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Density expansion of the energy of N close-to-boson excitons

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Abstract. Pauli exclusion between the carriers of N excitons induces novel many-body effects, quite different from the ones generated by Coulomb interaction. Using our commutation technique for interacting close-to-boson particles, we here calculate the Hamiltonian expectation value in the N-ground-state-exciton state. Coulomb interaction enters this quantity at first order only by construction; nevertheless, due to Pauli exclusion, subtle many-body effects take place, which give rise to terms in $(Na_x^3/\mathcal{V})^n$ with $n \geq 2$. An *exact* procedure to get these density dependent terms is given.

PACS. 71.35.-y Excitons and related phenomena

It is known that excitons being made of two fermions are not exact bosons. Their underlying fermionic character is however a major difficulty which has been overcomed very approximately up to quite recently. An approach [1,2] which has looked reasonable for years is to assume that excitons are exact bosons provided that their close-to-boson character is included in an appropriate exciton-exciton interaction which is basically a Coulomb interaction dressed by exchange processes.

Very recently, we have developed a formalism which allows to include the close-to-boson character of the excitons *exactly*, through an extremely simple and physically quite transparent algebra [3]. Using this "commutation technique", we have already shown [4], by calculating the correlations of *two* excitons, that Pauli exclusion between the two electrons and the two holes of these two excitons, enters their Coulomb terms in such a subtle way that a naïve bosonic Hamiltonian for excitons [1,2,5] cannot produce these terms correctly beyond first order in Coulomb interaction, reducing considerably the impact of such an effective Hamiltonian.

A way to physically understand the problem is to realize that excitons feel each other through both Coulomb interaction *and* Pauli exclusion between their components. Consequently, besides the usual many-body effects resulting from Coulomb interaction, the excitons do have very unusual ones coming from Pauli exclusion. These two kinds of many-body effects, being utterly independent, enter the various quantities of physical interest quite differently. So that there is no reason, for the exchange processes resulting from Pauli exclusion, to dress the Coulomb interaction in an unique way. In other words, there is no reason to describe the physics of interacting excitons by *one* dressed exciton-exciton interaction only, as assumed in the effective bosonic Hamiltonian.

In the present work, we calculate the semiconductor Hamiltonian expectation value in the N-ground-state-exciton state. In the absence of Coulomb interaction *and* Pauli exclusion, this Hamiltonian expectation value $\langle H\rangle_N$ should be equal to NE_0 with E_0 being the ground state energy of one exciton. Due to Coulomb interaction, which by construction enters this quantity at first order only, we should find *one* additional term resulting from the average Coulomb energy in this N-exciton state, and which should be $Na_x^3/\mathcal{V}$ smaller than the main energy NE_0, a_x being the exciton Bohr radius and $\mathcal{V}$ the sample volume. The exact calculation shows that the Hamiltonian expectation value also contains terms in $(Na_x^3/\mathcal{V})^n$ with $n \geq 2$, which originate from many-body effects between the N excitons induced by Pauli exclusion. Using our commutation technique, we show how we can derive these many-body effects in a systematic way, at any order in $\eta = Na_x^3/\mathcal{V}$.

Let us stress that the N-ground-state-exciton state $(B_0^\dagger)^N|v\rangle$ considered here is *not* the ground state of N electron-hole pairs. If this were the case, $\langle H\rangle_N$ would not be the Hamiltonian expectation value in this state, but barely the N-electron-hole-pair ground state energy. $(B_0^\dagger)^N|v\rangle$ is nevertheless a physically relevant state as it is the N-pair ground state at lowest order in the interactions (Coulomb and Pauli), so that $\langle H\rangle_N$ is part of the N-pair ground state energy. Moreover, as excitons – and not more complex structures like biexcitons – are coupled to light, $(B_0^\dagger)^N|v\rangle$ is the relevant "initial" state after the absorption of N photons tuned to the exciton ground state energy. In the time evolution of this initial state – from which follow the lifetime and scattering rates – this expectation value $\langle H\rangle_N$ also plays a crucial role.

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For the sake of simplicity, we here forget about the spin degrees of freedom of the excitons. Their inclusion is formally straightforward following reference [6]. They however lead to quite cumbersome equations which tend to hide the physics we want to point out here.

The paper is organized as follows. In Section 1, we recall the basic relations of our commutation technique and use them to calculate the expectation value of the Hamiltonian in the N-ground-state-exciton state, $\langle H\rangle_N$. In Section 2, we derive the recursion relation satisfied by the matrix elements which appear in the expression of $\langle H\rangle_N$, and we iterate this relation to obtain the density leading terms of these matrix elements. In Section 3, we calculate the three first terms of the $\eta = Na_x^3/\mathcal{V}$ expansion of $\langle H\rangle_N$ explicitly. In the conclusion, we discuss the obtained result and relate it to the new criterion for bosonic behavior of excitons we recently proposed [7].

1 Expectation value of the Hamiltonian using our commutation technique

The semiconductor Hamiltonian expectation value in the N-ground-state-exciton state reads

$$\langle H\rangle_N = \frac{\langle v|(B_0)^N H (B_0^\dagger)^N|v\rangle}{\langle v|(B_0)^N (B_0^\dagger)^N|v\rangle}\ , \tag{1}$$

where $|v\rangle$ is the electron-hole pair vacuum state and $B_0^\dagger$ the (exact) creation operator of one ground state exciton, *i.e.* exciton with a center of mass momentum $\mathbf{Q}_0 = \mathbf{0}$ and a relative motion in its ground state φ_{ν_0}. The algebraic calculation of $\langle H\rangle_N$ is quite easy through our commutation technique.

