## On the N-exciton normalization factor

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**Abstract.** The N-ground-state-exciton normalization factor, namely  $\langle v | B_0^N B_0^{\dagger N} | v \rangle = N! F_N$ , with  $B_0^{\dagger}$  the exact ground state exciton creation operator, differs from N! because the excitons are not perfect bosons. The quantity  $F_N$  turns out to be crucial for problems dealing with interacting excitons. Indeed, the excitons feel each other not only through the Coulomb interaction but also through Pauli exclusion between their components. A quite novel purely Pauli contribution exists in their many-body effects, which relies directly on  $F_N$ . Following procedures used in the commutation technique we recently introduced to treat interacting close-to-bosons, and in the BCS theory of superconductivity, we rederive important relations verified by the  $F_N$ 's. We also give new explicit expressions of  $F_N$  valid for  $\eta = N a_x^3 / \mathcal{V}$  small but  $N^2 a_x^3 / \mathcal{V}$  large, as  $F_N$ does not read in terms of  $\eta$  but  $N\eta$ , the exciton number N being possibly huge in macroscopic samples. Due to this superextensivity,  $F_N$  does not appear alone in physical quantities, but through ratios like  $F_{N+p}/F_N$ . We end this work by giving the  $\eta$  expansion of these ratios, useful for all purely Pauli many-body effects.

PACS. 71.35.Lk Collective effects (Bose effects, phase space filling, and excitonic phase transitions)

### **1** Introduction

In the low density limit, N electron-hole (e-h) pairs in a semiconductor are known [1] to form N excitons. However, as these composite particles are not perfectly bosonic, many-body effects between them [2] are quite tricky to handle properly: Indeed, all many-body theories [3] existing up to now were designed to deal with perfect fermions or perfect bosons. We have recently developed a new theory [4–10], called "commutation technique", to treat many-body effects between close-to-boson excitons. In addition to Coulomb interaction between their electrons and holes, these particles feel each other through Pauli exclusion between their electrons and between their holes. The interplay between Coulomb interaction and Pauli exclusion gives rise to all kinds of sophisticated Coulomb exchange processes. However, even in the absence of any Coulomb interaction, purely Pauli contributions to the exciton interaction must exist. They are related to the fact that, due to possible carrier exchanges in forming the excitons, N-exciton states, unlike perfect boson states, are not orthogonal. In other words, if we look for many-body effects between excitons, *i.e.*, terms in  $\eta = N a_x^3 / \mathcal{V}$ , where N is the exciton number in a volume  $\mathcal{V}$ , and  $a_x$  the exciton Bohr radius, they come from Coulomb interaction dressed by exchange processes, but also from the consequences of Pauli exclusion in scalar products of N-exciton states.

As the ground state exciton enters most problems of physical interest, one of these scalar products is of particular importance, namely

$$\langle v|B_0^N B_0^{\dagger N}|v\rangle = N! F_N , \qquad (1)$$

where  $|v\rangle$  is the vacuum state with no electron-hole pair, and  $B_0^{\dagger}$  is the creation operator of the ground state exciton,

$$B_0^{\dagger} = \sum_{\mathbf{k}} \phi_{\mathbf{k}} \, a_{\mathbf{k}}^{\dagger} \, b_{-\mathbf{k}}^{\dagger} \, , \qquad (2)$$

with  $\phi_{\mathbf{k}}$  being the relative motion wave function in  $\mathbf{k}$ space.

If the excitons were perfect bosons, we would have  $F_N = 1$ . For true excitons in large samples,  $F_N$  turns out to be extremely small [4], behaving as  $\exp(-N\eta)$ . This  $N^2$ dependence, which can be surprising at first, originates from the intrinsic N-body character of Pauli exclusion, which acts "at once" between the constituents of all the N excitons, being N-body by essence and thus conceptually quite different from the two-body Coulomb interaction. The superextensive behavior of  $F_N$  cannot appear, of course, in real physical quantities. Actually,  $F_N$  enters these quantities as ratios such as  $F_{N+p}/F_N$ . However, because these ratios behave as  $1 + O(\eta)$ , the contribution of

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their  $\eta$  dependent terms are as important in many-body effects between excitons as the one coming from Coulomb scatterings.

