Resonating Hartree-Fock studies on magnetic states in the Hubbard model on the uniform triangular lattice

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Abstract. We investigate the quantum fluctuations in magnetic states of the half-filled Hubbard model on the uniform triangular lattice, by means of the resonating Hartree-Fock approximation where a many-body wavefunction is constructed by non-orthogonal multi-Slater determinants. It is shown that the quantum fluctuations are described by large deviations from the 120°Néel order even at U/t=10, which results in significant reduction of the spin correlations.

1. Introduction
Spin structures on the triangular lattice have been attracting much interest since discovery of the non-magnetic insulating state in \(\kappa-\text{(BEDT-TTF)}_2\text{Cu}_2\text{(CN)}_3\).[1] So far, the path integral renormalization group (PIRG) theory has pointed out such non-magnetic insulating phase.[2, 3] Now, what we need would be much more detailed information on quantum fluctuations. Conventional numerical methods give physical information mainly through the correlation functions, and we cannot see how and why such electronic structures are realized. Such information would be important also for materials design using the complicated strongly correlated systems. In this research, we describe the spin structures on the uniform triangular lattice by means of a resonating Hartree-Fock (Res-HF) method. We will give physics to large quantum fluctuations in this system.

This paper is organized as follows. A brief review on the Res-HF method is given in §2. Our results on the quantum fluctuations and spin correlation function are shown in §3. A short summary is given in §4.

2. Res-HF method
How to describe strongly correlated electron systems has been one of the central subjects in solid state physics. Especially, it has been quite difficult to give reasonable physics to such large quantum fluctuations. To overcome this difficulty, we introduce the Res-HF method, where a many electron wavefunction is constructed by superposition of non-orthogonal Slater determinants, such as

\[
|\Psi> = \sum_{f=1}^{N_S} C_f \sum_G P^G|f>.
\]
All the orbitals of the Slater determinants $|f>$, as well as superposition coefficients $C_f$, are variationally determined. Details of this orbital optimization are given in ref. [4]. In this research, to describe the coplanar spin state, the Slater determinants have general spin orbits (GSO), which are characterized by the unitary transformation,

$$
(c_1, \ldots, c_n, c_{n+1}, \ldots, c_{2n}) = (a_{1\uparrow}, \ldots, a_{n\uparrow}, a_{1\downarrow}, \ldots, a_{n\downarrow}) \begin{pmatrix} U_{\uparrow\uparrow} & U_{\uparrow\downarrow} \\ U_{\downarrow\uparrow} & U_{\downarrow\downarrow} \end{pmatrix}.
$$

Restricted HF orbitals correspond to $U_{\uparrow\downarrow} = U_{\downarrow\uparrow} = 0$ and $U_{\uparrow\uparrow} = U_{\downarrow\downarrow}$, while different orbitals for different spins (DODS) correspond to $U_{\uparrow\downarrow} = U_{\downarrow\uparrow} = 0$ and $U_{\uparrow\uparrow} \neq U_{\downarrow\downarrow}$. GSO allow non-zero off-diagonal terms, that is, $(U_{\uparrow\downarrow})^\dagger = U_{\downarrow\uparrow} \neq 0$. As a result, dimension of the matrices become double. In addition, GSO-type Slater determinants break the original symmetries of the system, such as a translation and rotation. As shown below, this is very important to visualize the quantum fluctuations, but we have to recover the original symmetries of the system for the wavefunction. For this purpose, we adopt symmetry projections for each constituting S-det, which are symbolically denoted by $P^G$ in eq. (1). The symmetry projection corresponds to superposition of the Goldstone set for each symmetry broken state.

The most important feature of this method is that we can visualize the quantum fluctuations by analyzing the structures of the optimized Slater determinants.

We apply this method to the Hubbard model on the uniform triangular lattice, whose Hamiltonian is given by

$$
H = -t \sum_{<i,j>_{\sigma=\uparrow\downarrow}} (a_{i\sigma}^\dagger a_{j\sigma} + a_{j\sigma}^\dagger a_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow},
$$

where $t$ and $U$ represent the transfer integral between the nearest neighbor sites and the on-site Coulomb interaction, respectively. In the following calculations, the system size is $6 \times 6$, and a periodic boundary condition is imposed. This system has a $D_6$ rotational symmetry as well as a translational symmetry.