Two important relations of this commutation technique are [3]

$$\left[H, B_i^\dagger\right] = E_i B_i^\dagger + V_i^\dagger\ , \tag{2}$$

$$\left[V_i^\dagger, B_j^\dagger\right] = \sum_{mn} \xi^{\mathrm{dir}}_{mnij} B_m^\dagger B_n^\dagger\ , \tag{3}$$

where E_i is the i exciton energy and $B_i^\dagger$ the (exact) creation operator of an i exciton, i standing for $(\nu_i, \mathbf{Q}_i)$. The operator $V_i^\dagger$ comes from the Coulomb interactions between the i exciton and the rest of the system, while the parameter $\xi^{\mathrm{dir}}_{mnij}$ corresponds to the direct Coulomb scattering of the (i,j) excitons into the (m,n) states (see Fig. 1a). In $\mathbf{r}$ space, $\xi^{\mathrm{dir}}_{mnij}$ reads [3]

$$\begin{aligned}\xi^{\mathrm{dir}}_{mnij} = \xi^{\mathrm{dir}\,*}_{ijmn} = \frac{1}{2}\int & d\mathbf{r}_{e_1}\, d\mathbf{r}_{h_1}\, d\mathbf{r}_{e_2}\, d\mathbf{r}_{h_2} \\ & \times \phi_m^*(e_1,h_1)\phi_n^*(e_2,h_2) \\ & \times [V_{e_1e_2} + V_{h_1h_2} - V_{e_1h_2} - V_{e_2h_1}] \\ & \times \phi_i(e_1,h_1)\phi_j(e_2,h_2) + (i \leftrightarrow j)\ ,\end{aligned} \tag{4}$$

where $\phi_i(e,h)$ is the total wave function of the i exciton, *i.e.* the product of the relative motion wave function $\varphi_{\nu_i}(\mathbf{r}_e - \mathbf{r}_h)$, and the center of mass wave function $\mathrm{e}^{\mathrm{i}\mathbf{Q}_i\cdot(\alpha_e\mathbf{r}_e+\alpha_h\mathbf{r}_h)}/\sqrt{\mathcal{V}}$, with $\alpha_e = 1-\alpha_h = m_e/(m_e+m_h)$.

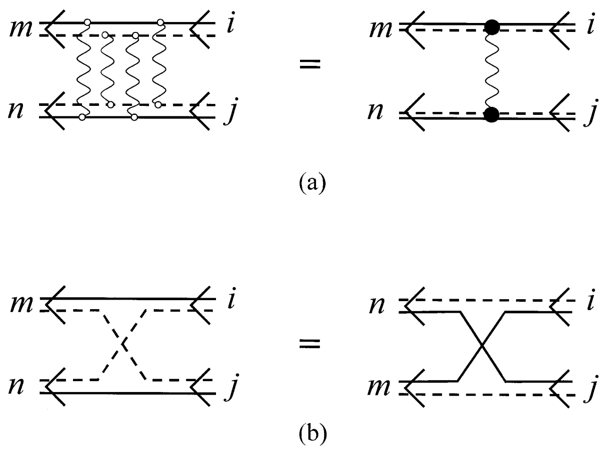

Fig. 1. (a) Direct Coulomb interaction $\xi^{\mathrm{dir}}_{mnij}$ between two excitons which are scattered from the (i,j) states to the (m,n) states, the "in" and "out" excitons being made with the same electron-hole pairs. (b) Coupling between (i,j) and (m,n) excitons induced by the fact that two electrons and two holes can be coupled in two different ways to form two excitons.

Using equations (2,3), it is straightforward to prove by induction that

$$\begin{aligned}\left[H, (B_0^\dagger)^N\right] = N E_0 (B_0^\dagger)^N + \frac{N(N-1)}{2} \\ \times \sum_{mn} \xi^{\mathrm{dir}}_{mn00} B_m^\dagger B_n^\dagger (B_0^\dagger)^{N-2} + N (B_0^\dagger)^{N-1} V_0^\dagger\ ,\end{aligned} \tag{5}$$

so that, as $H|v\rangle = 0 = V_0^\dagger|v\rangle$, we get with H acting on the left

$$\begin{aligned}\langle H\rangle_N = N E_0 + \frac{N(N-1)}{2} \\ \times \sum_{mn} \xi^{\mathrm{dir}}_{00mn} \frac{\langle v|(B_0)^{N-2} B_m B_n (B_0^\dagger)^N|v\rangle}{\langle v|(B_0)^N (B_0^\dagger)^N|v\rangle}\ .\end{aligned} \tag{6}$$

As expected, Coulomb interaction enters $\langle H\rangle_N$ at first order only, as $\langle H\rangle_N$ is linear in the Coulomb scatterings $\xi^{\mathrm{dir}}_{00mn}$.