We have seen this  $F_N$  factor appearing for the first time in our attempt to determine a criterion for bosonic behavior of N excitons [4]. By introducing the deviationfrom-boson operator defined as

$$\left[B_i, B_j^{\dagger}\right] = \delta_{ij} - D_{ij} , \qquad (3)$$

it appears reasonable to impose that the expectation value

$$\langle D \rangle_N = \langle v | B_0^N D_{00} B_0^{\dagger N} | v \rangle / \langle v | B_0^N B_0^{\dagger N} | v \rangle$$
(4)

must be small for N ground state excitons to behave as bosons. This expectation value turns out [4] to be  $2(1-F_{N+1}/F_N)$ . It is proportional to  $\eta$ , as expected. However the prefactor we find is surprisingly large, being of the order of 100 for 3D and 2D systems: This makes the excitons lose their bosonic character much before the Mott criterion makes them disappear. Let us recall that, while our criterion for bosonic behavior relies on a "clean" calculation, the Mott criterion uses two quantities calculated in limits which exclude each other: The ladder diagrams for excitons, valid at small density only, and the RPA for Coulomb screening, valid at high density only.

This  $F_N$  factor also plays a crucial role in the calculation of the expectation value of the Hamiltonian in the Nground-state-exciton state [8]. While Coulomb interaction appears at first order by construction in this quantity,  $\eta^n$ terms with  $n \ge 2$  are found, which physically come from purely Pauli many-body effects and can be traced back to ratios like  $F_{N+p}/F_N$ .

More generally, all physical quantities appear as matrix elements, and all matrix elements between N-exciton states, with most of them in the ground state, do have  $F_N$  factors. Our new derivation of the exciton-exciton scattering rate [11] relies on  $F_N$ , through scalar products of  $B_{i_1}^{\dagger} \cdots B_{i_p}^{\dagger} (B_0^{\dagger})^{N-p} |v\rangle$  states with  $i_j \neq 0$ .  $F_N$  factors also enter the new determination of the N electron-hole-pair ground state in the small density limit we are currently studying.

 $F_N$  is the crucial quantity for the purely Pauli part of many-body effects between excitons which results from their close-to-boson character. Consequently, it is worth a detailed study.

In Section 2, we use our commutation technique [5,6] to derive the recursion relation between the  $F_N$ 's given in our previous work (Ref. [4]). This commutation technique relies on two parameters  $\xi_{mnij}^{\text{dir}}$  and  $\lambda_{mnij}$ . The first one plays no role in the calculation of  $F_N$  as it corresponds to the (direct) *Coulomb* scattering of two excitons when the "in" and "out" excitons are made with the same pairs  $(e_1, h_1)$  and  $(e_2, h_2)$ . On the opposite, the second parameter  $\lambda_{mnij}$ , which originates from the composite nature of the excitons, *i.e.*, from the fact that two excitons can be made either with  $(e_1, h_1)$   $(e_2, h_2)$  or with  $(e_1, h_2)$   $(e_2, h_1)$ , appears in  $F_N$ . Using these  $\lambda_{mnij}$ 's, we can recover the recursion relation between the  $F_N$ 's as given in equation (12)

of reference [4]. From it, we derive a new expression of  $F_N$  valid for  $\eta = N a_x^3 / \mathcal{V}$  small but  $N (N a_x^3 / \mathcal{V})^n$  large, as these are the usual conditions of interest for N interacting excitons. We finally obtain the  $\eta$  expansion of ratios like  $F_{N+p}/F_N$  which are the quantities appearing in manybody effects between excitons.

Beside excitons, there are other quite well-known closeto-boson particles: the Cooper pairs. For a deeper understanding of many-body effects between excitons, it can be interesting to make a link between the well-known BCS theory of superconductivity [12,13] and our new commutation technique. In Section 3, we recover the recursion relation between the  $F_N$ 's using a procedure inspired by the BCS formalism. We also derive an explicit expression of  $F_N$  from which we recover the  $\eta$  expansion of  $F_{N+p}/F_N$ using a saddle point method.

In Section 4, we give some numerical results on  $F_N$  and  $F_{N+1}/F_N$  obtained for rather small N, namely  $N \leq 200$ , in order for the calculations to be numerically tractable.

#### $2 F_N$ using the commutation technique

#### 2.1 Recursion relation between the $F_N$ 's

Our commutation technique [5,6] turns out to be quite convenient for calculating quantities dealing with interacting excitons. For this reason, it is worthwhile to detail a calculation of  $F_N$  using this method.

