Possible anomalous spin dynamics of the Hubbard model on a honeycomb lattice

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Abstract
In this paper, the Hubbard model on a honeycomb lattice is investigated by using an O(3) nonlinear σ model. A possible candidate for a quantum non-magnetic insulator in a narrow parameter region is found near the metal–insulator transition. After studying the magnetic properties of the quantum non-magnetic insulator, anomalous spin dynamics is shown. In addition, we find that this region could be widened by hole doping.

1. Introduction
The Fermi liquid paradigm has been very successful as a basis for understanding the physics of conventional solids including metals and (band) insulators. For the band insulators, the chemical potential lies inside the energy gap. Due to the energy gap, the charge degree of freedom is frozen. If the spin rotation symmetry can be broken spontaneously, the elementary excitations are gapless spin waves and gapped quasi-particles (electrons or holes) that carry both spin and charge quantum numbers. However, unlike conventional insulators, the elementary excitations carrying fractional quantum numbers of an electron may exist in certain insulators. Such a nontrivial quantum state of an insulator with electron-fractionalization is usually called a quantum spin liquid state [1].

Various approaches show that quantum spin liquids may exist in a two-dimensional (2D) \( S = 1/2 \) \( J_1-J_2 \) model or the Heisenberg model on a kagome lattice. In these models, the quantum disordered ground states are accessible (in principle) by appropriate frustrating interactions. On the other hand, some researchers have found that the quantum spin liquid ground states may be realized in an organic material \( \kappa-(\text{bis(ethylenedithio)tetrathiafulvalene})_2\text{Cu}_2\text{(CN)}_3 \) \( (\kappa-(\text{BEDT-TTF})_2\text{Cu}_2\text{(CN)}_3) \) [2–4]. Such a type of quantum spin liquid lies on the insulating side of metal–insulator (MI) transition. Because the spin liquid is adjacent to the MI transition, one may guess it is the local charge fluctuations rather than frustrations that disrupt spin ordering and drive the ground state to a spin liquid state. Such a type of spin liquid can be described by the Hubbard model in the intermediate coupling region. Motivated by experiments, a \( U(1) \) slave-rotor theory of the Hubbard model was formulated on the triangular lattice [5] and its \( SU(2) \) generalization on the honeycomb lattice has been established [6].

In this paper we will focus on the antiferromagnetic (AF) insulator of the Hubbard model on a honeycomb lattice. It is known that these AF insulating states belong to a special class of AF ordered state-nodal AF insulator (NAI); an AF order with relativistically massive fermionic excitations. For this reason, the situation differs from that in the traditional Hubbard model on a square lattice. The simplest approach to study the honeycomb Hubbard model is the Hartree–Fock (HF) mean field method, from which a semi-metal–insulator (MI) transition at a critical value \( (U/t)_c \approx 2.23 \) between a semi-metal (SM) and an AF insulator was obtained [7]. In the weak interaction region \( U/t < (U/t)_c \), the ground state is SM with nodal Fermi-points. In the strong interaction region \( U/t > (U/t)_c \), the ground state becomes an insulator with massive fermionic excitations. However, HF theory does not maintain spin rotation symmetry by fixing the spins along the \( \hat{z} \)-axis. So the results are not reliable.

Besides the mean field theory, different values of the MI transition have been obtained by numerical approaches: \( (U/t)_c \approx 4.5 \pm 0.5 \) by Monte Carlo (MC) simulations in [7–9] as well as \( 5.0 < (U/t)_c < 5.1 \) by quantum MC in [10]; \( (U/t)_c \approx 4 \) by series expansion techniques in [9]; \( (U/t)_c \approx 3.1 \) by a slave boson approach in [11]; \( (U/t)_c \approx 13.3 \) by dynamical mean field theory (DMFT) adopting the iterated perturbation theory for a single-site problem in [12] and \( (U/t)_c \approx 10 \) in [13] by DMFT at finite temperature. Another issue here is the nature of the insulator state. By the \( SU(2) \)
slave-rotor theory, a quantum spin liquid was predicted in the region of $1.26 < U/t < 1.30$, lying on the insulating side of the MI transition, due to strong local charge fluctuations [6]. Such a type of spin liquid near the MI transition could be described by the Hubbard model in the intermediate coupling region.

In this paper, instead of studying the MI transition to obtain an accurate critical value, we focus on the following issue: whether the insulator has long range AF order or not. We will investigate the two-dimensional honeycomb Hubbard model by an approach proposed in [1, 14–18] that maintains spin rotation symmetry. In this way, we find anomalous spin dynamics near the critical point of the MI transition: there may exist a narrow non-magnetic insulator and such a narrow non-magnetic insulator will favor hole doping. Such types of non-magnetic insulator in bipartite lattices are not driven by frustration, as has been done in various spin models. Instead, they come from quantum fluctuations of relatively small effective spin moments near the Mott transition.

