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Realizing Topological Mott Insulators from the RKKY Interaction

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We engineer topological insulating phases in a fermion-fermion mixture on the honeycomb lattice, without resorting to artificial gauge fields or spin-orbit couplings and considering only local interactions. Essentially, upon integrating out the fast component (characterized by a larger hopping amplitude) in a finite region of dopings, we obtain an effective interaction between the slow fermions at half-filling, which acquires a Haldane mass with opposite parity in the two valleys of the Dirac cones, thus triggering a quantum anomalous Hall effect. We carefully analyze the competition between the induced Semenoff-type mass (producing charge density wave orders in real space) versus the Haldane mass (QAH), as a function of the chemical potential of the fast fermions. If the second species involves spin-1/2 particles, this interaction may induce a quantum spin Hall phase. Such fermion-fermion mixtures can be realized in optical lattices or in graphene heterostructures.

The quest of topological phases in the absence of a net uniform magnetic field, has attracted a great attention recently in the field of condensed matter physics, in connection with the spin-orbit coupling and artificial gauge fields¹⁻⁴. The realization of such phases has become important due to their physical properties such as the edge transport and potential applications for spintronics⁵. The HgTe quantum well and three-dimensional Bismuth analogues have been a perfect area for the quantum spin Hall effect and topological band insulators⁶⁻⁹. In addition, the quantum anomalous Hall effect and its version on the honeycomb lattice, the Haldane model¹⁰, have been observed with photons^{11,12}, cold atom systems¹³ and magnetic topological insulators¹⁴. Synthetic gauge fields and spin-orbit couplings are currently vastly investigated in optical lattices¹⁵ and photon analogues¹⁶. Engineering topological phases through interactions is also interesting on its own. Interactions may also localize the charge, through Mott physics. The transition between topological band insulator and Mott phase has been largely addressed¹⁷⁻²². An example of topological band insulators induced by interactions, resulting in topological Mott insulators, has also been proposed by Raghu et al.²³ on the honeycomb lattice. This scenario requires however that the next-nearest-neighbour interaction exceeds the nearest-neighbour repulsion²³⁻²⁵. In addition, recent numerical works have questioned the existence of a topological phase within this model^{26,27}. In this Letter, we envision a fermion-fermion mixture comprising local interactions, for the realization of such topological Mott insulators. The idea here is that one copy of the mixture is much faster than the other, inducing an exotic Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction²⁸ on the partner copy. We will show below that the long-range aspect of the RKKY interaction can contribute to frustrate the charge density wave orders.

This class of topological Mott insulators, which refers to topological band insulators induced by interaction effects²³, must be distinguished from the other class of (three-dimensional) topological Mott insulators, which

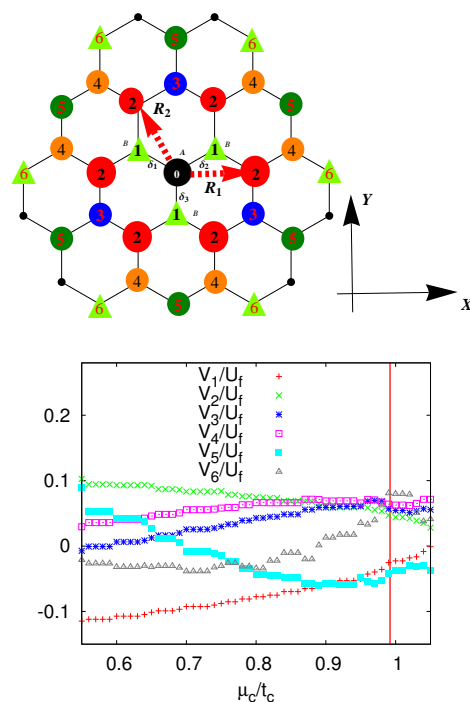


FIG. 1. (Color online) *Upper panel*: Graphene honeycomb lattice with the two sublattices A and B. We introduce 1, 2, 3... 6 to label the six nearest-neighbour partners of the site 0. *Lower panel*: The ratio of interaction V_i/U_f ($i=1,2,3,4,5,6$) as a function of the chemical potential of the fast fermions, where i refers to the definition of sites in the upper panel with U_f the onsite interaction.

corresponds to a Mott phase where the spin sector is embodied by a band structure of a topological band insulator giving rise to purely neutral spin edge modes¹⁷. Known examples of topological Mott phases also exist in one dimension^{29,30}. Topological aspects of Kondo materials have been recently addressed theoretically and observed experimentally³¹⁻³³.

