Magnetism in the two-dimensional t-t' Hubbard model: From low- to over-doping

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Based on quantum Monte Carlo calculations, we shall discuss the regime where ferromagnetic correlation is dominant in the two-dimensional t-t' Hubbard model at a finite temperature. In this model, ferromagnetism competes with antiferromagnetism and we reveal how crossover occurs between them at a finite temperature by the bias-free method. We shall investigate the data in the context of the so-called "low-density ferromagnetism." The weak-coupling result is also shown and the data are compared with the "Nagaoka ferromagnetism."

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I. INTRODUCTION

The Hubbard model is a basic model to study phenomena due to correlation effects in the electron system, e.g., itinerant ferromagnetism. Exact results have been accumulated in one and infinite dimensions, but many problems are left to be solved in other dimensions.[1] Generally speaking, quantum fluctuation is large in lower dimensions, which leads to many fascinating properties. Therefore the two-dimensional (2D) Hubbard model is one of the central issues in modern condensed matter physics. In this paper, we discuss magnetic properties in one of the prototypes, 2D Hubbard models on a square lattice with the nearest (t) and next-nearest neighbor (t') hopping, which we call "t-t' Hubbard model" in this paper. Our main focus is on the itinerant ferromagnetism.

Recently the t-t' Hubbard model was studied with the filling at the "Van-Hove density" and appearance of itinerant ferromagnetism was suggested in the ground state at $t'/t=0.47$ (Ref. 2) (note that it contrasts with a previous conclusion in, e.g., Ref. 3). We call it "low-density ferromagnetism" in this paper.[4,5] A variational study has also been performed for a more extended parameter window in the phase diagram.[6] Superconducting properties have also been studied.[7] Further, quantum spin phase has been discovered at half filling in Ref. 8. However, bias-free systematic data on the global properties are left to be revealed (as a function of, e.g., filling and t'/t) and it is what we want to study in this paper.

Since the itinerant ferromagnetism is one of the longstanding, classical problems in condensed matter physics (see, for example, Refs. 9–12), it is crucial to shed light on the magnetism in the t-t' Hubbard model by a bias-free method. In this paper, we reveal the magnetic properties in the t-t' Hubbard model from low- to over-doping, based on an approximation-free method: finite-temperature auxiliary-field quantum Monte Carlo (AFQMC).[13–15] In some cases, however, we have to reach the temperature regime with a severe negative-sign problem (see, e.g., Ref. 16) for the study of the itinerant ferromagnetism. In order to overcome the difficulty, we employ an algorithm which has been proposed recently, constrained path QMC (CPQMC).[17]

II. MODEL

The t-t' Hubbard model is described by the following Hamiltonian on a square lattice with a periodic boundary condition:

$$\begin{aligned}\mathcal{H} = &-t\sum_{\langle i,j\rangle\in\text{n.n.},\sigma}(c^\dagger_{i\sigma}c_{j\sigma}+\text{H.c.})\\ &+t'\sum_{\langle k,l\rangle\in\text{n.n.n.},\sigma}(c^\dagger_{k\sigma}c_{l\sigma}+\text{H.c.})\\ &+U\sum_i(n_{i\uparrow}-1/2)(n_{i\downarrow}-1/2)-\mu\sum_i n_i,\end{aligned}\tag{1}$$

where $c^\dagger_{i\sigma}/c_{i\sigma}$ creates/annihilates an electron at the site i and $n_{i\sigma}=c^\dagger_{i\sigma}c_{i\sigma}$. The $t(t')$ denotes the nearest (next-nearest neighbor) hopping amplitude and U the strength of the on-site Coulomb interaction. The μ is the chemical potential, which controls the filling $n=N^e/\Omega$ (N^e is the electron number and Ω is the site number) and we also use a notation $\tilde{\mu}=\mu+U/2$. In the following, we set both t and t' to be positive (see also the discussion later which concerns the sign of t and t').

