Quantum Anomalous Hall Effect in $Hg_{1-y}Mn_yTe$ Quantum Wells

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The quantum Hall effect is usually observed when a two-dimensional electron gas is subjected to an external magnetic field, so that their quantum states form Landau levels. In this work we predict that a new phenomenon, the quantum anomalous Hall effect, can be realized in $Hg_{1-y}Mn_yTe$ quantum wells, without an external magnetic field and the associated Landau levels. This effect arises purely from the spin polarization of the Mn atoms, and the quantized Hall conductance is predicted for a range of quantum well thickness and the concentration of the Mn atoms. This effect enables dissipationless charge current in spintronics devices.

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When a two-dimensional electron gas is subjected to a high magnetic field, electronic states form Landau levels. When the temperature is low compared to the spacing between Landau levels, quantized Hall conductance can be observed. In the quantum Hall (QH) regime, electric current flows unidirectionally along the edge of the sample without any dissipation due to the absence of backscattering. The breaking of time reversal symmetry (TRS) is a necessary condition for the Hall effect; however, an external magnetic field (MF) is not required. Soon after the observation of the Hall effect, Hall also observed the anomalous Hall effect [1], where an additional Hall resistance arises from the spin-orbit interaction between electric current and magnetic moments. In the extreme case, an anomalous Hall effect can occur without the external MF as long as the system breaks TRS spontaneously. Given the experimental observation of the QH effect, it is natural to ask whether the anomalous Hall effect can also be quantized without external MF and the associated Landau levels. Such a question is not only of great academic interest, but also has important practical implications. Realizing dissipationless charge current through the quantum anomalous Hall (QAH) effect without an external MF could enable a new generation of quantum electronic devices.

Some years ago, Haldane [2] constructed a theoretical toy model in the honeycomb lattice to show that QH effect is in principle possible without Landau levels. This model breaks TRS but conserves lattice translation symmetry. Haldane's model was extended to include localization physics in Ref. [3]. Unfortunately, this model is mostly academic, and cannot be realized in the recently discovered graphene system. Later, the work on the intrinsic anomalous Hall effect of a ferromagnetic semiconductor in a metallic regime [4–6] showed the relation between Berry's phase and Hall conductance. Qi *et al.* [7] constructed a tight-binding model of electron spin-orbit coupled to the polarized magnetic moments, and showed that Hall conductance can be quantized in appropriate parameter regimes. This model breaks TRS due to magnetic moments rather than Landau levels, and provides another example of the QAH effect. More recently, a closely related topological phenomenon known as the quantum spin Hall (QSH) effect has been theoretically predicted and experimentally observed in HgTe quantum wells (QW) [8,9]. In this work, we show that when the HgTe QW are doped with magnetic Mn atoms, the QAH effect can be realized within an experimentally accessible parameter regime. We propose an experiment to demonstrate that the quantized Hall conductance indeed arises from magnetic moments rather than Landau levels.

As a starting point, we first briefly review the physics of the QSH effect in HgTe QW. HgTe has an inverted band structure, where the p-type Γ_8 band has higher energy compared to the s-type Γ_6 band at the Γ point. For HgTe/CdTe QW, there exists a topological quantum phase transition across some critical well thickness d_c where the band structure changes from the normal to the inverted character. The novel QSH effect occurs in the inverted regime $d > d_c$ [8]. In order to describe the physics near d_c, an effective four-band model is introduced as

$$H_0(k) = \begin{pmatrix} h_+(\mathbf{k}) & 0 \\ 0 & h_-(\mathbf{k}) \end{pmatrix}, \tag{1}$$

where $h_+(\mathbf{k}) = \epsilon_\mathbf{k} + \mathcal{M}(\mathbf{k})\sigma_z + A(k_x\sigma_x - k_y\sigma_y)$ and $\sigma_{x,y,z}$ is the Pauli matrix. $h_-(\mathbf{k}) = h_+^*(-\mathbf{k})$ is required by TRS. $\epsilon_\mathbf{k}$ and $\mathcal{M}(\mathbf{k})$ are expanded as $\epsilon_k = C_0 + C_2k^2$ and $\mathcal{M}(k) = M_0 + M_2k^2$. This effective model is expressed in the subspace containing the states $|E1, \pm\rangle$ and $|H1, \pm\rangle$, where $|E1, \pm\rangle$ is a superposition of $|\Gamma_6, \pm\frac{1}{2}\rangle$ and $|\Gamma_8, \pm\frac{1}{2}\rangle$, while $|H1, \pm\rangle$ is formed by $|\Gamma_8, \pm\frac{3}{2}\rangle$. Here $\pm$ denotes the two spin states which are degenerate due to the Kramers theorem. The diagonal block $h_\pm(\mathbf{k})$ describes a Dirac model in 2 + 1 dimensions, which at half filling carries a Hall conductance of $\pm e^2/h$, respectively [2,7,8]. Thus the net Hall conductance of the inverted QW system vanishes, while the spin Hall conductance, defined as the difference between the two blocks, is still nonzero. Therefore the QSH effect can be viewed as two copies of the QAH effects, with the opposite quanta of Hall conductances.