The paper is organized as follows. In section 2, the semi-metal–insulator transition is studied by a HF mean field approach. In section 3, an effective O(3) nonlinear $\sigma$ model (NL$\sigma$M) is obtained to investigate properties of the honeycomb Hubbard model. In section 4, a global phase diagram is given and magnetic properties of the insulator state are studied based on the NL$\sigma$M. In section 5, we discuss how to observe anomalous spin dynamics in experiments. In section 6, we show the doping effect on the magnetic properties of the ground state. Finally, our conclusions are given in section 7.

2. Metal–insulator transition

As a starting point, the Hamiltonian of the Hubbard model on honeycomb lattice is given by

$$\mathcal{H} = -t \sum_{\langle i,j \rangle} (\hat{c}_i^\dagger \hat{c}_j + \text{h.c.}) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \mu \sum_i \hat{c}_i^\dagger \hat{c}_i. \quad (1)$$

Here $\hat{c}_i = (\hat{c}_{i\uparrow}, \hat{c}_{i\downarrow})^T$ and $\hat{c}_{i\sigma}^\dagger, \hat{c}_{j\sigma}$ are electronic creation and annihilation operators. $t$ is the hopping integral. $U$ is the onsite Coulomb repulsion. $\sigma$ are the spin indices representing spin-up ($\sigma = \uparrow$) and spin-down ($\sigma = \downarrow$) for electrons. $\mu$ is the chemical potential, which is $\frac{1}{2}$ in half-filling. $\langle i, j \rangle$ denotes two sites on a nearest-neighbor link. $\hat{n}_{i\uparrow}$ and $\hat{n}_{i\downarrow}$ are the number operators of electrons with up-spin and down-spin, respectively.

Because the honeycomb lattice is a bipartite lattice (see figure 1), we divide the system into two sublattices, A and B. Performing the Fourier transformations, the electronic annihilation operators on two sublattices are written as

$$\hat{c}_{i \in A, \sigma} = \frac{1}{\sqrt{N_s}} \sum_k e^{-ik \cdot R} \hat{a}_{k\sigma},$$
$$\hat{c}_{i \in B, \sigma} = \frac{1}{\sqrt{N_s}} \sum_k e^{-ik \cdot R} \hat{b}_{k\sigma}, \quad (2)$$

where $N_s$ denotes the number of unit cells. For free fermions, the Hamiltonian could be transformed in the momentum space as

$$\mathcal{H} = \sum_{k, \sigma} (\hat{a}_{k\sigma}^\dagger \hat{b}_{k\sigma}^\dagger + \text{h.c.}) \left( \begin{array}{cc} 0 & \xi_k \sigma \\ \xi_k^* \sigma & 0 \end{array} \right) \left( \begin{array}{c} \hat{a}_{k\sigma} \\ \hat{b}_{k\sigma} \end{array} \right). \quad (4)$$

where the energy of free fermions is

$$|\xi_k| = -t \sum_i e^{ik \cdot R_a} \left| c_i \right|$$

$$= t \sqrt{3} + 2 \cos(\sqrt{3} k_x) + 4 \cos(3k_x/2) \cos(\sqrt{3} k_y/2). \quad (5)$$

Here we define the vectors of nearest neighbors as

$$\delta_1 = \frac{a}{2}(1, \sqrt{3}), \quad \delta_2 = \frac{a}{2}(1, -\sqrt{3}), \quad \delta_3 = (-a, 0) \quad (6)$$

where $a$ is the length of the hexagon side and chosen to be unity. The spectrum for free electrons is then obtained as $E_k = \pm |\xi_k|.$

Next we use the path-integral formulation of electrons with spin rotation symmetry to study the on-site repulsive interaction in the Hubbard model [1, 14–18]. The interaction term can be handled by using an $SU(2)$ invariant Hubbard–Stratonovich (HS) decomposition in the arbitrary on-site unit vector $\Omega_i$:

$$\hat{n}_{i\uparrow} \hat{n}_{i\downarrow} = \frac{\hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger}{4} - \frac{1}{4} [\Omega_i \cdot \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}]^2 \quad (7)$$

where $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ is the Pauli matrix. Then the HS transformation for the interaction term is

$$e^U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} = \int \prod_i d\Delta_x \prod_i d\Delta_i \prod_i d\Omega_i \exp \left( \sum_i \left[ \frac{1}{U} (\Delta_x^2 + \Delta_i^2) + i \Delta_x \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow} - \Delta_i \hat{c}_{i\sigma}^\dagger \Omega_i \cdot \sigma \hat{c}_{i\sigma} \right] \right). \quad (8)$$

