Interaction and spin–orbit effects on a kagome lattice at 1/3 filling*

Liu Hai-Di(刘海迪)†, Chen Yao-Hua(陈耀桦), Lin Heng-Fu(林恒福),
Tao Hong-Shuai(陶红帅), and Wu Jian-Hua(武建华)

Institute of Physics, Chinese Academy of Sciences, Beijing 100190, *China*

(Received 20 January 2014; revised manuscript received 19 February 2014; published online 15 May 2014)

We investigate the competing effects of spin–orbit coupling and electron–electron interaction on a kagome lattice at 1/3 filling. We apply the cellular dynamical mean-field theory and its real-space extension combined with the continuous time quantum Monte Carlo method, and obtain a phase diagram including the effects of the interaction and the spin–orbit coupling at $T = 0.1t$, where T is the temperature and t is the hopping energy. We find that without the spin–orbit coupling, the system is in a semi-metal phase stable against the electron–electron interaction. The presence of the spin–orbit coupling can induce a topological non-trivial gap and drive the system to a topological insulator, and as the interaction increases, a larger spin–orbit coupling is required to reach the topological insulating phase.

Keywords: kagome lattice, spin–orbit coupling, Hubbard interaction

PACS: 71.10.–w, 05.30.Rt, 71.10.Fd **DOI:** 10.1088/1674-1056/23/7/077101

1. Introduction

Topological insulators (TIs), which exhibit gapless edge states while the bulk remains gapped and are characterized by a Z_2 topological invariant, have attracted great attention in recent years.[1–8] The TI can be well understood in a single-particle picture and the time-reversal symmetry is essential in defining the Z_2 topological invariant. In the presence of the time-reversal symmetry, back scattering of the edge states is forbidden and the TI is topologically protected against weak perturbations like non-magnetic disorders or weak interactions.[9,10] When interactions are stronger and cannot be treated as perturbations, the interplay between the TI and many-body interactions becomes unclear and needs to be further examined.[11–18]

We carry out an investigation on this topic by considering interacting electrons on a kagome lattice. The kagome lattice is a triangular lattice with three sites per unit cell as illustrated in Fig. 1(a). It is a prototype of a geometrically frustrated electron system, which is suggested to be a candidate to host the quantum spin liquid phase[19–22] and is thus actively studied in the field of strongly correlated electron systems.[23–25] The density of states (DOS) of the tight-binding model with nearest neighborhood hoppings on a 1/3 filling kagome lattice is shown in Fig. 1(d) and the corresponding band structure is illustrated in Fig. 1(c). It can be seen that there are two inequivalent Dirac points locating at the corners of the first Brillouin zone (BZ) and the system is a Dirac semi-metal, an analogue to the half-filling honeycomb lattice. Similar to the Kane–Mele model[26] on honeycomb lattices, the spin–orbit coupling (SOC) can open a non-trivial gap at the Dirac points and drive the system to a TI phase.[27,28] Based on this proposal, we further consider the Hubbard interactions to study the interplay of the spin–orbit coupling and the electron–electron interaction on the kagome lattice. Besides, the interactions can also induce a TI phase as a result of the spontaneous symmetry breaking in certain systems,[29–31] which is different from the case we consider in this paper.