When the TRS is broken, two spin blocks are no longer related, and their charge Hall conductances no longer cancel exactly. The key idea of this work is to identify the parameter space where one spin block is in the normal regime, while the other spin block is in the inverted regime. The normal regime gives a topologically trivial insulator with vanishing Hall conductance, while the inverted regime gives a topologically nontrivial insulator with one quantum unit of Hall conductance; therefore, the whole system becomes a QAH state. Now we return to the four-band effective Hamiltonian (1) and address what kind of term can induce QAH effect. To describe the spin splitting induced by magnetization, a phenomenological term is introduced as

$$H_s = \begin{pmatrix} G_E & 0 & 0 & 0 \\ 0 & G_H & 0 & 0 \\ 0 & 0 & -G_E & 0 \\ 0 & 0 & 0 & -G_H \end{pmatrix}, \qquad (2)$$

where spin splitting is $2G_E$ for the $|E1, \pm\rangle$ band and $2G_H$ for the $|H1, \pm\rangle$ band. Then the energy gap is given by $E_g^+ = 2M_0 + G_E - G_H$ for the up spin block while $E_g^- = 2M_0 - G_E + G_H$ for down spin block. In order to obtain QAH effect, we require that (i) the state with one kind of spin is in the inverted regime while the other goes into the normal regime, namely $E_g^+ E_g^- < 0$, (ii) the entire system is still in the insulating phase with a full bulk gap, which requires that $|E1, +\rangle$ ($|E1, -\rangle$) and $|H1, -\rangle$ ($|H1, +\rangle$) do not cross each other, leading to the condition $(2M_0 + G_E + G_H)(2M_0 - G_E - G_H) > 0$. Combining the above two conditions, we arrive at $G_E G_H < 0$, which requires that the spin splittings for $|E1, \pm\rangle$ and $|H1, \pm\rangle$ must have the opposite sign. This condition is illustrated in Fig. 1(a). We can also understand the physics from the edge state picture [Fig. 1(b)]. On the boundary of a QSH insulator there are counterpropagating edge states carrying opposite spin. When the spin splitting term increases, spin-down edge states penetrate much deeper into the bulk due to the decreasing gap, and eventually disappear, leaving only spin-up edge states bound more strongly to the edge. Thus the system has only spin-up edge states and transforms from a QSH state to a QAH state.

Therefore the key condition $G_E G_H < 0$ is identified for the QAH effect. We may ask whether or not it is true in the realistic material. Fortunately, in HgTe QW doped with Mn, *sp-d* exchange coupling indeed gives the opposite signs for G_E and G_H, a fact which is well established in the literature [10,11]. From a standard perturbative treatment of the eight-band Kane model [8,12], we find the coefficients G_E, G_H in Eq. (2) can be expressed as $G_E = -(3AF_1 + BF_4)$ and $G_H = -3B$ in which A, B are given by [11,13] $A = \frac{1}{6}N_0\alpha y\langle S\rangle$ and $B = \frac{1}{6}N_0\beta y\langle S\rangle$. F_1, F_4 are