Here $\Delta_c$ and $\Delta_i$ are the auxiliary fields. By replacing the electronic operators $\hat{c}_{i\sigma}^\dagger$ and $\hat{c}_{i\sigma}$ with Grassmann variables $c_{i\sigma}^*$ and $c_{i\sigma}$, we can rewrite the Hamiltonian in the Grassmann variables as

$$\mathcal{H} = \sum_{k, \sigma} (\hat{a}_{k\sigma}^\dagger \hat{b}_{k\sigma}^\dagger + \text{h.c.}) \left( \begin{array}{cc} 0 & \xi_k \sigma \\ \xi_k^* \sigma & 0 \end{array} \right) \left( \begin{array}{c} \hat{a}_{k\sigma} \\ \hat{b}_{k\sigma} \end{array} \right). \quad (4)$$
and $c_{i,\sigma}$, the effective Lagrangian in terms of the Grassmann variables $c_{i,\sigma}^\dagger$ and $c_{i,\sigma}$ is then obtained as

$$\mathcal{L}_{\text{eff}} = \sum_{i,\sigma} c_{i,\sigma}^\dagger \partial_\tau c_{i,\sigma} - \sum_{\langle ij \rangle} (t_{ij} c_{i,\sigma}^\dagger c_{j,\sigma} + \text{h.c.})$$

$$- \sum_i \Delta_i c_i^\dagger \hat{\Omega}_i \cdot \sigma c_i$$

$$+ \sum_i \left[ \frac{1}{U} (\Delta_i^2 + \Delta_i^4) + (i\Delta_i - \mu) c_i^\dagger c_i \right].$$

(9)

The ground state of the honeycomb Hubbard model is known to be long range AF order in the large $U$ limit. Such an order can be described by a simple saddle-point Lagrangian by fixing the direction vector field $\Omega_i$ to $\hat{z}$-axis $\Omega_i = (-1)^i \hat{z}$ and choosing the amplitude as

$$i\Delta_i = \frac{U}{2} (c_i^\dagger c_i) = \frac{Un}{2}$$

(10)

$$\Delta_i = \frac{U}{2} (c_i^\dagger \sigma_i c_i) = (-1)^i \frac{UM}{2} = (-1)^i \Delta$$

(11)

where $n$ is the average on-site electron density. $M$ is the staggered magnetization and $\Delta = \frac{UM}{2}$ is the energy band gap. The effective Lagrangian becomes

$$\mathcal{L}_{\text{eff}} = \sum_{i,\sigma} c_{i,\sigma}^\dagger \partial_\tau c_{i,\sigma} - \sum_{\langle ij \rangle} (t_{ij} c_{i,\sigma}^\dagger c_{j,\sigma} + \text{h.c.})$$

$$- \sum_i (-1)^i \Delta_i c_i^\dagger \sigma_i c_i + \frac{UN_n}{4} (M^2 - 1).$$

(12)

One obtains the spectrum of the electrons as

$$E_k = \pm \sqrt{\xi_k^2 + \Delta^2}.$$  

(13)

Finally we derive the self-consistency equation for $M$ by minimizing the free energy at temperature $T$ in the Brillouin zone as

$$1 = \frac{1}{N_i} \sum_k \frac{U}{2E_k} \tanh(\beta E_k/2).$$  

(14)

Here $\beta = \frac{1}{k_B T}$.

From figure 2, one can find that MI transition occurs at a critical value of about $U/t \approx 2.23$ at zero temperature. In the weakly coupling limit ($U/t < 2.23$), the ground state is a SM with nodal Fermi-points. In the strong coupling region ($U/t > 2.23$), due to $M \neq 0$, the ground state becomes an insulator with massive fermionic excitations. However, finite $M$ merely implies the existence of effective spin moments rather than a long range AF order, since this result is obtained in a mean field level by fixing the spins along the $\hat{z}$-axis. Thus one needs to examine the stability of magnetic order against quantum fluctuations of effective spin moments by maintaining spin rotation symmetry.

3. Effective nonlinear $\sigma$ model in the insulator state

In this section, we will derive an effective $\text{NL}_\sigma M$ of spin fluctuations with spin rotation symmetry in the honeycomb Hubbard model beyond the above mean field theory.
In the continuum limit, we denote

\[ S_{\text{eff}} = \frac{1}{2} \int_0^\beta d\tau \sum_i \left[ -4\zeta(a_0(i) - \Delta \sigma \cdot \mathbf{l})^2 + 4\rho_\sigma a_i^2 + \frac{2\Delta^2}{U} \right] \]

(20)

where \( \rho_\sigma \) and \( \zeta \) are two parameters.

