are characterized by a \( Z_2 \) topological number \([6,7,8,9,10,11,12]\). Excitingly, experimental evidence for the QSH insulating states has been found \([13,14]\).

Anomalous Hall (AH) effect describes the dependence of the Hall current on the spin magnetization not the external magnetic field, whose mechanism has been debated for a long time, including the anomalous velocity from the interband matrix element \([15]\), screw scattering \([16]\), and side jump \([17]\). Recently, a new perspective on the AH effect has been developed from the topological Berry curvature of the band structure which is a combined effect from spin-orbit coupling and spin polarization \([18,19]\). Its quantum version, topological insulators arising from spin magnetization has been proposed and investigated in semiconductor systems \([20,21,22]\).

The current development of cold atom physics has provided another new opportunity to investigate the QH effect. Several methods have been proposed including globally rotating the trap or optical lattice, or introducing effective gauge potential generated by laser beams \([23,24,25,26,27]\). However, the rotating angular velocity cannot be large enough otherwise the centrifugal potential will throw atoms away. It is also difficult to make the light induced gauge potential strong in a large region.

In this article, we propose an orbital analogue of the quantum anomalous Hall (QAH) effect in solid state systems, i.e., the QAH effect arising from orbital angular momentum polarization without LLs. This can be achieved by rotating each optical site around its own center which is an experimentally feasible technique \([28]\). The lift of the degeneracy between \( p_x \pm ip_y \) orbitals gives rise to non-trivial topological band structures, and provides a natural way to realize Haldane’s model. Increasing rotation angular velocity induces topological phase transition by changing the Chern number of the band structure. We also consider the QH effect arising with LLs in such systems.

The experiment to rotate each site in the lattice around its own site center has been performed by Gemelke et al. \([28]\). Electro-optic phase modulators are applied to the laser beams forming the lattice, which results in a periodical overall translation of the lattice at a radio-frequency \( \omega_{RF} \) but without the internal lattice distortions. \( \omega_{RF} \) is hundreds of times larger than the harmonic frequency \( \omega_L \) of each site, thus atoms only feel an averaged potential with a small distortion along the oscillation axis. This axis can be controlled to rotate at an audio frequency \( \Omega_z \), which induces the rotation of each site around its own center at such a frequency. \( \Omega_z \) can be much larger than the overall parabolic trapping frequency and reach a few kilo-Hertz. This technique has been applied in the triangular lattice described in Ref. \([28]\).

Let us consider to apply this technique to the honeycomb lattice which has been constructed quite some ago \([29]\). We study the \( p_{x,y} \)-orbital band filled with spinless fermions described in Ref. \([30,31,32]\) with the new ingredient of rotation as

\[
H_0 = t_{||} \sum_{\vec{r} \in A} \{ p_{x}^\dagger \hat{r}_{x} + p_{y}^\dagger \hat{r}_{y} + h.c. \} - \mu \sum_{\vec{r}} n_{\vec{r}},
\]

\[
H_L = \sqrt{\Omega_z} \sum_{\vec{r}} \{ p_{x}^\dagger \hat{r}_{x} p_{y}^\dagger \hat{r}_{y} - p_{y}^\dagger \hat{r}_{y} p_{x}^\dagger \hat{r}_{x} \},
\]

