



# Reply to "Comment on 'Ground State of the Strong-coupling Hubbard Hamiltonian: A Numerical Diagonalization Study'"

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## Reply to "Comment on 'Ground state of the strong-coupling Hubbard Hamiltonian: A numerical diagonalization study'"

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We establish the correctness of our exact diagonalization results for the ground state of the effective strong-coupling Hubbard Hamiltonian, and the consistency of their interpretation within the finite-size system studied. We discuss why comparison of our results to calculations by S. Tang and J. E. Hirsch (preceding Comment) is misleading and inconclusive. The possible importance of finite-size effects has already been pointed out.

Tang and Hirsch (TH)<sup>1</sup> question our interpretation of the staggered magnetization distribution (SMD), as obtained by exact diagonalization of the effective strong-coupling Hubbard Hamiltonian on a finite system of ten sites.<sup>2</sup> They also raise the issue of finite-size effects in establishing long-range order. In this Reply, we show both from general arguments and by comparison to an analytically solvable example that our earlier findings about the behavior of the SMD are correct, and they are consistent with our conclusions concerning magnetic properties of the system studied. The possible importance of finite-size effects has been mentioned before<sup>2</sup> and is reiterated here.

We wish to point out that TH have not found different results by reproducing our calculations on the effective strong-coupling Hamiltonian, but infer that our results may be incorrect by comparing them to calculations on the Heisenberg and Hubbard models. We discuss why this comparison is not valid for the cases of interest. The apparent discrepancy may be due to numerical error in the calculations of TH. Alternatively, it is possible that the Hubbard model and the effective strong-coupling Hamiltonian, studied in Ref. 2, give rise to qualitatively different physics for a range of the parameters, which would be an interesting nonperturbative effect.

Rotational invariance in spin space of the effective strong-coupling Hubbard Hamiltonian, invoked by TH to challenge our results, is irrelevant for the case of a system with an odd number of electrons. The  $x=0.1$  case for the ten-site system has an odd number (nine) of electrons and the ground state is necessarily characterized by half-integer values of  $S_z$ . Accordingly, the ground state does not possess rotational invariance in spin space, which is broken by the orientation of the spin along the chosen  $z$  axis. The SMD for this case can, in principle, exhibit double peaks. By contrast, the ground state of the Heisenberg model is characterized by  $S=0$  for a finite system with an even number of electrons (this is equivalent to the effective strong-coupling Hubbard Hamiltonian at half filling). The ground state for this system is necessarily rotationally invariant in spin space, and as a result the SMD does not exhibit double peaks. This simply means that the SMD is not the optimal method to discern the possible ex-

istence of antiferromagnetic (AF) order in the case of an even number of electrons. Comparison of the SMD for these two inequivalent cases is not meaningful.

Having established from general arguments that it is possible for a finite system with an odd number of electrons to exhibit double peaks in the SMD, we proceed to show that this is exactly the case for the ground state of the effective strong-coupling Hamiltonian, for appropriate values of the constants. First, we prove this point for an analytically solvable example. Consider the limiting case of the Heisenberg model (that is  $t \rightarrow 0$  and  $t^2/U$  constant, thus keeping only the  $H_2$  part of the effective Hamiltonian of Ref. 2). In order to provide an analytic solution to this problem we investigate a four-site system with periodic boundary conditions, containing three electrons. The possible states of this system in the  $S_z = \frac{1}{2}$  subspace are shown in Fig. 1 (they are denoted by  $|i, \chi\rangle$ , where  $i=1, \dots, 4$  is the position of the empty site and  $\chi = \alpha, \beta, \gamma$  is the spin environment). A translationally invariant ground state of this system can be constructed analytically and is given by

$$|\psi_k\rangle = \frac{1}{\sqrt{24}} \sum_{i=1,4} e^{ik \cdot r_i} (2|i, \alpha\rangle - |i, \beta\rangle - |i, \gamma\rangle).$$

The SMD of this ground state exhibits off-center peaks, as shown in Table I. Thus, we have proven by a trivial example that the ground state of the Heisenberg model in a finite system with an odd number of electrons has double-peaked SMD. This is the relevant comparison to more elaborate treatments. Similar behavior is found in the ten-site system with mobile holes at large values of  $t/U$ , where the spin-spin correlations are consistent with AF

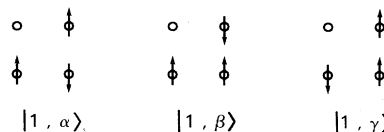


FIG. 1. The possible states of a four-site system with three electrons (see text for discussion).

TABLE I. Staggered magnetization distribution for the ground state of a four-site, three-electron Heisenberg model at the allowed values of the staggered magnetization  $m_z$  in the  $S_z = \frac{1}{2}$  subspace. The SMD exhibits off-center peaks (see text).

