Electron-hole asymmetry in magnetic properties of lightly doped high-T_C superconductors: a quantum Monte Carlo study

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Abstract

Using a recently developed variational quantum Monte Carlo method, magnetic properties of high-T_C superconductors are studied at zero temperature (T), by numerical simulations on the 2D t-J model. Our focus here is to explore the difference in the properties of p-type and n-type cuprates as a function of the carrier concentrations close to half filling. As observed experimentally, it is found that the antiferromagnetically ordered phase persists even for a small, yet finite amount of carrier doping, and that this phase is more robust in the electron doped case.

Key words: high-T_C cuprate; t-J model; quantum Monte Carlo; spin correlation

There have been stimulating studies on high-T_C superconductors to explore the underlying mechanism and unusual normal state properties. Experimentally much attention has been recently devoted to rather lightly doped p- and n-type cuprates [1]. This is partially because high quality samples have become now available, and because it is now clear that understanding the evolution of the electronic state with carrier doping from undoped Mott insulator is crucial to clarify the nature of the systems. Theoretically it is still in the middle of extensive debate. It is widely accepted however that a 2D t-J-like model can describe low-energy physics of cuprates defined by the following Hamiltonian [2];

$$H = J\sum_{\langle i,j\rangle}(\mathbf{S}_i\cdot\mathbf{S}_j - n_in_j/4) - t\sum_{\langle i,j\rangle\sigma}\left(\tilde{c}^\dagger_{i,\sigma}\tilde{c}_{j,\sigma} + \text{H.c.}\right) - t'\sum_{\langle\langle i,j\rangle\rangle\sigma}\left(\tilde{c}^\dagger_{i,\sigma}\tilde{c}_{j,\sigma} + \text{H.c.}\right). \quad (1)$$

Here the notation is conventional (see *e.g.*, Ref [3]). Introduction of next nearest-neighbor hopping t' deserves some explanation; small cluster calculations have shown that the t-J model indeed capture low energy physics of more involved multi-band models with t'/t negative (positive) for hole-doped (electron-doped) case, at least for small carrier densities x [4]. We remind that this sign difference originates from the fact that the parent cuprates are charge transfer insulators, and therefore a "carrier" represents in the model a Zhang-Rice singlet (an inert Cu d^{10} configuration) for the hole (electron) doped system. It is also now widely accepted that, in the half-filling undoped case, the model shows antiferromagnetic (AFM) long-range order at $T = 0$. It is very interesting therefore to study theoretically how strong this AFM phase is against carrier doping and how the robustness of the phase depends on the nature of doped carriers.

There exist several numerical studies on small clusters (≤ 26 sites) indicating that at finite x close to half-filling positive (negative) t'/t enhances (degrades) AFM correlations compared to $t' = 0$ [5]. Although these results might give the correct trend at short distances, it is difficult within such small cluster calculations to really assess the existence of long-range order. For this purpose we have studied this issue using quantum Monte Carlo techniques, which allows much larger sizes ($\simeq 100$ sites).

To study ground sate properties of the 2D t-t'-J

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model (1), we employ a recently developed variational quantum Monte Carlo method by Sorella [3,6]. Results presented here are computed by variational and fixed node methods (VMC and FN, respectively), and the details on how to minimize the energy for a variational wave function with many parameters are found in Ref. [3]. We just mention here that we employ the most general singlet variational wave function of the Jastrow-BCS form, with a pairing function of d-wave symmetry. The Jastrow factor, which includes the Gutzwiller projector, makes the wave function of the RVB type. After all the possible variational parameters are optimized, we obtain a fairly good guiding function that is used for FN. Also note that the variational energy of FN is lower than the one of VMC [6].

Main results are summarized in Figs. 1 and 2 where real-space spin-spin correlation functions are given for various t'/t and doped carrier concentrations x [7] at $J/t = 0.3$. These results provide clear evidence that strong spin correlations remain finite at the largest distances for finite carrier concentrations x. The critical x_c above which long range order disappears apparently depends on the parameters used; for the present set of $t'/t = -0.2$, 0, and 0.2, $x_c \simeq 0.06$, 0.08, and 0.12, respectively. Of particular interest is the result that the spin correlations are enhanced (degraded) when positive (negative) t'/t is incorporated into the model, corresponding to electron (hole) doing. Our results are consistent with the previous studies [5,8] and experimental observations [9].

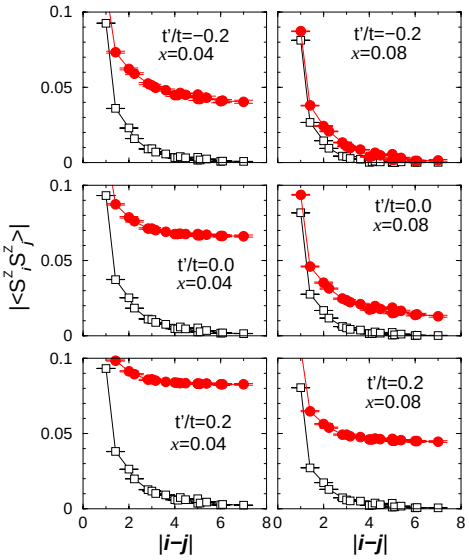

Fig. 1. Absolute value of real-space spin correlation functions for 2D t-t'-J model with $J/t = 0.3$ and $t'/t = -0.2$ (top), 0.0 (middle), and 0.2 (bottom). Carrier densities x are 0.04 (left) and 0.08 (right) on a tilted square lattice of $\sqrt{98} \times \sqrt{98}$. Open squares and solid circles are for VMC and FN, respectively.

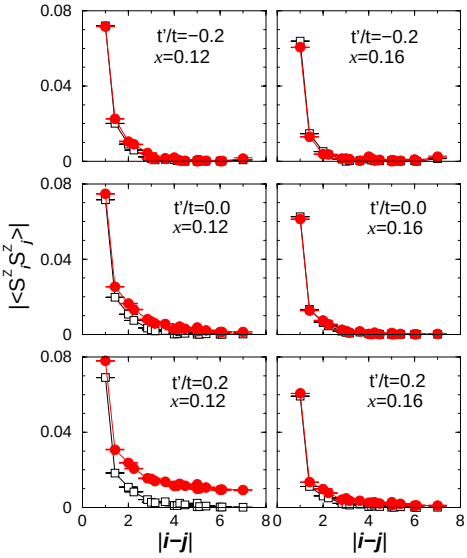

Fig. 2. Same as in Fig. 1, but $x = 0.12$ (left) and 0.16 (right).

In conclusion, magnetic properties of the lightly doped 2D t-J model with next nearest neighbor hopping t' are numerically studied to understand the different behaviors as a function of carrier concentrations for hole ($t'/t < 0$) and electron ($t'/t > 0$) doping. Our large cluster calculations clearly show that AFM long-range order exists away from half-filling and is more robust for the electron doped case. These results compare very well with experimental observations. More detailed analyses and other properties will be presented in a separate paper [10].

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