Interaction-induced merging of Dirac points in non-Abelian optical lattices

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We study the properties of an ultracold Fermi gas loaded in a square optical lattice and subjected to an external and classical non-Abelian gauge field. We calculate the energy spectrum of the system and show that the Dirac points in the energy spectrum will remain quite stable under on-site interaction of certain strength. Once the on-site interaction grows stronger than a critical value, the Dirac points will no longer be stable and merge into a single hybrid point. This merging implies a quantum phase transition from a semimetallic phase to a band insulator. The on-site interaction between ultracold fermions could be conveniently controlled by Feshbach resonances in current experiments. We propose that this interaction-induced merging of Dirac points may be observed in the ultracold-Fermi-gas experiments.

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I. INTRODUCTION

One of the most interesting properties of graphene [1], a single layer of carbon atoms packed in a honeycomb lattice, lies in the fact that the low-energy excitations obey a linear dispersion relation [2] around the so-called Dirac points and thus can be used as a test bed for relativistic quantum electrodynamics. Consequently, it is now possible to observe many remarkable phenomena in table-top experiments, such as Klein tunneling [3,4] and the relativistic extension of Landau levels [5–7], which usually only occur in high-energy physics [8]. This advantage of graphene has stimulated great interest in the investigation of Dirac points [8] in many other systems. In particular, ultracold atoms in optical lattices provide a versatile playground where the properties of condensed-matter systems can be simulated [9,10] in a highly controllable manner, such as the superfluid-Mott insulator transitions of Hubbard models [11–13]. A quantum-optical analog of graphene can be achieved by loading ultracold fermionic atoms such as ^{40}K or ^{6}Li [12,13] into a hexagonal optical lattice [14]. The effects of Dirac points were discussed in the context of ultracold atoms in honeycomb lattice [14] and T_3 (rhombic) lattices [15]. Moreover, much more intriguing phenomena arise when these systems are subjected to artificial non-Abelian gauge fields [16–18], such as the non-Abelian Aharonov-Bohm effect [17], non-Abelian atom optics [19], quasirelativistic effects [20], or exotic topological phase transitions [21].

Here we would like to emphasize a fact that the non-Abelian artificial gauge field also provides an interesting setup where Dirac points emerge in a square optical lattice [22], which is originally limited to staggered fields [23,24]. In this article, we consider a similar system in which two-component (two-color) ultracold fermionic atoms are trapped in a square optical lattice. And the dramatic difference between these two systems comes from the repulsive on-site interaction introduced into the model by us. References [21,22] mentioned above mainly dwelled on free Fermi gases on two-dimensional (2D) optical lattices. We study the effects of repulsive on-site interaction on the energy spectrum of the 2D Fermi gas loaded into a square optical lattice and subjected to a non-Abelian artificial gauge field. Implementing a self-consistent mean-field theory, we show that the Dirac points in the energy spectrum remain quite stable under repulsive on-site interaction of certain strength. When the on-site interaction grows stronger than a critical value, the Dirac points will no longer be stable and two Dirac points merge into a single point. This merging indicates a quantum phase transition between a semimetallic phase and a band insulator [14,25–31]. And one thing worthy to be mentioned here is that once the two Dirac points merge, the final dispersion relation becomes quite exotic—it is linear in one direction but parabolic in the other orthogonal direction. Very recently, a well-designed experiment has been carried out by Leticia *et al.* [32], in which the creating, moving, and merging of Dirac points has been realized with a Fermi gas loaded into a tunable honeycomb lattice. While the creating, moving and merging of Dirac points in the experiment [32] is generated by designing complex lattice geometries, the merging of the Dirac points in our model is induced by strong repulsive on-site interaction. Since pairwise interactions could be conveniently controlled by means of Feshbach resonances [33], we propose that the interesting merging of Dirac points in our model may be experimentally observed and characterized in non-Abelian optical lattices. The non-Abelian optical lattice could be prepared by generalizing the recent experiment [16], as proposed in Refs. [17,18].