Cold atom graphene systems³⁴ and heterostructures on the honeycomb lattice may be relevant for experimental realizations and the adjustability of the interactions among the mixture^{35,36} will allow for the exploration of various quantum phases. Mixtures of ultra-cold atoms have already attracted some attention for the realization of topological phases and supersolid phases³⁷. The RKKY interaction has already been shown to be efficient to engineer topological superconductors³⁸.

We propose a model on the honeycomb lattice with two species of fermions (c and f) among which there is one *spinless* species of fermions c and one spin-1/2 (or spinless) species f . The two species of fermions are coupled together via a repulsive interaction characterized by the coupling constant g_{cf} . In the case of spins-1/2 f fermions, we also consider the effect of an on-site Hubbard interaction U_f , resulting in the Hamiltonian:

$$H = -t_f \sum_{\langle i,j \rangle, \sigma} f_{i\sigma}^\dagger f_{j\sigma} + \mu_f \sum_{j, \sigma} f_{j\sigma}^\dagger f_{j\sigma} + U_f \sum_i f_{i\uparrow}^\dagger f_{i\uparrow} f_{i\downarrow}^\dagger f_{i\downarrow} - t_c \sum_{\langle i,j \rangle} c_i^\dagger c_j + \mu_c \sum_j c_j^\dagger c_j + \sum_{j, \sigma} g_{cf} f_{j\sigma}^\dagger f_{j\sigma} c_j^\dagger c_j. \quad (1)$$

We take the lattice spacing to be 1. The three vectors indicating the nearest neighbors are $\delta_1 = (-\frac{\sqrt{3}}{2}, \frac{1}{2})$, $\delta_2 = (\frac{\sqrt{3}}{2}, \frac{1}{2})$, $\delta_3 = (0, -1)$. Both the fermions f and fermions c have the band structure of a graphene system. We can diagonalize the band structure of fermions c on the honeycomb lattice by introducing the isospin of the two sublattice fermions $\Phi_c = (c_{A\mathbf{k}}, c_{B\mathbf{k}})^T$:

$$H_c = -t_c \sum_{\langle i,j \rangle} c_i^\dagger c_j + \mu_c \sum_i c_i^\dagger c_i = \sum_k \Phi_c^\dagger \mathcal{H}_k^c \Phi_c \quad (2)$$

$$\mathcal{H}_k^c = \begin{pmatrix} \mu_c & -t_c g^*(\mathbf{k}) \\ -t_c g(\mathbf{k}) & \mu_c \end{pmatrix},$$

in which $g(\mathbf{k}) = \sum_{j=1,2,3} e^{i\mathbf{k} \cdot \delta_j}$. We obtain two bands of fermions with the energy levels: $\epsilon_\pm(\mathbf{k}) = \mu_c \pm t_c |g(\mathbf{k})|$ and the related annihilation operators $\Phi_{c\pm} = \frac{1}{\sqrt{2}}(c_{A\mathbf{k}} \pm c_{B\mathbf{k}} e^{i\phi_{\mathbf{k}}})$, $\phi_{\mathbf{k}} = \arg(g(\mathbf{k}))$.

Below, we consider the case where the fermions c are much faster than the fermions f ($t_c \gg t_f$), justifying the formal Gaussian integration of the fermions- c . For simplicity, we assume that the fermions c are spin-polarized (one-component). The induced dynamical RKKY susceptibility involves the Lindhard function:

$$\chi_{IJ}(\Omega, \mathbf{q}, \mu_c) = - \sum_{\mathbf{k}} \lim_{\eta \rightarrow 0} \frac{n_f(\epsilon_-(\mathbf{k} + \mathbf{q})) - n_f(\epsilon_-(\mathbf{k}))}{\Omega + \epsilon_-(\mathbf{k} + \mathbf{q}) - \epsilon_-(\mathbf{k}) + i\eta} \alpha_{IJ}(\mathbf{k}, \mathbf{q}), \quad (3)$$

