Spin and charge response to magnetic frustration in strongly correlated itinerant electron systems

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We investigate the effects of magnetic frustration on spin and charge dynamics in strongly correlated itinerant electron systems by using the exact diagonalization technique. A Hubbard model with adjustable degree of magnetic frustration is constructed. Static and dynamic spin and charge correlation functions show different dependence on the degree of magnetic frustration in the system. With increasing magnetic frustration, the spin and charge correlation function spectra become more sparse, indicating a decreased level of mixing of the spin and charge degrees of freedom or a partial spin-charge separation.

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Magnetic frustration is known to play an important role in determining the material properties of magnetic systems. The Heisenberg model is extensively used to represent insulating magnetic materials that are treated as a collection of interacting local magnetic moments. Magnetic frustration is well defined and understood in such systems and has far-reaching consequences on their properties.[1] An extension to conducting materials requires the inclusion of the itinerant aspects of the material. A widely used formalism for strongly correlated itinerant electron systems is the t-J model[2] where electron hopping is included but the magnetic coupling between spin moments remains essentially the same as in the Heisenberg model. This allows a clear definition and characterization of magnetic frustration in the system.[3] However, the t-J model has certain limitations and is not applicable to materials where the electron correlation is strong but not enough to project out the double occupancy entirely. A more general formalism is offered by the Hubbard model[4] which under certain conditions (near half-filling in the strong interaction limit) can be transformed to the t-J model.[5] Since electrons are totally itinerant and are not explicitly described as local spin moments, magnetic frustration in the Hubbard model is not as intuitive as in the t-J and Heisenberg models. There is a lack of systematic understanding of magnetic frustration and its effects on the spin and charge dynamics in Hubbard systems.

In this paper, we report on an exact diagonalization study of a periodic cluster Hubbard model with magnetic frustration. A continuous change of the degree of magnetic frustration is allowed. The objective is to gain a systematic understanding of the behavior of magnetic frustration in strongly correlated itinerant electron systems and its effect on spin and charge dynamics. Magnetic frustration in the Hubbard model can be introduced by two general methods. The first is to introduce an external field and use constrained system geometries.[6] The second method is to explore the inherent properties of the system itself. A commonly used method of the latter kind is to introduce and adjust electron hopping beyond the nearest neighbors.[7] This yields competing exchange effects that cause magnetic frustration in the system. In the present work we adopt the second method.

The model Hamiltonian is defined on an eight-site cluster, as a part of a square lattice, with periodic conditions as shown in Fig. 1. It is written as

$$H=-t\sum_{(ij)\sigma} c_{i\sigma}^{\dagger}c_{j\sigma}-2s\sum_{\langle ij\rangle\sigma} c_{i\sigma}^{\dagger}c_{j\sigma}+U\sum_{i} c_{i\uparrow}^{\dagger}c_{i\uparrow}c_{i\downarrow}^{\dagger}c_{i\downarrow}. \tag{1}$$

All notation is standard in the Hubbard formalism. Here we consider the first and second nearest-neighbor (1NN and 2NN) hopping with amplitude $-t$ and $-s$, respectively. The factor of 2 in the second term is due to the renormalization introduced by the periodical boundary conditions.

In the above Hamiltonian, there is a parameter-dependent symmetry which determines the degree of geometric (magnetic) frustration in the system. When the ratio of the 2NN and 1NN hopping parameters, $s/t=0.5$, the system is topologically equivalent to a connected triangular ring structure (a tetrahedron), i.e., a magnetically frustrated system.[8] By

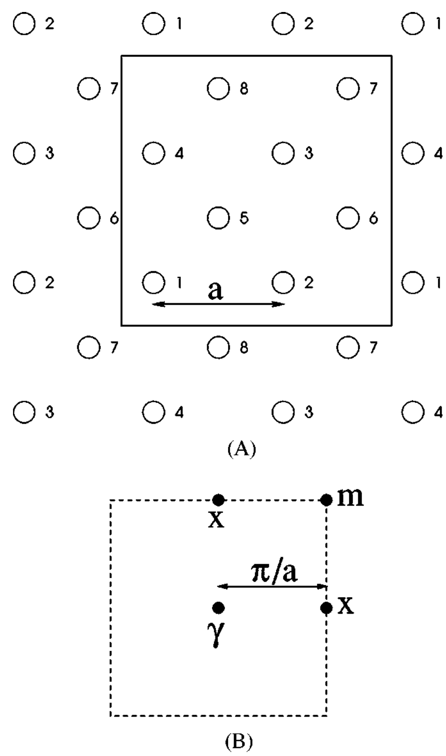

FIG. 1. (a) The eight-site cluster with periodic boundary conditions. (b) The corresponding high-symmetry points sampled in the first Brillouin zone.