Staggered magnetization $m_z$	Staggered magnetization distribution
-0.375	0.33333
-0.125	0.16667
0.125	0.16667
0.375	0.33333

order. To illustrate the point, we show in Fig. 2 the SMD for the  $x=0.1$  case at different values of  $t/U$ . It is obvious from Fig. 2 that as  $t/U$  increases, the SMD develops off-centered shoulders and finally, for large enough values of  $t/U$ , a double peak. The appearance of the double peak coincides with AF spin-spin correlations extending to the longest possible distance in our finite system. This indicates a tendency for AF ordering in the ten-site lattice (perfect AF order corresponds to two peaks at the largest absolute values of the staggered magnetization).

We next discuss why the comparisons of the numerical results made by TH (Fig. 1 of Ref. 1) are not valid. TH have performed calculations on the Hubbard model and obtained results which (assuming they are free of numerical errors) apparently contradict our calculations. However, the Hubbard model has a Hilbert space with many more states than the corresponding effective strong-coupling Hamiltonian, studied in Ref. 2. It is likely that this enlarged Hilbert space considerably reduces the tendency for AF ordering. At the values of  $t/U$  where we observe AF ordering (e.g.,  $t/U=0.15$ ), there may be substantial mixing between the two subbands of the Hubbard model, in which case the single occupancy of each site (an inherent assumption in the effective strong-coupling Hamiltonian) no longer holds. Hirsch<sup>3</sup> has shown that the Hubbard model and the effective strong-coupling Hamiltonian exhibit very different behavior in the charge-density correlations for  $t/U=0.15$  (or  $U=6.67t$ , see Fig. 1 of Ref. 3). Thus, comparing the Hubbard model directly to the effective strong-coupling Hamiltonian at these values of  $t/U$  (Fig. 1 of Ref. 1), is unjustified and misleading. The effective strong-coupling Hamiltonian remains an interesting model in itself, however, and the fact that it can be derived from the Hubbard model in the large  $U$  limit serves only to motivate its relevance.

Finally, the issue of finite-size effects in establishing the existence of long-range order remains an open question.

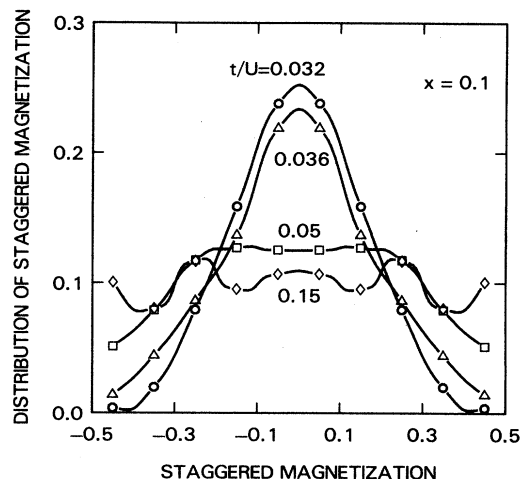


FIG. 2. Staggered magnetization distribution for a ten-site system with nine electrons, in the ground state of the effective strong-coupling Hamiltonian, for various values of  $t/U$ . At the two highest values of  $t/U$  there is tendency for AF order, extending to the longest possible distance of our finite system.

This was carefully pointed out in our earlier work, where it is observed that the persistence of AF order up to the longest possible distance in the ten-site system at nonzero doping, “will be an interesting result if it survives in the limit of an infinite system.”<sup>2</sup> In the absence of sufficient data to perform finite-size scaling, our previous work attempted to draw plausible conclusions about the behavior of the system. In fact, finite-size effects (as well as other numerical problems associated with fermion statistics and the approach to zero temperature) are also present in Monte Carlo calculations cited by TH,<sup>1</sup> in support of their claims.

In conclusion, we have shown from general arguments and by comparison to an analytically solvable example, that the ground state of the effective strong-coupling Hamiltonian for a finite system with an odd number of electrons exhibits double-peaked SMD. Our numerical results for the SMD of the  $x=0.1$  case for the ten-site cluster (studied in Ref. 2) are correct and do not violate any symmetry principles. The existence of double peaks in the SMD for appropriate values of the constants is consistent with tendency for AF order extending to the longest possible distance in our finite system.

We thank T. D. Schultz and T. M. Rice for useful discussions.

<sup>1</sup>S. Tang and J. E. Hirsch, preceding Comment, Phys. Rev. B **40**, 2594 (1989).

<sup>2</sup>E. Kaxiras and E. Manousakis, Phys. Rev. B **37**, 656 (1988).

<sup>3</sup>J. E. Hirsch, Phys. Rev. Lett. **54**, 1317 (1985).