### 3. Results and Discussion

The phase diagram of the triangular Hubbard model has intensively been investigated by PIRG. The purpose of the present work is not a follow-up of PIRG results, but to explicitly show the quantum fluctuations in this system. Figure 1 shows the spin correlation function at $U/t = 10$, where the PIRG concluded that the ground state is the $120^\circ$ Neel state. We can see a significant peak at $(2\pi/3, 2\pi/3)$, which suggests a triple periodicity of the spin structure. This is consistent with the PIRG result. However, all the correlation function say is that the system has a triple periodicity of the spin structure.

**Figure 1.** Spin correlation function at $U/t = 10$. There exits a significant peak at $(2\pi/3, 2\pi/3)$, which corresponds a triple periodicity of the spin structure.
periodicity and we cannot conclude that such spin structure is certainly a $120^\circ$ Néel state. Furthermore, the peak at $(2\pi/3, 2\pi/3)$ is significantly reduced, compared to the uniform $120^\circ$ Néel state. The origin of this reduction is also unclear.

Before showing the Res-HF results, we briefly discuss the unrestricted HF (UHF) ground and low energy excited states. As shown in Fig.2(a), the UHF ground state at $U/t = 10$ is the $120^\circ$ Néel state. On the other hand, the excited states have one (b) or two (c) flipped spins marked by circles, and the $120^\circ$ Néel structure is modified around the flipped spins.

![Figure 2. Spin structures of UHF ground (a), and excited states (b, c) at $U/t = 10$.](image)

Now, we show in Fig.3 the structures of two typical Slater determinants generating the Res-HF wavefunction. We can see that $120^\circ$ Néel state is largely modified, especially around spins marked by circles. This modulation is much large and wide ranging compared to the UHF excited states. Thus, we can conclude that the modulation from the $120^\circ$ Néel spin structure makes dominant quantum fluctuations in the triangular Hubbard model and these quantum fluctuations reduce the uniform $120^\circ$ Néel spin structure. At the same time, we can say that the triple periodicity in the spin correlation function actually comes from the $120^\circ$ Néel structure. On the other hand, we should be careful to conclude that this spin correlation is really long-ranged, since this correlation is largely reduced, compared to the UHF result. We need larger systems to be investigated. In addition, the spin structure in the non-magnetic phase is another interesting subject. These challenging researches will be done in the near future.

![Figure 3. Spin structures of two typical Slater determinants generating the Res-HF wavefunction at $U/t = 10$.](image)

Finally, it might be meaningful to see how superposition of such Slater determinants lowers the energy compared to the uniform UHF ground state. For convenience, we denote the UHF ground state by $|UHF\rangle$, while Slater determinants having defects or deviations from the uniform UHF spin structure, as in Fig.3, are denoted by $|S1\rangle$, $|S2\rangle$, ... . The UHF ground state corresponds to the state having the lowest diagonal component $<UHF|H|UHF\rangle$. However, it does not lower the energy by the off-diagonal components, such as $<UHF|HP^G|UHF\rangle$, 


Table 1. \( N_S \)-dependence of the ground state energies by the Res-HF method at \( U/t = 10 \). UHF ground state energy is -15.226.

| \( N_S \) | Energy   |
|---------|----------|
| 1       | -16.224  |
| 3       | -16.468  |
| 5       | -16.574  |
| 7       | -16.636  |
| 9       | -16.671  |

or \( < UHF|H|S1 > \), because the UHF ground state has a uniform spin structure. On the other hand, the Slater determinants, shown in Fig.3, have large off-diagonal components, such as \( < S1|HPG|S1 > \), or \( < S2|H|S1 > \). Our results indicate that such off-diagonal components are important to lower the many-body ground state energy. We show how the Res-HF energy depends on the number of generating Slater determinants (\( N_S \)) in Table 1. The Res-HF energy is slightly lower than the PIRG result[3] when \( N_S \) is larger than 7.

4. Summary

The Res-HF method has been applied to the Hubbard model on the uniform triangular lattice. The spin correlation function shows the triple periodicity of the spin structure, and we have shown that such periodicity really comes from the 120° Néel structure. Furthermore, we have explicitly shown the deviations from the 120° Néel structure make quantum fluctuations in the triangular Hubbard model. The 120° Néel spin correlation is significantly reduced by these quantum fluctuations.

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References

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