Reply to Comment on Perturbative calculations of quantum spin tunneling in effective spin systems with a transversal magnetic field and transversal anisotropy

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Hereby we want to give a reply to the comment by Garg on our manuscript ‘Perturbative calculations of quantum spin tunneling in effective spin systems with a transversal magnetic field and transversal anisotropy’. Within our work [1] we presented a perturbative solution for the resonant tunnel splitting energy \( \Delta E \) of an arbitrary effective single spin system described by the following Hamiltonian:

\[
\hat{H} = -K_x \hat{S}_x^2 - \hat{S}_y \hat{B}_x + \hat{K} (\hat{S}_x^2 - \hat{S}_y^2). \tag{1}
\]

We obtained two formulas for the ground doublet energy splitting, one for the integer spins and one for the half-integer. For the integer spin case the formula has the following structure:

\[
\Delta E_{\text{split}} = \left| \frac{2 \prod_{j=1}^{s} (S_{x,j} + S_{y,j}) \cdot (\Delta B_x + \Delta B_K)}{\Pi_{j=1}^{2s-1} |(E_{x-j} - E_{y-j})|} \right|
\]

\[
\Delta B_x = B_x^{2s}
\]

\[
\Delta B_K = (-1)^{2s-1} \prod_{j=1}^{s} |(E_{x-(2j-1)} - E_{y-(2j-1)})|
\]

\[
\Delta B_{K} = \sum_{i=1}^{s} \sum_{j=1}^{s} \sum_{j_i,j_{i-1},j_{i+1}} |(E_{x-j} - E_{y-j})|
\]

\[
(S_{x,j_{i,j_{i+1}}}) = \frac{1}{2} \sqrt{(s + 1) 2j - j(j + 1)}
\]

\[
|E_{x-j} - E_{y-j}| = |j^2 - 2s \cdot j|K_x
\]

and for the half-integer spin case:

\[
\Delta E_{\text{split}} = \left| \frac{2 \prod_{j=1}^{s} (S_{x,j} + S_{y,j}) \cdot (\Delta B_x + \Delta B_{K})}{\Pi_{j=1}^{2s-1} |(E_{x-j} - E_{y-j})|} \right|
\]

\[
\Delta B_x = B_x^{2s}
\]

\[
\Delta B_K = \sum_{n=0}^{s} B_x^{2n+1} \cdot K \gamma = s + \frac{1}{2} \cdot (-1)^{2s+1} \prod_{j=1}^{s} \sum_{j_i,j_{i-1},j_{i+1}} |(E_{x-j} - E_{y-j})|.
\]

Further, we investigated the influence of the transversal magnetic field on the energy splitting for higher integer quantum spins and we introduced an exact formula, obtained by the ratio \( \lim_{s \to \infty} |\Delta B_{K,i} / \Delta K| = 1 \),

\[
\frac{1}{\alpha_m K_x} \cdot B_x^2 = K
\]

\[
\alpha_m = 2 + \sum_{n=0}^{m} 16n, \quad m \in \mathbb{N}_0
\]

\[
\alpha_m \in [2, 18, 50, 98, 162,...]
\]

which defines values of the transversal magnetic field, the transversal anisotropy and the uniaxial anisotropy where the contribution of the transversal magnetic field to the energy splitting is at least equal to the contribution of the transversal anisotropy.

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The comment by Garg on our manuscript ‘Perturbative calculations of quantum spin tunneling in effective spin systems with a transversal magnetic field and transversal anisotropy’ contains two points. First, the author of the comment introduces a more compact version of our formula equations (2) and (3) for the tunnel splitting energy.

\[
\Delta E = \frac{4s}{2^{2s}(2s - 1)!K^2} \prod_{n=1}^{2s-1} (B_x - (2s + 1 - 2n)B_n)
\]

\[
B_n = \sqrt{2KK_x}.
\]

(5)

Which agrees very well with our formula in equation (2) (see table 1).

We disagree with the implication by the author of the comment that his formula in equation (5) should replace ours (equations (2) and (3)), because our intention was not to generate a compact formula, but rather to derive formulas which can distinguish between mixed \(\Delta B_K\) and pure \(\Delta B_x\) tunneling paths. We have chosen this approach in order to obtain a mathematical structure which enables us to make relations between the tunneling paths, without any further transformations.

To obtain a similar separated expression of the tunneling paths (like in our formalism) based on equation (5) by the author of the comment, one should have to do some transformations, which would make the formula less compact.

Second, the author of the comment disagrees with our interpretation of equation (4) regarding the energy splitting values. The author of the comment shows that the values of \(\Delta E\), generated by the parameters which fulfills our equation (4), leads to the energy splitting \(\Delta E = 0\).

Here we agree with the comment of the author that our interpretation of equation (4) is not exact, because in our technical numerical procedure the tunneling terms do not cancel each other completely out as predicted by equation (4). The conclusion by the author of the comment is correct that these special values of \(B_n\) lead to quenched tunneling points [2], where the energy splitting is exactly zero. This means that our formula in equation (4) generates parameters (\(B_n\) and \(K\) and \(K_x\)) where we obtain shared quenching points \(\Delta E = 0\) for all quantum spin numbers.

Vanishing of mixed \(\Delta B_{s,K}\) paths

In order to show further advantages of the mathematical structure of equations (2) and (3) we want to use this opportunity to present an effect which is not related to the quenched tunnel splitting [2], but can be made visible by our perturbative approach. This effect describes a unique situation where no mixing of tunneling paths \(\Delta B_{s,K}\) term in equation (2)) occurs, but instead only pure paths \(\Delta B_s\) and \(\Delta K_x\) exist. By plotting the \(\Delta B_{s,K}\) term against the transversal magnetic field demonstrated in figures 1(a) and (b) we see that the mixed \(\Delta B_{s,K}\) paths are vanishing under certain values of \(B_n\). In figure 1(a) we show a spin \(s = 3\) system, which is the smallest possible system where this effect appears. We see that under the value of \(B_n = 0.021\) (arb. units), which depends on the parameters of \(K_x\) and \(K\), the mixed \(\Delta B_{s,K}\) paths are vanishing. The spin \(s = 13\) system in figure 1(b) demonstrates that the number of these critical values of \(B_n\) where the mixed \(\Delta B_{s,K}\) paths are vanishing, depends on the spin quantum number. It is important to mention that the number of these \(B_n\) values has the tendency to increase with increasing spin quantum number. Moreover, this increase seems not to be monotonous: for spin \(s = 7\) there are three critical values of \(B_n\), but for spin \(s = 8\) only two.

These values differ for each spin number. They are also different from the values of the quenched tunnel splitting, and lead to a linear combination of two pure paths \(\Delta B_s\) and \(\Delta K\) (see equation (2)) for integer spins and to the single contribution \(\Delta B_s\) (see equation (3)) for the half integer spins. This leads to the conclusion that in contrast to the quenched tunnel splitting, where the energy splitting is vanishing and so the quantum spin tunneling, our formalism reveals a situation where quantum spin tunneling occurs but the influence of the transversal magnetic field is drastically reduced, both for integer and half-integer spins. We can interpret this
situation as the destructive interference of the $\Delta B_{x,K}$ paths, which occurs because of the alternating series structure for positive $K$.

References

[1] Krizanac M, Vedmedenko E Y and Wiesendanger R 2017 New J. Phys. 19 010303
Krizanac M, Vedmedenko E Y and Wiesendanger R 2017 New J. Phys. 19 029501
[2] Garg A 1993 Europhys. Lett. 22 205