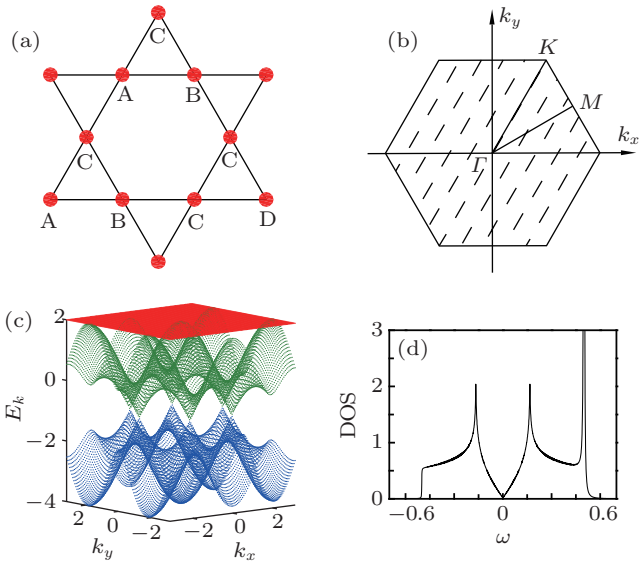


Fig. 1. (color online) (a) Sketch of the kagome lattice. Each unit cell of the kagome lattice has three sites labelled A, B, and C. (b) The first Brillouin zone of the kagome lattice, here K, M, and Γ denote points with different symmetries. (c) The tight-binding band structure of the kagome lattice at 1/3 filling. (d) DOS of the kagome lattice at 1/3 filling with $U = 0$.

We do a numerical analysis of the interplay between SOC and electron–electron interactions on the 1/3 filling kagome

*Project supported by the National Basic Research Program of China (Grant Nos. 2011CB921502 and 2012CB821305) and the National Natural Science Foundation of China (Grant Nos. 61227902, 61378017, and 11311120053).

†Corresponding author. E-mail: hdliu@iphy.ac.cn

© 2014 Chinese Physical Society and IOP Publishing Ltd

lattice by applying the cluster dynamical menn-field theory (CDMFT)[32] and its real-space extension[33,34] combined with the continuous-time quantum Monte Carlo (CTQMC) simulation.[35]

2. Model

The model we are considering on the kagome lattice can be described by the following Hamiltonian:

$$H = -t\sum_{\langle ij\rangle\sigma} c^{+}_{i\sigma}c_{j\sigma} + \mathrm{i}\lambda_{\mathrm{so}}\sum_{\langle ij\rangle\alpha\beta} \nu_{ij}c^{+}_{i\alpha}\sigma^{z}_{\alpha\beta}c_{i\beta} + U\sum_{i} n_{i\uparrow}n_{i\downarrow}, \quad (1)$$

where $c^{+}_{i\sigma}$ ($c_{i\sigma}$) is the creation (annihilation) operator of an electron with spin σ on lattice site i, the sum of $\langle ij\rangle$ runs over all the nearest neighbors, and $n_{i\sigma} = c^{+}_{i\sigma}c_{i\sigma}$ is the electron number operator. The first term in Eq. (1) is the kinetic energy representing the nearest neighborhood hopping with hopping energy $-t$. The second term is the SOC, where λ_{so} is the SOC strength, $\nu_{ij} = 1$ or -1 depending on the hopping direction as shown in Fig. 2(a) (a clockwise (anti-clockwise) hopping gives a minus (plus) sign),[26,28] and σ^{z} is the third Pauli matrix. It is clear that the SOC term does not mix the two spin species and the mirror symmetry is reserved. The third term is the on-site Hubbard interaction. For the non-interacting case where $U = 0$, the energy spectrum can be obtained via directly diagonalizing the Hamiltonian. We perform a calculation for a system with a strip geometry, which is infinite in the x direction and has 16 unit cells (i.e., 16×3 sites) in the y direction. The result for $\lambda_{\mathrm{so}} = 0.1t$ is shown in Fig. 2(b), where we can see the edge states connecting the bulk bands. At 1/3 filling, there are helical edge states propagating at opposite directions for different spin species on different edges, which is a characteristic feature of the TI states.