in which $n_f(\epsilon_-(\mathbf{k}))$ is the Fermi-Dirac distribution of the fermions c with energy of the lower band and IJ are the indices for the sublattices A and B. $\alpha_{AB}(\mathbf{k}, \mathbf{q}) = e^{i(\theta_{\mathbf{k}+\mathbf{q}} - \theta_{\mathbf{k}})}$, $\alpha_{BA}(\mathbf{k}, \mathbf{q}) = e^{-i(\theta_{\mathbf{k}+\mathbf{q}} - \theta_{\mathbf{k}})}$ and $\alpha_{AA} = \alpha_{BB} = 1$. We denote the susceptibility on the same lattice as $\chi_{II}(\Omega, \mathbf{q}, \mu_c)$ and the susceptibility on the different sublattices as $\chi_{AB}(\Omega, \mathbf{q}, \mu_c)$ and $\chi_{BA}(\Omega, \mathbf{q}, \mu_c)^*$.

The RKKY interaction between the fermions f , depends strongly on μ_c , which we can adjust. One example is when the static RKKY susceptibility peaks at wave vectors that are nesting vectors graphene system close to quarter-filling ($\mu_c = 0.992t_c$) with Van Hove singularities (Fig. 2). We have also represented the RKKY interaction in the direct space as shown in Fig. 1 upper panel as a function of chemical potential. A similar two-fluid model has been previously proposed on the honeycomb lattice³⁹, however our model insists on the honeycomb band structure of the fast fermion c : this leads to an RKKY interaction with long range interaction and negative nearest-neighbour interaction, which suppresses other orders like charge density wave and Semenoff mass⁴¹. To illustrate these two points, we first proceed to write down the Green function for the slow fermions f , and the RKKY interaction induced by the fermion c will bring about an interaction between the fermion f . To evaluate the influence of the RKKY interaction on the (bare) Green's function $G_0(\omega, \mathbf{k})$ of a fermion- f , we use a standard Hartree-Fock decoupling of the interaction. If we write the spinor $\Psi_{fk}^\dagger = (f_{kA}^\dagger, f_{kB}^\dagger)$, then the Green function and the Schwinger-Dyson equation for the fermion f will be represented as:

$$G_f(\omega, \mathbf{k})_{IJ}^{-1} = G_0(\omega, \mathbf{k})_{IJ}^{-1} - i \sum_{\Omega, \mathbf{q}} \frac{g_{cf}^2}{2} \chi_{IJ}(\Omega, \mathbf{q}, \mu_c) G_f(\omega + \Omega, \mathbf{k} + \mathbf{q})_{JI} \quad (4)$$

$$\simeq G_0(\omega, \mathbf{k})_{IJ}^{-1} + \sum_{\mathbf{q}} \frac{g_{cf}^2}{2} \chi_{IJ}(0, \mathbf{q}, \mu_c) [2P f_{JI}(\mathbf{k} + \mathbf{q}) - \delta_{JI}]$$

$$G_0(\omega, \mathbf{k})^{-1} = \omega - t_f(\tau_x \Re e + \tau_y \Im m)g(\mathbf{k}),$$

in which τ_x , τ_y and τ_z are Pauli matrices in sublattices subspace. We have checked that the peaks of $\chi_{IJ}(\Omega, \mathbf{q}, \mu_c)$ varies less than 20% when $|\Omega| < 0.3t_c$, we have therefore made the adiabatic approximation in the

second equality of Eq. 4, which consists of replacing the dynamical RKKY susceptibility by the static susceptibility: $\chi_{IJ}(\Omega, \mathbf{q}, \mu_c) \simeq \chi_{IJ}(0, \mathbf{q}, \mu_c)$. $P f_{JI}(\mathbf{k} + \mathbf{q})$ is the projector to the lower band for the fermion f .

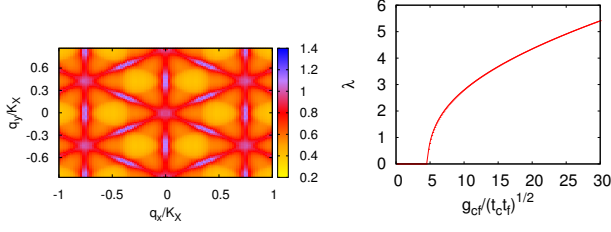


FIG. 2. (Color online) *Left panel*: The static RKKY susceptibility on the same sublattice $\chi_{II}(0, \mathbf{q}, \mu_c = 0.992t_c)$ as a function of $\mathbf{q} = \frac{\mathbf{Q}}{2}$ as defined in Eq. 3. *Right panel*: The amplitude of the spontaneous spin-orbit coupling λ as a function of g_{cf} when $\mu_c = 0.992t_c$.

