

## Comments

Comments are short papers which criticize or correct papers of other authors previously published in the *Physical Review*. Each Comment should state clearly to which paper it refers and must be accompanied by a brief abstract. The same publication schedule as for regular articles is followed, and page proofs are sent to authors.

### Comment on "Magnetic susceptibility of the two-dimensional Hubbard model"

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The observed magnetic spin susceptibility of high-temperature superconductors such as  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  increases when  $x$  increases from zero, i.e., as one dopes away from half-filling. Recent Monte Carlo simulations of A. Moreo [Phys. Rev. B **48**, 3380 (1993)] suggest that this behavior can be reproduced by the two-dimensional Hubbard model only at large coupling, namely,  $U/t$  of order 10. Using longer runs, our Monte Carlo simulations show that the same behavior as for  $U/t=10$  is obtained even in the intermediate coupling regime ( $U/t=4$ ), as long as the temperature is low enough ( $T=t/6$ ) that strong antiferromagnetic correlations are building up at half-filling. These results are consistent with the fact that in two dimensions, the generalized random phase approximation should fail in the parameter range where it predicts a magnetic phase transition.

One of the main puzzles in establishing the applicability of the one-band Hubbard model to high-temperature superconductors is the behavior of the uniform magnetic spin susceptibility as obtained, say, by Knight-shift measurements.<sup>1</sup> While the maximum as a function of temperature is easy to understand qualitatively from the behavior of the Hubbard model at half-filling in the strong-coupling (Heisenberg) regime, the behavior away from half-filling and in the intermediate- or weak-coupling regime is theoretically much more uncertain. The limiting low-temperature value of the magnetic susceptibility experimentally increases as a function of doping, a behavior which at first glance can be reproduced within perturbative approaches only in models which include second-neighbor hopping.<sup>2</sup> With only nearest-neighbor hopping, nonperturbative effects, such as pseudogaps<sup>3</sup> are usually invoked.

To numerically check under what conditions the one-band nearest-neighbor Hubbard model reproduces the experimentally observed behavior,<sup>1</sup> Moreo<sup>4</sup> has studied the magnetic spin susceptibility using determinantal quantum Monte Carlo techniques.<sup>5,6</sup> Moreo has shown that on a  $4\times 4$  lattice at inverse temperature  $\beta=4/t$  the susceptibility has a maximum at half-filling and decreases with doping in the intermediate-coupling regime  $U/t=4$ , while in the strong-coupling regime  $U/t=10$ , the susceptibility increases with hole doping near half-filling, resembling the experimental results<sup>1</sup> obtained for  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ . Moreo suggests that experimental results can be reproduced only when the coupling is quite large, namely,  $U/t=10$  or more.

We have used the same quantum Monte Carlo technique on a  $4\times 4$  lattice for  $U/t=4$  but at lower tempera-

ture, namely,  $k_B T=t/6$ , or inverse temperature  $\beta=6/t$ . As shown in Fig. 1, we find that at this lower temperature, the susceptibility has qualitatively the same behavior as that observed for larger coupling ( $U/t=10$ ) and larger temperature ( $\beta=4/t$ ) by Moreo. We measured the structure factor instead of the uniform magnetic susceptibility but these quantities are easily related using the fluctuation-dissipation theorem. To obtain the results of Fig. 1, one must perform much longer runs than is usually done. Typically, to obtain one point on the curve we have used  $\Delta\tau=\frac{1}{15}$  and 100 000 warm-up sweeps of the whole space-time lattice before the measurements were taken. Measuring the static structure factor after

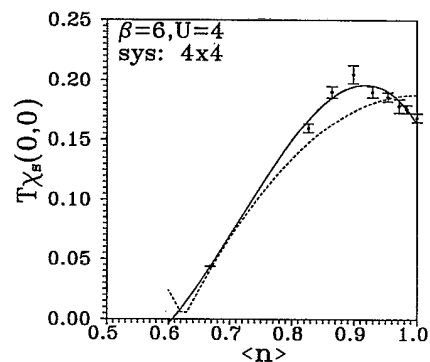


FIG. 1. The static magnetic spin susceptibility  $\chi_s$ , multiplied by temperature  $T$  is plotted as a function of band filling  $\langle n \rangle$ . The units are  $t=1$ ,  $k_B=1$ ,  $\hbar=2$ . Monte Carlo results are shown by points and error bars. The solid line is a guide to the eye. The dotted line shows the result for the free case ( $U=0$ ) for the same system size and temperature.

every update of the lattice in space, and doing no measurement every other update of the whole space-time lattice, we have made of order 10 000 000 measurements, using blocks of 10 000 measurements to eliminate the effect of sticking<sup>7</sup> on the estimation of the statistical error. It takes almost one week of computing time to obtain one point in Fig. 1 with a processor executing 27 million floating-point operators per second.<sup>8</sup>