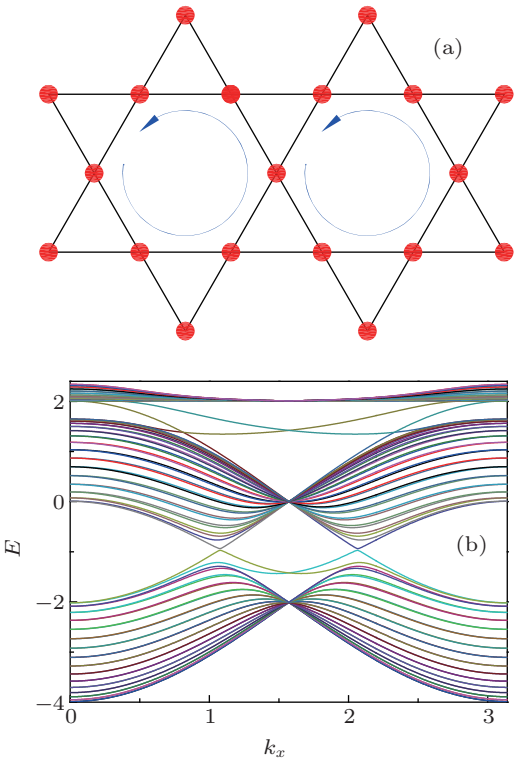


Fig. 2. (color online) (a) Schematic diagram of the nearest-neighbor SOC in a 2D kagome lattice strip. The blue arrows mark the direction for $\nu_{ij} = 1$, and the hoppings along the opposite direction corresponds to $\nu_{ij} = -1$. (b) Band structure of the kagome lattice strip with $\lambda_{\mathrm{so}} = 0.1t$ and $U = 0$.

3. Method: CDMFT and its real-space extension

We apply the cluster dynamical mean-field theory and its real-space extension combined with the continuous-time quantum Monte Carlo simulation to treat the correlated electrons in this strongly correlated system at 1/3 filling.

The essential idea of the dynamical mean-field theory (DMFT) is to map the lattice model onto a single-site quantum impurity model.[36] The CDMFT is a cluster extension of the DMFT and can treat short-range spatial correlations by mapping the lattice model onto a self-consistent embedded cluster,[33,34,36] which is successfully used to study strongly correlated systems.[37–39] Practically, we map the kagome lattice onto an N_{c}-site effective cluster model, and the system becomes a superlattice of clusters. The bulk property of the 1/3 filling kagome lattice can be obtained by the standard CDMFT procedure.[32,36]

For the purpose of investigating the edge states, we need to consider a strip of kagome lattice. We apply the periodic boundary condition in the x direction and the open boundary condition in the y direction. Since the translation symmetry in the y direction is broken, it is required to employ the real-space extension of the CDMFT,[14,33,34] the infinite superlattice in the CDMFT becomes a superlattice ribbon as illustrated in Fig. 3. The coarse-grained Dyson equation in the real-space CDMFT can be written as

$$g^{-1}_{\mathrm{c}}(\mathrm{i}\omega) = \left[\sum_{\tilde{k}_x}\frac{1}{\mathrm{i}\omega+\mu-t(\tilde{k}_x)-\Sigma(\mathrm{i}\omega)}\delta_{I,J}\right]^{-1} + \Sigma(\mathrm{i}\omega), \quad (2)$$

where $t(\tilde{k}_x)$ is the hopping matrix for the supperlattice ribbon, the summation of $\tilde{k}_x$ is taken over the reduced first Brillouin zone, $g_{\mathrm{c}}(\mathrm{i}\omega)$ and $\Sigma(\mathrm{i}\omega)$ are the block diagonal matrices with block size N_{c} (we chose $N_c = 3$), I, J are the block indices, and μ is the chemical potential. The $t(\tilde{k}_x)$ can be calculated using the inter-cluster Fourier transform, which is defined as

$$c_m(X,n) = \frac{1}{\sqrt{N_x}}\sum_{\tilde{k}_x} \mathrm{e}^{-\mathrm{i}\tilde{k}_x n}c_m(X,\tilde{k}_x),$$

$$\frac{1}{N_x}\sum_{n} \mathrm{e}^{-\mathrm{i}(\tilde{k}_x-\tilde{k}'_x)n} = \delta_{\tilde{k}_x,\tilde{k}'_x}.$$

Here $c_m(X,n)$ is the annihilation operator, where $X =$ A, B, or C represents one of the three sites within a cluster, and (n,m)

is the coordinate of a cluster with unit vectors $(1,\sqrt{3})a$ and $(2,0)a$, with a being the distance between the nearest sites as illustrated in Fig. 3.