To find the properties of the low-energy physics, we study the continuum theory of the effective action in equation (20). In the continuum limit, we denote \( \mathbf{n}, \mathbf{l} \), \( i a_{ij} \approx U_i^\dagger U_j - 1 \) and \( a_0(i) = U_i^\dagger \partial_\tau U_i \) by \( \mathbf{n}(x, y), \mathbf{l}(x, y), U_i^\dagger \partial_\tau U_i \) (or \( U_i^\dagger \partial_\tau U_i \) and \( U_i^\dagger \partial_\tau U_i \), respectively. From the relations between \( U_i^\dagger \partial_\tau U_i \) and \( \partial_\mu \mathbf{n} \),

\[ a_i^2 = a_{i,1}^2 + a_{i,2}^2 = -\frac{i}{2}(\partial_\rho \mathbf{n})^2, \quad \tau = 0, \quad (21) \]

\[ a_\mu^2 = a_{\mu,1}^2 + a_{\mu,2}^2 = \frac{i}{2}(\partial_\rho \mathbf{n})^2, \quad \mu = x, y, \quad (22) \]

\[ a_0 \cdot \mathbf{l} = -\frac{1}{2}(\mathbf{n} \times \partial_\rho \mathbf{n}) \cdot \mathbf{l}, \quad (23) \]

the continuum formulation of the action in equation (20) becomes

\[ S_{\text{eff}} = \frac{1}{2} \int_0^\beta d\tau \int d^2r \left[ \zeta(\partial_\rho \mathbf{n})^2 + \rho_\sigma(\nabla \mathbf{n})^2 - 4i\Delta \zeta(\mathbf{n} \times \partial_\rho \mathbf{n}) \cdot \mathbf{l} + \left( \frac{2\Delta^2}{U} - 4\Delta^2 \zeta \right) \right] \]

(24)

where the vector \( \mathbf{a}_0 \) is defined as \( \mathbf{a}_0 = (a_{0,1}, a_{0,2}, 0) \).

Finally, we integrate the transverse canting field \( \mathbf{l} \) and obtain the effective NL\( \sigma \)M as

\[ S_{\text{eff}} = \frac{1}{2g} \int_0^\beta d\tau \int d^2r \left[ \frac{1}{c}(\partial_\rho \mathbf{n})^2 + c(\nabla \mathbf{n})^2 \right] \]

(25)

with a constraint \( \mathbf{n}^2 = 1 \). The coupling constant \( g \) and spin wave velocity \( c \) are defined as

\[ g = \frac{\zeta}{\rho_\sigma}, \quad c^2 = \frac{\rho_\sigma}{\chi^2}, \quad \chi^2 = \left( \frac{1}{\zeta} - 2U \right)^{-1}. \quad (26) \]

Here \( \rho_\sigma \) is the spin stiffness,

\[ \rho_\sigma = \frac{1}{N_0} \sum_k \frac{e^2}{4(\Delta k)^2 + \Delta^2 \zeta} \]

(27)

where the corresponding coefficient \( e^2 \) is

\[ e^2 = \frac{1}{4} T^2 \left[ 6\Delta^2 + 27\zeta^2 + (2\Delta^2 + 27\zeta^2) \cos(\sqrt{3}\zeta k) 
+ 36\zeta^2 \cos(3\zeta k/2) \cos(\sqrt{3}\zeta k) 
+ 2(5\Delta^2 + 27\zeta^2) \cos(3\zeta k/2) \cos(\sqrt{3}\zeta k/2) 
+ 9\zeta^2 \cos(3\zeta k)(1 + \cos(\sqrt{3}\zeta k)) \right]. \quad (28) \]

\( \chi^2 \) is the transverse spin susceptibility, of which \( \zeta \) is

\[ \zeta = \frac{1}{N_0} \sum_k \frac{\Delta^2}{4(\Delta k)^2 + \Delta^2 \zeta}. \quad (29) \]

One can see detailed calculations of \( \rho_\sigma \) and \( \zeta \) in the appendix.

The numerical results of \( \rho_\sigma \) and \( c \) are illustrated in figure 3, where one can find that \( c = 0.168901985t = 1.055637J \) in the strongly coupling limit \( U = 25t \) match the earlier result, \( c = 1.06066J \). (32)

In this section we will use the effective NL\( \sigma \)M to study the magnetic properties of the insulator state. The Lagrangian of NL\( \sigma \)M with a constraint \( \mathbf{n}^2 = 1 \) using a Lagrange multiplier \( \lambda \) becomes

\[ \mathcal{L}_{\text{eff}} = \frac{1}{2c^2} (\partial_\rho \mathbf{n})^2 + c^2 (\nabla \mathbf{n})^2 + i\lambda(1 - \mathbf{n}^2) \]

(31)

where \( i\lambda = m^2 \) and \( m \) is the mass gap of the spin fluctuations.