II. MODEL AND HAMILTONIAN

We consider a two-component (two-color) Fermi gas trapped on a square optical lattice and subjected to an artificial non-Abelian gauge potential. Fermionic atoms in the system are interacting with a repulsive on-site interaction. It is well known that this pairwise interaction can be freely tuned by means of Feshbach resonances [33] in ultracold-atom experiments nowadays. The Hamiltonian of the system reads

$$H = -t \sum_{\langle \mathbf{r}\mathbf{r}' \rangle} \sum_{\tau,\tau'} \left(c^{\dagger}_{\mathbf{r}\tau} e^{-i \int_{\mathbf{r}'}^{\mathbf{r}} \mathbf{A}\cdot d\mathbf{l}} c_{\mathbf{r}'\tau'} + \text{H.c.} \right) + V \sum_{\mathbf{r}} n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow}, \quad (1)$$

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where t is the hopping amplitude, $c_{\mathbf{r},\tau}$ ($c^{\dagger}_{\mathbf{r},\tau}$) is the fermionic annihilation (creation) operator at site $\mathbf{r}$ of the square optical lattice, $\tau = \uparrow, \downarrow$ can be regarded as a pseudospin index, $\langle \mathbf{r}\mathbf{r}' \rangle$ denotes that the sum is over nearest neighbors and V is the strength of the on-site interaction between fermionic atoms. The coordinate of a fermion is given by $\mathbf{r} = (ma, na)$, where m,n are integers and a is the lattice constant of the square optical lattice. Here we set $\hbar = e = 1$. The external gauge potential has the following form, $\mathbf{A} = \frac{B_0}{2}(-y,x) + a(B_\alpha \sigma_y, B_\beta \sigma_x)$, in which B_0, B_α, B_β are experimentally controllable parameters and $\sigma_{x,y}$ are the Pauli matrices. This intriguing artificial gauge field can be realized following the proposals [17,18,34] along the lines of the recent experiment [16]. After some algebra, the original Hamiltonian (1) becomes

$$H = -t \sum_{\langle \mathbf{r}\mathbf{r}' \rangle} \sum_{\tau,\tau'} (c^{\dagger}_{\mathbf{r}\tau} [U_{\mathbf{r}\mathbf{r}'}]_{\tau\tau'} c_{\mathbf{r}'\tau'} + \text{H.c.}) + V \sum_{\mathbf{r}} n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow}, \tag{2}$$

where $U_{\mathbf{r}\mathbf{r}'}$ is the matrix form of a nontrivial unitary operator accompanying the hopping between lattice site $\mathbf{r}$ and its nearest neighbor $\mathbf{r}'$. If the hopping is along x axis, $U_{\mathbf{r}\mathbf{r}'} = U_x(m) = e^{-i\pi\Phi m} e^{i\Phi_\alpha \sigma_y}$. If the hopping is along the y axis, $U_{\mathbf{r}\mathbf{r}'} = U_y(n) = e^{-i\pi\Phi n} e^{i\Phi_\beta \sigma_x}$. $\Phi = B_0 a^2$ is the Abelian magnetic flux, and $\Phi_{\alpha,\beta} = B_{\alpha,\beta} a^2$ is the non-Abelian flux. Fermions hopping around an elementary plaquette undergo a unitary transformation [22] $U = U_x(m) U_y(n+1) U_x^{\dagger}(m+1) U_y^{\dagger}(n)$. The boundary between Abelian regime and non-Abelian regime is well defined by the gauge-invariant Wilson loop [22,34] $W = \text{tr}U$. Here we constrain ourselves to the non-Abelian regime, where the Wilson loop fulfills $|W| < 2$ and we set the Abelian flux $\Phi = 0$.

