

van den Brink, Khaliullin, and Khomskii Reply: In the preceding Comment [1], Shen points out that the on-site Coulomb interaction, that can cause charge order in half-doped manganites [2], also destabilizes the magnetic CE phase observed in these systems.

This is a valid observation, but it is not *a priori* clear whether in the relevant parameter regime the *C* phase is indeed lower in energy than the CE phase within our model [2]. From the exact diagonalization of a 16-site ring, Shen finds a ground-state energy for the CE phase as a function of U , which is compared to the energy of an *infinite* ring in the *C* phase, in order to find a critical coupling $U_c = 5t$ above which the *C* phase is stable. In order to determine the critical coupling, however, one should handle finite-size effects in both phases on equal footing and compare the CE-phase energy with the energy of a 16-site *C*-phase ring, which is $E_{16}^C = -0.628t$. Using this value for the energy, we can estimate from Fig. 1 in Ref. [1] that $U_c \approx 10t$, which is in the relevant parameter regime for the half-doped manganites.

As Shen states, other interactions, which are neglected in the model could very well compensate for the small energy differences between the *C* and the CE phases. We wish to point out, in particular, that coherent and incoherent hopping between two sites with opposite spin orientation lowers the kinetic energy of the CE phase appreciably.

The main aim of our model is to explain the observed charge and orbital order, *given* the CE magnetic structure. As to the stability of the phases, indeed not all physical relevant effects are taken into account. Especially, the contribution of lattice distortions, which we neglected, is important [3]. Also, for instance, anharmonic effects that favor occupation of elongated orbitals [4], which may stabilize the CE phase, are not incorporated into the model.

Moreover, one should also take into account that the hopping between two sites with antiferromagnetically coupled core spins is not completely blocked. For a finite Hund's rule coupling (J_H) an electron can hop coherently from a high spin state to lower spin states on a neighboring site, but even for an infinitely large J_H , there exists quantum effects which allow hopping that preserves the total high spin state $S + 1/2$, but with different projections $S^z = S + 1/2$ and $S - 1/2$ at different sublattices [5]. Such electron hopping processes between *C*-type chains or between CE zigzag chains modify the total energy. One can easily estimate the coherent contribution to the kinetic energy in second order perturbation theory. The contribution from hopping between two chains in the *C* phase is

then $\delta E_C = -\frac{3}{8} \frac{t^2}{\Delta}$ and in the CE phase is $\delta E_{CE} = -\frac{5}{8} \frac{t^2}{\Delta}$. This difference is due to the fact that in the CE phase also the $x^2 - y^2$ orbital on the corner site is partially occupied. As typically $\Delta \approx J_H$ and J_H is in the order of $5t$, the energy lowering of the CE phase due to this effect would be larger than the energy loss due to the on-site Coulomb interactions in the CE phase. The incoherent contributions that change the spin projections on different sublattices are more involved to calculate, but they would certainly lower the energy of the CE phase with respect to the *C* phase as the interchain hopping integrals are larger in the former.

We therefore conclude that the model of Ref. [2], which correctly captures the interplay of spin, charge, and orbital degrees of freedom in the half-doped manganites and gives a reasonable description of their electronic structure, is by itself not sufficient for the precise determination of the regions of stabilities of different phases. For this, several other factors, in particular those mentioned above, should be taken into account.

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