Using the large-\( N \) approximation we rescale the field \( \mathbf{n} \rightarrow \sqrt{N} \mathbf{n} \) and obtain the saddle-point equation of motion as

\[ (n_0)^2 - k_B T \sum_{n_0, n \neq 0} \Pi(n, j_n) = 1. \quad (32) \]

In equation (32), \( n_0 \) is the mean field value of \( \mathbf{n} \) and \( \Pi(n, j_n) = -\frac{c^2}{a_n + n_0 - m} \) is the propagator of the spin fluctuations \( \mathbf{n} \rightarrow \mathbf{n} - n_0 \). Here \( a_n = 2\pi nk_B T, n = \text{integers}. \)

At finite temperature, the solution of \( n_0 \) is always zero that is consistent with the Mermin–Wagner theorem. From equation (32), we may get the solution of \( m \) as

\[ m = 2k_B T \sinh^{-1} \left[ e^{-\frac{m}{2k_B T}} \sinh \left( \frac{c \Delta}{2k_B T} \right) \right]. \quad (33) \]
In the limit $T \ll \Lambda$, equation (33) can be rewritten as
\[
m = 2k_B T \sinh^{-1}\left(\frac{1}{2} \exp \left[ -\frac{2\pi c}{k_B T} \left( 1 - \frac{1}{g_c} \right) \right] \right)
\] (34)
where
\[g_c = \frac{4\pi}{\Lambda}.\] (35)

Therefore, at zero temperature the solutions of $n_0$ and $m$ of equation (32) are determined by the dimensionless coupling constant $\alpha = g\Lambda$. In particular, there exists a critical point $\alpha_c = 4\pi$ (or $g_c = \frac{4\pi}{\Lambda}$): For the case of $\alpha < 4\pi$, we get solutions of $n_0$ and $m$:
\[n_0 = \left( 1 - \frac{g}{g_c} \right)^{1/2}, \quad m = 0.\] (36)

For the case of $\alpha > 4\pi$, we get solutions of $n_0$ and $m$:
\[n_0 = 0, \quad m = 4\pi c \left( 1 - \frac{g}{g_c} \right).\] (37)

So we calculate the dimensionless coupling constant $\alpha = g\Lambda$ and show the results in figure 4. The quantum critical points corresponding to $\alpha_c = 4\pi$ become $(U/t)_{c2} \approx 2.88$ and $(U/t)_{c3} \approx 2.93$, which divide the insulator state into three phases—a quantum disordered state (QD) in the region of $2.88 < U/t < 2.93$ and two long range AF order in the regions of $2.23 < U/t < 2.88$ and $U/t > 2.93$. The reentrant character of AF order when one increases the interaction strength is due to the nonlinear relationship between the dimensionless coupling constants $\alpha$ and $M$.

In the regions $2.23 < U/t < 2.88$ and $U/t > 2.93$ (where $\alpha < \alpha_c$), at low temperature the mass gap $m$ of spin fluctuations is determined by
\[m \approx k_B T \exp \left[ -\frac{2\pi c}{k_B T} \left( 1 - \frac{1}{g_c} \right) \right].\] (38)

Because the energy scale of the mass gap $m$ is always much smaller than the temperature, i.e., $m \ll k_B T$ (or $\omega_0$), quantum fluctuations become negligible in a sufficiently long-wavelength and low-energy regime ($m < |\omega| < k_B T$). Thus in this region one may only consider the purely static (semiclassical) fluctuations. So we call it the renormalized classical (RC) region.

At zero temperature, the mass gap $m$ vanishes (see figure 5), which means that long range AF order appears. To describe the AF order, we introduce a spin order parameter $\mathcal{M}_0$ [22–24]:
\[\mathcal{M}_0 = \frac{M}{2n_0} = \frac{M}{2} \left( 1 - \frac{g}{g_c} \right)^{1/2}.\] (39)

As shown in figure 6, the ground state of the AF ordered phase has a finite spin order parameter.

In the region $2.88 < U/t < 2.93$ (where $\alpha > \alpha_c$), there is a finite mass gap of spin fluctuations at zero temperature (see figure 5):
\[m = 4\pi c \left( 1 - \frac{g}{g_c} \right).\] (40)

Therefore, the ground state of the insulator in this region does not have long range AF order. Instead, it is a quantum
disordered state (or non-magnetic insulator state) with a zero spin order parameter $\mathcal{M}_0 = 0$ in a narrow non-magnetic window (see figure 6).

Based on the above results, we get the global phase diagram shown in figure 7. One can see that at finite $T$, there are four crossover lines, $T_{\text{HF}}$, $T_\rho$, $T_v$ (two lines of $T_v$), separating five regions.

