Eur. Phys. J. B **24**, 415 (2001)
DOI:

THE EUROPEAN PHYSICAL JOURNAL B
EDP Sciences

Erratum

Microscopic interactions in $CuGeO_3$ and organic Spin-Peierls systems deduced from their pretransitional lattice fluctuations

J.-P. Pouget[a]

Laboratoire de Physique des Solides[b], Université Paris-Sud, bâtiment 510, 91405 Orsay Cedex, France

Eur. Phys. J. B **20**, 321–333 (2001)

I - Column 3 of Table 1 quotes incorrect values of the 3D singlet-triplet gap Δ_σ for the organic Spin-Peierls (SP) systems. One should replace the values indicated by the activation energy of the spin susceptibility or of the NMR relaxation rate below T_{SP}. This leads to $\Delta_\sigma/k_B \approx 56$ K, 70–90 K and 100 K for MEM$(TCNQ)_2$, $(TMTTF)_2PF_6$ and $(BCPTTF)_2PF_6$ respectively.

II - The ratio (expression (2)) which relates the SP gap at 0° K (Δ_σ^{MF}) to the SP critical temperature (T_{SP}^{MF}) in the mean field theory (with respect to the lattice degrees of freedom) of the SP transition of the Heisenberg chain is not an universal quantity. It varies with the alternation parameter δ of the exchange integral in the SP phase (defined by $J(1 \pm \delta)$) because of the presence of logarithmic corrections in δ, especially for Δ_σ. If one follows the original derivation of Schulz (Ref. [43]) where the singlet-triplet gap is written under the form:

$$\Delta_\sigma = BJ\delta^{2/3}, \tag{1}$$

the parameter B varies with δ. With the recent numerical calculations of reference [52] one should take $B \approx 1.5$ for δ in the range 0.05–0.15 corresponding to the SP systems considered in the paper. With this B value the expression (2) of the paper becomes:

$$\Delta_\sigma^{MF} \approx 2.3 T_{SP}^{MF}. \tag{2}$$

In consequence all the values of Δ_σ^{MF} given column 5 of Table 1 must be modified, leading to $\Delta_\sigma^{MF}/k_B \approx 140$ K, 90 K, 180 K and 230 K for $CuGeO_3$, MEM$(TCNQ)_2$, $(TMTTF)_2PF_6$ and $(BCPTTF)_2PF_6$ respectively.

Accordingly, at the end of Section 5.2 the relationship between Δ_σ^{MF} and the spin-phonon coupling α must be also changed into:

$$\Delta_\sigma^{MF} \approx 0.6\alpha^2/\Omega_0. \tag{3}$$

In that context, it is interesting to note that the dependence of Δ_σ with δ, numerically calculated in reference [52], can be reproduced with an accuracy of few percent by the analytical Hartree-Fock expression derived for the magnetic susceptibility of an alternating system of spins [L.N. Bulaevskii, Soviet Physics-Solid State, **11**, 921 (1969)]:

$$\Delta_\sigma = J\delta\{1 + [4/\pi(1+\delta)]K[(1-\delta)/(1+\delta)]\}, \tag{4}$$

where $K[x]$ is the complete elliptic integral of the first kind.

Finally, the use of a linear relationship between Δ_σ and δ introduced in the totally mean-field treatment of the SP transition of the Heisenberg chain:

$$\Delta_\sigma = pJ\delta, \tag{5}$$

with $p = 1 + 2/\pi$, always underestimates Δ_σ, at a given δ, by a factor two.

III - The low temperature behavior of the inverse reduced correlation length of the SP chain is given in the WKB approximation (see T. Schneider, E. Stoll, Phys. Rev. B **22**, 5317 (1980)) by:

$$(\xi_c/\xi_0)^{-1} = 2(2T_{SP}^{MF}/\pi T)^{1/2}\exp - (4T_{SP}^{MF}/3T).$$

Accordingly, the expression (4) of the paper must be corrected by this expression (work done in collaboration with C. Bourbonnais).

IV - In Section 5.4 two possibilities were suggested for the pressure dependence of the singlet-triplet dispersion curve. This is the scenario (ii), where the mid-band value of the dispersion along b^*, identified at Δ_σ in the paper, increases under pressure, which is the correct one (see Fig. 4.22 in O. Cépas, thesis (Université Joseph Fourier-Grenoble I, 2000)).

[a] e-mail: pouget@lps.u-psud.fr
[b] CNRS-UMR 8502