If the excitons were exact bosons, the ratios in the sum would be 1 for $m = n = 0$, and 0 otherwise, so that we would get $\langle H\rangle_N = NE_0 + N(N-1)\xi^{\mathrm{dir}}_{0000}/2$. We can then note that for $n = i = j$, equation (4) reduces to

$$\begin{aligned}\xi^{\mathrm{dir}}_{miii} = \frac{1}{\mathcal{V}^2}\int d\mathbf{r}_{e_1}\, d\mathbf{r}_{h_1}\, d\mathbf{r}_{e_2}\, d\mathbf{r}_{h_2}\, \mathrm{e}^{\mathrm{i}(\mathbf{Q}_i-\mathbf{Q}_m)\cdot(\alpha_e\mathbf{r}_{e_1}+\alpha_h\mathbf{r}_{h_1})} \\ \times \varphi^*_{\nu_m}(\mathbf{r}_{e_1}-\mathbf{r}_{h_1})\varphi_{\nu_i}(\mathbf{r}_{e_1}-\mathbf{r}_{h_1})\,|\varphi_{\nu_i}(\mathbf{r}_{e_2}-\mathbf{r}_{h_2})|^2 \\ \times\left(\frac{e^2}{|\mathbf{r}_{e_1}-\mathbf{r}_{e_2}|} + \frac{e^2}{|\mathbf{r}_{h_1}-\mathbf{r}_{h_2}|} - \frac{e^2}{|\mathbf{r}_{e_1}-\mathbf{r}_{h_2}|} - \frac{e^2}{|\mathbf{r}_{e_2}-\mathbf{r}_{h_1}|}\right) = 0,\end{aligned} \tag{7}$$

as can be seen by exchanging $\mathbf{r}_{e_2}$ and $\mathbf{r}_{h_2}$. Consequently, strangely enough, if we forgot about the close-to-boson character of the excitons, $\langle H\rangle_N$ would be equal to NE_0 as if the excitons were not interacting at all!

Of course, excitons are not exact bosons. Let us now show how we can calculate the matrix elements appearing in the sum of equation (6) for exact excitons. Here again, two important relations of our commutation technique make their calculation quite easy, namely [3]

$$\left[B_i, B_j^\dagger\right] = \delta_{ij} - D_{ij} \tag{8}$$

$$\left[D_{mi}, B_j^\dagger\right] = 2\sum_n \lambda_{mnij} B_n^\dagger \ . \tag{9}$$

D_{ij} is the deviation-from-boson operator, while the parameter λ_{mnij} describes the fact that there are two ways to couple two electrons (e_1, e_2) and two holes (h_1, h_2) to make two excitons, either $(e_1, h_1)(e_2, h_2)$ or $(e_1, h_2)(e_2, h_1)$ (see Fig. 1b). In $\mathbf{r}$ space λ_{mnij} reads [3]

$$\begin{aligned}\lambda_{mnij} = \lambda^*_{ijmn} = \frac{1}{2}\int & \mathrm{d}\mathbf{r}_{e_1}\,\mathrm{d}\mathbf{r}_{h_1}\,\mathrm{d}\mathbf{r}_{e_2}\,\mathrm{d}\mathbf{r}_{h_2} \\ & \times \phi^*_m(e_1, h_1)\phi^*_n(e_2, h_2)\phi_i(e_1, h_2)\phi_j(e_2, h_1) \\ & + (i \leftrightarrow j) \ .\end{aligned} \tag{10}$$

Equations (8–10) are the key equations which allow an easy calculation of the matrix elements appearing in $\langle H\rangle_N$.

2 Calculation of the matrix elements appearing in $\langle \mathrm{H}\rangle_{\mathrm{N}}$

From equations (8, 9), it is straightforward to prove by induction that

$$\begin{aligned}\left[B_m, (B_0^\dagger)^N\right] = {} & N\delta_{m0}(B_0^\dagger)^{N-1} - N(N-1) \\ & \times \sum_p \lambda_{mp00} B_p^\dagger (B_0^\dagger)^{N-2} - N(B_0^\dagger)^{N-1} D_{m0}.\end{aligned} \tag{11}$$

Before calculating the matrix elements of $\langle H\rangle_N$, with two excitons possibly outside the ground state, let us first consider the simpler ones, with only one exciton outside the ground state, namely

$$\mathcal{A}_m^{(N)} = \langle v \mid (B_0)^{N-1} B_m (B_0^\dagger)^N \mid v\rangle / N! \ . \tag{12}$$

As $D_{ij} \mid v\rangle = 0$, we get from equation (11) that $\mathcal{A}_m^{(N)}$ verifies the recursion relation

$$\mathcal{A}_m^{(N)} = \delta_{m0}\mathcal{A}_0^{(N-1)} - (N-1)\sum_p \lambda_{mp00}\left(\mathcal{A}_p^{(N-1)}\right)^* \ , \tag{13}$$

which is shown in Figure 2a. If we iterate this equation, and note that $\mathcal{A}_0^{(N)}$ is nothing but the quantity F_N defined in reference [7],

$$\mathcal{A}_0^{(N)} = F_N = \langle v \mid (B_0)^N (B_0^\dagger)^N \mid v\rangle / N! \ , \tag{14}$$

