Erratum: Heisenberg and Dzyaloshinskii-Moriya interactions controlled by molecular packing in trinuclear organometallic clusters [Phys. Rev. B **95, 094432 (2017)]**

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The forms of the intermolecular spin-orbit coupling discussed in Secs. IV A and IV B of our recent paper do not have the C_3 symmetry of the underlying molecular system. In particular, $\lambda_{\mu\nu;ij}$ is a pseudovector; our original treatment did not properly account for this. Below, we give the correct C_3 -symmetric forms of these interactions and describe the changes in our results when this is corrected.

In Sec. IV A, we studied the case where the intramolecular spin-orbit coupling only couples equivalent Wannier orbitals ($i = j$) on neighboring molecules (μ and ν) by setting $\lambda_{\mu\nu;ij} = \lambda_{\mu\nu}\delta_{ij}$. The correct C_3 -symmetric form is

$$\lambda_{\mu\nu;ij} = (\lambda_1 \cos \phi_j - \lambda_2 \sin \phi_j, \lambda_2 \cos \phi_j + \lambda_1 \sin \phi_j, \lambda_3)\delta_{ij}, \quad (1)$$

where $\phi_j = 2\pi(j-1)/3$ and λ_1, λ_2 , and λ_3 are constants. Importantly, this form of the intermolecular spin-orbit coupling correctly accounts for the mixing of the x and y components of $\lambda_{\mu\nu;ij}$ under the threefold rotations about the z axis. Thus, $\sum_{i,j=1}^3 \lambda_{\mu\nu;ij}^x = \sum_{i,j=1}^3 \lambda_{\mu\nu;ij}^y = 0$. It then follows immediately from Eqs. (27) that $D_{\mu\nu}^x = D_{\mu\nu}^y = 0$. Thus, Eq. (28) should be replaced by

$$\mathbf{D}_{\mu\nu} = \hat{\mathbf{z}} \frac{8t_{\mu\nu}\lambda_3}{9(J_c - 2t_c)}, \quad (2)$$

where $\hat{\mathbf{z}} = (0, 0, 1)$.

In Sec. IV.B, we allowed orbitals to couple to every orbital on neighboring molecules. The most general C_3 -symmetric form of the coupling constant is

$$\lambda_{\mu\nu;ij} = [\lambda_1(i-j)\cos\phi_j - \lambda_2(i-j)\sin\phi_j, \lambda_2(i-j)\cos\phi_j + \lambda_1(i-j)\sin\phi_j, \lambda_3(i-j)], \quad (3)$$

where now the functions $\lambda_1(i-j)$, $\lambda_2(i-j)$, and $\lambda_3(i-j)$ only depend on the difference of i and j modulo 3. Again, one has $D_{\perp}^x = D_{\perp}^y = 0$; indeed this could have been anticipated from the C_3 symmetry of the problem [1]. Thus, Eq. (29) should be replaced by

$$\mathbf{D}_{\perp} = \hat{\mathbf{z}} \frac{8}{9(J_c - 2t_c)} \sum_{ij} t^{(i)}\lambda_3(j). \quad (4)$$

These errors have important consequences for $\text{Mo}_3\text{S}_7(\text{dmit})_3$: One finds that $\mathbf{D}_{\perp}/J_{\perp} = 0.019\hat{\mathbf{z}}$; similarly, Fig. 9 should be replaced by Fig. 1 below (the curves for $D_{\perp}^z$ and $J_{\perp}$ are unchanged but $D_{\perp}^x = D_{\perp}^y = 0$).

FIG. 1. Effective interlayer Dzyaloshinskii-Moriya and exchange interactions in $\text{Mo}_3\text{S}_7(\text{dmit})_3$ as a function of the interaction strength. Here we have set $J_c = 4t_c^2/U$ and taken all other parameters from first-principles calculations [2,3]. Note that the perturbation theory breaks down as $U \rightarrow 2t_c$.

Finally, we note that the above discussion implies that the quantization axis (z) in Eq. (32) is parallel to the crystallographic c axis of $\text{Mo}_3\text{S}_7(\text{dmit})_3$.

Except as discussed above, the results and conclusions of the paper are unchanged.

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