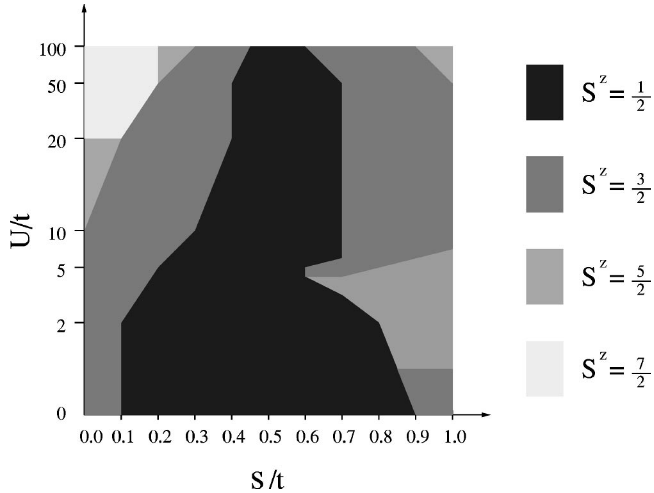

FIG. 2. Ground-state phase diagram of the Hubbard model for the nearly half-filled $(n=7)$ case. The ground-state magnetization is shown as functions of the on-site interaction strength and the degree of magnetic frustration in the system. Notice that the vertical axis is in logarithmic scale.

changing the s/t ratio, we can adjust the degree of magnetic frustration in the system, allowing a systematic study of the spin and charge response to the magnetic frustration. Due to the change of this hopping parameter-dependent symmetry, the hypotheses of the Nagaoka theorem[9] are not satisfied when the ratio s/t is nonzero. As a result, the ground state of the system is not always ferromagnetic even in the large-U limit. In particular, in the fully frustrated phase with $s/t=0.5$, the ground-state magnetization is always 1/2, i.e., spin minimally aligned. However, it should be noted that when s/t is large, the Nagaoka results will return.

The theoretical method used in this work is the small-cluster approach.[10] We consider in this work the case of seven electrons in the eight-site cluster, i.e., a nearly half-filled, highly correlated electron system. With two (one for each spin) orbitals on each site, there are 16 orbitals in the cluster shown in Fig. 1(A). Simple combinatorial arguments yield 11 440 many-body states in the cluster. The symmetries inherent in the Hamiltonian are exploited to diagonalize the complete many-body Hamiltonian matrices. A full sysmetry analysis of the eight-site Hubbard model is given by Freericks and Falicov.[11] In this work we only implemented partial symmetry analysis in the calculations. After the symmetry analysis, the largest block to diagonalize is of order 294.

We first examine the ground-state magnetization S^Z in the s/t-U/t phase space, as shown in Fig. 2, to characterize the magnetic frustration in the system. It is seen that the system undergoes a transition from high-spin states to low-spin states as s/t approaches 0.5. Several trends are clearly seen here. First, the system is fully ferromagnetic or nearly so when the interaction is strong and s/t is away from 0.5; it moves toward the fully frustrated state with $S^Z=1/2$ when $s/t=0.5$ is approached. It is also clear that with increasing short-range Coulomb interaction U, it becomes harder to achieve the spin-minimally-aligned (i.e., fully frustrated) state in the system. Another observation is that the effect of the change in s/t on the ground-state magnetization is asymmetric about the $s/t=0.5$ point.