An important point is that the Hartree term and certain contributions from the Fock term will change the chemical potential of the fermion f . Here, we evaluate:

$$\begin{aligned} \tilde{\mu}_f = & \mu_f + g_{cf}^2 [\Re \chi_{II}(0, 0, \mu_c) - \sum_{q \neq 0} \Re \chi_{II}(0, q, \mu_c)] \langle n_k \rangle \\ & + \frac{g_{cf}^2}{2} \sum_q \Re \chi_{II}(0, q, \mu_c). \end{aligned} \quad (5)$$

We find numerically that $\tilde{\mu}_f - \mu_f$ is negligible (ranging from $0.03t_f$ to $0.09t_f$) for $g_{cf} < 20\sqrt{t_c t_f}$. This justifies our consideration of the half-filled case for the fermion f .

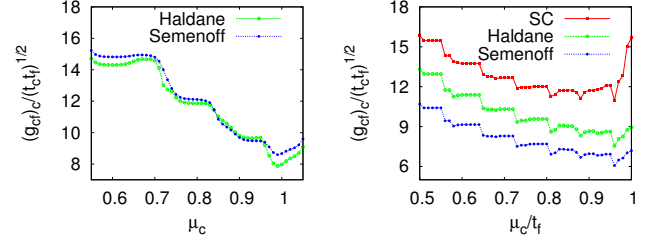


FIG. 3. (Color online) *Left panel*: Critical value of g_{cf} as a function of μ_c such that Eq.(10) has a non trivial solution respectively in the odd sector (Haldane mass) and the even sector (Semenoff mass). *Right panel*: Critical value of g_{cf} as a function of μ_c respectively for the instability of superconductivity, Haldane phase and Semenoff phase by limiting the RKKY interaction within nearest-neighbour and next-nearest neighbour interaction. The dominance of the Semenoff phase demonstrates the necessity of the long tail of the RKKY interaction for the emergence of the Haldane phase.

At a mean-field level, we can solve the Green's function $G_f(\omega, \mathbf{p})$ by using the Ansatz: $G_f(\omega, \mathbf{p})^{-1} = \omega - a(\mathbf{p})\tau_x - b(\mathbf{p})\tau_y - c(\mathbf{p})\tau_z$ such that $a(\mathbf{p}), b(\mathbf{p}), c(\mathbf{p}) \in \mathbf{R}$. Then, we are able to find self-consistent equations for the real function $a(\mathbf{p}), b(\mathbf{p}), c(\mathbf{p})$. If we denote $E(\mathbf{k}) = t_f |g(\mathbf{k})|$, the projector to the lower band then becomes:

$$P_{fJI}(\mathbf{k}+\mathbf{q}) = \frac{1}{2} \left[1 + \frac{a(\mathbf{k}+\mathbf{q})\tau_x + b(\mathbf{k}+\mathbf{q})\tau_y + c(\mathbf{k}+\mathbf{q})\tau_z}{E(\mathbf{k}+\mathbf{q})} \right] \quad (6)$$

By inserting Eq. 6 into Eq. 4, we obtain three coupled non-linear equations, which are hard to resolve. By replacing $a(\mathbf{p}), b(\mathbf{p})$ on the right hand side of the self-consistent equation by $\Re g(\mathbf{p})$ and $\Im g(\mathbf{p})$, we have the 1st order corrections of the bare Green function:

$$a(\mathbf{p}) = t_f \Re g(\mathbf{p}) + \frac{g_{cf}^2}{2} \sum_{\mathbf{q}} \frac{\Re(t_f \chi_{AB}(0, \mathbf{q}, \mu_c) g(\mathbf{p}+\mathbf{q}))}{E(\mathbf{p}+\mathbf{q})} \quad (7)$$

$$b(\mathbf{p}) = t_f \Im g(\mathbf{p}) + \frac{g_{cf}^2}{2} \sum_{\mathbf{q}} \frac{\Im(t_f \chi_{AB}(0, \mathbf{q}, \mu_c) g(\mathbf{p}+\mathbf{q}))}{E(\mathbf{p}+\mathbf{q})} \quad (8)$$

$$c(\mathbf{p}) = -\frac{g_{cf}^2}{2} \sum_{\mathbf{q}} \frac{\chi_{II}(0, \mathbf{q}, \mu_c)}{E(\mathbf{p}+\mathbf{q})} c(\mathbf{p}+\mathbf{q}). \quad (9)$$