In the noninteracting limit of Hamiltonian (1), i.e., the case in which fermions hop freely between neighboring sites without any interaction, Hamiltonian of the system is of quadratic form and can be analytically solved by Bogoliubov transformations. The energy spectrum of this case has been beautifully analyzed in the literature [22], where the fermion gas becomes a collections of noninteracting quasiparticles. The spectrum of the system develops four independent Dirac points at $K_D \in \{(0,0), (\frac{\pi}{a},0), (0,\frac{\pi}{a}), (\frac{\pi}{a},\frac{\pi}{a})\} \in BZ$ in the neighborhood of the π-flux point (i.e., $\Phi_\alpha, \Phi_\beta = \pi/2$). However, once the on-site interaction is taken into account in Hamiltonian (1), it is not of quadratic form any more and therefore cannot be solved by a Bogoliubov transformation directly. This is the case we consider in this article. We study the repulsively interacting fermions on a square optical lattice subjected to a non-Abelian gauge field by means of self-consistent mean-field theory. Our starting point is Eq. (2).

III. MEAN-FIELD THEORY

We mainly consider the repulsive interaction regime in this paper. As the on-site interaction grows stronger and stronger, fermionic atoms with different colors on the square lattice tend to repel each other and avoid staying on the same lattice site. Once the interaction strength is over a critical point, the square optical lattice at half-filling will enter a phase in which each site of the lattice is occupied by a single atom [see Fig. 1(b)]. Therefore, we define $\Delta_{\mathbf{r}} = V \langle c^{\dagger}_{\mathbf{r}\uparrow} c_{\mathbf{r}\downarrow} \rangle$ as our order parameter.

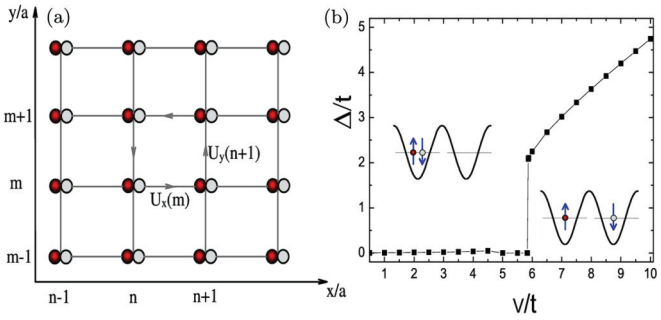

FIG. 1. (Color online) (a) Two-component (two-color) ultracold fermionic atoms trapped in a square optical lattice and subjected to a non-Abelian artificial gauge field. The circle filled with red (gray) color denotes internal atom state $|\uparrow\rangle$ ($|\downarrow\rangle$). $U_x(m)$ and $U_y(n+1)$ are unitary operators induced by the external artificial gauge field. (b) The self-consistent mean-field order parameter Δ vs on-site interaction V. The system size is 24×24 and we set the convergence criterion to 10^{-4}.

Under this mean-field approximation, the Hamiltonian (2) can be written in quadratic form,

$$H_{\text{MF}} = -t \sum_{\langle \mathbf{r}\mathbf{r}' \rangle} \sum_{\tau\tau'} (c^{\dagger}_{\mathbf{r}\tau} [U_{\mathbf{r}\mathbf{r}'}]_{\tau\tau'} c_{\mathbf{r}'\tau'} + \text{H.c.}) - \sum_{\mathbf{r}} (\Delta_{\mathbf{r}} c^{\dagger}_{\mathbf{r}\downarrow} c_{\mathbf{r}\uparrow} + \text{H.c.}) + \frac{VN}{2} + \frac{1}{V} \sum_{\mathbf{r}} |\Delta_{\mathbf{r}}|^2. \tag{3}$$