III. WEAK-COUPLING APPROACH

In this section, we study the t-t' Hubbard model through the weak-coupling approach. In the beginning, let us study the case of free fermion

$$\begin{aligned}\mathcal{H}_0 = &-\sum_{\langle i,j\rangle\in\text{n.n.},\sigma}t(c^\dagger_{i\sigma}c_{j\sigma}+\text{H.c.})\\ &+\sum_{\langle k,l\rangle\in\text{n.n.n.},\sigma}t'(c^\dagger_{k\sigma}c_{l\sigma}+\text{H.c.}).\end{aligned}\tag{2}$$

Defining the Fourier transformation by $c_{j\sigma}=1/\sqrt{L_xL_y}\Sigma_k\exp(ikj)\overline{c_{k\sigma}}$ and $k=(k_x,k_y)$ (the system size is $L_x\times L_y$), we get

$$\begin{aligned}\mathcal{H}_0 &= -\sum_{k,\sigma}2t(\cos k_x+\cos k_y)\overline{c^\dagger_{k\sigma}}\,\overline{c_{k\sigma}}\\ &\quad+\sum_{k,\sigma}4t'\cos k_x\cos k_y\overline{c^\dagger_{k\sigma}}\,\overline{c_{k\sigma}}\\ &=\sum_{k,\sigma}\epsilon(\boldsymbol{k})\overline{c^\dagger_{k\sigma}}\,\overline{c_{k\sigma}}.\end{aligned}\tag{3}$$

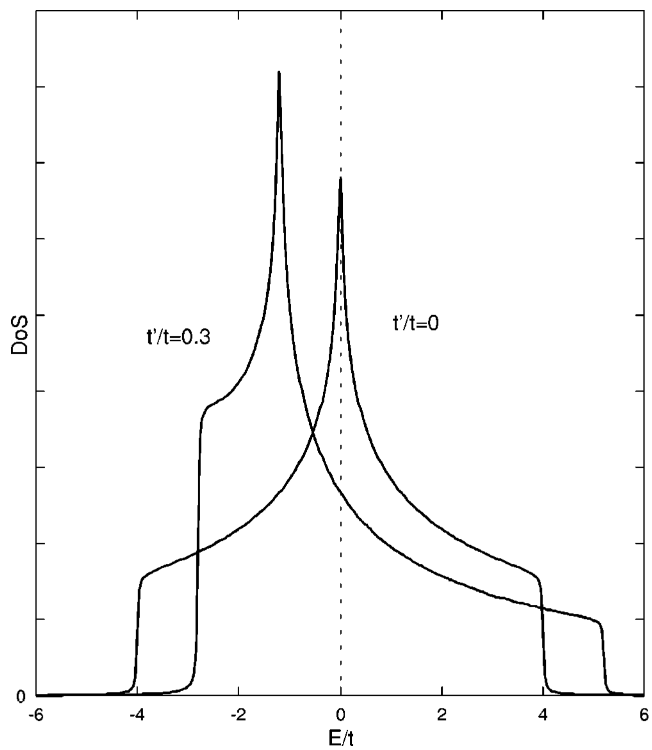

FIG. 1. DoS without interaction for $t'/t=0,0.3$.

The density of states (DoS) has a support of $[-4(t-t'),4(t+t')]$ $(t'/t \leqslant 0.5)$ and shows a diverging behavior at the Van-Hove energy (see Fig. 1).