where \( \hat{e}_{i,1,2} = \frac{\tau_{\vec{r}}}{2} \hat{e}_{x} + \frac{1}{2} \hat{e}_{y} \) and \( \hat{e}_{3} = -\hat{e}_{y} \) are the unit vectors pointing from a site in the \( A \)-sublattice to its three neighbors in the \( B \)-sublattice; \( p_{i} \equiv (p_{x} \hat{e}_{x} + p_{y} \hat{e}_{y}) \cdot \hat{e}_{i} (i = 1 \sim 3) \) are the projections of the \( p \)-orbitals along the \( \hat{e}_{i} \) direction; \( \mu \) is the chemical potential; \( a \) is the near-
est neighbor bond length. Since there is no overall lattice rotation, the vector potential due to the Coriolis force and the centrifugal potential across the entire lattices do not appear. The effect is to break the degeneracy between \( p_x \pm ip_y \) as described by \( H_L \). \( \Omega \) can easily reach the order of the recoil energy \( E_R \), and \( t_i \) can be tuned one order smaller than \( E_R \) \cite{31}, thus we have a large flexibility of tuning \( \Omega \parallel \parallel \). The band structure of Eq. 1 is presented as follows. Under the chiral transformation \( P \), i.e., \( p_{r_a,x,y} \rightarrow -p_{r_a,x,y} \), \( p_{r_B,x,y} \rightarrow -p_{r_B,x,y} \), combined by the time-reversal transformation \( T \), Eq. 1 transforms as \( (TP)^{-1} (H_0 + H_L) (TP) = -(H_0 + H_L) \), thus its spectra are symmetric with respect to the zero energy. At \( \Omega_z = 0 \) it exhibits two dispersive bands touching at Dirac cones located at \( K_{1,2} = (\pm \frac{\Omega_z}{\sqrt{3} \Omega}, 0, 0) \) and other two flat bands \cite{30,31}. The dispersive bands touch the flat bands at the Brillouin zone (BZ) center \( K_0 = (0, 0, 0) \). We define the 4-component spinor as \( \psi(k) = (p_{A,x}(k), p_{A,y}(k), p_{B,x}(k), p_{B,y}(k))^T \), and the two bases for the dispersive bands as \( \phi_1(k) = \sqrt{\frac{N_O}{N_0}} \left\{ f_{12}(k), -\frac{i}{\sqrt{3}} f_{23}(k) - f_{31}(k) \right\} , \) and \( \phi_2(k) = \sqrt{\frac{N_O}{N_0}} \left\{ 0, 0, f_{12}(k), -\frac{i}{\sqrt{3}} f_{23}(k) - f_{31}(k) \right\} \), where \( f_{ij} = e^{i k \cdot \hat{e}_i} - e^{-i k \cdot \hat{e}_j} \) and \( N_0(k) \) is the normalization factor. At nonzero \( \Omega_z \), gaps open between different bands. The Dirac cones become gapped with \( \Delta = \Omega_z \), and the masses are of the opposite sign at \( K_{1,2} \). The bottom band is no longer flat at nonzero \( \Omega_z \). Its minimum at \( K_0 \) is pushed down by a value of \( \frac{2}{3} \Omega_z \) and that of the second band is pushed up by \( \frac{\Omega_z}{3} \). This opens a gap of \( 3 \Omega_z \). A similar analysis applies to the top and the third bands.

As \( \Omega_z \) approaches \( \frac{\Omega_z}{\parallel \parallel} \), the middle two bands at \( K_0 \) are pushed to zero from both up and below respectively, and form a single gapless Dirac cone in the BZ as depicted in Fig. 1 B. Let us define another two bases as \( \phi_1' = \frac{1}{2} \{ 1, i, -1, -i \} \), and \( \phi_2' = \frac{1}{2} \{ 1, -i, 1, -i \} \) for the Dirac cone at \( K_0 \), and the Hamiltonian matrix becomes

\[
H_2(k) = \begin{pmatrix}
-\frac{1}{2} \Omega_z - \frac{i}{2} t_y & \frac{1}{2} \Omega_z + \frac{i}{2} t_y \\
\frac{1}{2} \Omega_z + \frac{i}{2} t_y & -\frac{1}{2} \Omega_z - \frac{i}{2} t_y
\end{pmatrix}.
\]

(2)

We notice that a single Dirac cone of the chiral fermion is allowed in the 2D bulk lattice systems, which actually does not contradict to the fermion doubling theory proved for 3D lattices \cite{33}.

As \( \Omega_z \) goes even larger, the lower and upper two pairs of bands are projected into the single orbital bands of \( p_x \pm ip_y \) respectively. The lower two are described by the \( p_x + ip_y \) orbital with a nearest neighbor hopping of \( \frac{t_j}{2} \). Furthermore, a Haldane type next nearest neighbor hopping is generated as depicted in Fig. 1 D: one particle at site \( A \) in the \( p_x + ip_y \) orbital hops to the high energy orbital of \( p_x - ip_y \) at its nearest neighbor \( B \), and hops back into the \( p_x + ip_y \) state at the next nearest neighbor site \( A' \). Along the directions indicated by arrows, this hopping amplitude can be calculated from the second order perturbation theory as \( t_{nn} = \frac{t_j^2}{2 \Omega_z} e^{\frac{i \pi}{4}} \). As pointed out in Ref. \cite{32}, this generates two massive Dirac cones with gap \( \Delta = \frac{t_j^2}{2 t_{nn}} \), at \( K_{1,2} \) of masses with opposite signs.

