Magneto-transport through single-molecule magnets: Kondo-peaks, zero-bias dips, molecular symmetry and Berry's phase

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Corrigendum

Magneto-transport through single-molecule magnets: Kondo-peaks, zero-bias dips, molecular symmetry and Berry's phase

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In the paper [1] we reviewed transport through molecular magnets in dependence of magnetic anisotropy and external magnetic fields. Unfortunately, several of the numerical results of this paper are not correct. In particular, in the exchange interaction $J\mathbf{S}\cdot\mathbf{s}$, coupling the SMM to the first site on the Wilson chain in the NRG algorithm, the term $JS_z s_z$ was inadvertently implemented incorrectly. As a result, we did not account for matrix elements of the z-component of the SMM spin operator $\langle i|S_z|j\rangle$ with $i \neq j$, while accounting for those with $i = j$. Here $|i\rangle, |j\rangle$ denote eigenstates of the SMM part of our Hamiltonian $\mathcal{H}_{\mathrm{SMM}} = -DS_z^2 + \frac{1}{2}\sum_{n=1,2} B_{2n}(S_+^{2n} + S_-^{2n}) + H_x \cdot S_x + H_z \cdot S_z$ with $D > B_2, B_4$. Thus, the NRG algorithm was applied correctly but using incorrect matrix elements, thereby not capturing the transitions into SMM excited states. This leads to incorrect results only when two conditions are met: (i) the excited states of the SMM are relevant, i.e. J is large enough compared to the largest anisotropy splitting $\Delta = (2S-1)D$, and additionally, (ii) there is transverse anisotropy (B_2, B_4) or a transverse magnetic field. Both conditions (i) and (ii) have to apply at the same time for quantitative errors to occur. Importantly, in the weak exchange limit, i.e. where J is sufficiently weak compared to Δ, condition (i) does not apply: all the results in section 3.1 of [1] are therefore correct. This we checked by explicit recalculation of the results with the corrected code [2]. However, the result in section 3.2 of [1] for large J requires correction. For this we refer to the erratum [2] to [3]. For a very large magnetic field $H_z \gg D, B_2$ the anisotropy becomes unimportant and the eigenstates approach spin eigenstates. Also in this limit, the paper [1] reports the correct suppression and splitting of the Kondo peak. For the above reasons the problem could not be detected in the numerous checks we performed against known results for the Kondo effect for various spins S in a magnetic field but without magnetic anisotropy.

Recalculation of the results of sections 4 and 5 of [1] confirms one of the central conclusions, namely, that the excited states can indeed be involved in the Kondo effect. However, the correct order of magnitude of T_K is much smaller, see [2], and the re-entrant behavior of the

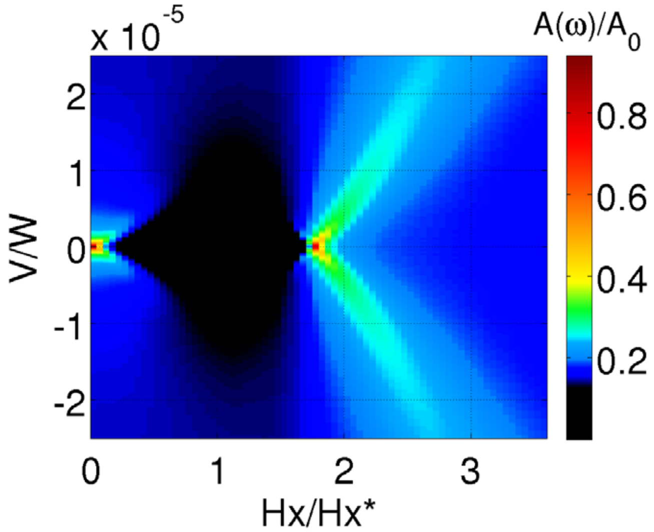

Figure 1. Plot of the spectral function A (normalization $A_0 = \pi^2/4$) as a function of the frequency ω, set equal to the bias voltage V, and the magnetic field energy H_x in units of the diabolical scale $H_x^* = \sqrt{2B_2(D+B_2)}$ for half-integer spin $S = 3/2$ and $D = 10^{-4}$ W and $B_2/D = 0.1$. The value of $J = 0.15$ W is chosen somewhat smaller than the original $J = 0.2$ to reduce the renormalization effect of the positions of the diabolical points.