Based on the mean-field theory for the ferromagnetism, a naive expectation is that, when the Fermi energy is set near the Van-Hove energy, the ferromagnetic correlation is dominant. But this picture does not hold even in the weak-coupling approach especially near half-filling. Actually let us

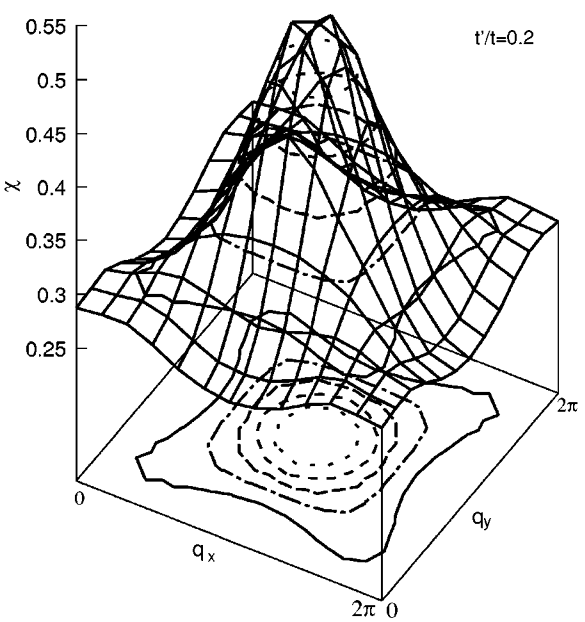

FIG. 2. Magnetic susceptibility $\chi(\boldsymbol{q})$ by the RPA ($t'/t=0.2$, $U/t=1$, $T/t=0.3$) on a 12×12 lattice.

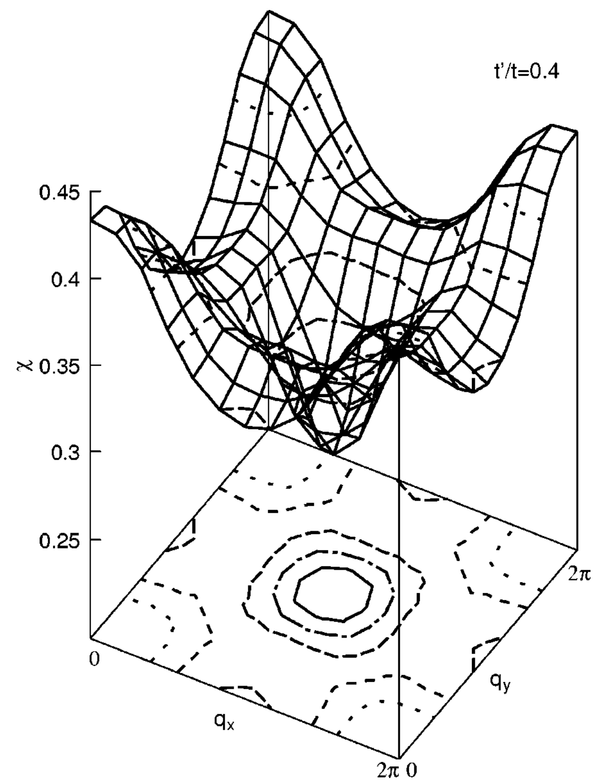

FIG. 3. Magnetic susceptibility $\chi(\boldsymbol{q})$ by the RPA ($t'/t=0.4$, $U/t=1$, $T/t=0.3$) on a 12×12 lattice.

show the weak-coupling results by the random phase approximation (RPA). In the RPA, the magnetic susceptibility $\chi(\boldsymbol{q})$ is given by

$$\chi(\boldsymbol{q}) = \chi_0(\boldsymbol{q})[1 - U\chi_0(\boldsymbol{q})]^{-1} \tag{4}$$

and

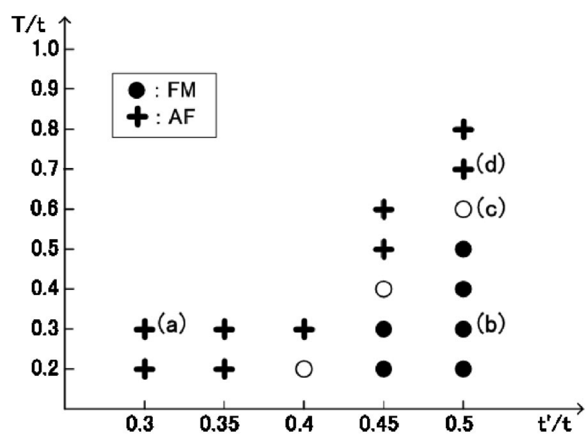

FIG. 4. t'/t-T/t phase diagram which shows the magnetic property for the t-t' Hubbard model on a 12×12 lattice with $U/t=4$. The Fermi energy is set at the Van-Hove energy of the free fermion. It shows competition between ferromagnetism (Fm) and antiferromagnetism (AFm), as t'/t and the temperature (T) is varied. FM(AFM) means that the system is (anti)ferromagnetic(like) respectively (see Sec. IV for the precise definition of this terminology).