A reduction in ground-state magnetization is a strong indication of magnetic frustration in the system. To further support this point, we examine the following magnetic correlation functions: $L_k=(1/L)\Sigma_{kNN}\langle S_i^Z S_j^Z\rangle$ where L_k is the kth nearest-neighbor (kNN) magnetic correlation ($k=0$ gives the on-site correlation with $i=j$), L the number of sites in the cluster, and $\langle\cdots\rangle$ the ground-state expectation value. In the cluster studied in this work there is a sum rule $L_0+2L_1+2L_2+2L_3=S^{Z2}/N$.

We have calculated these correlation functions for various interaction and hopping parameters and found that when the interaction is strong (e.g., $U/t=50$–100), L_1 totally vanishes and $L_2=-0.125$ at $s/t=0.5$, indicating a completely frustrated 1NN coupling and an antiferromagnetic 2NN coupling. Results under other interaction parameters show similar but less pronounced features.[12] When s/t is in a range close to 0.5 (0.3–0.8), the system shows alternating weak antiferromagnetic and ferromagnetic 1NN and 2NN correlations. These are characteristic of magnetically frustrated system.

The calculated results also indicate that L_0 decreases with U/t. This raises an interesting question about the suitability of the t-J model as the large-U version of the Hubbard model. In other words, what value of U is large enough to justify the use of the effective t-J model instead of the more realistic Hubbard model.[13] To address this question, we notice that in the large-U limit, when all double-occupied states are projected out as in the case of the t-J model, the on-site magnetic correlation function satisfies the sum rule $L_0=(1/L)\Sigma_i\langle S_i^Z S_i^Z\rangle=n/(4L)=7/32=0.2188$. Here $n=7$ is the number of electrons and $L=8$ is the number of sites in the cluster. The calculated results show that at $U/t=100$ this sum rule is essentially satisfied with only slight deviation when s/t increases. However, when we lower U/t to values still considered to be large to moderate, there is significant change in the value of L_0. For example, at $U/t=10$, the calculated L_0 is below the sum rule value by nearly 6%; at $U/t=5$, it is below by about 15%. Since the sum rule (5) still has to be satisfied here, other magnetic correlation functions also will be affected. Therefore, caution should be exercised in using the t-J model to interpret magnetic properties of the Hubbard systems. This may also apply to the interpretation of other physical properties.

To investigate the spin and charge response to the magnetic frustration in the system, we calculate static and dynamic spin and charge correlation functions. The static (equal-time) spin and charge correlation functions are defined as $S(Q)=(1/L)\langle\phi_0|S_{-Q}^Z S_Q^Z|\phi_0\rangle$ and $N(Q)=(1/L)\langle\phi_0|N_{-Q}N_Q|\phi_0\rangle$ with $S_Q^Z=\Sigma_i e^{iQR_i}S_i^Z$ and $N_Q=\Sigma_i e^{iQR_i}n_i$ where R_i is the lattice vector, Q the k vector, n_i the number of electron on site i, $|\phi_0\rangle$ the ground state, and L the total number of sites in the cluster. These correlation functions contain information on the spin and charge order in the system.

The calculated results show that the static charge correlation has little dependence on the degree of magnetic frustra-

