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Reply

Reply to the Comment by S. Rombouts *et al.* on "New criteria for bosonic behaviour of excitons"

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We agree with Rombouts, Van Neck and Pollet (RVNP) that the problem of interacting close-to-boson particles like excitons is not trivial. For this reason, notations must be accurate so as to avoid confusion and/or misleading interpretations. We call N the number of electron-hole (e-h) pairs in the system and $B_i^\dagger$ the creation operator of the exact exciton i, defined by $(H - E_i)B_i^\dagger|v\rangle = 0$, where H is the exact semiconductor Hamiltonian written in terms of fermions (electrons and holes). These exact excitons differ from bosons because $[B_i, B_j^\dagger] \neq \delta_{ij}$. Those willing to treat excitons as bosons from the start, introduce *other* exciton operators $\bar{B}_i^\dagger$ such that $[\bar{B}_i, \bar{B}_j^\dagger] = \delta_{ij}$. Using these operators, they replace H by an effective bosonic Hamiltonian $H_{\rm eff} = \bar{H}_0 + \bar{V}$, the non-interacting part reading $\bar{H}_0 = \sum_i E_i \bar{B}_i^\dagger \bar{B}_i$.

We now consider RVNP's Comment. They call the "e-h pair number" and the "boson number" with the *same* letter N, which is misleading since the problem is precisely to find the number of e-h pairs which can be considered as bosons. Their $\hat{B}^\dagger$ is clearly our ground-state exciton creation operator $B_0^\dagger$. On the opposite, the meaning of the *other* operator $B^\dagger$ appearing in their Hamiltonian (3) is unclear. In view of the effective Hamiltonian $\bar{H}_0$, we are led to think that $B^\dagger = \bar{B}_0^\dagger$, so that their Hamiltonian would just correspond to *one* term of the non-interacting part of the effective bosonic Hamiltonian. However, RVNP's previous work [1] —which is an extended version of this Comment— leads us to believe that $\hat{B}^\dagger$ and $B^\dagger$ are in fact identical (in spite of the fact that $B^\dagger$, written $b_0^\dagger$ in their letter, reads in terms of electrons $a_{\boldsymbol{k}}^\dagger a_{-\boldsymbol{k}}^\dagger$ and not in terms of electrons and holes $a_{\boldsymbol{k}}^\dagger b_{-\boldsymbol{k}}^\dagger$ as it should). This uncertainty on the precise meaning of $B^\dagger$ does not help to discuss their results, since the issue is essentially to know to which extent we can consider that $B_0^\dagger \simeq \bar{B}_0^\dagger$, *i.e.*, $\hat{B}^\dagger \simeq B^\dagger$ if $B^\dagger \equiv \bar{B}_0^\dagger$. RVNP introduce a "boson occupation number $N_{\rm c}$", which they call "exciton occupation number" later on —although excitons are not always bosons. This $N_{\rm c}$ is first defined as the expectation value of $\hat{B}^\dagger \hat{B}$, which is then replaced by $B^\dagger B$. There is no doubt that, if $B^\dagger \equiv \bar{B}_0^\dagger$, the operator $B^\dagger B$, *i.e.* $\bar{B}_0^\dagger \bar{B}_0$, is the ground-state boson number operator. On the opposite, if $B^\dagger$ is not $\bar{B}_0^\dagger$ but $B_0^\dagger$, the physical meaning of $B^\dagger B$ is not clear. *One of the goals of our letter was precisely to determine to which extent $B_0^\dagger B_0$ may be considered as a boson number operator.*