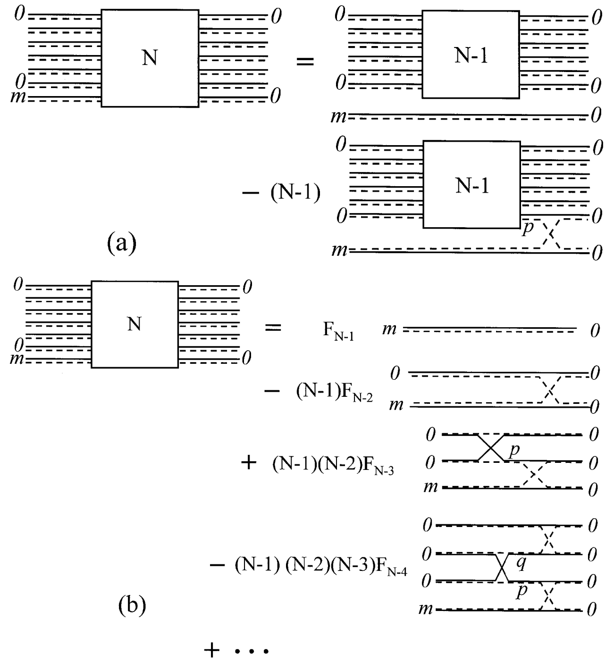

Fig. 2. Overlap $\mathcal{A}_m^{(N)}$, as defined in equation (12), between two N-exciton states, when one of the N excitons is in a state m, instead of the ground state 0. (a) Diagrammatic representation of the integral equation (13) which links $\mathcal{A}_m^{(N)}$ to $\left(\mathcal{A}_p^{(N-1)}\right)^*$. The cross represents the λ_{mp00} exchange process. (b) Density expansion of $\mathcal{A}_m^{(N)}$ as given in equation (15). The quantity F_N, defined in equation (14), differs from 1 because the excitons are not exact bosons.

we find that $\mathcal{A}_m^{(N)}$ expands as

$$\begin{aligned}\mathcal{A}_m^{(N)} = {} & F_{N-1}\delta_{m0} - (N-1)F_{N-2}\lambda_{m000} \\ & + (N-1)(N-2)F_{N-3}\sum_p \lambda_{mp00}\lambda_{00p0} \\ & -(N-1)(N-2)(N-3)F_{N-4}\sum_{pq}\lambda_{mp00}\lambda_{00pq}\lambda_{q000} + \cdots \ ,\end{aligned} \tag{15}$$

(see Fig. 2b). By expliciting the λ's, it is possible to show that, for $m = 0$, equation (15) is nothing but the recursion relation between the F_N's given in reference [7], namely

$$\begin{aligned}F_N = {} & F_{N-1} - (N-1)\,\sigma_2\,F_{N-2} \\ & + (N-1)(N-2)\,\sigma_3\,F_{N-3} - \cdots \ ,\end{aligned} \tag{16}$$

with

$$\begin{aligned}\sigma_n &= \sum_{\mathbf{k}} |\Phi_{\nu_0}(\mathbf{k})|^{2n} \\ &= \frac{16(8n-5)!!}{(8n-2)!!}\,(64\pi a_x^3/\mathcal{V})^{n-1} \ ,\end{aligned} \tag{17}$$

in 3D, $\Phi_{\nu_0}(\mathbf{k})$, given in the appendix, being the Fourier transform of $\varphi_{\nu_0}(\mathbf{r})$.

Let us now turn to the matrix elements with two excitons possibly outside the ground state, namely

$$\mathcal{B}_{mn}^{(N)} = \langle v \mid (B_0)^{N-2} B_m B_n (B_0^\dagger)^N \mid v\rangle / N! \,. \tag{18}$$

From equation (9), we get

$$\left[D_{mi}, (B_0^\dagger)^N\right] = 2N \sum_q \lambda_{mqi0} B_q^\dagger (B_0^\dagger)^{N-1} \,, \tag{19}$$

easy to prove by induction. Using equations (11, 18, 19), we find that $\mathcal{B}_{mn}^{(N)}$ verifies the recursion relation,

$$\begin{aligned}\mathcal{B}_{mn}^{(N)} &= F_{N-2}(\delta_{m0}\delta_{n0} - \lambda_{mn00}) - (N-2)\sum_q \left(\mathcal{A}_q^{(N-2)}\right)^* \\ &\times \left\{ \left(\delta_{m0}\lambda_{nq00} - \sum_p \lambda_{mp00}\lambda_{nqp0} \right) + (m \leftrightarrow n) \right\} \\ &+ (N-2)(N-3) \sum_{pq} \left(\mathcal{B}_{pq}^{(N-2)}\right)^* \lambda_{mp00}\lambda_{nq00} \,, \end{aligned} \tag{20}$$

shown in Figure 3a. We can then use equation (15) for $\mathcal{A}_q^{(N)}$ and iterate equation (20). The three first terms of the expansion of $\mathcal{B}_{mn}^{(N)}$ are obtained by replacing $\mathcal{A}_q^{(N-2)}$ by the two first terms of equation (15) and $\mathcal{B}_{pq}^{(N-2)}$ by the first term of equation (20). This leads to

$$\begin{aligned}\mathcal{B}_{mn}^{(N)} &= F_{N-2}(\delta_{m0}\delta_{n0} - \lambda_{mn00}) - (N-2)F_{N-3} \\ &\times \left\{ \left(\delta_{m0}\lambda_{n000} - \sum_p \lambda_{mp00}\lambda_{n0p0} \right) + (m \leftrightarrow n) \right\} \\ &+ (N-2)(N-3)F_{N-4} \\ &\times \Bigg\{ \left[\left(\delta_{m0}\sum_p \lambda_{np00}\lambda_{00p0} - \sum_{pq} \lambda_{mp00}\lambda_{nqp0}\lambda_{00q0} \right) + (m \leftrightarrow n) \right] \\ &+ \lambda_{m000}\lambda_{n000} - \sum_{pq} \lambda_{mp00}\lambda_{nq00}\lambda_{00pq} \Bigg\} + \cdots \end{aligned} \tag{21}$$

The meaning of all these terms is easier to grasp from their diagrammatic representation shown in Figure 3b. We see that the first term of $\mathcal{B}_{mn}^{(N)}$ corresponds to all Pauli couplings between *two* ground state excitons $(0,0)$ and the two (m,n) excitons; the second term of $\mathcal{B}_{mn}^{(N)}$ corresponds to all Pauli couplings between *three* ground state excitons $(0,0,0)$ and the three $(m,n,0)$ excitons; the third term couples the $(0,0,0,0)$ excitons to the $(m,n,0,0)$ excitons, and so on ...