It is easy to check by recurrence that

$$B_{m}, B_{0}^{\dagger N} = \delta_{m0} N B_{0}^{\dagger N-1} - N(N-1) \\ \times \sum_{n} \lambda_{mn00} B_{n}^{\dagger} B_{0}^{\dagger N-2} - N B_{0}^{\dagger N-1} D_{m0}, \quad (5)$$

where the  $\lambda_{mnij}$  coefficients of the commutation technique are such that

$$\left[D_{mi}, B_j^{\dagger}\right] = 2\sum_n \lambda_{mnij} B_n^{\dagger} , \qquad (6)$$

 $D_{mi}$  being defined in equation (3). Equation (5) can be used to obtain  $B_0 B_0^{\dagger N} |v\rangle$ . As  $B_m |v\rangle = 0 = D_{m0} |v\rangle$ , which results from their definitions, we find

$$\langle v | B_0^N B_0^{\dagger N} | v \rangle = N \langle v | B_0^{N-1} B_0^{\dagger N-1} | v \rangle - N(N-1)$$
  
 
$$\times \sum_m \lambda_{m000} \langle v | B_0^{N-1} B_m^{\dagger} B_0^{\dagger N-2} | v \rangle.$$
 (7)

The same equation (5) can also be used to obtain the bra  $\langle v|B_0^{N-1} B_m^{\dagger}$  appearing in the sum. This leads to

$$F_{N} = F_{N-1} - (N-1)\lambda_{0000} F_{N-2} + \frac{N(N-1)^{2}(N-2)}{N!} \times \sum_{mn} \lambda_{00mn} \lambda_{m000} \langle v | B_{0}^{N-3} B_{n} B_{0}^{\dagger N-2} | v \rangle, \quad (8)$$

since  $\lambda_{mnij} = (\lambda_{ijmn})^* = \lambda_{nmij}$  (as can be seen from the explicit value of  $\lambda_{mnij}$  given below in Eq. (12)). If we keep

using equation (5), we generate a recursion relation for  $F_N$ which reads

$$F_N = \sum_{n=1}^{N} a_n^{(N)} F_{N-n}.$$
 (9)

According to equation (8), the first two coefficients are simply

$$a_1^{(N)} = 1$$
,  $a_2^{(N)} = -(N-1)\lambda_{0000}$ , (10)

while the following ones are found to be

$$a_3^{(N)} = (N-1)(N-2) \sum_m \lambda_{000m} \lambda_{m000},$$
  

$$a_4^{(N)} = -(N-1)(N-2)(N-3) \sum_{mn} \lambda_{00mn} \lambda_{m000} \lambda_{n000},$$
(11)

and so on ... Since  $\langle v|B_0^N B_0^{\dagger N}|v\rangle$  can only depend on the ground state exciton characteristics ( $\mathbf{Q}_0 = \mathbf{0}, \nu_0$ ), it must be possible to rewrite the sums appearing in  $a_n^{(N)}$  in terms of  $\langle \mathbf{k} | x_{\nu_0} \rangle = \phi_{\mathbf{k}}$  only. In order to show it, we can use [5,6]

$$\lambda_{mnij} = \frac{1}{2} \int d\mathbf{r}_{e_1} \, d\mathbf{r}_{e_2} \, d\mathbf{r}_{h_1} \, d\mathbf{r}_{h_2} \, \varPhi_m^*(e_1, h_1) \\ \times \, \varPhi_n^*(e_2, h_2) \, \varPhi_i(e_1, h_2) \, \varPhi_j(e_2, h_1) + (m \leftrightarrow n), \quad (12)$$

where  $\Phi_n(e,h) = \langle \mathbf{r}_e - \mathbf{r}_h | x_{\nu_n} \rangle \mathcal{V}^{-1/2} \exp[\mathrm{i} \mathbf{Q}_n \cdot (\alpha_e \mathbf{r}_e +$  $\alpha_h \mathbf{r}_h$ ] is the *n* exciton wave function, and  $\alpha_{e,h}$  =  $m_{e,h}/(m_e + m_h)$ . By taking the Fourier transform of  $\langle \mathbf{r} | x_{\nu} \rangle$ ,  $\lambda_{mnij}$  also reads [6]