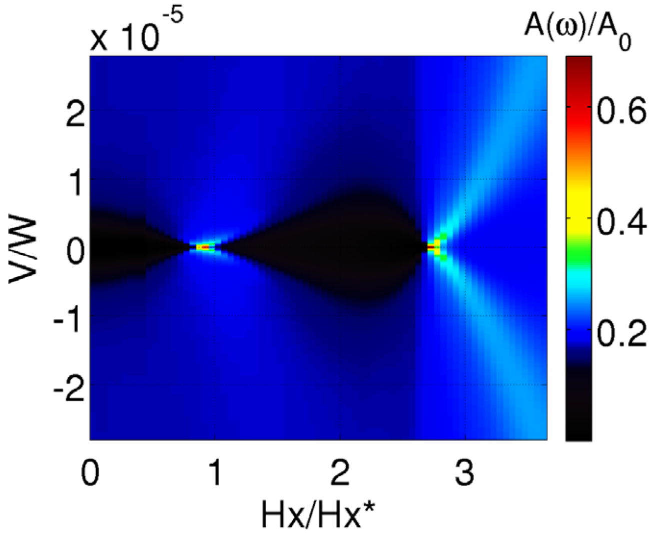

Figure 2. The same as figure 1 except for spin $S = 2$ and anisotropy $D = 2 \times 10^{-4}$ W.

Kondo effect as a function of a longitudinal magnetic field of figures 4, 5 and 7 of [1] is not present. Recalculation of the results of section 5 of [1] confirms the Berry-phase oscillations in the conductance as a function of the external transverse magnetic field H_x (in units of $g\mu_B = 1$). However, at the crossing points of these oscillations, a re-entrant Kondo effect is found, contrary to our statement at the end of section 5.1 of [1]. This instead agrees with the predictions by

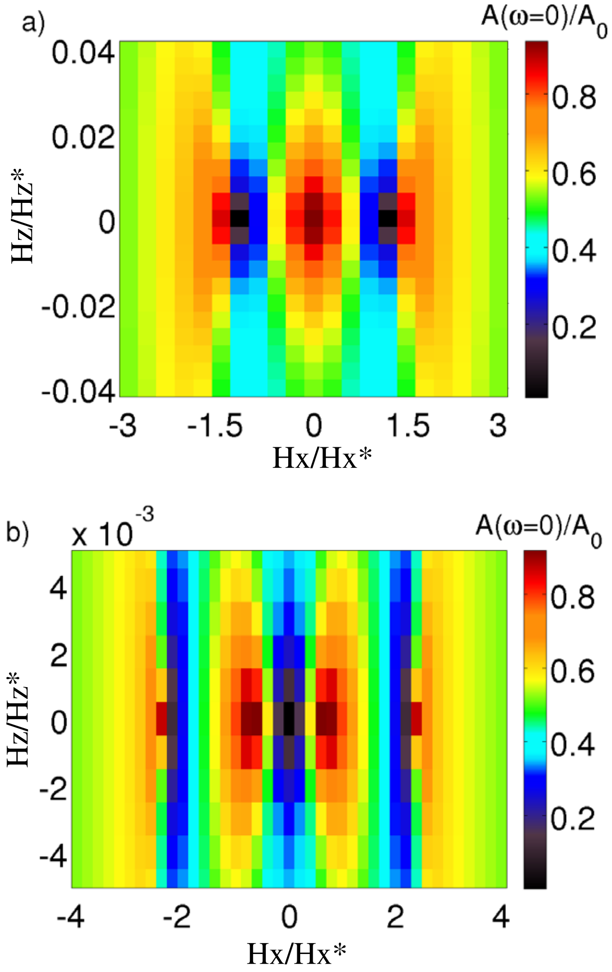

Figure 3. Maps of the spectral function A (normalization $A_0 = \pi^2/4$) evaluated at zero frequency as a function of the longitudinal (H_z) and transverse magnetic fields (H_x) in units of the diabolical scales $H_x^* = \sqrt{2B_2(D+B_2)}$ and $H_z^* = \sqrt{D^2 - B_2^2}$. (a) Spin $S = 3/2$ anisotropy $D = 10^{-4}$ W and other parameters as in figure 1. (b) Spin $S = 2$ and anisotropy $D = 2 \times 10^{-4}$ W and other parameters as in (a).

Leuenberger and Mucciolo [4] in the high-temperature limit that were obtained by a poorman scaling analysis. In figures 1 and 2, we exemplify the corrected results by showing the dependence of the spectral function on the transverse field for half-integer spin $S = 3/2$ and integer spin $S = 2$, respectively. For the (half-)integer S, the Kondo effect occurs close to odd (even) multiples of the Berry-phase scale $H_x^* = \sqrt{2B_2(D+B_2)}$ up to $2S - 1$, the positions being renormalized due to the large value of J. Similar corrections apply to the zero-bias conductance maps as a function of the longitudinal and transverse fields shown in figure 7 of [1]. In figure 3, we show a representation of the corrected maps demonstrating that the Berry-phase oscillations are suppressed with increasing longitudinal field.

Finally, we mention that the results of [5] are affected only quantitatively [6]. For clarity, we point out that the results of the authors on transport through SMMs other than those mentioned here are not affected in any way by the issue reported here.

Acknowledgment

All of the new calculations above were performed by F May when working at the Institut Für Theoretische Physik, Johann Wolfgang Goethe-Universität, 60438 Frankfurt/Main, Germany. By all means he should be considered to be the first author of the corrigendum, which is however not possible within the policies of *New Journal of Physics*.

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