3 Density expansion of $\langle \mathrm{H} \rangle_\mathrm{N}$

Let us now return to the expectation value of the Hamiltonian $\langle H\rangle_N$. Using equations (6, 14, 18, 21), and the fact that $\xi_{000m}^{\mathrm{dir}}=0$ (see Eq. (7)), we find that $\langle H\rangle_N$ reads

$$\langle H\rangle_N = N(E_0 + \Delta) \,, \tag{22}$$

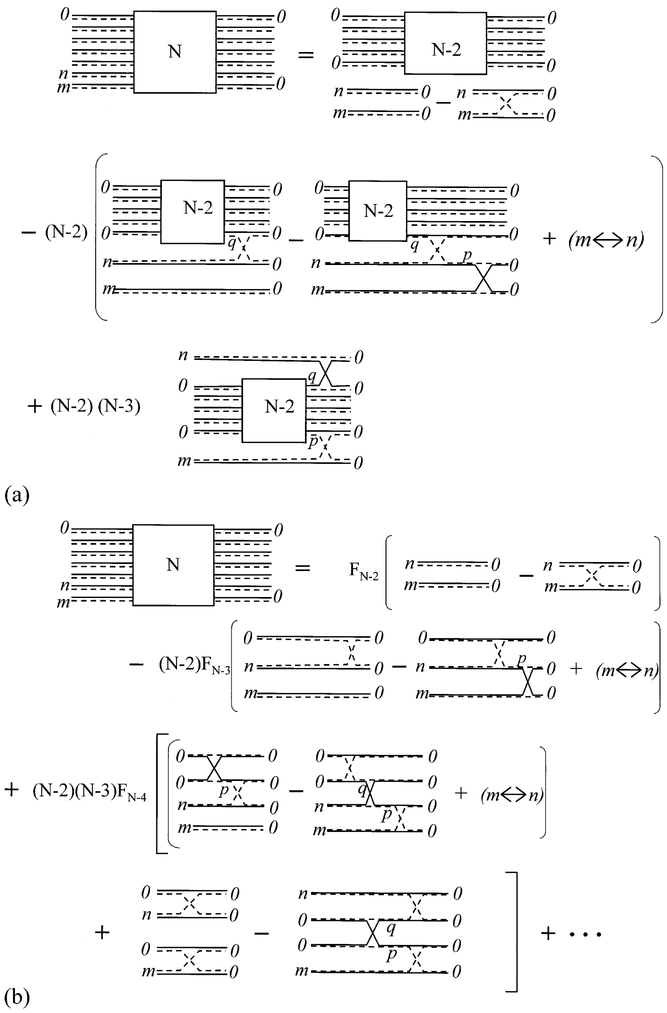

Fig. 3. Overlap $\mathcal{B}_{mn}^{(N)}$, as defined in equation (18), between two N-exciton states when two of the N excitons are in the states (m,n) instead of the ground state 0. (a) Diagrammatic representation of the integral equation (20) which links $\mathcal{B}_{mn}^{(N)}$ to $\left(\mathcal{A}_q^{(N-2)}\right)^*$ and $\left(\mathcal{B}_{pq}^{(N-2)}\right)^*$. The cross of the first line corresponds to λ_{mn00} while the two crosses of the last line correspond to λ_{nq00} and λ_{mp00}. (b) Density expansion of $\mathcal{B}_{mn}^{(N)}$ as given in equation (21). F_N is defined in equation (14).

where the three first terms of Δ are given by

$$\begin{aligned}\Delta &= -(N-1)\frac{F_{N-2}}{F_N}\frac{S_1}{2} + (N-1)(N-2)\frac{F_{N-3}}{F_N} S_2 \\ &- (N-1)(N-2)(N-3) \\ &\times \frac{F_{N-4}}{F_N}\left(S_3 + \frac{S_3'}{2} - \frac{S_3''}{2}\right) + \cdots \,, \end{aligned} \tag{23}$$

the expressions of the various sums S_n in terms of ξ^{dir}'s and λ's being given below.

By looking at Figure 4a, or by using equations (4, 10), it is easy to see that the first sum S_1 reads in $\mathbf{r}$ space

$$\begin{aligned} S_1 &= \sum_{mn} \xi^{\rm dir}_{00mn} \lambda_{mn00} \\ &= \int \mathrm{d}\mathbf{r}_{e_1}\,\mathrm{d}\mathbf{r}_{h_1}\,\mathrm{d}\mathbf{r}_{e_2}\,\mathrm{d}\mathbf{r}_{h_2}\,\phi_0^*(e_1,h_1)\phi_0^*(e_2,h_2) \\ &\times (V_{e_1e_2} + V_{h_1h_2} - V_{e_1h_2} - V_{e_2h_1})\phi_0(e_1,h_2)\phi_0(e_2,h_1)\ , \end{aligned} \tag{24}$$

which is nothing but $\xi^{\rm right}_{0000} \equiv \xi^{\rm exch}_{0000}$ defined in our previous works dealing with the matrix elements of H in the two-exciton subspace [3]. This term is also the usual exchange Coulomb term of the effective bosonic Hamiltonian for excitons [2,8].