The highest crossover line is $T_{\text{HF}}$, which is obtained from equation (14) and denotes the establishment of the effective spin moments. Above $T_{\text{HF}}$, it is metal phase with no energy gap $\Delta = 0$. The crossover line $T_\rho \sim \rho_0$ denotes the validity of the NL$\sigma$M, where $\rho_0$ is the energy scale of spin stiffness. In the region $T_\rho < T < T_{\text{HF}}$, free spin moments are established (denoted by $M \neq 0$) that show a Curie–Weiss behavior. In this region one cannot use the effective NL$\sigma$M. Below $T_\rho$, short range spin-correlation exists and the effective NL$\sigma$M is valid. The region below $T_\rho$ is dominated by the crossover lines $T_v \sim \rho_0|1 - g/g_c|$ together with two quantum critical points (QCP) at $(U/t)_{\lambda_2} = 2.88$ and $(U/t)_{\lambda_3} = 2.93$ which represent the QCP of $g = g_c$ in the NL$\sigma$M [22, 24]. In the region $T_v < T < T_\rho$, when $g$ approaches $g_c$, the spin-correlation length has a general scaling as

$$\xi \sim |g - g_c|^{-1}. \quad (41)$$

At the QCP of $g = g_c$, $T \neq 0$, the spin-correlation length has a power law temperature-dependence given by [22, 24]

$$\xi(T) \sim \frac{1}{T^{(1/2)}} \quad (42)$$

where $\varepsilon = 2.12$. So we call this region the quantum critical (QC) region. Below $T_c$, we get two RC regions and a narrow QD region.

5. Spin–spin correlations

In order to make our theoretical predictions verifiable, we discuss the detection of the anomalous spin dynamics via spatial spin–spin correlations $\langle S(r, t) \cdot S(0, 0) \rangle = \langle c_d^+(r, t) \sigma_c c(r, t) \cdot c_d^+(0, 0) \sigma_c c(0, 0) \rangle$ or dynamic spin susceptibility $\chi''(q, \omega)$. Here $\chi''(q, \omega)$ is defined as

$$\chi''(q, \omega) = \frac{1}{\pi} \int dt \int d\omega \ e^{i(q\cdot r - \omega t)} \langle S(r, t) \cdot S(0, 0) \rangle. \quad (43)$$

One may also observe the dynamic spin susceptibility $\chi''(q, \omega)$, which reveals the spin–spin correlations by NMR measurement. Consequently, it determines the spin–spin correlation in the real space as $\cos(Q_0 \cdot r) e^{-|q|/\xi}$, with the correlation length $\xi$ and the AF wavevector $Q_0 = (\pm \frac{\pi}{\sqrt{2}}, \pm \frac{\pi}{\sqrt{2}})$. To show clearly the anomalous spin dynamics, we calculate the spin–spin correlation $\langle S(r, t) \cdot S(0, 0) \rangle$. The dynamic spin susceptibility at $Q_0$ is determined by $n$ fields

$$\chi(q, \omega) = (n_\sigma(q, \omega) n_\sigma(-q, -\omega)) = \frac{g c}{q^2 + \omega^2 + m^2} \quad (44)$$

where we have introduced the momentum $q$. The equal-time spin–spin correlation function is proportional to $e^{-|q|/\xi}$, where the spin-correlation length $\xi$ is therefore given by $\frac{\pi}{n}$. As equation (43) indicates, the spin dynamic structure factor as well as the dynamic spin susceptibility function may reflect the effective short range magnetic correlation length $\xi$.

In figure 8, we give the spin-correlation length defined as $\xi = \frac{\sqrt{\xi}}{m}$ at $T = 0.02t$, $0.1t$, $0.2t$, respectively. From figure 8, taking $T = 0.02t$ as an example, one can see that the spin-correlation length increases quickly with increasing interaction $U/t$. However, the spin-correlation length does not increase monotonically with $U/t$—it will decrease and reach a minimum value near the MI transition $U/t_{\lambda_2} \sim (U/t)_{\lambda_3} \sim (U/t)_{\lambda_3}$. When one increases the interaction further, the spin-correlation revives and finally decreases in the strongly interacting limit due to $J \rightarrow 0$. For other cases with higher temperature, $T = 0.1t, 0.2t$, there exists a similar dip structure of the spin-correlation length with $U/t$, which means that it may be possible to observe the anomalous spin dynamics more easily in experiments. In particular, one can see that the narrow non-magnetic insulator is sensitive to the choice of the cutoff
The dip structure of the spin-correlation length via $U/t$ is robust. Thus, in the future, it may be possible to simulate the Hubbard model on a honeycomb lattice by using a two-component mixture of repulsive cold fermionic atoms on an optical lattice and then observing the anomalous spin dynamics [25–27].

