Reply to "Comment on 'Fe magnon dispersion curve calculated with the frozen spin-wave method'"

Leonard Kleinman and Qian Niu
Department of Physics, The University of Texas, Austin, Texas 78712-1081
(Received 3 September 2002; published 21 January 2003)

We argue that the frozen spin-wave energy (either total or internal) is a second-order quantity. The force theorem approximation, whether in the form disscussed, but not used by us, or in the form used by Nicholson and Brown, is accurate only to first order. We agree that they *now* get agreement with our first-principles calculations and experiment in spite of this.

DOI: 10.1103/PhysRevB.67.016402 PACS number(s): 75.25.+z, 75.50.Bb

In the preceding Comment,[1] Nicholson and Brown stressed the usefulness of the frozen potential approximation (FPA) by general theoretical arguments and by presenting their new results on the magnon dispersion of Fe, which are in agreement with our results[2] and with experiment. In their earlier calculations of magnon dispersions, there was about a factor of 2 error for Fe (compare Fig. 1 of the preceding Comment with Fig. 1 of Ref. 3) and a smaller but still significant error apparent in their Co dispersion curve. We suspected that the FPA might be the cause of such big errors, and presented our analysis on an inherent problem with FPA.[2] We now learn that such errors were actually due to computational mistakes.[4] It remains to be understood why FPA can produce reasonable results despite an inherent second-order error in this approximation.

The commonly given reason for FPA is the force theorem, which states that to first order in a small perturbation, the change in the energy of a system is given by the change in the sum of occupied level energies. However, there are second-order terms in the perturbation that cannot be accounted for by the change of level energies. This is true for both the total energy and the internal energy. When one considers a second-order effect such as in the evaluation of the magnon energy, a second-order mistake in the system energy can lead to a zero order error relative to the quantity of interest.

The preceding Comment now makes it clear that FPA can be justified by applying the force theorem with respect to a different quantity of small perturbation: not the constraining potentials but rather the deviation from the true Kohn-Sham potential in the FPA. There are still second-order corrections, but these are second-order terms of a quantity smaller than the constraining potentials. In particular, these second-order corrections vanish in the long wavelength limit, and can start to contribute only to fourth order in the wave vector. Their (corrected) numerical results for Fe still seem to be good beyond the immediate neighborhood of small wave vectors. Further work needs to be done to establish more precisely the domain of validity of FPA in the general case. We observe, based on earlier work on spiral spin-density waves,[5] that the magnetization direction in transition metals tends to have most of its variation in the outer part of the unit cell where the spin density is small. Thus the rigid rotation of the spin within the Wigner-Seitz sphere used in FPA is a better approximation than one might have expected.

This work has been supported by the NSF under Grant Nos. DMR-0073546 and DMR- 0071893 and by the Welch Foundation.

[1] D.M.C. Nicholson and R. H. Brown, preceding paper, Phys. Rev. B **67**, 016401 (2003).
[2] D.M. Bylander, Qian Niu, and Leonard Kleinman, Phys. Rev. B **61**, 11 875 (2000).
[3] R.H. Brown, D.M.C. Nicholson, Xingdong Wang, and T.C. Schulthess, J. Appl. Phys. **85**, 4830 (1999).
[4] D.M.C. Nicholson (private communication).
[5] D.M. Bylander and Leonard Kleinman, Phys. Rev. B **58**, 9207 (1998).

