Erratum: Charge and spin ordering in the mixed-valence compound $LuFe_2O_4$ [Phys. Rev. B 81, 134417 (2010)]

A. B. Harris and T. Yildirim

(Received 27 June 2010; published 27 July 2010)

DOI: 10.1103/PhysRevB.82.029902 PACS number(s): 75.25.−j, 75.10.Jm, 75.40.Gb, 99.10.Cd

Note typographic errors in Eqs. (9) and (10). In each of these equations the final square brackets should have an exponent 1/2, as one easily sees from Eq. (8). In view of the correction below, change three lines below Eq. (28) where it was stated that "Δ is positive for $U_4<0$" to read "Δ is positive for $U_2U_3>0$."

The significant error is that the algebra leading to the result given in Eq. (26) for the difference between the mean-field transition temperatures for ferroelectric and antiferroelectric ordering, $\Delta T \equiv T_{\mathrm{MF,F}} - T_{\mathrm{MF,AF}}$, is incorrect, and as written is inconsistent with the rest of the paper. This inconsistency is removed by this erratum which shows that the correct result is that ΔT is positive for $U_2U_3>0$, as stated elsewhere in the paper. To correct this error replace the text starting from, just before Eq. (20), "We have that…" and continuing down to and including Eq. (26), by the following.

Here $T_{\mathrm{MF,F}}$ is obtained by minimizing $\mu(q_z=0,\phi)$ with respect to ϕ and $T_{\mathrm{MF,AF}}$ is obtained by minimizing $\mu(q_z=3\pi/c,\phi)$ with respect to ϕ. In calculating ΔT we will assume that U_4 is much less than either U_2 or U_3, which are both much less than U_1. We determine ΔT to first order in U_4 in which case Eq. (11) gives

$$T_{\mathrm{MF,F}} = \mathrm{Max}_\phi\{3U_1 + (U_4/U_1)\cos(\phi)\sqrt{U_2^2+U_3^2+2U_2U_3\cos(2\phi)} + [U_2^2+U_3^2+2U_2U_3\cos(2\phi)]/(4U_1)\} \tag{20}$$

and

$$T_{\mathrm{MF,AF}} = \mathrm{Max}_\phi\{3U_1 - (U_4/U_1)\cos(\phi)\sqrt{U_2^2+U_3^2-2U_2U_3\cos(2\phi)} + [U_2^2+U_3^2-2U_2U_3\cos(2\phi)]/(4U_1)\}. \tag{21}$$

We first treat the case $U_2U_3>0$, in which case the expression for $T_{\mathrm{MF,F}}$ is maximized at $\phi=0$ for $U_4>0$ and at $\phi=\pi$ for $U_4<0$. The expression for $T_{\mathrm{MF,AF}}$ is maximized at $\phi=\pi/2+\epsilon$, where ϵ denotes a quantity proportional to U_4. The results to first order in U_4 can be obtained by setting $\epsilon=0$. Then

$$T_{\mathrm{MF,F}} = 3U_1 + |U_4||U_2+U_3|/U_1 + (U_2+U_3)^2/(4U_1), \tag{22}$$

$$T_{\mathrm{MF,AF}} = 3U_1 + (U_2+U_3)^2/(4U_1), \tag{23}$$

so that

$$\Delta T = |U_4||U_2+U_3|/U_1. \tag{24}$$

For $U_2U_3<0$ a similar analysis yields

$$\Delta T = -|U_4||U_2-U_3|/U_1. \tag{25}$$

These results are consistent with $T_{\mathrm{MF,F}}$ being higher (lower) than $T_{\mathrm{MF,AF}}$ for U_2U_3 positive (negative) *independent of the sign of* U_4. (The sign of U_4 was determined in the preceding section by comparison with the experimental data.) These results for ΔT are consistent with the results of Table I and Figs. 7–10 which show that in the paraelectric phase ferroelectric fluctuations are dominant for $U_2U_3>0$ irrespective of the sign of U_4. As mentioned, we choose $U_2U_3>0$ and since we suppose $|U_3| \ll |U_2|$, we have that

$$\Delta T \approx |U_2U_4|/U_1 = \frac{(2)(30)}{500} = 0.12\ \mathrm{K}. \tag{26}$$