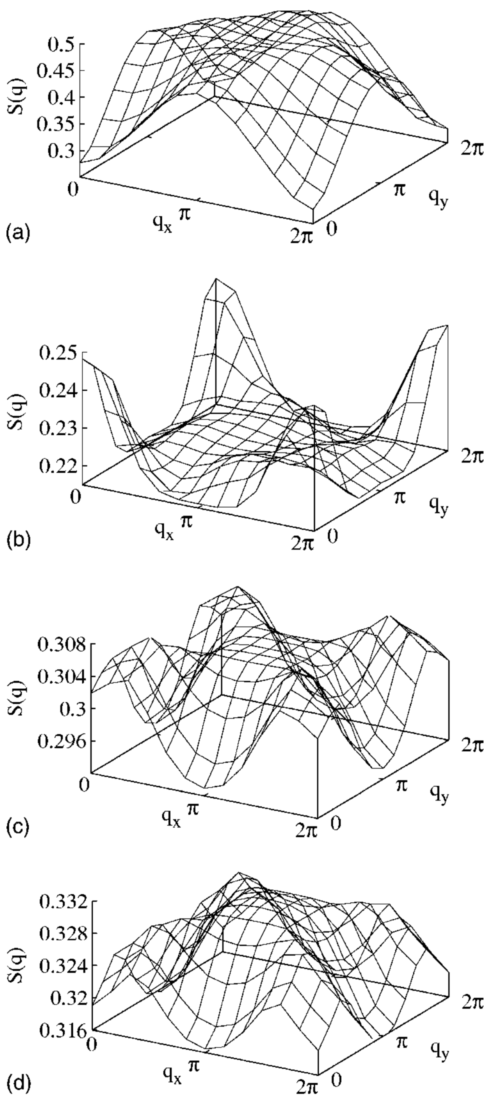

FIG. 5. Spin structure factor $S(\boldsymbol{q})$ on a 12×12 lattice with $U/t=4$. The Fermi energy is at the Van-Hove energy: (a) $t'/t=0.3$, $T/t=0.3$, (b) $t'/t=0.5$, $T/t=0.3$, (c) $t'/t=0.5$, $T/t=0.6$, and (d) $t'/t=0.5$, $T/t=0.7$. In (a), there is a peak around $\boldsymbol{q}=(\pi,\pi)$ (antiferromagneticlike). In (b), there is a peak at $\boldsymbol{q}=(0,0)$ (ferromagnetic). As the temperature (T) is increased [from (b) to (d)], crossover occurs from ferromagnetic to antiferromagneticlike correlation.

$$\chi_0(\boldsymbol{q}) = -\frac{1}{\Omega}\sum_{\boldsymbol{k}} \frac{f[\overline{\epsilon}(\boldsymbol{k}+\boldsymbol{q})] - f[\overline{\epsilon}(\boldsymbol{k})]}{\overline{\epsilon}(\boldsymbol{k}+\boldsymbol{q}) - \overline{\epsilon}(\boldsymbol{k})}, \qquad (5)$$

where the summation is over $[0,2\pi)\times[0,2\pi)$, $\overline{\epsilon}(\boldsymbol{k})=\epsilon(\boldsymbol{k})-(\mu+U/2)=\epsilon(\boldsymbol{k})-\tilde{\mu}$ and $f(x)=1/[\exp(\beta x)+1]$ ($\beta=1/T$ and T is the temperature). The results are shown in Figs. 2 and 3 where the Fermi energy is at the Van-Hove energy. It tells us that ferromagnetic correlation competes severely with antiferromagneticlike one near half-filling (low-doping regime) in the t-t' Hubbard model. But, far away from half-filling (over-doping regime), the results suggest that the ferromagnetic correlation dominates. As is well known, however, the ferromagnetic correlation is overestimated in the weak-coupling approach. Then, in order to get approximation-free results, we shall apply the QMC method in the next section.