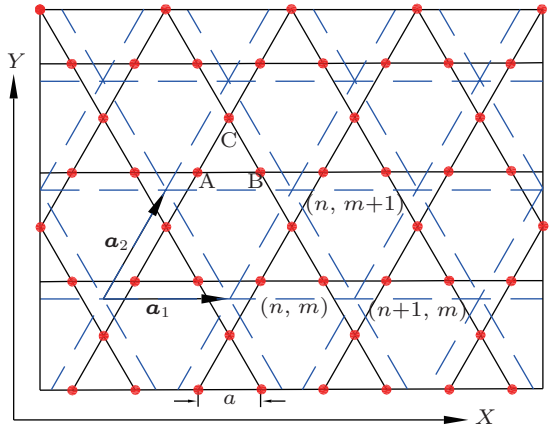


Fig. 3. (color online) Sketch of a kagome strip, where (n,m) is the label of the cluster, n corresponds to the infinite x direction, and m corresponds to the limited y direction. The entire lattice is tiled with identical clusters of size $N_c = 3$, A, B, and C represent three sites within a cluster, and its unit vectors are $\boldsymbol{a}_1 = (1,\sqrt{3})a$ and $\boldsymbol{a}_2 = (2,0)a$, where a is the distance between the nearest sites.

The self-energy is approximated to be within each cluster, which is used to calculate the Green's function and then various physical properties of the system. The main focus of our numerical analysis is to obtain the self-energy, which can be realized iteratively. With an initial input of self-energy $\Sigma(\mathrm{i}\omega)$, we can obtain the effective Weiss field $g_c(\mathrm{i}\omega)$ for a cluster via the coarse-grained Dyson's equation in Eq. (2). Then the impurity model including the cluster and the Weiss field is solved using the CTQMC to obtain the cluster Green's function G_c. Once G_c is determined, we can renew the self-energy by Dyson's equation $\Sigma(\mathrm{i}\omega) = g_c^{-1}(\mathrm{i}\omega) - G_c^{-1}(\mathrm{i}\omega)$ to close the iteration. In our calculation, we set $t = 1$ as the energy unit and $a = 1$ as the length unit. We also need to tune the chemical potential μ to put the system at 1/3 filling, i.e., $\langle n\rangle = 1/3$. All the calculations are done at $T = 0.1t$, where T is the temperature.

4. Results

We first consider the effect of the electron–electron interaction and set $\lambda_{so} = 0$. The density of states can be obtained by employing the maximum entropy method,[40] and the result is shown in Fig. 4 for different interaction strengths at $T = 0.1t$. It can be seen that when U increases from 1 to 13, there is no gap opened, which means that the system remains a semi-metal in a large range of interaction strengths. This is different from the case at 1/2 filling where the Mott transition takes place when the interaction reaches a certain value.[25] At 1/3 filling, the localization of electrons is not necessary to avoid the on-site energy cost. We also calculate the evolutions of magnetic order parameter M and double occupancy D_o when the interaction increases as shown in Fig. 5. Here M and D_o are defined as

$$M = \frac{1}{N_c}\sum_i \mathrm{sign}(i)(\langle n_{i\uparrow}\rangle - \langle n_{i\downarrow}\rangle),$$
$$D_o = \langle n_{i\uparrow} n_{i\downarrow}\rangle,$$

where

$$\mathrm{sign}(i) = \begin{cases} 1, & i = \mathrm{A\ or\ B}, \\ -1, & i = \mathrm{C}. \end{cases}$$

When $U = 0$ at 1/3 filling, $D_o = \langle n_{i\uparrow} n_{i\downarrow}\rangle|_{U=0} = 1/3 \times 1/3 = 0.11$. As the interaction increases, there is no magnetic order in our system and D_o is decreasing, which suggests that the system is always in a paramagnetic semi-metal phase.

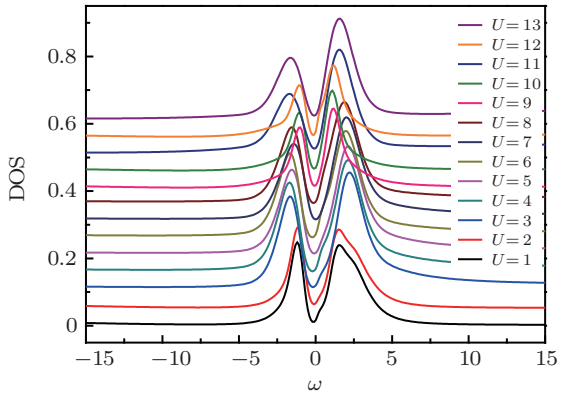


Fig. 4. (color online) DOS at 1/3 filling. Here $T = 0.1$ and $\lambda_{so} = 0$.

