Nematic Ferromagnetism on the Lieb lattice

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We discuss the properties of possible ferromagnetic orders on the Lieb lattice. We show that the presence of a quadratic-flat band crossing point (QFBCP) at half filling will dramatically affect the magnetic ordering. In the presence of a weak on-site repulsive interaction, we find the ground state is a nematic ferromagnetic order with simultaneously broken of time-reversal and rotational symmetries. When the interaction strength increases, the rotational symmetry will restore at some critical value, and the system enters a conventional ferromagnetic regime. We also point out that the spin gap in both the nematic and conventional ferromagnetic phases is of the order of interaction. This observation suggests that these magnetic orders can be realized and detected in cold atomic systems with present technology.

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The investigation on ferromagnetism is one of the central topics in condensed matter physics, and has attracted attention for nearly a century since the early age of quantum theory. Heisenberg showed that a system of localized spins would favor a fully polarized state by gaining exchange energy. [1] However, the same argument can not be simply applied in itinerant fermions, where the kinetic energy of the underlying system has to be considered on an equal footing with the interaction effect.

The discussion on the stability of itinerant ferromagnetism in a lattice system dates back to 1960’s. Thouless [2] and Nagaoka [3] pointed out that a ferromagnetic ground state can be stabilized in any finite bipartite lattice with infinite on-site repulsive interaction. Lieb showed that the stable region of ferromagnetism can be extended to arbitrary repulsive interaction, provided that the number of sites are different for the composite sublattices. [4] The key ingredient in Lieb’s argument is the existence of a non-dispersive, or briefly flat, band. When the flat band is partially filled, fermions tend to be spin polarized to minimize the interaction energy, without any cost in the kinetic energy. In other words, since states in the flat band consists of localized Wannier functions, the ferromagnetic states can benefit from the exchange interaction as pointed out by Heisenberg. Subsequent studies confirm the stability of ferromagnetism in various models [2, 6], and generalize the idea to nearly-flat-band cases [7]. Experimental realization of the (nearly-) flat-band ferromagnetism has been proposed in a class of physical systems including atomic quantum wires [8], quantum-dot super-lattices [9], and organic polymers [10].

Rapid progress in cold atom experiments has paved a new route toward the exploration of ferromagnetism in itinerant fermions. Thank for the extraordinary controllability of lattice potentials and interaction, several proposals has been made to realize (nearly) flat-band ferromagnetism [11] [12]. In particular, Noda et al. investigated two-component cold fermions loaded into a two-dimensional (2D) generalized Lieb lattice, and suggested that a ferromagnetic order can be stabilized in a wide parameter region. [12] The 2D generalized Lieb lattice consists of two square lattices (sublattice A and B), and has three sites per unit cell, as shown in Fig. 1. With only nearest-neighbor hopping, the lattice topology supports a flat band in the middle of two dispersive bands, hence can stabilize ferromagnetism when it is partially filled.

Apparently, a sole flat band does not exist in any realistic physical system. In all proposed model lattices for...
flat-band ferromagnetism, the flat band is always associated with dispersive bands, and the effect of their accompany is not fully understood. As a typical example, if the two composite sublattices of the Lieb lattice have the same depth, the flat band degenerates with the two linearly dispersive bands at the $\mathbf{M} = (\pi, \pi)$ point. On the other hand, in general cases where the depth of sublattice $A$ is different from that of sublattice $B$, the flat band can touch only one of the two dispersive bands at the $\mathbf{M}$-point, as illustrated in Fig. 1(d), leading to a quadratic-flat band crossing point (QFBCP).

In this manuscript, we show that the ferromagnetic order is dramatically affected by the existence of the QFBCP. In the non-interacting level, the QFBCP is protected by the time reversal (TR) and $C_4$ rotational symmetries. When a repulsive on-site interaction is present, since the 2D density of state (DOS) is singular, the QFBCP becomes marginally unstable, leading to a spontaneous broken of the TR and/or $C_4$ rotational symmetries. We find that in the weak coupling limit the ground state of the system is a nematic ferromagnetic (NFM) order, characterized by a broken of $C_4$ point group down to $C_2$. The $C_4$ rotational symmetry will restore with increasing interaction, via a second or first order phase transition, depending on the value of $V_b$. Within a mean-field calculation, we further map out the phase diagram at half filling and identify three phases including: (i) a semimetal phase with conventional FM order, (ii) a band insulator with conventional FM order, and (iii) a band insulator with conventional FM order. These magnetic orders have the potential to be realized and detected in cold fermions loaded in optical lattices with present technology.