The second sum of equation (23) involves three excitons as can be seen from Figure 4b. It reads

$$\begin{aligned} S_2 &= \sum_{mnp} \xi^{\rm dir}_{00mn} \lambda_{mp00} \lambda_{n0p0} \\ &= \int \mathrm{d}\mathbf{r}_{e_1}\,\mathrm{d}\mathbf{r}_{h_1}\,\mathrm{d}\mathbf{r}_{e_2}\,\mathrm{d}\mathbf{r}_{h_2}\,\mathrm{d}\mathbf{r}_{e_3}\,\mathrm{d}\mathbf{r}_{h_3} \\ &\times \phi_0^*(e_1,h_1)\phi_0^*(e_2,h_2)\phi_0^*(e_3,h_3) \\ &\times [V_{e_1e_2} + V_{h_1h_2} - V_{e_1h_2} - V_{e_2h_1}] \\ &\times \phi_0(e_1,h_2)\phi_0(e_2,h_3)\phi_0(e_3,h_1)\ . \end{aligned} \tag{25}$$

The three sums of the third term of equation (23) involves four excitons. The first sum S_3, shown in Figure 4c, reads

$$\begin{aligned} S_3 &= \sum_{mnpq} \xi^{\rm dir}_{00mn} \lambda_{mp00} \lambda_{nqp0} \lambda_{00q0} \\ &= \int \mathrm{d}\mathbf{r}_{e_1}\,\mathrm{d}\mathbf{r}_{h_1}\,\mathrm{d}\mathbf{r}_{e_2}\,\mathrm{d}\mathbf{r}_{h_2}\,\mathrm{d}\mathbf{r}_{e_3}\,\mathrm{d}\mathbf{r}_{h_3}\,\mathrm{d}\mathbf{r}_{e_4}\,\mathrm{d}\mathbf{r}_{h_4} \\ &\times \phi_0^*(e_1,h_1)\phi_0^*(e_2,h_2)\phi_0^*(e_3,h_3)\phi_0^*(e_4,h_4) \\ &\times [V_{e_1e_2} + V_{h_1h_2} - V_{e_1h_2} - V_{e_2h_1}] \\ &\times \phi_0(e_1,h_2)\phi_0(e_2,h_3)\phi_0(e_3,h_4)\phi_0(e_4,h_1). \end{aligned} \tag{26}$$

The sum S_3' defined as $S_3' = \sum_{mnpq} \xi^{\rm dir}_{00mn} \lambda_{mp00} \lambda_{nq00} \lambda_{00pq}$ and shown in Figure 4d, reads as equation (26) except for the four ϕ_0's which are replaced by

$$\phi_0(e_1,h_3)\phi_0(e_2,h_4)\phi_0(e_3,h_2)\phi_0(e_4,h_1)\ .$$

The last sum S_3'' defined as $S_3'' = \sum_{mn} \xi^{\rm dir}_{00mn} \lambda_{m000} \lambda_{n000}$, and shown in Figure 4e, reads as equation (26) except for the four ϕ_0's which are now replaced by

$$\phi_0(e_1,h_3)\phi_0(e_2,h_4)\phi_0(e_3,h_1)\phi_0(e_4,h_2)\ .$$

This sum is in fact equal to zero as easily seen by exchanging $(\mathbf{r}_{e_2} \leftrightarrow \mathbf{r}_{h_2})$, and $(\mathbf{r}_{e_4} \leftrightarrow \mathbf{r}_{h_4})$, in the integral.

It is physically important to note that all these sums contain the *same Coulomb coupling between only two excitons* made with (e_1,h_1) and (e_2,h_2). Couplings between more than two excitons appearing in $S_{n\geq 2}$, result from many-body effects induced by the close-to-boson character of the excitons.

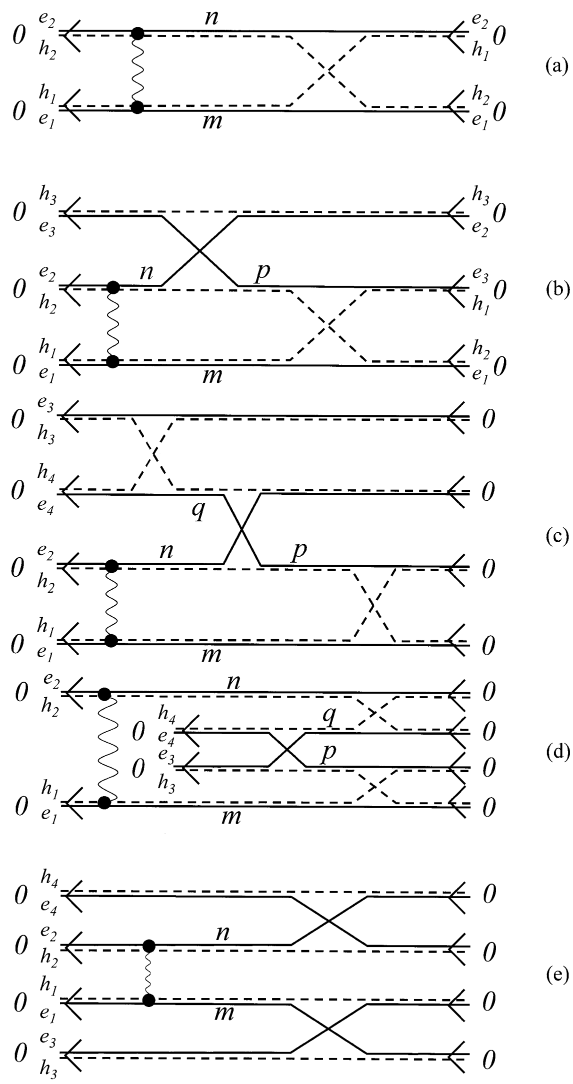

Fig. 4. (a) The sum S_1 defined in equation (24) with one exchange process λ_{mn00} which transforms the $(0,0)$ excitons into (m,n) excitons, followed by one direct Coulomb interaction $\xi^{\rm dir}_{00mn}$ which scatters these (m,n) excitons back into the ground state $(0,0)$. (b) The sum S_2, defined in equation (25), with two exchanges and one direct Coulomb scattering. (c) (d) (e) The sums S_3, S_3' and S_3'', defined in equation (26) and below, with three exchanges and one direct Coulomb scattering.