Through a canonical transformation, the above Hamiltonian can be diagonalized by solving the following Bogoliubov–de Gennes (BdG) equation [35]:

$$\sum_{\mathbf{r}'} \begin{pmatrix} h_{\mathbf{r}\mathbf{r}',\uparrow} & O_{\mathbf{r}\mathbf{r}'} \\ O^{*}_{\mathbf{r}\mathbf{r}'} & h_{\mathbf{r}\mathbf{r}',\downarrow} \end{pmatrix} \begin{pmatrix} u^n_{\mathbf{r}'} \\ v^n_{\mathbf{r}'} \end{pmatrix} = E_n \begin{pmatrix} u^n_{\mathbf{r}'} \\ v^n_{\mathbf{r}'} \end{pmatrix}, \tag{4}$$

where $h_{\mathbf{r}\mathbf{r}',\tau} = -t[U_{\mathbf{r}\mathbf{r}'}]_{\tau\tau}$, $O_{\mathbf{r}\mathbf{r}'} = -\Delta_{\mathbf{r}} \delta_{\mathbf{r}\mathbf{r}'} - t[U_{\mathbf{r}\mathbf{r}'}]_{\uparrow\downarrow}$, and $(u^n_{\mathbf{r}}, v^n_{\mathbf{r}})$ is the eigenvector corresponding to the eigenenergy E_n. The self-consistent equation of the order parameter is

$$\Delta_{\mathbf{r}} = V \sum_{n} u^n_{\mathbf{r}} v^{n*}_{\mathbf{r}} \tanh\left(\frac{E_n}{2k_B T}\right). \tag{5}$$

We solve the set of BdG equations self-consistently via the exact diagonalization method in real space. The system size of 24×24 is used in the calculation and the convergence criterion of $\Delta_{\mathbf{r}}$ is set to be 10^{-4} in units of the nearest-neighbor hopping t. We find that the order parameter is uniform ($\Delta_{\mathbf{r}} = \Delta$, where Δ is real) in the vicinity of the π-flux regime. Our calculations [see Fig. 1(b)] show that as the on-site interaction V increases from zero, the order parameter turn out to be nonzero at $V_c \approx 5.88t$ and the system undergoes a quantum phase transition from a semimetallic phase to a band insulator.

IV. INTERACTION-INDUCED MERGING OF DIRAC POINTS

By the above-mentioned self-consistent mean-field theory, we transform the original Hamiltonian into the quadratic form (3). Implementing appropriate Fourier transformations, Eq. (3) can be easily diagonalized in momentum space. The corresponding energy spectra are shown in Fig. 2. As the mean-field order parameter Δ grows stronger, the two

