Comment on "Spin-wave theory for anisotropic Heisenberg antiferromagnets"

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We point out that as their main result Soukoulis, Datta, and Lee's Néel temperature result in random-phase approximate [Phys. Rev. B **44**, 446 (1991)] is valid only for classical spins, and then give the quantum result for spin $\frac{1}{2}$. Besides we make some other comments on their paper.

Soukoulis, Datta, and Lee claimed in their paper[1] to model the magnetic properties of the undoped cuprates by an anisotropic quantum Heisenberg antiferromagnetic model (QHAFM) defined on three-dimensional (3D) simple-cubic lattice with in-plane coupling $J_{\parallel}>0$ and interplane coupling $J_{\perp}=\delta J_{\parallel}$, i.e., a quasi-2D QHAFM. The Hamiltonian reads

$$H=\sum_{\langle ij\rangle} J_{ij} S_i \cdot S_j \ , \tag{1}$$

where $\langle ij\rangle$ represents a bond between the nearest neighboring i and j sites, $J_{ij}=J_{\parallel}$ or $J_{ij}=J_{\perp}$ if $\langle ij\rangle$ is parallel or perpendicular to the CuO_2 plane, respectively. Here we plan to make some comments on their paper.

First, we point out that their expressions (7) and (8) for the Néel temperature T_N in the random-phase approximate (RPA) are correct only for classical spins, i.e., the $S\rightarrow\infty$ case. It is well known that spin is $\frac{1}{2}$ for the undoped cuprates. Generally, to deal with QHAFM one uses the so-called sublattice approach to divide the lattice into two or more sublattices. In this approach the $\frac{1}{2}$-spin RPA Néel temperature expression should read[2-4]

$$T_N=\frac{J_{\parallel}Z}{4W}\ , \quad W=\frac{2}{N}\sum_k{}' \frac{1}{1-r_k^2}\ , \tag{2}$$

where $Z=4+2\delta$, $r_k=(2/Z)(\cos k_x+\cos k_y+\delta\cos k_z)$, and the primed k summation here is carried out on the reduced Brillouin zone. On the other hand, the T_N result can be derived without the sublattice postulation. The consistent equation of sublattice spin s reads

$$\tfrac{1}{2}=\frac{1}{N}\sum_k \frac{s}{\sqrt{1-r_k^2}}\coth\frac{\beta\omega_k}{2}\ . \tag{3}$$

When T approaches T_N, s tends to zero so that we can expand Eq. (3) in terms of s. s as a function of T is given by

$$s=\left[\frac{12W}{J_{\parallel}^2Z^2}T\left[T-\frac{J_{\parallel}Z}{4W}\right]\right]^{1/2}, \tag{4}$$

where W is given by the latter expression of (2). From (3) we see $T_N=J_{\parallel}Z/4W$. It is the correct T_N expression in (2).

If $\delta=0$, the T_N expression in (2) gives $T_N=0$. When δ tends to zero, T_N has an asymptotic behavior:

$$T_N\sim\pi J_{\parallel}/\ln(1/\delta) \tag{5}$$

in contrast with expression (8) in Ref. 1. If $\delta=1$, expression (2) gives $T_N=0.989J_{\parallel}$. This is in excellent agreement with the high-temperature series expansion result $T_N=0.951J_{\parallel}$,[5,7] but is considerably smaller than $1.36J_{\parallel}$ obtained by Sukoulis *et al.* Figure 1 shows our T_N values as functions of the anisotropy parameter δ.

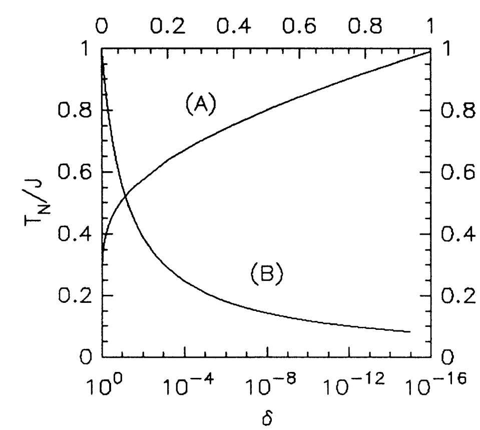

FIG. 1. T_N's as functions of δ in the RPA. The (A) line has its δ scale on the upper edge of the frame, the (B) line on the lower edge. $T_N/J_{\parallel}=0.989$ and 0 for $\delta=1$ and 0, respectively.

In their paper, Soukoulis *et al.* claimed that their T_N result (7) (Ref. 1) was obtained in a RPA for the general spin S for the anisotropic Heisenberg model. As has been discussed above, the $\frac{1}{2}$ spin T_N for the undoped cuprates should be given by our expression (2). Their T_N expression (7) is equivalent to the $S\rightarrow\infty$ limit value of Tahir-Kheli and ter Harr's *ferromagnetic* Curie temperature[8] divided by S^2. This means that their result is classical. It is not appropriate for them to use their $S\rightarrow\infty$ classical result for the $s=\frac{1}{2}$ quantum antiferromagnetic case of undoped cuprates.

As for modeling the undoped cuprates by the quasi-2D QHAFM defined on a sc lattice, it had been done by the author[2] in 1989 and by Singh *et al.*[6] in 1990.

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