The sums S_1, S_2, S_3, S_3' are calculated in the Appendix (see Eqs. (A.9–A.12)). Although not obvious at first, S_1, S_2 and $S_3 + S_3'/2$ are in fact real even if Φ_{ν_0} is not, as necessary to have a real energy change Δ resulting from these Coulomb and Pauli couplings.

The F_{N-p}/F_N ratios also generate density dependent terms in Δ. These ratios differ from 1 due to the close-to-boson character of the excitons. Their η expansion can be obtained from the recursion relation (16), which also reads

$$\frac{F_N}{F_{N-1}} = 1 - (N-1)\,\sigma_2\,\frac{F_{N-2}}{F_{N-1}} + (N-1)(N-2)\,\sigma_3\,\frac{F_{N-3}}{F_{N-1}} + \cdots \tag{27}$$

As σ_n is in $(a_x^3/\mathcal{V})^{n-1}$ (see Eq. (17)), we can iterate equation (27) to obtain the ratio F_N/F_{N-1}, for $N \gg 1$, as an expansion in powers of the parameter $\eta = Na_x^3/\mathcal{V}$. We get

$$\frac{F_N}{F_{N-1}} = 1 - N\sigma_2 + N^2(\sigma_3 - \sigma_2^2) + O(\eta^3). \tag{28}$$

As for large N, $F_{N-p}/F_N \simeq (F_{N-1}/F_N)^p$, the ratios appearing in equation (23) are given by

$$\begin{aligned}\frac{F_{N-2}}{F_N} &= 1 + 2N\sigma_2 + N^2(5\sigma_2^2 - 2\sigma_3) + O(\eta^3)\\ \frac{F_{N-3}}{F_N} &= 1 + 3N\sigma_2 + O(\eta^2)\\ \frac{F_{N-4}}{F_N} &= 1 + O(\eta).\end{aligned} \tag{29}$$

By inserting equation (29) into equation (23), we obtain the following expansion of the energy change Δ in powers of η:

$$\begin{aligned}\Delta = &-N\frac{S_1}{2} + N^2[S_2 - \sigma_2 S_1]\\ &+ N^3\left[-S_3 - \frac{S_3'}{2} + 3\sigma_2 S_2 - \frac{S_1}{2}(5\sigma_2^2 - 2\sigma_3)\right] + O(\eta^4).\end{aligned} \tag{30}$$

Using equations (17, A.9–A.12) and putting everything together, we finally find that the Hamiltonian expectation value in the N-ground-state-exciton state expands in powers of $\eta = Na_x^3/\mathcal{V}$ as

$$\begin{aligned}\langle H\rangle_N &= NE_0\left(1 - \frac{13\pi}{3}\eta + \frac{73\pi^2}{20}\eta^2 - \frac{3517\pi^3}{210}\eta^3 + O(\eta^4)\right)\\ &= NE_0\left(1 - 1.4\times 10^1\,\eta + 3.6\times 10^1\,\eta^2 - 5.2\times 10^2\,\eta^3 + O(\eta^4)\right).\end{aligned} \tag{31}$$

Let us again stress that terms in η^n with $n \geq 2$ come from many-body effects induced by Pauli exclusion, since Coulomb interaction enters $\langle H\rangle_N$ at first order only.

4 Conclusion

We have calculated the expectation value $\langle H\rangle_N$ of the exact semiconductor Hamiltonian in the N-ground-state-exciton state $(B_0^\dagger)^N|v\rangle$, using the commutation technique we recently introduced. Due to novel many-body effects induced by the close-to-boson character of the excitons, $\langle H\rangle_N$ appears as an expansion in powers of the density through $\eta = Na_x^3/\mathcal{V}$, Coulomb interaction entering this quantity at first order only by construction. Higher order terms in η^n, with $n \geq 2$, result from both, sophisticated exchange processes in which the Coulomb interaction appears at first order only (see Fig. 4), and purely Pauli many-body effects which make $\langle v|(B_0)^N(B_0^\dagger)^N|v\rangle$ to differ from its exact boson value $N!$

From the result given in equation (31), we see that the prefactors of the expansion of $\langle H\rangle_N$ are rather large so that $\eta = Na_x^3/\mathcal{V}$ has to be much smaller than 1 for $\langle H\rangle_N$ to be equal to the energy of N non-interacting boson-excitons NE_0. In a previous work [7], we have already shown that, while the Mott criterion corresponds to $\eta = Na_x^3/\mathcal{V} \simeq 1$ for the electron-hole pairs to be bound in excitons, *i.e.* for the excitons to exist in spite of screening, the criterion for the excitons to behave as bosons is more like $100Na_x^3/\mathcal{V} \simeq 1$. As the η expansion of $\langle H\rangle_N$ is physically linked to many-body effects induced by the close-to-boson character of the excitons, it is after all reasonable to find similar conditions for excitons to behave as bosons and for the Hamiltonian expectation value to be equal to the one of N non-interacting boson-excitons.