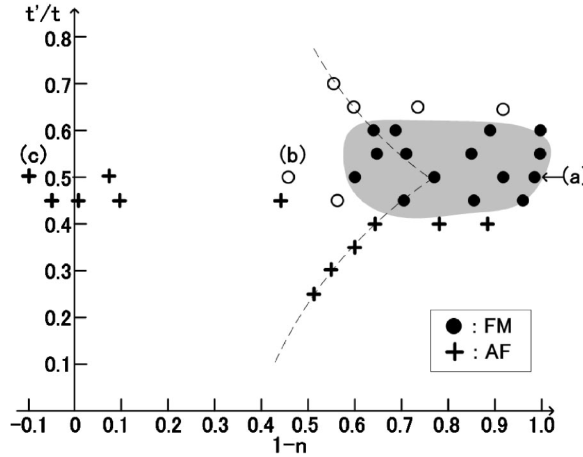

FIG. 6. n-t'/t phase diagram which shows the magnetic property for the t-t' Hubbard model on a 12×12 lattice with $U/t=4$ and $T/t=0.3$. Dashed line corresponds to the case when the Fermi energy is at the Van-Hove energy of the free system. The shaded region corresponds to the parameters where ferromagnetic correlation is dominant.

IV. QMC RESULTS

In this section, based on the QMC technique, we show our results on the magnetic properties for the t-t' Hubbard model. In order to discuss the magnetism, we adopt the spin structure factor

$$S(\boldsymbol{q}) = \frac{1}{\Omega}\sum_{j,k} \exp[-iq(j-k)]\langle S_j^z S_k^z\rangle, \qquad (6)$$

where $S_i^z=\frac{1}{2}(n_{i\uparrow}-n_{i\downarrow})$ and $\langle\cdots\rangle$ means the grand-canonical ensemble average at a finite temperature T.

In the beginning, we set the chemical potential μ to be at the Van-Hove energy of the free fermion. Figure 4 shows how the magnetic behavior changes as a function of t'/t and T/t with the system size 12×12 and $U/t=4$. Ferromagnetic correlation emerges only in the low temperature region around $t'\sim 0.5t$. It is based on the extrapolated spin structure factor for the Trotter decomposition in the imaginary time axis ($\Delta\tau\to 0$) from three data typically at $t\Delta\tau=0.100$, 0.050, and 0.033.

In this paper, “ferromagnetic correlation is dominant” (or simply “ferromagnetic”) means that the spin structure factor $S(\boldsymbol{q})$ has a peak just at $\boldsymbol{q}=(0,0)$ [and “antiferromagneticlike” means the peak is *around* $\boldsymbol{q}=(\pi,\pi)$] apart from the statistical error in the QMC. Note that all of the correlation in this paper is short ranged due to finite-temperature effects. Typical spin structure factor is shown in Figs. 5(a)–5(d), which correspond to data points (a)–(d) in Fig. 4.