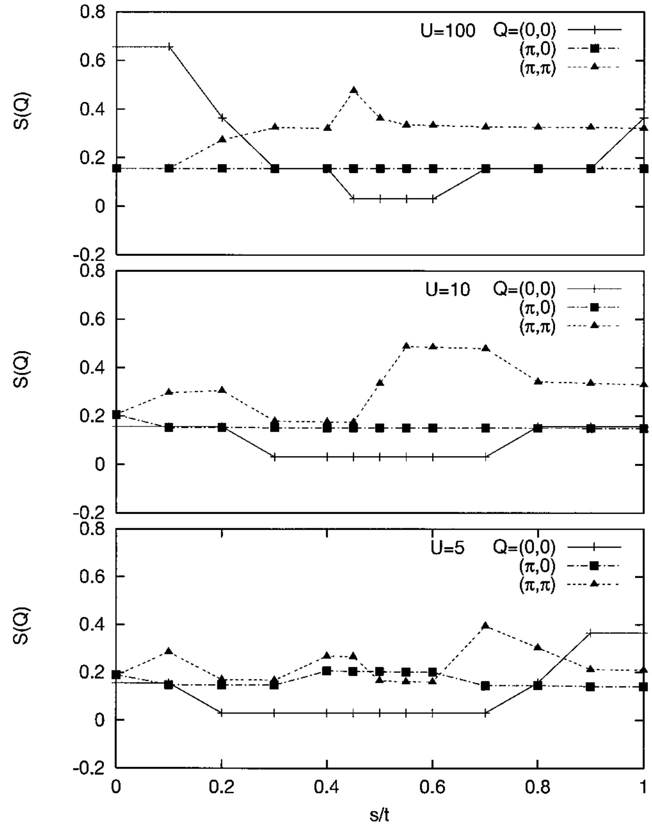

FIG. 3. The static spin correlation function vs s/t at the three k points sampled in the calculation for $U/t=5$, 10, and 100.

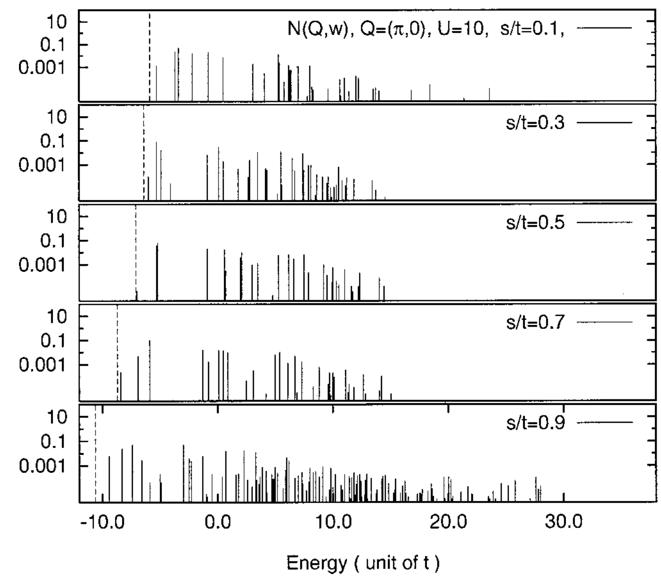

FIG. 4. The dynamic charge correlation function spectrum at the $X\ [Q=(\pi,0)]$ point for $U/t=10$ and various s/t values. The vertical dashed lines indicate the position of the ground-state energy of the system.

tion in the system, whereas the static spin correlation is quite sensitive to the change in magnetic frustration. This is consistent with the expectation that magnetic frustration will have more profound effect on the magnetic (spin) order in the system, and consequently the spin and charge degrees of freedom respond differently to the change in magnetic frustration. At the γ point $[Q=(0,0)]$, the static correlation function equals $n^2/L=6.125$, independent of the Hamiltonian parameters. At the other two k points $[Q=(\pi,0)$ and $(\pi,\pi)]$, the static correlation function stays essentially flat close to zero for all parameter choices, indicating that there is no charge density order in the system. The static spin correlation function is shown in Fig. 3. It has large values of $S[Q=(0,0)]$ near $s/t=0$ and 1 and small values (close to zero) when s/t is in a range close to 0.5. This range decreases with increasing U. This result reflects the magnetic order or lack of it in various part of the parameter space shown in Fig. 2. An interesting observation in the static spin correlation function is the large peak in the magnetically frustrated region for $Q=(\pi,\pi)$. It indicates a 3NN ferromagnetic coupling in the system under certain Hamiltonian parameter choices.

Since conclusions based on static structure factors $S(Q)$ and $N(Q)$ are highly indirect and sometimes unable to reveal and distinguish important features,[14] an investigation of the dynamic spin and charge response is highly desirable. The dynamical spin and charge correlation functions are defined as $S(Q,\omega)=(1/L)\Sigma_v|\langle v|S_Q^Z|\phi_0\rangle|^2\delta(\omega-E_v+E_0)$ and $N(Q,\omega)=(1/L)\Sigma_v|\langle v|N_Q|\phi_0\rangle|^2\delta(\omega-E_v+E_0)$ where $|v\rangle$ is the vth eigenstate with energy E_v.