We consider spin $1/2$ fermions loaded in the 2D Lieb lattice

$$H = -t \sum_{\langle i,j \rangle, \alpha} c_{i\alpha}^\dagger c_{j\alpha} + V_b \sum_i n_i + U \sum_i n_i^\uparrow n_i^\downarrow,$$

(1)

where $t$ is the hopping matrix, $c_{i\alpha}^\dagger (c_{i\alpha})$ is the creation (annihilation) fermionic operator, $V_b$ is the chemical potential offset for the sublattice $B$ (i.e., the relative shift of the two sublattices), and $U$ is the on-site interaction. In the context of cold atoms, $V_b$ can be easily controlled by varying the relative intensity of optical lattices, and a repulsive interaction $U > 0$ can be achieved and tuned via an adiabatic ramping to the upper branch on the BEC side of a Feshbach resonance.

In the non-interacting case, the Hamiltonian can be diagonalized in momentum space, leading to a band structure consisting of three bands as shown in Fig. 1(d). One of the three bands is completely flat, as required by the bipartiteness of the Lieb lattice. The flat band has Bloch wavefunction $\propto [0, -\cos(k_x), \cos(k_y)]$ on the three sites within a unit cell, indicating the presence of local Wannier functions residing on the sublattice $B$ and having opposite amplitudes between sites 2 and 3. When the chemical potential offset $V_b = 0$, the three bands are degenerate at the $\mathbf{M} = (\pi, \pi)$ point, where the two linearly dispersive bands intersect with the flat band. In general cases of $V_b \neq 0$, depending on the sign of $V_b$, one of the two massive bands breaks the $\mathbf{M}$-point degeneracy, and the flat band only touches the other dispersive band as illustrated in Fig. 1(d). As a consequence, the $\mathbf{M}$-point becomes a quadratic-flat band crossing point (QFBCP). Around this point, the effective two-band Hamiltonian reads

$$H_0^{\text{eff}} = \frac{2t^2}{V_b} \left[ |\delta k_x|^2 \left( \frac{\delta k_x^2}{|\delta k|^2} \right) + O(\delta k^4), \right]$$

(2)

where $\delta \mathbf{k} = \mathbf{k} - \mathbf{M}$ and $\delta \mathbf{k}_\perp = \delta k_x \pm i\delta k_y$. From this effective Hamiltonian, it is clear that the cases of positive and negative chemical potential offset $V_b$ are equivalent via a particle-hole transformation. Thus, we focus on systems with $V_b > 0$ without loss of generality in the following discussion.

The presence of a QFBCP at the $\mathbf{M}$-point is the central feature of the Lieb lattice. This band crossing point (BCP) is protected by the time reversal (TR) and $C_4$ rotational symmetries in the non-interacting case, and is characterized with a nontrivial topological index $2\pi$. Such a putative topologically stable BCP becomes marginally unstable against infinitesimal repulsive interaction $U > 0$, leading to a spontaneous broken of TR and/or $C_4$ rotational symmetries, which drives the system toward a magnetic and/or nematic phase. Besides, since the BCP consists of a non-dispersive band, the infinite density of state (DOS) allows the possibility of filling the high momentum states with one single spin species without gaining any kinetic energy. As a consequence, if the on-site interaction $U$ is repulsive, the system could easily favor a ferromagnetic phase for filling factors between $1/3$ and $2/3$.

Next, we focus on the case of repulsive Hubbard $U > 0$ with half filling, and investigate the magnetic and nematic magnetic order within a mean-field (MF) level. The magnetic order is characterized by on-site magnetization $\mathbf{B}_1$ and $\mathbf{B}_2$ for sublattices $A$ and $B$, respectively. By minimizing the MF energy functional, we find that the system is stabilized by a staggered ferromagnetic order with $\mathbf{B}_1$ and $\mathbf{B}_2$ both oriented along the out-of-plane $z$-axis. In the weakly interacting limit $U \ll t$, the magnetization on sublattice $A$ is quadratically dependent on $U$ with $B_{1z} \approx \alpha_2 U^2/9t$, where $\alpha_2 = (2/\pi^2) \int d^2k [\cos^2(k_x) + \cos^2(k_y)]/[V_b^2/t^2 + 4 \cos^2(k_x) + 4 \cos^2(k_y)]^{3/2}$, and the magnetization on sublattice $B$ is linearly dependent on the interaction with $B_{2z} \approx -U/6$. In the strongly coupling limit $U \gg t$, the interaction turns to be the only relevant energy scale, and both $B_{1z}$ and $B_{2z}$ are linearly dependent on $U$ with $B_{1z,2z} = \pm U/3$, respectively. Here, we set $B_3$ to be along the positive $z$-axis without loss of generality.