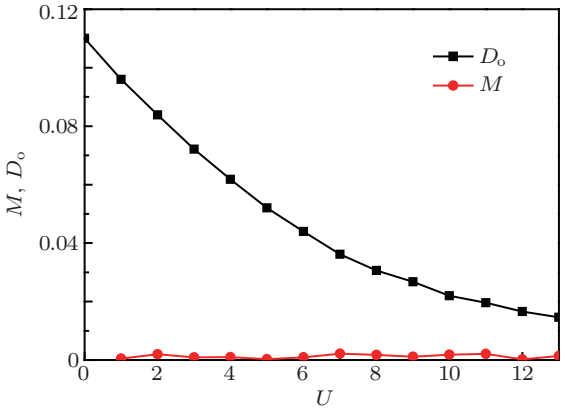


Fig. 5. (color online) The evolutions of magnetic order M and double occupancy D_o on the 1/3 filling kagome lattice.

Then we move to the case with both the electron–electron interaction and the SOC. Figure 6 shows the DOS at different SOC strengths when $U = 2$ and 8. It can be seen that at a fixed U, a gap will emerge when λ_{so} increases and the system goes into an insulating phase. In order to identify whether the insulator phase driven by the SOC is topologically non-trivial, we calculate the spectral function $A(k_x,\omega)$ on the corresponding kagome strip using the real-space CDMFT. The results are

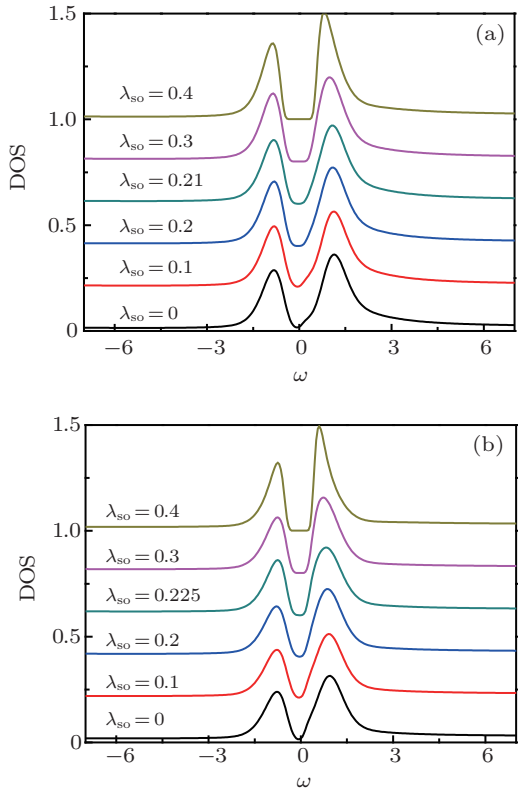


Fig. 6. (color online) DOS for different λ_{so} when (a) $U = 2$ and (b) $U = 8$ at $T = 0.1$ on the 1/3 filling kagome lattice. It is found that $\lambda_{so} = 0.21$ and $\lambda_{so} = 0.255$ are the transition points from semi-metal to TI.