In Eqs. 7 and 8, the RKKY interaction renormalizes the graphene band structure, and we have checked that the modification is of one order smaller than the function $a(\mathbf{p})$ and $b(\mathbf{p})$. In Eq. 9, the RKKY interaction opens a gap in the system with the function $c(\mathbf{p})$. We remark that Eq. 9 has always a trivial solution $c(\mathbf{p}) = 0, \forall \mathbf{p}$ for any values of g_{cf} . However, when g_{cf} is larger than one critical value $(g_{cf})_c$ to be determined, there can exist a non-trivial solution for the function $c(\mathbf{p})$. It is reasonable

to make the approximation of $E(\mathbf{k}+\mathbf{q}) = t_f |g(\mathbf{k}+\mathbf{q})|$ before this instability onset. In order to study the instability onset of the function $c(\mathbf{p})$, we take the limit $c(\mathbf{p}) \rightarrow 0$, and therefore obtain a solvable linear equation:

$$c(\mathbf{p}) = -\frac{g_{cf}^2}{2} \sum_{\mathbf{q}} \frac{\chi_{II}(0, \mathbf{q}, \mu_c)}{t_f |g(\mathbf{p}+\mathbf{q})|} c(\mathbf{p}+\mathbf{q}), \quad (10)$$

We discretize the first Brillouin zone and Eq. 10 in-

volves a real matrix with the dimension as the number of discretization points. Eq. 10 then turns into:

$$[V_\chi] = M_\chi[V_\chi], \quad (11)$$

in which V_χ is the column vector representing the discretized function $c(\mathbf{p})$. The criticality occurs when the largest eigenvalue of the matrix M_χ attains 1. Eigenvectors of the matrix M_χ has two subspaces, the odd parity subspace $c(\mathbf{p}) = -c(-\mathbf{p})$ and the even parity subspace $c(\mathbf{p}) = c(-\mathbf{p})$ knowing that M_χ is invariant under the parity symmetry since $\chi_{II}(0, \mathbf{q}, \mu_c) = \chi_{II}(0, -\mathbf{q}, \mu_c)$. In contrast to the $t - V_1 - V_2$ model²⁷, we can tune the chemical potential of the fermion c in order to adjust the threshold of criticality of the emergence of Haldane and Semenoff mass. In Fig. 3 left panel, we see that when $\mu_c = 0.992t_c$, the critical threshold of g_{cf} for the emergence of the Haldane mass reaches its minimum: $(g_{cf})_c = 7.88\sqrt{t_c t_f}$.

If we denote the renormalized eigenvector for the biggest eigenvalue of the matrix M_χ in the odd parity sector as VO_χ , then beyond the instability threshold $g_{cf} > (g_{cf})_c$ the Haldane mass should have the similar behavior as VO_χ : $c(\mathbf{p}) = \lambda VO_\chi(\mathbf{p})$. The amplitude of the Haldane mass λ is determined by minimizing the following energy as a function of λ :

$$E_0(\lambda) = - \sum_{\mathbf{p}} \sqrt{[a(\mathbf{p})]^2 + [b(\mathbf{p})]^2 + [\lambda VO_\chi(\mathbf{p})]^2} \quad (12)$$

$$+ g_{cf}^2 \sum_{\mathbf{p}, \mathbf{q}} \chi_{IJ}(0, \mathbf{q}, \mu_c) \frac{\lambda^2 VO_\chi(\mathbf{p}) VO_\chi(\mathbf{p} + \mathbf{q})}{[E(\mathbf{p})E(\mathbf{p} + \mathbf{q})]},$$

in which $E_0(\lambda)$ is the energy of the half-filled fermion f under the RKKY interaction. The amplitude λ is plotted as a function of g_{cf} in Fig. 2 right panel.