Next, away from the Van-Hove energy, we study how the “ferromagnetic regime” extends as the filling (n) and t'/t are varied at the temperature $T/t=0.3$ on a 12×12 lattice. As shown in Fig. 6, the ferromagnetic regime extends even

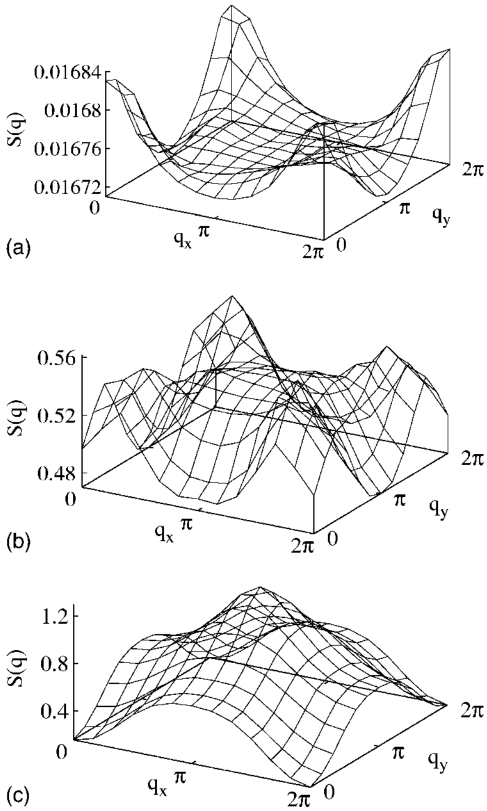

FIG. 7. Spin structure factor $S(\boldsymbol{q})$ on a 12×12 lattice with $t'/t=0.5$, $U/t=4$, and $T/t=0.3$. (a) $n=0.02$, (b) $n=0.54$, (c) $n=1.10$. Crossover from ferromagnetic to antiferromagneticlike correlation is observed, when we approach the half filling $n=1$ [from (a) to (c)].

away from the Van-Hove "line" on which the Fermi energy is set at the Van-Hove energy of the free fermion. It is the "low-density ferromagnetism" discussed in Ref. 2 and its extension. We also varied $T/t(\sim0.3)$ and found that the ferromagnetic regime is robust and the phase diagram is the same qualitatively, so far as we have studied. We also confirmed that the sign of t and t' is irrelevant around the Van-Hove line. Typical spin structure factor $S(\boldsymbol{q})$ is shown in Figs. 7(a)–7(c), which correspond to data points (a)–(c) in Fig. 6. Further we revealed that the regime expands, when U/t is increased (see Figs. 8 and 9). In the case when both t and t' is positive, the Nagaoka's theorem holds and the

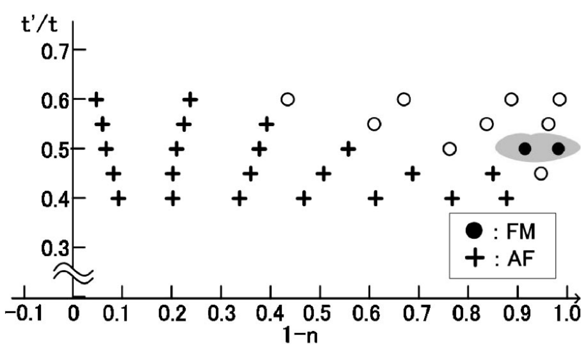

FIG. 8. The same as Fig. 6 with $U/t=2$.

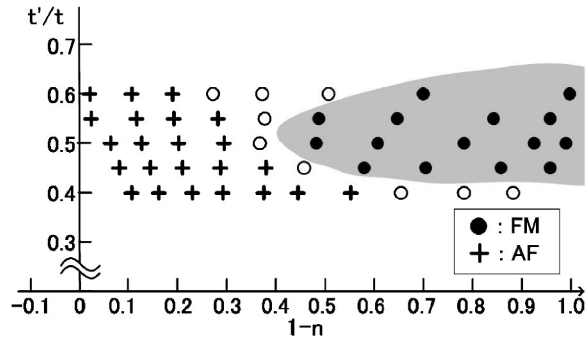

FIG. 9. The same as Fig. 6 with $U/t=5$.

ground state is expected to be ferromagnetic (or near to it) in the vicinity of the half-filling.[18] Therefore, based on the present results, we conjecture that the ferromagnetic regime finally connects to the "Nagaoka ferromagnetism" in the strong-coupling regime (large U/t). It is difficult, however, to study the regime by the present method due to numerical instabilities and it is the beyond the scope of this paper.