Let us recall the spirit of our approach: In the low-density limit, N e-h pairs in their ground state $|\psi^{(N)}\rangle$ are close to N ground-state excitons. To lowest order in $\eta = Na_{\mathrm{X}}^3/V$, $\langle\psi^{(N)}|H|\psi^{(N)}\rangle \simeq NE_0 \simeq \langle v|B_0^N H B_0^{\dagger N}|v\rangle/\langle v|B_0^N B_0^{\dagger N}|v\rangle$ (see [2,3]). Although the basis for N e-h pairs made of the N-exciton states $B_{i_1}^\dagger \cdots B_{i_N}^\dagger|v\rangle$ is overcomplete and non-orthogonal [4], it can be used to expand $|\psi^{(N)}\rangle$. It leads to $|\psi^{(N)}\rangle \simeq B_0^{\dagger N}|v\rangle$ at lowest order in η, in agreement with Keldysh and Koslov [5]. We know that, when $H = H_0 + V$, the Coulomb interaction V between N-fermion states is unimportant for $\langle 0|V|0\rangle \ll \langle 0|H_0|0\rangle$, $|0\rangle$ being the N-fermion state *in the absence of interactions*. In the same way, we can use $B_0^{\dagger N}|v\rangle$, the zeroth-order exciton state in η, *i.e.*, in Coulomb *and* Pauli interactions, to estimate when N pairs deviate from N ground-state bosons. This deviation is physically linked to the Pauli part of these X-X interactions. There is however a formal difficulty to assess when it is small, since this Pauli part is not characterized by a potential V_{Pauli}. We may see $[B_0, B_0^\dagger] = 1 - D_{00}$ as being the equivalent of $H = H_0 + V$ with respect to this Pauli part. This led us to impose $\langle v|B_0^N D_{00} B_0^{\dagger N}|v\rangle \ll \langle v|B_0^N B_0^{\dagger N}|v\rangle$. We can also view $B_0^\dagger B_0$ as representing the number of bosons if $[B_0, B_0^\dagger] \simeq 1$, *i.e.*, if $B_0^\dagger \simeq \bar{B}_0^\dagger$. This led us to $\langle v|B_0^N (B_0^\dagger B_0) B_0^{\dagger N}|v\rangle$ close to its exact boson value $N\langle v|B_0^N B_0^{\dagger N}|v\rangle$. The first criterion gives $100\eta \ll 1$ while the second one gives $50\eta \ll 1$: These results are consistent with each other [6].

In their Comment, RVNP claim that the number of bosons is the expectation value of $B^\dagger B$ in an appropriate ground state, supposedly "exact". This is correct if and only if $B^\dagger = \bar{B}_0^\dagger$. However, within this boson framework, the excitons are viewed as bosons from the start, so that there is no way to assess when they deviate. On the opposite, if $B^\dagger$ is not $\bar{B}_0^\dagger$ but $B_0^\dagger$, we have shown that $B^\dagger B$ can be associated to the ground-state boson number for $50\eta \ll 1$ only, so that we contest the meaning of their result for $\eta \simeq 1/4\pi$. Moreover, we question the validity of results obtained using their eq. (3) instead of the exact H. Either $B^\dagger = \bar{B}_0^\dagger$, and again excitons are considered as bosons from start, or $B^\dagger = B_0^\dagger$ and we do not know any *clean* procedure to transform the *exact* H into their eq. (3): The exciton *vs.* boson problem is too subtle to trust results obtained from uncontrolled approximations, guesses and/or wishful thinkings.

To conclude, our aim is to find the properties of N e-h pairs in their ground state *as an expansion* in $\eta = Na_{\mathrm{X}}^3/V$. The η terms come from both Coulomb interaction and Pauli exclusion, the last one being physically linked to the close-to-boson character of the excitons. Contrary to RVNP's claim, the state $B_0^{\dagger N}|v\rangle$ is definitely relevant: It is the N-pair ground state at lowest order in η. Moreover, $B_0^\dagger B_0$ can be associated to a boson number operator for $50\eta \ll 1$ only, so that we contest using it up to $\eta \simeq 1/4\pi$. We wish to stress that our criterion for bosonic behavior of excitons does not mean that excitons cannot undergo Bose-Einstein condensation, but just that, above say $\eta \simeq 1/100$, the critical density for BE condensation cannot be taken as that for non-interacting bosons: Excitons do exist according to the Mott criterion, but their interactions (Pauli and Coulomb) must be taken into account.

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[6] Being of course valid as leading-order corrections in η, they should not be used beyond their validity range, as performed by RVNP in fig. 1 of their Comment.