Reply to "Comment on 'Electronic structure of spin-$\frac{1}{2}$ Heisenberg antiferromagnetic systems: $Ba_2Cu(PO_4)_2$ and $Sr_2Cu(PO_4)_2$' "

S. Salunke, M. A. H. Ahsan,* R. Nath, A. V. Mahajan, and I. Dasgupta
Department of Physics, Indian Institute of Technology Bombay, Mumbai 400076, India
(Received 16 October 2008; published 6 March 2009)

In the following we respond to the comments by Rosner *et al.* [Phys. Rev. B **79**, 127101 (2009)].

DOI: 10.1103/PhysRevB.79.127102 PACS number(s): 71.20.−b, 71.70.Gm, 75.10.Pq

The first comment pertains to the magnitude of the leading hopping parameter t_1 obtained by Salunke *et al.*[1] This hopping is somewhat underestimated in the work by Salunke *et al.*[1] in comparison to the work by Johannes *et al.*[2] and the authors of the comment, by a series of full-potential density-functional calculations, argue that this is due to the use of tight-binding linear muffin tin orbital (TB-LMTO) method within atomic sphere approximation (ASA) for the calculation of the band dispersion in Ref. 1. Johannes *et al.*[2] employed full-potential method to calculate the band dispersion followed by a fitting scheme to extract various hopping parameters. Although for the systems considered here with an isolated Cu $d_{x^2-y^2}$ band, an accurate full-potential calculation followed by the fitting scheme, may provide very reliable magnitudes for the various hopping parameters, it does not provide as much insight into the origin of these tight-binding parameters as the *N*th order muffin tin orbital (NMTO) downfolding approach. It is also to be noted that in the absence of a reliable scheme to obtain U_{eff}, an accurate evaluation of the hopping parameters for these strongly correlated Heisenberg antiferromagnetic (HAF) systems is presently less important as it does not provide accurate enough estimate for the exchange integrals J_{ij} crucial to model these systems. In view of the above, the main emphasis of the work by Salunke *et al.*[1] has been to understand the origin of the dominant nearest-neighbor hopping parameter (t_1) crucial for the unique one-dimensional properties of these systems, using an *ab initio* scheme where the use of TB-LMTO ASA method is found to be adequate for the description of band dispersion. Using NMTO downfolding scheme in the framework of TB-LMTO ASA, Salunke *et al.*[1] not only filter out the low-energy band dispersion but also obtain the corresponding Wannier functions that give rise to these bands thereby providing a direct access to the origin of the various hopping integrals crucial to understand the physics of these systems. The second comment by Rosner *et al.*[3] is on the exact diagonalization studies in Ref. 1. Salunke *et al.*[1] merely speculated that small interchain hoppings may be important for the low-temperature properties of these compounds. They tried to verify the above speculation using exact diagonalization studies on small systems which has been criticized by the authors of the comment. However, the exact diagonalization studies carried out by the authors of the comment do not rule out the importance of the small interchain couplings for the low-temperature properties of these systems as anticipated by Salunke *et al.*[1]

*Present address: Jamia Millia Islamia, New Delhi 110025, India.

[1] S. S. Salunke, M. A. H. Ahsan, R. Nath, A. V. Mahajan, and I. Dasgupta, Phys. Rev. B **76**, 085104 (2007).
[2] M. D. Johannes, J. Richter, S.-L. Drechsler, and H. Rosner, Phys. Rev. B **74**, 174435 (2006).
[3] H. Rosner, M. Schmitt, D. Kasinathan, A. Ormeci, J. Richter, S.-L. Drechsler, and M. D. Johannes, preceding Comment, Phys. Rev. B **79**, 127101 (2009).