The above band structures exhibit non-trivial topological properties. The Berry curvature \( F_{xy}(\vec{k}) \), or the gauge field strength, in the momentum space for the \( n \)-th band \( (n = 1 \sim 4) \) is defined as \( F_{n,xy}(\vec{k}) = \partial_{k_y} A_{n,y}(\vec{k}) - \partial_{k_x} A_{n,x}(\vec{k}) \), where \( A_{n,i}(i = x, y) \) is gauge potential defined as \( A_{n,i}(i = x, y) \). The eigenstates of the lower two bands are related to those of the upper two by the transformation \( |\psi_{4-n}(\vec{k})\rangle = (TP) |\psi_{n}(\vec{k})\rangle (n = 1, 2) \), thus the Berry curvature satisfies \( F_{4-n,xy}(\vec{k}) = -F_{n,xy}(\vec{k}) \). The field strength \( F_{xy} \) of the lower two band is depicted in Fig. 2 at different angular
velocities. \( F_{n,xy} \) mainly distributes at wavevectors \( \vec{k} \) with small gap values of \([E_{n\pm1}(\vec{k}) - E_n(\vec{k})]\). The total flux in the BZ for each band is quantized known as the Chern number \( C_n = \frac{1}{2\pi} \int d^2k \; F_{n,xy}(\vec{k}) \) [1, 2]. At all values of \( \Omega_z > 0 \), the Chern number of band 1 is quantized to 1, in spite of a significant change of distribution of \( F_{xy} \) as increasing \( \Omega_z \), as depicted in Fig. 2 A, C and E. The maximal of \( F_{xy} \) are distributed among a ring around the BZ center at small values of \( \Omega_z \), and are pushed to the two vertexes \( K_{1,2} \) of BZ as \( \Omega_z \) increases. The Chern number of band 2 is more subtle. At small \( \Omega_z \), each of two massive Dirac points at \( K_{1,2} \) approximately contribute a flux of \( \frac{1}{2} \). As \( \Omega_z/t_\parallel \rightarrow \frac{1}{2} \) from below, the maximum of \( F_{xy} \) is shifted to the new Dirac point at the BZ center, which approximately contributes the flux of \( \frac{1}{4} \). However, these contributions are canceled by the background negative flux at \( \Omega_z/t_\parallel < \frac{1}{2} \), and thus the Chern number is zero. A topological quantum phase transition occurs at \( \Omega_z/t_\parallel \rightarrow \frac{1}{2} \) beyond which the flux from the Dirac point \( K_0 \) flips the sign to \( -\frac{1}{2} \). Combined with the background contribution, the Chern number of \( C_2 \) changes to \(-1\). In analogy to electron systems, the transverse conductivity can be defined as the ration between the mass flow and the potential gradient as \( \sigma_{xy} = -J_x/\partial_y V \). When the Fermi level lies in the band gap, \( \sigma_{xy} \) is quantized as the sum of the Chern numbers of the occupied bands.

The above band structure with non-vanishing Chern numbers gives rise to topological stable gapless edge modes lying inside the band gap. Fig. 3 depicts the spectra with the open boundary condition on the zig-zag edges. The number of chiral edge modes inside the gap between \( n \) and \( n+1 \) band is the sum of Chern numbers from band 1 to \( n \), i.e., \( \sum_{i=1}^{n} C_i \). At \( \Omega_z < \frac{1}{2} t_\parallel \), the Chern numbers reads \( C_1 = -C_4 = -1 \) and \( C_2 = -C_3 = 0 \), thus edge modes exist in all of the three band gaps with the same chirality. At \( \Omega_z > \frac{3}{2} t_\parallel \), \( C_2 \) and \( C_3 \) change to \( C_2 = -C_3 = -1 \). Thus the edge modes between band 1 and 2, and that between band 3 and 4 are of the opposite chiralities. No edge mode appears between band 2 and 3. This agrees with the picture that Eq. 1 reduces to two copies of Haldane’s model at \( \Omega_z > t_\parallel \).