6. Doping effect

In this section we will leave half-filling and study the hole doping case. In the case of hole concentration $d = 1 - n$, the chemical potential $\mu$ is no longer $U/2$. The Hamiltonian becomes

$$\mathcal{H} = -\sum_{\langle ij \rangle} (t_{ij} c_i^\dagger c_j + \text{h.c.}) - \sum_i \Delta_i c_i^\dagger \Omega_i \cdot \sigma c_i + \sum_i \left( \frac{Un}{2} - \mu \right) c_i^\dagger c_i.$$  \hspace{1cm} (45)

In this case, we can obtain $M$, $\mu$, $\xi$, $\rho_s$, in a similar way to that of the half-filling case, at $T = 0$ as follows:

$$1 = \frac{1}{N_\varepsilon} \sum_{\varepsilon_{k<\mu}} \frac{U}{2E_k}, \quad 1 - d = \sum_{\varepsilon_{k<\mu}} 1,$$

$$\xi = \frac{1}{N_\varepsilon} \sum_{\varepsilon_{k<\mu}} \frac{\Delta^2}{4(|\xi_k|^2 + \Delta^2)^2},$$

$$\rho_s = \frac{1}{N_\varepsilon} \sum_{\varepsilon_{k<\mu}} \frac{\epsilon^2}{4(|\xi_k|^2 + \Delta^2)^2}.$$  \hspace{1cm} (46)

Given a certain hole concentration $d$, then $\rho_s$ and $c$ may be obtained. Compared with figure 9, one can see that the spin stiffness $\rho_s$ increases when the hole concentration increases.

7. Conclusion

In this paper, we investigated the two-dimensional honeycomb Hubbard model with an approach that maintains spin rotation symmetry. In this way, we found anomalous spin dynamics not far from the critical point of the MI transition: there may exist a narrow non-magnetic insulator in the region $2.88 < U/t < 2.93$ in the half-filling case and this non-magnetic insulator will favor hole doping. Recently such a
predicted non-magnetic insulator between a semi-metal and long range AF order near MI transition was indeed confirmed by the QMC method in [28], where the non-magnetic insulator was found to be in the region $3.5 < U/t < 4.3$ with a short range spin–spin correlation. The difference between our results and that from the QMC method is the existence of a long range AF order between the non-magnetic insulator and the semi-metal. Such a discrepancy may come from the fluctuated charge degree of freedom near the MI transition that we have ignored.

The possible non-magnetic insulator may give us the chance to pursue new kinds of order beyond Landau’s paradigm. So finally we discuss the nature of the non-magnetic insulator in the two-dimensional honeycomb Hubbard model. In [29], it was pointed out that by considering the fermionic nature of vortices (half-skymrions), a nodal spin liquid becomes the ground state of the non-magnetic insulator state in the $\pi$–flux Hubbard model on a square lattice. There exist three types of quasi-particles in nodal spin liquids: nodal fermionic spinons, gapped Bosonic spinons and a roton-like $U(1)$ gauge field. Following a similar approach, one may draw the same conclusion that the non-magnetic insulator in the two-dimensional honeycomb Hubbard model is another example of a nodal spin liquid with similar quasi-particles.

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Appendix. The detailed calculations of $\rho_s$ and $\zeta$

To give $\rho_s$ and $\zeta$ for calculation, we choose $U_i$ to be

$$U_i = \left( \begin{array}{cc} z_i^+ \sigma_1 & z_i^- \sigma_1 \\
                    -z_i^- \sigma_1 & z_i^+ \sigma_1 \end{array} \right)$$

(47)

where $n_i = \bar{z}_i \sigma_1 z_i$, $z_i = (z_{i1}, z_{i2})^T$, $\bar{z}_i z_i = I$. The spin fluctuations around $n_i = \bar{z}_i$ are

$$n_i = \bar{z}_i + \Re(\phi_i) \bar{\xi} + \Im(\phi_i) \bar{\eta}$$

(48)

$$z_i = \left( \begin{array}{c} \frac{1 - |\phi_i|^2}{\phi_i} / 8 \\
                    + O(|\phi_i|^3) \end{array} \right)$$

(49)

Then the quantities $U_j^+ U_j$ and $U_j^+ \partial_j U_i$ can be expanded in powers of $\phi_i - \phi_j$ and $\partial_j \phi_i$,

$$U_j^+ U_j = e^{\frac{\frac{\bar{z}_j \sigma_1}{2}}{8}}$$

(50)

$$U_j^+ \partial_j U_i = \left( \begin{array}{cc} 0 & -\frac{1}{2} \partial_j \phi_i \\
                    \frac{1}{2} \partial_j \phi_i & 0 \end{array} \right)$$

(51)

According to equation (18), the gauge field $a_{ij}$ and $a_{d0}(i)$ are given as

$$a_{ij} = \frac{1}{2}(\phi_i - \phi_j)\sigma_y$$

(52)