To study the possibility of nematic magnetic order with both TR and $C_4$ rotational symmetries broken, we allow the magnetization on sublattice $B$ to be different for sites 2 and 3, and map out the zero-temperature phase diagram as shown in Fig. 2(a). We find that the optimized magnetization $B_i = \pm 1, 2, 3$ are always along the $z$-
FIG. 2: (a) Zero temperature phase diagram for spin 1/2 Fermi system on the Lieb lattice at half filling. The nematic ferromagnetic (NFM) order is favored for weak interaction, and is separated from the ferromagnetic (FM) order by a second order (thin solid) or first order (thick solid) transition line. Within the NFM regime, the system is a semi-metal (SM) for small $U$ and $V_b$, and undergoes a second order (thin dashed) or first order (thick solid) transition to become a band insulator (BI) with increasing $U$ and $V_b$. An example of the band structure for different phases (red dots) are shown in Fig. 3 (a-c). For two typical values of $V_b/t = 1.5$ and 2.3 (dotted lines), the magnetization on the three sites are shown in (b) and (c), respectively.

axis, hence we consider only axial magnetic order in the following discussion.

In the weakly interacting limit, the nematic FM phase is always favorable with an exponentially small magnetization difference $|\delta| \equiv |B_{2z} - B_{3z}| \sim \exp(-\gamma t/U)$, where $\gamma$ is a positive parameter depending on $V_b$. This observation is also confirmed by a perturbative analysis by treating the magnetization difference as a perturbation to the existing FM order. When $U$ is increasing from the weakly interacting limit, the NFM phase remains stable up to a critical value $U_c$, above which the $C_4$ rotational symmetry restores and the system enters the conventional FM regime. For small values of $V_b < V_c \sim 1.7$, the phase transition between NFM and FM is of the second order, as identified by the condition $V_b = B_{1z} - B_{2z}$. By increasing $V_b > V_c$, the NFM-FM phase boundary becomes of the first order, resulting from the competition between the corresponding metastable states.

Within the NFM phase, the $C_4$ rotational symmetry is spontaneously broken down to $C_2$ by splitting the QFBCP into two Dirac points located along the direction of one of the principal axes for weak interactions. The two Dirac points have the same Berry flux $\pi$, in clear contrast to the case of graphene where the two Dirac points have Berry fluxes $\pi$ and $-\pi$. In this case, the system is an anisotropic semimetal (SM) at half filling, with the Fermi surface shrinks to the two Dirac points as shown in Fig. 3(a). By increasing $U$, the two Dirac points move toward the boundary of the Brillouin zone, and eventually disappear when the magnetization difference $\delta = |B_{2z} - B_{3z}|$ between sites 2 and 3 exceeds the bandwidth of the first excited dispersive band. As a result, a full gap is open and the system becomes an anisotropic band insulator (BI) as depicted in Fig. 3(b). When the system enters the FM regime, the magnetization is large enough such that a finite gap is always present, and the system is a band insulator as shown in Fig. 3(c).

Note that in both the NFM and FM phases, the spin gap remains in the order of the interaction strength $U$ [See Fig. 3(d)]. This observation suggests that the magnetic order on the Lieb lattice is robust against thermal fluctuations. Although the Mermin-Wigner theorem excludes the possibility of any 2D ferromagnetic order at finite temperature in the thermodynamic limit, the existence of such an order in a finite size system is perfectly allowed, provided that the coherence length
is comparable or exceeding the system size. Specifically, the coherence length of the magnetic order is \( \xi \sim \hbar c \exp(\rho_s/T)/(k_B T) \), where \( c \) is the spin-wave velocity at zero temperature, and the phase stiffness \( \rho_s \) is in the same order of the MF transition temperature \( T_{MF} \). Since the spin gap \( \Delta_s \) increases linearly with \( U \), and the interaction can be tuned to be fairly large via an \( s \)-wave Feshbach resonance, the temperature required to observe the FM and NFM phases could be reachable within present technique. [17]