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Appendix

We start from the expressions of S_1, S_2, S_3 and S_3' in $\mathbf{r}$ space given in equations (24–26), and we rewrite them by using the Fourier transforms of the exciton wave function and Coulomb potential. For $\mathbf{Q}_0 = \mathbf{0}$, we have

$$\phi_0(e,h) = \frac{1}{\mathcal{V}}\sum_{\mathbf{k}} \Phi_{\nu_0}(\mathbf{k})\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{r}_e - \mathbf{r}_h)}\ , \tag{A.1}$$

$$\frac{e^2}{r} = \sum_{\mathbf{q}} V_{\mathbf{q}}\,\mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{r}}\ , \tag{A.2}$$

with $V_{\mathbf{q}} = 4\pi e^2/\mathcal{V}q^2$ in 3D.

If we insert equations (A.1, A.2) into S_1 given in equation (24), and we perform the integrals over the $\mathbf{r}$'s, we get

$$S_1 = 2\sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k}-\mathbf{k}'}|\Phi_{\nu_0}(\mathbf{k})|^2\left[|\Phi_{\nu_0}(\mathbf{k}')|^2 - \Phi_{\nu_0}^*(\mathbf{k})\,\Phi_{\nu_0}(\mathbf{k}')\right]\ . \tag{A.3}$$

By using the Schrödinger equation for the exciton relative motion,

$$(\hbar^2\mathbf{k}^2/2\mu - \epsilon_{\nu_0})\Phi_{\nu_0}(\mathbf{k}) - \sum_{\mathbf{k}'} V_{\mathbf{k}-\mathbf{k}'}\,\Phi_{\nu_0}(\mathbf{k}') = 0\ , \tag{A.4}$$

with $\epsilon_{\nu_0} = E_0 = -e^2/2a_x$, we can check that S_1 is real.

If we now insert equations (A.1, A.2) into S_2 given in equation (25), and perform the integrals over the $\mathbf{r}$'s, we get

$$\begin{aligned}S_2 = \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k}-\mathbf{k}'}\,\big[&2|\Phi_{\nu_0}(\mathbf{k})|^4\,|\Phi_{\nu_0}(\mathbf{k}')|^2\\ &-|\Phi_{\nu_0}(\mathbf{k})|^4\,\Phi_{\nu_0}^*(\mathbf{k})\,\Phi_{\nu_0}(\mathbf{k}')\\ &-\left(\Phi_{\nu_0}^{*2}(\mathbf{k})\Phi_{\nu_0}(\mathbf{k})\right)\left(\Phi_{\nu_0}^2(\mathbf{k}')\Phi_{\nu_0}^*(\mathbf{k}')\right)\big]\ .\end{aligned} \tag{A.5}$$

The second term of equation (A.5) is real due to equation (A.4), while the last term is real by $(\mathbf{k} \leftrightarrow \mathbf{k}')$.

For the third order sums, we obtain in the same way

$$S_3 = \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k}-\mathbf{k}'} \, |\Phi_{\nu_0}(\mathbf{k})|^4 \Big[\, 2|\Phi_{\nu_0}(\mathbf{k})|^2 \, |\Phi_{\nu_0}(\mathbf{k}')|^2 - |\Phi_{\nu_0}(\mathbf{k})|^2 \, \Phi^*_{\nu_0}(\mathbf{k}) \, \Phi_{\nu_0}(\mathbf{k}') - |\Phi_{\nu_0}(\mathbf{k}')|^2 \, \Phi_{\nu_0}(\mathbf{k}) \, \Phi^*_{\nu_0}(\mathbf{k}') \, \Big] \ , \tag{A.6}$$

$$S'_3 = 2 \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k}-\mathbf{k}'} \, |\Phi_{\nu_0}(\mathbf{k})|^4 \Big[\, |\Phi_{\nu_0}(\mathbf{k}')|^4 - |\Phi_{\nu_0}(\mathbf{k}')|^2 \, \Phi^*_{\nu_0}(\mathbf{k}) \, \Phi_{\nu_0}(\mathbf{k}') \, \Big] \ . \tag{A.7}$$

The energy shift Δ depending on $(S_3 + S'_3/2)$ as $S''_3 = 0$, we can check that this quantity is real due again to equation (A.4).

By inserting the 3D value of $\Phi_{\nu_0}(\mathbf{k})$, namely

$$\Phi_{\nu_0}(\mathbf{k}) = \frac{8\sqrt{\pi}}{(1 + a_x^2 k^2)^2} \left(\frac{a_x^3}{\mathcal{V}} \right)^{1/2} \ , \tag{A.8}$$

into equations (A.3, A.5–A.7), and by calculating the integrals over $\mathbf{k}$ and $\mathbf{k}'$, we obtain

$$S_1 = \frac{26\pi}{3} \left(\frac{a_x^3}{\mathcal{V}} \right) E_0 \ , \tag{A.9}$$

$$S_2 = \frac{2933\pi^2}{20} \left(\frac{a_x^3}{\mathcal{V}} \right)^2 E_0 \ , \tag{A.10}$$

$$S_3 = \frac{10795\pi^3}{2} \left(\frac{a_x^3}{\mathcal{V}} \right)^3 E_0 \ , \tag{A.11}$$

$$S'_3 = \frac{29601\pi^3}{28} \left(\frac{a_x^3}{\mathcal{V}} \right)^3 E_0 \ , \tag{A.12}$$

with $E_0 = -e^2/2a_x$.

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