Supposing $a_{ij}$ and $a_{d0}(i)$ to be a constant in space and denoting $\partial_i \phi_i = \mathbf{a}$ and $\partial_j \phi_j = iB_j$, we have

$$a_{ij} = -\frac{1}{2} \mathbf{a} \cdot (i - j) \sigma_y$$

(54)

$$a_{d0}(i) = -\frac{1}{2} B_j \sigma_y$$

(55)

The energy of the Hamiltonian of equation (20) becomes

$$E(B_y, \mathbf{a}) = \frac{1}{2} \zeta B_y^2 + \frac{1}{2} \rho_s a^2.$$

(56)

Then one can get $\zeta$ and $\rho_s$ from the following equations by calculating the partial derivative of the energy

$$\zeta = \frac{1}{N_s} \frac{\partial^2 E_0(B_y)}{\partial B_y^2} \bigg|_{B_y = 0}$$

(57)

$$\rho_s = \frac{1}{N_s} \frac{\partial^2 E_0(a)}{\partial a^2} \bigg|_{a = 0}.$$

(58)

Here $E_0(B_y)$, $E_0(a)$ are the energy of the lower Hubbard band

$$E_0(B_y) = \sum_k (E^\zeta_{+k} + E^\zeta_{-k})$$

(59)

$$E_0(a) = \sum_k (E^\rho_{+k} + E^\rho_{-k})$$

(60)

where $E^\zeta_{+k}$, $E^\zeta_{-k}$ and $E^\rho_{+k}$, $E^\rho_{-k}$ are the energies of the following Hamiltonians $\mathcal{H}^\zeta$ and $\mathcal{H}^\rho$:

$$\mathcal{H}^\zeta = -\sum_{i<j}(t_{i,j} \psi_i^\dagger \psi_j + \text{h.c.}) - \Delta \sum_i (-1)^i \psi_i^\dagger \sigma_z \psi_i$$

$$+ \sum_i \psi_i^\dagger a_{d0}(i) \psi_i$$

(61)

$$\mathcal{H}^\rho = -\sum_{i<j}(t_{i,j} \psi_i^\dagger e^{\delta i} \psi_j + \text{h.c.}) - \Delta \sum_i (-1)^i \psi_i^\dagger \sigma_z \psi_i.$$ (62)

Using the Fourier transformations for $\mathcal{H}^\zeta$, we have the spectrum of the lower band of $\mathcal{H}^\zeta$

$$E^\zeta_{\pm k} = -\sqrt{\left( \frac{\xi_k \pm B_y}{2} \right)^2 + \Delta^2}$$

(63)

where $\xi_k$ has been obtained in equation (5). Using equation (57), $\zeta$ is obtained as

$$\zeta = \frac{1}{N_s} \sum_k \frac{\Delta^2}{4(|\xi_k|^2 + \Delta^2)^2}$$

(64)

Similarly, using the Fourier transformations for $\mathcal{H}^\rho$, we obtain the spectrum of the lower band of $\mathcal{H}^\rho$

$$E^\rho_{\pm k} = -\sqrt{\Delta^2 + |\psi|^2 + |\mathbf{a}|^2 + 4|\Delta^2|/2} + (\psi^\dagger - \psi^\dagger \mathbf{a}^2)^2$$

(65)

where $\psi$ and $\mathbf{a}$ are defined as

$$\psi = -i \sum_k e^{ik\delta} \cos \left( \frac{1}{2} \mathbf{a} \cdot \delta \right)$$

(66)
\[ \psi = -t \sum \delta e^{i\mathbf{k} \cdot \mathbf{\delta}} \sin \left( \frac{1}{2} \mathbf{a} \cdot \mathbf{\delta} \right). \]  

Using equation (58), \( \rho_s \) is given as

\[ \rho_s = \frac{1}{N_s} \sum_k \epsilon^2 \left[ 4(\epsilon_k^2 + \Delta^2) \right]. \]  

The corresponding coefficient \( \epsilon^2 \) is

\[ \epsilon^2 = \frac{4t^2}{4\Delta^2 + 27t^2} \left[ 6\Delta^2 + 27t^2 + (2\Delta^2 + 27t^2) \cos(\sqrt{3}k_y) + 36t^2 \cos(3k_y/2) \cos(\sqrt{3}k_y) \cos(\sqrt{3}k_y/2) \right. \]
\[ + 2(5\Delta^2 + 27t^2) \cos(3k_y/2) \cos(\sqrt{3}k_y/2) \cos(\sqrt{3}k_y/2) \]
\[ \left. + 9t^2 \cos(3k_y)(1 + \cos(\sqrt{3}k_y)) \right]. \]

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