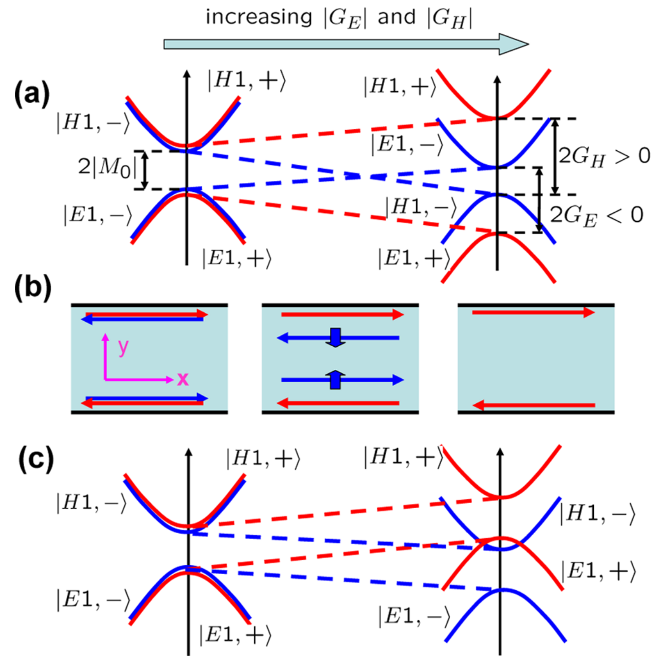

FIG. 1 (color online). Evolution of band structure and edge states upon increasing the spin splitting. For (a) $G_E < 0$ and $G_H > 0$, the spin-down states $|E1, -\rangle$ and $|H1, -\rangle$ in the same block of the Hamiltonian (1) touch each other and then enter the normal regime. But for (c) $G_E > 0$ and $G_H > 0$, gap closing occurs between $|E1, +\rangle$ and $|H1, -\rangle$ bands, which belong to different blocks of the Hamiltonian, and thus will cross each other without opening a gap. In (b) we show the behavior of the edge states during the level crossing in the case of (a).

the amplitudes of $|\Gamma_6, \pm\frac{1}{2}\rangle$ and $|\Gamma_8, \pm\frac{1}{2}\rangle$ components in the state $|E_1, \pm\rangle$, respectively, which can be extracted from the numerical calculation. N_0 is the number of unit cells per unit volume, y is Mn fraction, and $\langle S\rangle$ is spin polarization of Mn out of the QW plane. α and β describe *sp-d* exchange coupling strength for the *s*-band and the *p*-band electron, respectively, where the signs and magnitudes are crucial for the relative sign of G_E and G_H. For $Hg_{1-y}Mn_yTe$, these parameters are given by $N_0\alpha = 0.4$ eV, $N_0\beta = -0.6$ eV [11,13] and $F_1 = 0.57$, $F_4 = 0.43$, leading to the opposite signs for G_E and G_H. Combined with the previous analysis about the Hamiltonian (2), we conclude that QAH effect can occur in MnHgTe QW, as long as Mn magnetization $\langle S\rangle$ is large enough and perpendicular to the QW plane.

Although the above analysis already gives a clear explanation of the physical mechanism of the QAH effect, to obtain more quantitative predictions we perform a realistic electronic structure calculation based on the eight-band Kane model [12,13]. Our Hamiltonian takes into account the exchange term and bulk inversion asymmetry terms [12], in addition to the terms included in the original Kane model. In Fig. 2(a), the energy spectrum of the lowest subbands $|E1, \pm\rangle$ and $|H1, \pm\rangle$ at the Γ point is plotted as a function of QW thickness d. At a critical thickness $d_{c1} = 7.25$ nm, a level crossing "A" occurs between $|E1, -\rangle$ and

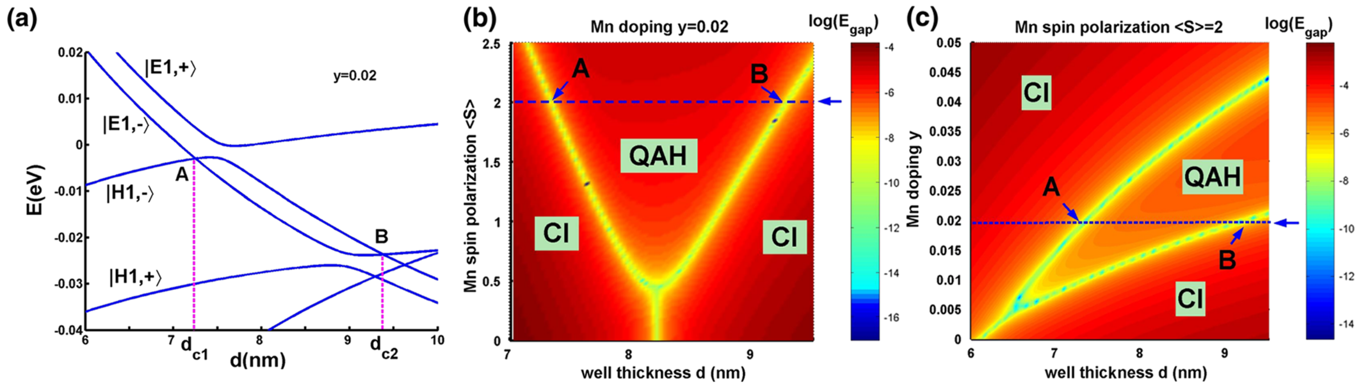

FIG. 2 (color online). (a) The energy levels for $|E1,\pm\rangle$ and $|H1,\pm\rangle$ are plotted as a function of the QW thickness. Two crossing points (A and B) are labeled in the figure. The energy gap ($\log(E_{\rm gap})$ used here) is plotted as a function of the well thickness d versus the Mn magnetic moment $\langle S\rangle$ in (b), versus the Mn doping concentration y in (c). Dashed blue line in (b) or (c) refers to the line along which (a) is plotted. The points "A" and "B" correspond to the two Dirac-type crossing points. Two different phases, conventional insulator (CI) with $\sigma_H = 0$ and QAH state with $\sigma_H = -e^2/h$, are separated by the gap closing line in the figures.