Finally, let us comment on the negative sign problem. In our data, there is no serious problem so far as when $T/t\geqslant0.3$ is satisfied. Below it, however, the AFQMC does not always work well due to the negative sign problem. In order to overcome it, we have applied the CPQMC technique and got data for $T/t\leqslant0.3$ (see also the Appendix).[17]

V. SUMMARY AND DISCUSSION

To summarize, based on the bias-free, QMC technique, we have found the regime where the ferromgnetic correlation is dominant in the 2D t-t' Hubbard model at a finite temperature. In this model, we revealed how crossover occurs between ferromagnetism and antiferromagnetism at a finite temperature. We investigated the data in the context of the so-called low-density ferromagnetism. The weak-coupling result is also shown and the data are compared with the Nagaoka ferromagnetism.

The ferromagnetic regime expands in the strong-coupling region (large U/t). Therefore it is an interesting open problem to study the strong-coupling region in more details and elucidates the connection with the Nagaoka ferromagnetism.[18] Moreover the correlation effects should be relevant near the ferromagnetic criticality. Then a quasiparticle structure might emerge in the vicinity of the Mott insulator.[19,20]

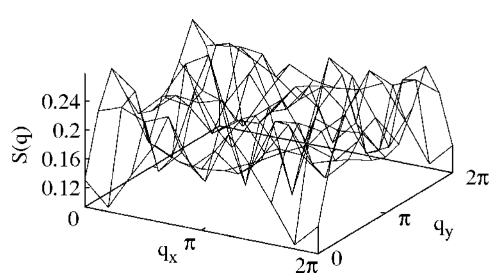

FIG. 10. Spin structure factor $S(\boldsymbol{q})$ by the AFQMC. The system size is 10×10, $t'/t=0.5$, $U/t=4$, and $T/t=0.2$.

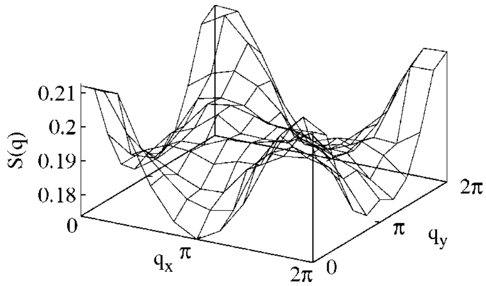

FIG. 11. Spin structure factor $S(\boldsymbol{q})$ by the CPQMC. The parameters are the same as Fig. 10.

In order to compare data with the t-t' Hubbard model, we have also studied the 2D Hubbard model on a triangular lattice by the AFQMC technique. In that model, we set the chemical potential near the Van-Hove energy of the free system (as in the t-t' Hubbard model). We expect the same physics as the t-t' Hubbard model discussed in this paper. However, no evidence for the ferromagnetism in that model is found, so far as can we study. But the strong-coupling regime on a triangular lattice is beyond our reach.

Further, it is challenging to shed light on the lower temperature regime than we studied. As the temperature is lowered, the tendency toward many kinds of order should appear and they may compete severely. There it is possible that superconducting correlation becomes dominant.

APPENDIX: CPQMC RESULTS

In this appendix we demonstrate the efficiency of the CPMC method. Note that we verified the validity of the CPQMC technique in comparison with the AFQMC method, in the region where both methods are available.

When $t'/t=0.5$ and $T/t=0.2$ on a 10×10 lattice for example, the negative sign problem is so severe that the statistical error washes out the fine structure of the magnetic properties (Fig. 10). By applying CPQMC to this, we found that the data is recovered (Fig. 11) and the result is consistent. It is to be noted, however, that the lower region (e.g., $T/t=0.1$) can not be reached even through the CPMC method due to notoriously severe negative-sign problem. Since it is possible that superconducting correlation wins there, it is interesting to explore the region.

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