Reply to "Comment on 'Excitons, trions, and biexcitons in transition-metal dichalcogenides: Magnetic-field dependence' "

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In the Comment, the authors state that the separation of the relative and center of mass variables in our work is not correct. Here we point out that there is a typographical error, i.e., q_i instead of $-e$, in two of our equations which, when corrected, makes the Comment redundant. Within the ansatzes mentioned in our paper all our results are correct, in contrast to the claims of the Comment.

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In the Comment [1] on our work [2], the authors state that the separation of the relative and center of mass variables in our work is not correct. We would like to thank the authors since this Comment made us realize that there is a typographical error, i.e., q_i instead of $-e$, in Eqs. (1) and (2) of our paper. This error probably caused the confusion and prompted the authors to write the Comment, and correcting it will make said Comment redundant. We will now explain this in more detail.

The kinetic part of the electron Hamiltonian in the presence of a magnetic field is given by $(\boldsymbol{p}+e\boldsymbol{A})^2$ (leaving out the prefactor for simplicity), with $\boldsymbol{p}$ the momentum, $\boldsymbol{A}$ the vector potential, and e the elementary charge. For a positively charged *real* particle, e.g., a proton, this becomes $(\boldsymbol{p}-e\boldsymbol{A})^2$ because of the opposite charge. Adding the Hamiltonians for a negatively charged and a positively charged particle leads to a total Hamiltonian of the form of Eq. (1) of the Comment. The single-particle angular momenta do not commute with the Hamiltonian and therefore cannot be set equal to zero. Therefore, in order to separate the relative and center of mass coordinates the procedure presented in the Comment, based on Refs. [4,5] of the Comment which treat real particles (i.e., atoms), should be used. However, a hole is *not* a real particle.

This brings us to the main point of our Reply. The hole Hamiltonian can be obtained from the electron Hamiltonian by taking its time reversal [3], which leaves the effective mass Hamiltonian invariant. This is because both the momentum and the vector potential change sign upon time reversal, while the charge does not (see for example Eq. (1) of Ref. [4]). Since the total magnetic momentum is squared, the hole Hamiltonian reduces to the electron Hamiltonian (see for example Eq. (2) of Ref. [5]). However, we inadvertently wrote q_i instead of $-e$ in Eqs. (1) and (2) of our paper, which may explain the confusion. When this is corrected, Eq. (1) of our paper becomes

$$H=\sum_{i=1}^{N}\frac{\hbar^2}{2m_i}\Big(\boldsymbol{k}_i+\frac{e}{\hbar}\boldsymbol{A}_i\Big)^2+\sum_{i<j}^{N}V_{ij}(|\boldsymbol{r}_i-\boldsymbol{r}_j|)+\sum_{i=1}^{N}V(r_i), \tag{1}$$

which agrees with Ref. [4]. Expanding the kinetic term for the case of excitons leads to

$$H_{\text{kin}}=\frac{\hbar^2k_e^2}{2m_e}+\frac{\hbar^2k_h^2}{2m_h}+\frac{e^2B^2}{8m_e}r_e^2+\frac{e^2B^2}{8m_h}r_h^2+\hat{A}, \tag{2}$$

with

$$\hat{A}=\frac{eB}{2m_e}\hat{L}_z^e+\frac{eB}{2m_h}\hat{L}_z^h. \tag{3}$$

The above expression now has a plus sign between the two terms, as compared to the minus sign as shown in the Comment. The operator $\hat{A}$ now commutes with the total Hamiltonian for equal electron and hole masses and can therefore be eliminated. Transforming to relative and center of mass coordinates then leads to Eq. (2) of the Comment [Eq. (11) of our paper]. The suggested approach in the Comment, i.e., that for real particles, leads to a diamagnetic term which is a factor 4 larger as compared to our result. The authors of the Comment suggest that this factor 4 might explain the discrepancy between our results and the experimental data for the diamagnetic shift, presented in Table V of our paper. However for WSe_2 and for B excitons for WS_2, for which our results are about a factor 2 smaller than the experimental results, incorporating this factor 4 would lead to results which are about a factor 2 larger than the experimental results.

This brings us to the last point of our report. For our simplified variational model we indeed assumed equal electron and hole masses in order to separate the center of mass part from the relative part. As stated in the Comment, density functional theory calculations have shown that there is in fact a small difference between the electron and hole effective masses. Nevertheless, equal effective masses are also often assumed in effective mass models [6], showing small quantitative differences, as well as implicitly in all works based on the Dirac model of Ref. [7]. We want to stress that we

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only used this approximation for the simplified variational model. For the SVM calculations for excitons, trions, and biexcitons we did not use this approximation since the relative and center of mass part of the Hamiltonian are numerically solved simultaneously. Therefore, the remark in the Comment about "the approximate exciton energies with a low accuracy shown in Table II" of our paper is in any case incorrect.

In summary, the Comment helped us realize that there is a notational error, i.e., q_i instead of $-e$, in Eqs. (1) and (2) of our paper, possibly indicating the need for an Erratum. When corrected, the Comment is redundant since the proposed procedure is not applicable to our Hamiltonian. Furthermore, we believe that the equal effective mass approximation is a nonissue because: (i) we only use it for the simplified variational model and not for the SVM results presented in Table II, (ii) the equal mass approximation is used in many different works in the literature, and (iii) it only gives small quantitative differences.

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