$$\lambda_{mnij} = \frac{1}{2} \,\delta_{\mathbf{Q}_m + \mathbf{Q}_n, \mathbf{Q}_i + \mathbf{Q}_j} \,F_{mnij} \left(\alpha_e(\mathbf{Q}_m - \mathbf{Q}_i), \alpha_h(\mathbf{Q}_n - \mathbf{Q}_i)\right) + (m \leftrightarrow n), \quad (13)$$

$$F_{mnij}(\mathbf{p}, \mathbf{p}') = \sum_{\mathbf{k}} \left\langle x_{\nu_m} \middle| \mathbf{k} - \frac{\mathbf{p} + \mathbf{p}'}{2} \right\rangle \left\langle x_{\nu_n} \middle| \mathbf{k} + \frac{\mathbf{p} + \mathbf{p}'}{2} \right\rangle$$
$$\times \left\langle \mathbf{k} + \frac{\mathbf{p} - \mathbf{p}'}{2} \middle| x_{\nu_i} \right\rangle \left\langle \mathbf{k} - \frac{\mathbf{p} - \mathbf{p}'}{2} \middle| x_{\nu_j} \right\rangle \cdot \quad (14)$$

The center of mass momentum conservation implies that all the (m, n...) exciton states appearing in the  $a_n^{(N)}$  sums have a zero momentum  $\mathbf{Q}$ . Consequently, all the  $(\mathbf{p}, \mathbf{p}')$  of  $F_{mnij}(\mathbf{p},\mathbf{p}')$  are equal to zero. The sums over (m,n...)can then be performed through closure relations between the  $|x_{\nu}\rangle$ 's, so that we finally get

$$F_N = F_{N-1} - (N-1)\sigma_2 F_{N-2} + (N-1)(N-2)\sigma_3 F_{N-3} -(N-1)(N-2)(N-3)\sigma_4 F_{N-4} + \cdots,$$
(15)

where following reference [4], we have set

$$\sigma_n = \sum_{\mathbf{k}} |\phi_{\mathbf{k}}|^{2n} = \sum_{\mathbf{k}} \left( \frac{64 \pi a_x^3}{\mathcal{V} (1 + k^2 a_x^2)^2} \right)^n, \qquad (16)$$

for 3D bulk excitons, the explicit calculation of these sums giving  $N^{n-1}\sigma_n = f(n)\tilde{\eta}^{n-1}$  with f(n) = 16(8n - 1)5)!!/(8n-2)!!, and

$$\tilde{\eta} = 64 \pi N a_x^3 / \mathcal{V} = 64 \pi \eta. \tag{17}$$

The recursion relation (15) is nothing but the one given in equation (12) of reference [4].

#### 2.2 Explicit expressions of $F_N$ for N large

A pedestrian calculation allows to check that equation (15) is fulfilled by the expansion

$$F_N \simeq \exp N \left[ -N \frac{\sigma_2}{2} + N^2 \left( \frac{\sigma_3}{3} - \frac{\sigma_2^2}{2} \right) -N^3 \left( \frac{\sigma_4}{4} - \sigma_2 \sigma_3 + \frac{5\sigma_2^3}{6} \right) + \cdots \right] , \quad (18)$$

for  $N(Na_x^3/\mathcal{V})^n$  small,  $\sigma_n$  being of order  $(a_x^3/\mathcal{V})^{n-1}$ . The above expression of  $F_N$  is also valid for  $N(N a_x^3/\mathcal{V})^n$  not small, which is what happens in usual experiments, as the existence of excitons requires  $N a_x^3 / \mathcal{V} \ll 1$ , but their number N is usually very large in a macroscopic sample. In order to derive equation (18), we can look for  $F_N$  as

$$F_N = \exp\left[-N(N-1)\beta_2 + N(N-1)(N-2)\beta_3 - N(N-1)(N-2)(N-3)\beta_4 + \cdots\right], \quad (19)$$

and enforce its validity for N = (2, 3, 4, ...), equation (19) already giving  $F_0 = F_1 = 1$ . For N = (2, 3, 4) we find

$$-\beta_{2} = \ln\left(F_{2}^{1/2}\right) \simeq \ln\left[1 - \frac{\sigma_{2}}{2} + \cdots\right] \simeq -\frac{\sigma_{2}}{2} + \cdots,$$
  