Now, we study the importance of the long-range aspect in the RKKY interaction. We compare the results of Fig. 3 left panel with those from an effective $V_1 < 0, V_2 > 0$ model, where for each μ_c , the parameters are extracted from the RKKY coupling, and we study the possible emergent instabilities. The superconducting instability entailed by the attractive nearest-neighbor interaction and the Haldane and Semenoff instability entailed by the repulsive next-nearest-neighbour interaction. The Semenoff mass, which shifts the chemical potential difference between the two sublattices, is connected to various charge density orders. After resolution of the self-consistent relations, we see from Fig. 3 right panel that superconductivity is not favored among the three and the QAH (Haldane) phase is never stable. The absence of superconductivity can be justified by the linear spectrum of the Dirac fermions at half-filling, suppressing the density of states at low energy. One needs the long tail of the RKKY interaction to frustrate the charge density wave (the Semenoff sector) from the V_2 interaction in agreement with recent numerical results²⁷. In this sense, the situation close to the Van Hove filling for the fast particles seems slightly better: all the longer range interaction channels are of the same order in magnitude.

Quantum Spin Hall (QSH) Effect- Next, we also consider the case of spin-1/2 f-fermions with $\mu_c = 0.992t_c$ and include the Hubbard interaction

$$H_f = \sum_{\mathbf{p}, \sigma} [(a(\mathbf{p}) + ib(\mathbf{p}))f_{a\mathbf{p}\sigma}^\dagger f_{b\mathbf{p}\sigma} + (a(\mathbf{p}) - ib(\mathbf{p}))f_{b\mathbf{p}\sigma}^\dagger f_{a\mathbf{p}\sigma}]$$

$$+ \sum_{\mathbf{p}, I, \sigma} c_I(\mathbf{p})(f_{a\mathbf{p}\sigma}^\dagger f_{a\mathbf{p}\sigma'} - f_{b\mathbf{p}\sigma}^\dagger f_{b\mathbf{p}\sigma'})\sigma_{\sigma\sigma'}^I + H_I \quad (13)$$

$$H_I = U \sum_i f_{i\uparrow}^\dagger f_{i\uparrow} f_{i\downarrow}^\dagger f_{i\downarrow},$$

in which σ^I ($I = 0, x, y, z$) are the Pauli matrices acting in spin space and σ^0 is the identity matrix. The functions $a(\mathbf{p})$ and $b(\mathbf{p})$ are renormalized amplitudes which are insensitive to the spin degrees of freedom. Here, the (bare) Hubbard interaction U also includes a renormalization from the RKKY contribution. The topological phase here mediated by the spin degrees of freedom can also be a quantum spin Hall (QSH) phase of Kane-Mele type⁶. Then, we introduce two order parameters: $c_0(\mathbf{p})$ and $c_I(\mathbf{p})$ related to the QAH and QSH phases respectively. Again, we adjust to zero the renormalized chemical potential of the f-fermions. Physically, if $c_0(\mathbf{q}) \neq 0$ then we are in a QAH phase, whereas when $c_I(\mathbf{q}) \neq 0$ with $I = (x, y, z)$ then we are in a QSH phase. Through a careful analysis of the quantum fluctuations²³, one establishes that the QSH phase is always favoured compared to the QAH phase for spinful fermions, due to the presence of Goldstone modes appearing from the breaking of the continuous rotational symmetry in the QSH phase. Therefore, we only take into account the order parameter $c_I(\mathbf{p})$. We find similar equations as in Eq. 9 and found that for $U = 0$, the critical value $(g_{cf})_c = 7.88\sqrt{t_c t_f}$ as the spinless case. By applying the slave-rotor technique⁴⁰, we find that the Mott transition out of the QSH phase occurs at a relatively large U_c in analogy to the Kane-Mele Hubbard model¹⁸.

To summarize, we have introduced a fermion-fermion mixture in graphene-type lattices, with one fast component characterized by a large tunneling strength. We have shown that the interaction produced on the alternative species allows to implement in realistic conditions a Quantum Anomalous Hall phase or a Quantum Spin Hall phase when we adjust the chemical potential for the fast fermion c either close to $\mu_c = 0.6t_c$ or close to the Van Hove filling factor, where more competing channels allow to frustrate charge density wave orders. In particular, the long-range aspect of the RKKY interaction allows to frustrate charge density wave orders. It should be noted that the induced relatively weak nearest-neighbor interaction here is attractive and other charge density wave orders are frustrated by the difference of chemical potentials between the fast and slow fermions, which should ensure the stability of the topological phase beyond the Hartree-Fock argument. This gives the opportunity to observe topological Mott insulators in ultracold mixtures of ⁶Li and ⁴⁰K.

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