We also study the QH effect on Eq. 1 arising from Landau levels (LL) by replacing the hopping part to

\[
H_{\text{hop}} = t_\parallel \sum_{\vec{r} \in A} \left\{ p_{\vec{r},i}^\dagger p_{\vec{r}+\vec{a}_i,\epsilon} e^{i f_{\vec{r}+\vec{a}_i} \vec{A} \cdot d\vec{r} + h.c.} \right\},
\]

where the vector potential-\( \vec{A} \) can be generated through another overall lattice rotation or by light induced gauge potential. We will take the flux per plaquette \( \Phi \) and \( \Omega_z \) as two independent variables. The spectra of the above Hamiltonian does not depend on the gauge choice but the physical wavefunctions differ by a gauge transformation. For the calculation convenience, we use the Landau gauge for an open boundary system along the zig-zag edge and take \( \Phi/(2\pi) = 0.05 \).

Due to the vector potential \( \vec{A} \), \((TP)(H_{\text{hop}} + \text{h.c.}) \rightarrow (TP)(H_{\text{hop}} - \text{h.c.}) \)
$H_L = -\epsilon \pi \delta_{ij} \delta_{kl} \mathbf{r}_i \cdot \mathbf{r}_j$ and $± \rho$, roughly symmetric to zero energy. Next let us look at the number of chiral edge modes between levels of $n$ to negative energy at the gap value around $\Omega_z$. The 0th LL is pushed to the zero energy arise from Dirac cones at $K_x = 0$. Landau levels close to the zero energy arise from Dirac cones at $K_z$ and $\Omega_z = 0.2t_{ll}$ as shown in Fig. 4. At small values of $\Omega_z$ (e.g., $\Omega_z = 0.2t_{ll}$ as shown in Fig. 4), gapless edge modes go through the entire spectra from the very band bottom to top. Landau levels close to the zero energy arise from Dirac cones at $K_{1,2}$ with opposite masses as shown in Eq. 3. The 0th LL is pushed to negative energy at the gap value around $-0.26t_{ll}$. The number of chiral edge modes between levels of $n = 0$ to $±1$ is 1 with opposite chirality and that between $n = ±1$ and $±2$ is 3. The energies of $n = ±1$ and $n = ±2$ appear roughly symmetric to zero energy. Next let us look at $\Omega_z = 3t_{ll}$ where a single gapless Dirac cone appears as shown in Eq. 3. Indeed the 0th LL appear close to the zero energy but with a small deviation, which is understandable as no exact symmetry to protect it right at the zero energy. It is tempting to think the appearance of the half-integer QH effect, but this is impossible in free fermion systems. Another half has to be contributed from the high energy part of the band structure. As a result, the number of chiral edge modes between LLs $n = 0$ and 1 is $1$, that between LLs $n = 0$ and $-1$ is $-1$. Thus the spectra from bottom to top become disconnected without edge modes connecting them. This disconnection actually begins to appear even earlier at $\Omega_z = 1.2t_{ll}$, and is enhanced as $\Omega_z$ goes larger. At large values of $\Omega_z$, the model reduces to two copies ($p_x, ± ip_y$) of Haldane’s model. The patterns of LLs between band 1 and 2, and between band 3 and 4 become those of the two massive Dirac cones with opposite mass signs. When Fermi level lies in between LLs, the transverse conductance $\sigma_{xy}$ is quantized at the number of chiral edge modes.

In summary, we propose to investigate the topological insulating states in the p-orbital systems in the honeycomb lattice, which can be realized by the current available experimental techniques. The orbital angular momentum polarization generates non-trivial Chern numbers in the band structure, which gives rise to the orbital counterpart of QAH effect without LLs. QH effect arising for LLs are also investigated, which shows quantitative different features from those in graphene.

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