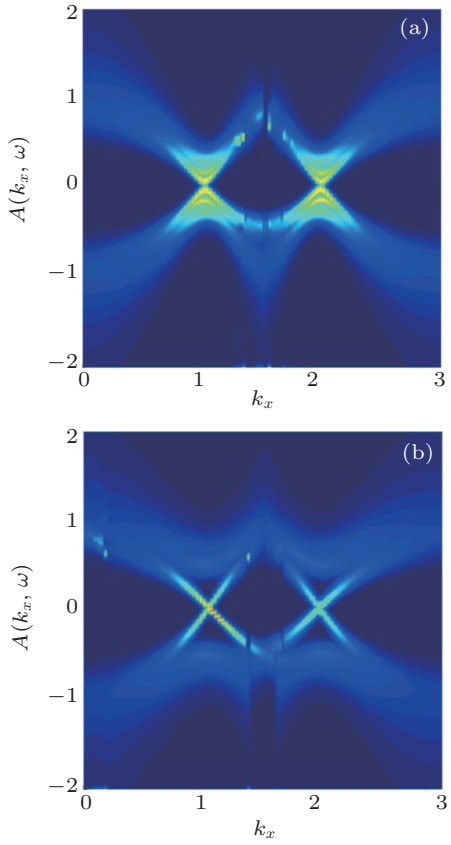


Fig. 7. (color online) The spectral function $A(k_x, \omega)$ on a kagome strip at $U = 2$ and $T = 0.1$ with $L = 48$, where L is the number of sites in the y direction: (a) semi-metal at $\lambda_{so} = 0.05$. (b) The helical edge states in the TI phase for $\lambda_{so} = 0.3$.

plotted in Fig. 7 with $\lambda_{so} = 0.05$ and 0.3 when $U = 2$, which correspond to the semi-metal and the insulating phases, respectively. It is shown in Fig. 7(a) that when $\lambda_{so} = 0.05$, there are no edge states coming out of the bulk states and the system remains a semi-metal. When $\lambda_{so} = 0.3$, as shown in Fig. 7(b), there are edge states isolated from the gapped bulk states, indicating that the system is in the TI state. We then can further obtain the phase diagram of the 1/3 filling kagome lattice with respect to λ_{so} and U as shown in Fig. 8. The system remains in the semi-metal phase at $\lambda_{so} = 0$, while a finite SOC drives the system to the TI phase. When the interaction becomes stronger, a larger SOC is needed for the system to reach the TI phase, and vice versa.

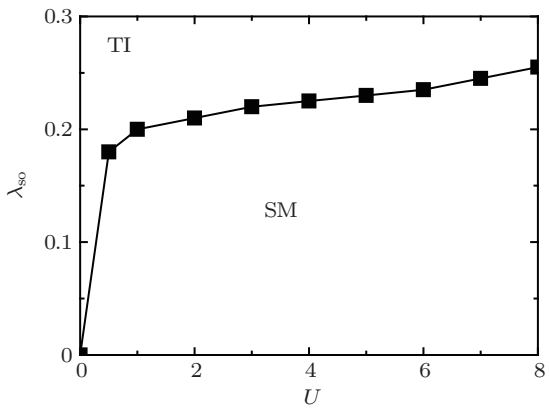


Fig. 8. The phase digram with SOC strength λ_{so} and on-site interaction U on the kagome lattice at 1/3 filling with $T = 0.1$. The line marks the transition from semi-metal to topological insulator with increasing λ_{so}.

5. Conclusion

We investigate the interplay between the electron–electron interactions and the SOC on a 1/3 filling kagome lattice by applying the cellular dynamical mean-field approximation and its real-space extension. We consider the effect of the interaction first and show that in the absence of the SOC, the system is in a semi-metal phase even with a strong interaction. Then by considering these two effects simultaneously, we obtain the phase diagram demonstrating the competing relation. With the increasing SOC, the system undergoes a phase transition from semi-metal to topological insulator, and as the interaction becomes stronger, a larger SOC is required for the transition.

References

[1] Hasan M Z and Kane C L 2010 *Rev. Mod. Phys.* **82** 3045
[2] Qi X L and Zhang S C 2011 *Rev. Mod. Phys.* **83** 1057
[3] Bernevig B A, Hughes T L and Zhang S C 2006 *Science* **314** 1757
[4] König M, Wiedmann S, Brüne C, Roth A, Buhmann H, Molenkamp L W, Qi X L and Zhang S C 2007 *Science* **318** 766
[5] Xia Y, Qian D, Hsieh D, Wray L, Pal A, Lin H, Bansil A, Grauer D, Hor Y S, Cava R J and Hasan M Z 2009 *Nat. Phys.* **5** 398
[6] Xiu F X and Zhao T T 2013 *Chin. Phys. B* **22** 96104
[7] Ding Y, Shen J, Pang Y, Liu G T, Fan J, Ji Z Q, Yang C L and Lü L 2013 *Acta Phys. Sin.* **62** 167401 (in Chinese)