Our results and those of Moreo<sup>4</sup> suggest that it is the presence of strong antiferromagnetic correlations at half-filling which yield a maximum in the magnetic susceptibility away from half-filling. Figure 3 of Ref. 6 shows that at  $U/t=4$  on a  $4\times 4$  lattice, the antiferromagnetic correlation length at half-filling has basically reached the size of the lattice<sup>9</sup> at the temperature we studied ( $\beta=6/t$ ), while it has not quite made it at the temperature ( $\beta=4/t$ ) studied by Moreo.<sup>4</sup> Evidently, at larger values of  $U/t$  the antiferromagnetic correlation length could reach the system size even at  $\beta=4/t$ . The results of Monte Carlo simulations on a related model also suggest the key role of strong antiferromagnetic correlations at half-filling: In the three-band model, Dopf, Muramatsu, and Hanke<sup>10</sup> have found a parameter range where the behavior observed experimentally is reproduced qualitatively and it seems that, in this parameter range, strong antiferromagnetic correlations are also present at half-filling.<sup>11</sup>

Whether these results of simulations on finite lattices have anything to do with the infinite system is a tricky question. A zeroth-order check consists in making sure that the  $U=0$  result has the same qualitative dependence on filling for both the finite and the infinite lattice. In Fig. 1, we plotted the  $U=0$  result for a  $4\times 4$  lattice with a dotted line. Clearly, the spin susceptibility decreases as the system is doped away from half-filling, in qualitative agreement with the infinite system. This kind of agreement is not true at all fillings since on a finite lattice the spin susceptibility is not a monotonous function of filling while it is for the infinite system. Moreo<sup>4</sup> has argued that finite-size effects should be smaller for larger interaction strengths because of localization effects. This is almost certainly true, unless interactions introduce some other effect, such as a phase transition. We can guess what should happen at  $U/t=4$  by using some analytical results. It has been shown<sup>12</sup> that the magnetic structure

factor obtained by Monte Carlo simulations is well described, not too close to half-filling, by the generalized random phase approximation (GRPA), if one takes into account two-particle correlations (Kanamori-Brueckner screening) by renormalizing the value of  $U$ . Using the renormalized value of  $U_m/t=2.2$  appropriate for the bare value  $U/t=4$ , we find that long-range order sets in for a filling about equal to that where the maximum appears in Fig. 1. This is consistent with the fact that in two dimensions, the GRPA should start to fail when it predicts a magnetic phase transition. Indeed, a better approximation would take into account Mermin-Wagner fluctuations which prohibit long-range order in two dimensions. How to include these fluctuations in itinerant electron theories is a problem which cannot presently be answered by Monte Carlo simulations but which is beginning to be successfully addressed analytically.<sup>13</sup> It would be reasonable to expect that in the regime where the mean-field transition found using the GRPA is suppressed by thermal fluctuations ( $T < T_{\text{GRPA}}^{(c)}$ ) the large antiferromagnetic fluctuations will nevertheless decrease the uniform spin susceptibility (at half-filling in Fig. 1, it is smaller than the noninteracting value). Because the tendency towards antiferromagnetism increases towards half-filling, the infinite-size two-dimensional Hubbard model would then show the same kind of behavior as the finite-size system of Fig. 1.<sup>14</sup> Consistency with experiment might then occur not only in the strong-coupling limit, but also at relatively smaller couplings as long as  $T_{\text{GRPA}}^{(c)}$  is not small compared with experimentally studied temperatures. In both the present work and that of Ref. 4 however, the system sizes are much too small to yield a definitive answer to the question of the infinite-size limit.

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<sup>7</sup>Liang Chen and A.-M.S. Tremblay, Int. J. Mod. Phys. B **6**, 547 (1992).

<sup>8</sup>Following J. E. Hirsch, Phys. Rev. B **35**, 1851 (1987), we used the transverse correlations as the estimator. As pointed out to us by Moreo, however, it turns out that for this problem the longitudinal estimator is less noisy. We have checked that it is indeed possible to obtain the same results with the

longitudinal estimator using runs which are five to ten times shorter.

<sup>9</sup>When the magnetic structure factor starts to scale with system size (as it does on the plateaus in Fig. 3 of Ref. 6) this indicates that the correlation length has reached the system size. This is why we take proximity to the plateau as an indication that the antiferromagnetic fluctuations are becoming strong. We are not interested in the zero-temperature limit per se.

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<sup>11</sup>G. Dopf, A. Muramatsu, and W. Hanke, Phys. Rev. B **41**, 9264 (1990). See Fig. 8 of this paper.

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<sup>13</sup>Y. Vilk (unpublished).

<sup>14</sup>Millis and Monien have recently argued in favor of such a spin-density-wave explanation of the uniform magnetic susceptibility in  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ : A. J. Millis and H. Monien, Phys. Rev. Lett. **70**, 2810 (1993).