$|H1,-\rangle$ bands. This is a Dirac-type level crossing, across which the Hall conductance jumps by $-e^2/h$. Since the system always remains gapped when Mn magnetization is adiabatically turned on, we know $\sigma_H = 0$ for $d < d_{c1}$ and $\sigma_H = -e^2/h$ for $d > d_{c1}$. The same analysis applies to the other critical thickness $d_{c2} = 9.4$ nm ["B" in Fig. 2(a)], where level crossing occurs between $|E1,+\rangle$ and $|H1,+\rangle$ bands and Hall conductance returns to 0. Therefore, for parameters $\langle S\rangle = 2$ and $y = 0.02$, the QAH effect appears in a QW thickness range $d_{c1} < d < d_{c2}$. The same calculation can be carried out to determine the whole phase diagram with three tunable parameters: QW thickness d, spin polarization $\langle S\rangle$, and Mn fraction y. In Figs. 2(b) and 2(c), the gap in the d-$\langle S\rangle$ plane and in the d-y plane are plotted, respectively. The line with bright color shows the phase boundary with vanishing gap. At zero $\langle S\rangle$ or zero y limit, TRS is recovered and the critical line terminates at the transition point between trivial and QSH insulators [8]. An important feature is that a minimal $\langle S\rangle$ (for fixed y) or minimal y (for fixed $\langle S\rangle$) is required to obtain QAH phase, which is a consequence of bulk inversion asymmetry. For example, for $y = 0.02$ we need $\langle S\rangle > 0.5$ for QAH phase.

We now discuss the experimental observation of the QAH effect in the $Hg_{1-y}Mn_yTe$ system. The main difficulty lies in the fact that with Mn doping $y = 0.02$, $Hg_{1-y}Mn_yTe$ is paramagnetic [14] rather than ferromagnetic. From the Curie-Weiss formula, we have

$$\langle S\rangle = -S_0 B_{5/2}\left(\frac{5g_{\rm Mn}\mu_B B}{2k_B(T+T_0)}\right), \tag{3}$$

where $S_0 = 5/2$, $B_{5/2}$ is the Brillouin function [12,13], and $T_0 > 0$ stands for a weak antiferromagnetic coupling between Mn spins. To generate the QAH effect, a small MF is needed to polarize Mn moments. In fact, some experiments have already shown quantized Hall conductance for MF less than 1 T [9,15]. Such magnitude of MF is achievable through the hybrid ferromagnetic-semiconductor structure with a magnetic layer deposited on the top of the semiconductor for device application [16]. However, since any small MF has an orbital effect, this experiment by itself cannot prove the existence of QAH. To solve this problem, we propose two different ways to polarize Mn spins without an orbital MF. The first approach is to apply a low-frequency polarized infrared light to provide the angular momentum required for aligning Mn moments. As the efficiency of the photoinduced Mn magnetization is quite low in experiment [17,18], we focus on another approach, time-resolved Hall measurement, which can provide a more dramatic demonstration of the QAH effect. First, a static MF is applied, which acts on itinerant electrons through three terms: the orbital effect $H_{\rm orb}$, the Zeeman term H_Z, and the exchange term $H_{\rm ex}$. In $H_{\rm ex}$, Mn spin polarization is determined by Eq. (3). Second, at time t_0 the MF is switched off within a time scale τ_B. As a result, Mn spin polarization will decay to zero in a spin-relaxation time τ_s. However, if $\tau_B \ll \tau_s$, there is a time window $t_0 + \tau_B < t \ll t_0 + \tau_s$ when the orbital and Zeeman effect of the MF already disappeared, but Mn spin polarization remains similar to the value before MF is removed. Consequently, within this time range there is no conventional QH based on Landau levels, so that pure QAH effect can be observed, if Mn spin polarization stays in the correct range.