[8] Guo J H, Qiu F, Zhang Y, Deng H Y, Hu G J, Li X N, Yu G L and Dai N 2013 *Chin. Phys. Lett* **30** 106801
[9] Wu C J, Bernevig B A and Zhang S C 2006 *Phys. Rev. Lett.* **96** 106401
[10] Xu C K and Moore J E 2006 *Phys. Rev. B* **73** 045322
[11] Yu S L, Xie X C and Li J X 2011 *Phys. Rev. Lett.* **107** 010401
[12] Hohenadler M, Lang T C and Assaad F F 2011 *Phys. Rev. Lett.* **106** 100403
[13] Lee D H 2011 *Phys. Rev. Lett.* **107** 166806
[14] Wu W, Rachel S, Liu W M and Le Hur K 2012 *Phys. Rev. B* **85** 205102
[15] Yuan J, Gao J H, Chen W Q, Ye F, Zhou Y and Zhang F C 2012 *Phys. Rev. B* **86** 104505
[16] Hohenadler M and Assaad F F 2013 *J. Phys.: Condens. Matter* **25** 143201
[17] Zheng D, Zhang G M and Wu C J 2011 *Phys. Rev. B* **84** 205121
[18] Maciejko J, Chua V and Fiete G A 2014 *Phys. Rev. Lett.* **112** 016404
[19] Wen X G 2002 *Phys. Rev. B* **65** 165113
[20] Colman R H, Sinclair A and Wills A S 2010 *Chem. Mater.* **22** 5774
[21] Fåk B, Kermarrec E, Messio L, Bernu B, Lhuillier C, Bert F, Mendels P, Koteswararao B, Bouquet F, Ollivier J, Hillier A D, Amato A, Colman R H and Wills A S 2012 *Phys. Rev. Lett.* **109** 037208
[22] Yan S M, Huse D A and White S R 2011 *Science* **332** 1173
[23] Nishimoto S, Nakamura M, O'Brien A and Fulde P 2010 *Phys. Rev. Lett.* **104** 196401
[24] Yamada A, Seki K, Eder R and Ohta Y 2011 *Phys. Rev. B* **83** 195127
[25] Ohashi T, Kawakami N and Tsunetsugu H 2006 *Phys. Rev. Lett.* **97** 066401
[26] Kane C L and Mele E J 2005 *Phys. Rev. Lett.* **95** 146802
[27] Guo H M and Franz M 2009 *Phys. Rev. B* **80** 113102
[28] Liu G C, Zhu S L, Jiang S J, Sun F D and Liu W M 2010 *Phys. Rev. A* **82** 053605
[29] Wen J, Rüegg A, Wang C C J and Fiete G A 2010 *Phys. Rev. B* **82** 075125
[30] Raghu S, Qi X L, Honerkamp C and Zhang S C 2008 *Phys. Rev. Lett.* **100** 156401
[31] Zhang Y, Ran Y and Vishwanath A 2009 *Phys. Rev. B* **79** 245331
[32] Kotliar G, Savrasov S Y, Pálsson G and Biroli G 2001 *Phys. Rev. Lett.* **87** 186401
[33] Kotliar G, Savrasov S Y, Haule K, Oudovenko V S, Parcollet O and Marianetti C A 2006 *Rev. Mod. Phys.* **78** 865
[34] Maier T, Jarrell M, Pruschke T and Hettler M H 2005 *Rev. Mod. Phys.* **77** 1027
[35] Rubtsov A N, Savkin V V and Lichtenstein A I 2005 *Phys. Rev. B* **72** 035122
[36] Georges A, Kotliar G, Krauth W and Rozenberg M J 1996 *Rev. Mod. Phys.* **68** 13
[37] Chen Y H, Tao H S, Yao D X and Liu W M 2012 *Phys. Rev. Lett.* **108** 246402
[38] Chen Y H, Wu W, Tao H S and Liu W M 2010 *Phys. Rev. A* **82** 043625
[39] Wu W, Chen Y H, Tao H S, Tong N H and Liu W M 2010 *Phys. Rev. B* **82** 245102
[40] Mand J and Gubernatis J E 1996 *Physics Reports* **269** 133