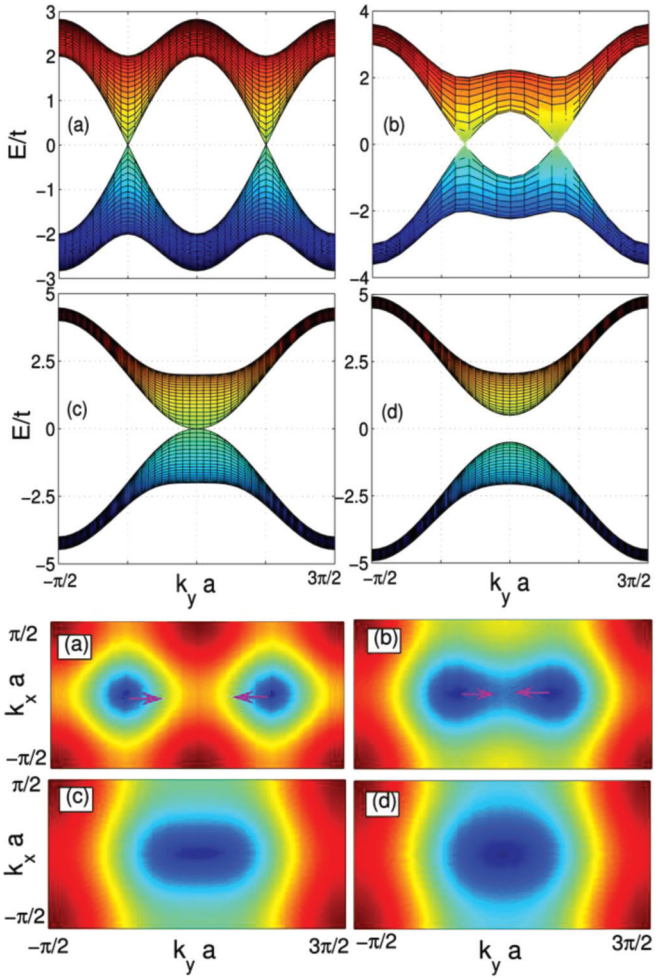

FIG. 2. (Color online) Merging of Dirac points in band structure of system as Δ grows stronger ($\Phi_\alpha = \Phi_\beta = \pi/2$). Top: portrait of the energy spectrum in k_x direction. Bottom: evolution of the two Dirac points. (a) $\Delta = 0$. There are two normal Dirac points. (b) $\Delta = 1.0$. The two Dirac points moves closer. (c) $\Delta = 2.0$. Two Dirac points merge into a single hybrid point, which signals the quantum phase transition. (d) $\Delta = 2.5$. A gap is opened.

originally separate Dirac points [Fig. 2(a)] will first move closer [Fig. 2(b)], then merge into a single hybrid point at $k_h = (\frac{\pi}{2a},0)$. Around this hybrid point $p = k - k_h$, the low-energy properties of the system are accurately described by a Dirac Hamiltonian

$$H_{\text{eff}} = \sum_p \Psi_p^\dagger H_D \Psi_p, \quad H_D = c_x \sigma_y p_x - c_y \sigma_x p_y^2, \tag{6}$$

where $\Psi_p = (c_{p\uparrow}, c_{p\downarrow})^T$ is the relativistic spinor, σ_x and σ_y are Pauli matrices and $c_x = 2at \sin\Phi_\alpha$, $c_y = at \sin\Phi_\beta$ represent the effective speed of light. From this Hamiltonian we can see that the energy spectrum is linear in the k_x direction but quadratic in the k_y direction [Fig. 2(c)]. The merging of the two Dirac points signals a quantum phase transition from the semimetallic phase to a band insulator [31,32]. If the order parameter Δ grows even stronger, a gap will be opened [Fig. 2(d)], which indicates a band-insulator phase. The self-consistent mean-field theory calculations show that the order parameter Δ remains zero as long as the on-site

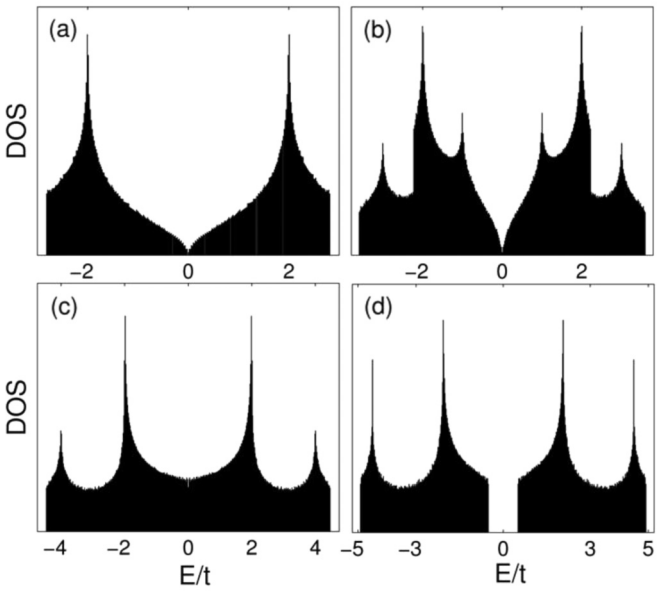

FIG. 3. Density of states (DOS) of system vs order parameter Δ. (a) $\Delta = 0$, (b) $\Delta = 1.0$, (c) $\Delta = 2.0$, (d) $\Delta = 2.5$.

interaction is smaller than $V_c = 5.88t$. Once the strength of the on-site interaction is over V_c, Δ will turn out to be a nonzero number which is not smaller than $\Delta_c = 2$. This can be easily seen in Fig. 1(b). Therefore, the spectrum shown in Fig. 2(b) will not be observed in reality. We give out this spectrum in Fig. 2 just for comparison.