To illustrate this proposal more clearly, we compare the band structure with and without Landau levels. In Figs. 3(a) and 3(b), the energy spectra is plotted as a function of MF for different thicknesses. The blue solid lines take into account $H_{\rm orb}$, H_Z, and $H_{\rm ex}$, corresponding to the spectra at time $t < \tau_B$ (setting $t_0 = 0$). In contrast, the red dashed lines are the conduction and valence band edges at time $\tau_B < t \ll \tau_s$, after the MF is switched off but Mn spin polarization remains the same. Since the energy spectrum is dispersive when the orbital effect of MF is absent, the system is insulating only when Fermi energy E_F lies between the two middle red dashed lines, i.e., between $|E1,-\rangle$ and $|H1,-\rangle$ for Fig. 3(a), or between $|E1,+\rangle$ and $|H1,+\rangle$ for Fig. 3(b). Depending on the initial values

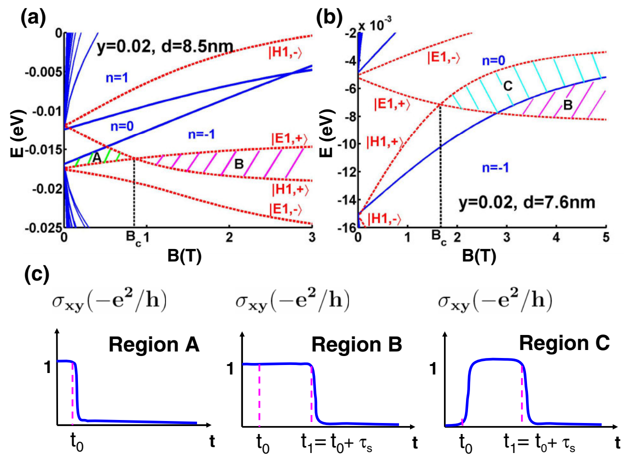

FIG. 3 (color online). Landau level spectra are plotted as a function of MF (blue solid line) for two different thicknesses (a) $d = 8.5$ nm and (b) $d = 7.6$ nm, taking into account exchange term, Zeeman splitting, and orbital effect. The corresponding red dashed lines show the band edge of the subbands $|H1, \pm\rangle$ and $|E1, \pm\rangle$ when the MF has been turned off but the Mn spin polarization remains. Without an external MF, the system is in a QSH insulator phase for (a), and a trivial insulator phase for (b). (c) shows schematically the predicted Hall conductances for the three different regions A, B, and C defined by shadows in (a) and (b).

of E_F and MF B, three different phenomenon can be observed. (i) When (E_F, B) is in region A of Fig. 3(a), the system has Hall conductance $\sigma_H = -e^2/h$ in the static MF and enters a trivial insulator phase after MF is switched off. Consequently, Hall conductance will drop to zero once the MF is removed. (ii) When (E_F, B) is in region B of Figs. 3(a) and 3(b), the system has Hall conductance $\sigma_H = -e^2/h$ for static field and enters a QAH phase with the same Hall conductance after the MF is switched off. Thus, Hall conductance will remain on the $-e^2/h$ plateau for a time $\sim\tau_s$ after turning off MF. (iii) When (E_F, B) is in region C of Fig. 3(b), the system has vanishing Hall conductance in the static field, but enters a QAH phase with $\sigma_H = -e^2/h$ after switching off MF. Consequently, we will observe the dramatic appearance of a ''pulse'' of Hall conductance in a time scale $\sim\tau_s$ even though the system is in the $\sigma_H = 0$ Hall plateau under a static field. Observation of this phenomenon gives the conclusive demonstration of the QAH effect. Because of the topological distinction between $\sigma_H = 0$ and $\sigma_H = -e^2/h$ states, the transition between them is always sharp at low temperature, even though Mn magnetization changes continuously. Consequently, the time dependence of σ_{xx} and σ_{xy} in this proposal should show the same critical behavior as the usual ''plateau transition'' in the QH effect.

Finally, we estimate the experimental conditions required to realize this proposal. First, both the switchoff time τ_B and Hall measurement time resolution δt [19] should be shorter than Mn spin relaxation time τ_s, which is of order 10–100 μs [20,21]. Second, the MF should be turned off slowly enough for electrons to stay in the instantaneous ground state during the switchoff operation (adiabatic condition), which requires $\tau_B \gg \hbar/E_g$, where E_g is energy gap and $\hbar/E_g \sim 10^{-12}$ s. Third, due to the gapless edge states, there will always be some excitation near the edge. Thus, we require that there is enough time for the electron to relax back to the equilibrium state after turning off MF. The time scale for relaxation is inelastic relaxation time, which is estimated to be 10^{-11} s [9]. Therefore, a MF of several tesla needs to be switched off within $10^{-11} \ll \tau_B \ll 10^{-4}$ s, and time resolution of transport measurement should satisfy $\delta t \ll 10^{-4}$ s.

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