The detection of the ferromagnetic orders can be implemented via an in-situ measurement [18, 19], which is able to extract single site density distribution for different spin species, and hence the local magnetization \( B_q \propto n_{i\uparrow} - n_{i\downarrow} \). If the system is prepared with equally populated two-component Fermi gas, we expect to see FM or NFM domains with opposite magnetizations, which are both resolvable within present experimental technology. Another possible detection scheme is to measure the single-particle dispersion with Bragg spectroscopy [20] or angle-resolved photoemission spectroscopy (ARPES) [21] to extract the spin gap.

In conclusion, we discuss the effect of a quadratic-fat band crossing point (QFBCP) on the ferromagnetic (FM) order. Taking the 2D Lieb lattice as an example, we show that the QFBCP is marginally unstable against infinitesimal repulsive interaction, given an infinite density of state of the flat band. In the weak interacting limit, the ground state is a nematic ferromagnetic (NFM) order with time-reversal and rotational symmetries broken. Within the NFM regime, the spontaneous generated magnetizations are different on sublattice B, and the QFBCP is broken into two Dirac points along one of the principal axes. In the strong coupling limit, the interaction \( U \) becomes the only relevant energy scale, and a conventional ferromagnetic (FM) phase with rotational symmetry restored is favored. We then map out the zero-temperature phase diagram within a mean-field analysis, and identify three regions including a semimetal with NFM order, a band insulator with NFM order, and a band insulator with FM order. We point out that the spin gap for all three phases is in the same order of interaction strength, which can be tuned via a Feshbach resonance. Thus, we expect these magnetic phases can be realized in two-component Fermi gases loaded in optical lattices at experimentally reachable temperatures, and can be distinguished via a species selective in-situ measurement.

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[1] W. Heisenberg, Z. Phys. 49, 619 (1928).
[2] D. J. Thouless, Proc. Phys. Soc. London 86, 893 (1965).
[3] Y. Nagaoka, Phys. Rev. 147, 392 (1966).
[4] E. H. Lieb, Phys. Rev. Lett. 62, 1201 (1989).
[5] A. Mielke, J. Phys. A 24, L73 (1991); 24, 3311 (1991); 25, 4335 (1992).
[6] H. Tasaki, Phys. Rev. Lett. 69, 1608 (1992); 75, 4678 (1995); A. Tanaka and H. Tasaki, ibid 98, 116402 (2007).
[7] H. Tasaki, J. Stat. Phys. 84, 535 (1996).
[8] R. Arita et al., Phys. Rev. B 57, R6854 (1998).
[9] H. Tamura, K. Shiraishi, T. Kimura, and H. Tasaki, Phys. Rev. B 65, 085324 (2002).
[10] Y. Suwa, R. Arita, K. Kuroki, and H. Aoki, Phys. Rev. B 68, 174419 (2003).
[11] L. Wang et al., Phys. Rev. A 78, 023603 (2008).
[12] K. Noda, A. Koga, N. Kawakami, and T. Pruschke, Phys. Rev. A 80, 063622 (2009).
[13] S. Zhang, H.-H. Hung, C. Wu, Phys. Rev. A 82, 053618 (2010).
[14] N. Goldman, D. F. Urban, and D. Bercioux, Phys. Rev. A 83, 063601 (2011).
[15] G.-B. Jo et al., Science 325, 1521 (2009).
[16] K. Sun, H. Yao, E. Fradkin, and S. A. Kivelson, Phys. Rev. Lett. 103, 046811 (2009).
[17] The on-site interaction depends on the lattice shape and depth. Thus, in the general case of \( V_b \neq 0 \), the interaction \( U_A \) on sublattice A is different from \( U_B \) on sublattice B. This site-dependent interaction will not change the phase diagram in a qualitative level, and the magnetic and nematic magnetic orders are still present. A detailed discussion in connection with realistic experimental setup will be found in a later publication.
[18] N. Gemelke, X. Zhang, C.-L. Hung, and C. Chin, Nature 460, 995 (2009).
[19] W. S. Bakr et al., Science 329, 547 (2010).
[20] P.T. Ernst et al., Nat. Phys. 6, 56 (2010).
[21] J. T. Stewart, J. P. Gaebler, and D. S. Jin, Nature 454, 744 (2008).