The calculated $S(Q,\omega)$ and $N(Q,\omega)$ at the $X\ [Q=(\pi,0)]$ point are shown in Figs. 4 and 5. The results at the $M\ [Q=(\pi,\pi)]$ point show similar behavior. We first notice that both show broad continuum spectra with the same energy scale. This indicates substantial spin-charge interaction in the system,[14] which couples the charge and spin excitations to the full Hilbert space, yielding a relatively dense spectrum even for a small (eight-site) cluster size that usually

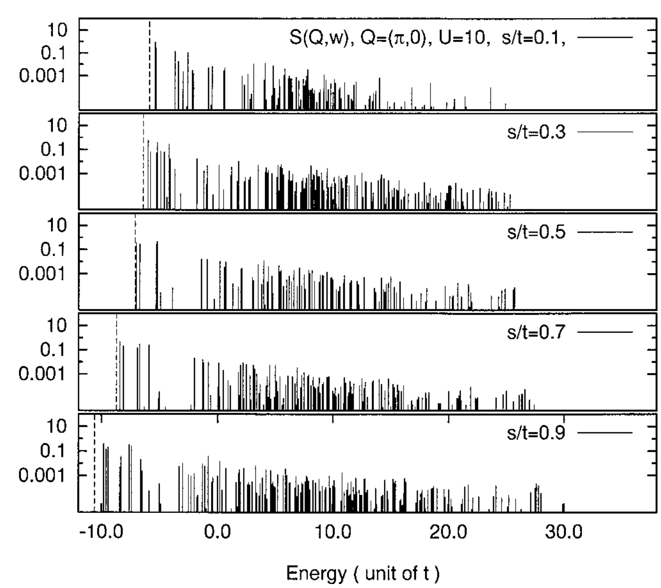

FIG. 5. The dynamic spin correlation function spectrum at the $X\ [Q=(\pi,0)]$ point for $U/t=10$ and various s/t values. The vertical dashed lines indicate the position of the ground-state energy of the system.

produces very sparse spectral peaks as a result of the relatively small number of degrees of freedom included in the calculation. However, when s/t approaches 0.5, the spectra become more sparse, indicating a reduced level of spin-charge mixing or a partial spin-charge separation in the system.[14,15] This result is consistent with the conclusion drawn from the analysis of the static spin and charge correlation functions, that they respond differently to the change in magnetic frustration. We see a spectral narrowing in the dynamic charge correlation function as s/t approaches 0.5, but no such narrowing is observed in the corresponding dynamic spin correlation function. It indicates that high-energy charge excitations are suppressed as magnetic frustration increases. A detailed analysis of the calculated dynamic correlation functions reveals that as s/t approaches 0.5, spectral weight is transferred from high-energy scale to low-energy scale. This can be understood as the consequence of the increase of low-energy spin excitation induced by increasing magnetic frustration in the system.

We have performed the calculations for other values of U/t and have found the conclusions given above remain valid for a broad range of U/t ($U/t=5-100$ tested). Differences are only quantitative; qualitative trends are the same. The only point worth mentioning here is that in large-U cases, a distinct satellite structure is observed in the high-energy scale in both $N(Q,\omega)$ and $S(Q,\omega)$, and increasing magnetic frustration suppresses spin excitations in the satellite structure very effectively but works to a much less degree of effectiveness in the charge excitation case. Again, this can be understood by realizing that magnetic frustration favors low-energy spin excitation.

In summary, we have constructed a Hubbard model with adjustable degree of magnetic frustration in the context of a periodic small-cluster approach and have studied the effects of magnetic frustration on the magnetic order and spin and charge dynamics, using the exact diagonalization technique. We have found that spin and charge degrees of freedom respond very differently to the change in magnetic frustration in the system. The calculated static charge correlation results indicate a lack of charge density order in the system while the static spin correlation results reveal the sensitivity and change of magnetic order in the system in response to the presence of magnetic frustration. A correlation between the degree of spin-charge mixing and magnetic frustration is observed in the calculated dynamic spin and charge correlation functions. Increasing magnetic frustration leads to a partial separation of the spin and charge degrees of freedom. This may justify an effective spin Hamiltonian for the description of the low-energy magnetic properties of frustrated itinerant electron systems.

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