To characterize the merging of Dirac points more clearly, we calculate the density of states (DOS) and cyclotron mass m_c for different strengths of on-site interaction (i.e., different values of Δ, correspondingly). The results are shown in Figs. 3 and 4. For the density of states in Fig. 3, we find that dramatic difference appeared at the occasion when two Dirac points merge into a hybrid one. While the DOS displays two peaks for the case of $\Delta = 0$ [Fig. 3(a)], there are four peaks in the case

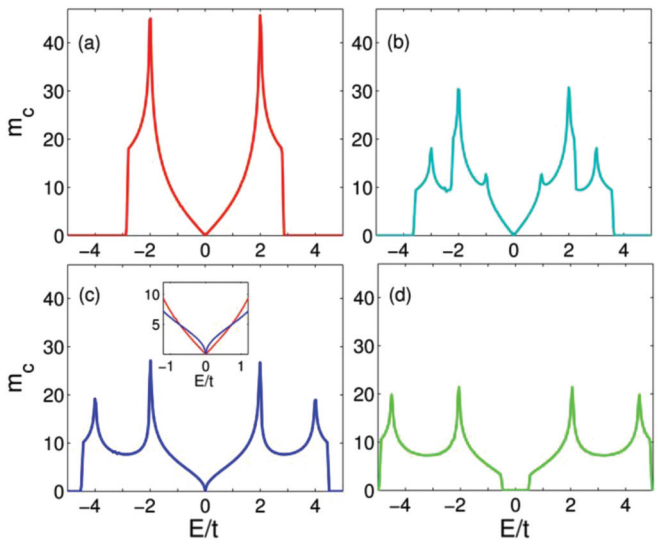

FIG. 4. (Color online) Cyclotron mass m_c vs Δ. (a) $\Delta = 0$, (b) $\Delta = 1.0$, (c) $\Delta = 2.0$, (d) $\Delta = 2.5$. Inset: comparison between (a) and (c) around the zero-energy point.

of $\Delta = 2$ [Fig. 3(c)]. Moreover, for $\Delta = 2$ [Fig. 3(c)], DOS turns out to be nonzero at $E = 0$. These differences would serve as an indication of the merging of the Dirac points. In Fig. 4, we give out the cyclotron mass m_c for different values of Δ and, correspondingly, for different strengths of on-site interaction. Comparing Figs. 4(a) and 4(c), we find that besides the difference in the numbers of peaks, the curve of m_c changes from concave to convex around the zero-energy point as shown in the inset of Fig. 4(c). This change signals a quantum phase transition between the semimetallic phase and band-insulator phase.

From Fig. 1(b), we can find that the mean-field order parameter can be tuned by increasing the strength of the on-site interaction. Therefore, this exotic merging of the Dirac points induced by the on-site interaction may be observed in ultracold-Fermi-gas experiments. This is quite different from the works of Refs. [31,32], where they engineer Dirac points by tuning the nearest-neighbor tunneling [31] or by tuning the geometry of the optical lattices [32]. For the concrete realization of the experiment, one may use ^{40}K atoms in $F = 9/2$ or $F = 7/2$ hyperfine manifolds or ^{6}Li with $F = 1/2$.

V. SUMMARY

The Dirac point plays a crucial role in many interesting phenomena in condensed-matter physics; for example, the massless electrons in graphene. In this article, we investigate a two-component(color) ultracold Fermi gas which is loaded in a square optical lattice. The addition of non-Abelian artificial gauge field gives rise to Dirac points in the energy spectrum of the system. We study the stability of Dirac points against the repulsive on-site interaction. Our calculations show that the Dirac points can be very stable under on-site interactions smaller than $V_c = 5.88t$. At V_c, the Dirac points turn out to be nonstable and merge into a hybrid point. The final hybrid point is linear in one direction but quadratic in the perpendicular direction. This merging of the Dirac points denotes a quantum phase transition from semimetallic phase to a band insulator. This exotic phenomena may be observed in ultracold-Fermi-gas experiments nowadays.

Note added in proof. Recently, we noticed another work [36] considering the interaction effects in Hofstadter problem.

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