$$\beta_{3} = \ln\left(F_{3}^{1/6}F_{2}^{-1/2}\right)$$
  

$$\simeq \ln\left[1 + \left(\frac{\sigma_{3}}{3} - \frac{\sigma_{2}^{2}}{2}\right) + \cdots\right] \simeq \left(\frac{\sigma_{3}}{3} - \frac{\sigma_{2}^{2}}{2}\right) + \cdots,$$
  

$$-\beta_{4} = \ln\left(F_{4}^{1/24}F_{3}^{-1/6}F_{2}^{1/4}\right)$$
  

$$\simeq \ln\left[1 + \left(\frac{\sigma_{4}}{4} - \sigma_{2}\sigma_{3} + \frac{5\sigma_{2}^{3}}{6}\right) + \cdots\right],$$
 (20)

in which we have used  $F_2 = 1 - \sigma_2$ ,  $F_3 = 1 - 3\sigma_2 + 2\sigma_3$ , and  $F_4 = 1 - 6\sigma_2 + 8\sigma_3 - 3\sigma_2^2 - 6\sigma_4$  (see Eq. (7) of Ref. [4]) as well as the fact that, for macroscopic volumes, the  $\sigma_n$ 's are always much smaller than 1. Note that the  $\beta_n$ 's given in equation (20) are in  $(a_x^3/\mathcal{V})^{n-1}$ , while the dropped terms are in  $(a_x^3/\mathcal{V})^n$ .

By expliciting the  $\sigma_n$ 's as given in equation (16), we get

$$F_N \simeq \exp N \left[ -\frac{f(2)}{2} \tilde{\eta} + \left( \frac{f(3)}{3} - \frac{f^2(2)}{2} \right) \tilde{\eta}^2 - \left( \frac{f(4)}{4} - f(2)f(3) + \frac{5f^3(2)}{6} \right) \tilde{\eta}^3 + \cdots \right]$$
$$\simeq \exp N \left[ -\frac{33}{256} \tilde{\eta} + \frac{233}{24576} \tilde{\eta}^2 - \frac{19617}{16777216} \tilde{\eta}^3 + \cdots \right]$$
$$\simeq \exp N \left[ -2.6 \, 10^1 \, \eta + 3.8 \, 10^2 \, \eta^2 - 9.5 \, 10^3 \, \eta^3 + \cdots \right]. \tag{21}$$

#### 2.3 $\eta$ expansion of $F_{N+p}/F_N$

Actually, the quantities appearing in many-body effects between excitons are not  $F_N$ , due to its superextensivity, but ratios like  $F_{N+p}/F_N$ . From equation (21) we find that

$$\frac{F_{N+p}}{F_N} \simeq \exp p \left[ -2 \left( \frac{f(2)}{2} \right) \tilde{\eta} + 3 \left( \frac{f(3)}{3} - \frac{f^2(2)}{2} \right) \tilde{\eta}^2 -4 \left( \frac{f(4)}{4} - f(2)f(3) + \frac{5f^3(2)}{6} \right) \tilde{\eta}^3 + \cdots \right] \\
\simeq \left( \frac{F_{N+1}}{F_N} \right)^p \cdot$$
(22)

(Note that, when calculating  $F_{N+p}/F_N$  from Eq. (21), we should not forget that  $\tilde{\eta}$  also depends on N.)  $\tilde{\eta}$  being small, equation (22) thus leads to

$$\frac{F_{N+1}}{F_N} \simeq 1 - f(2)\tilde{\eta} + (f(3) - f^2(2))\tilde{\eta}^2 - (f(4) - 3f(3)f(2) + 2f^3(2))\tilde{\eta}^3 + \cdots \simeq 1 - \frac{33}{128}\tilde{\eta} + \frac{2021}{32768}\tilde{\eta}^2 - \frac{3897}{262144}\tilde{\eta}^3 + \cdots \simeq 1 - 5.2 \,10^1 \,\eta + 2.5 \,10^3 \,\eta^2 - 1.2 \,10^5 \,\eta^3 + \cdots$$
(23)

We see that  $F_{N+1}/F_N$  is close to 1 for exciton densities such that  $\eta = na_x^3 < 10^{-2}$ . Let us recall that, for such densities,  $F_N$  is extremely small for macroscopic samples, since typical N's are of the order of  $10^6$ .

#### $3 F_N$ using a BCS procedure

We now turn to the derivation of various expressions of  $F_N$  given in reference [4], following a BCS-like procedure [12,13].

#### 3.1 Compact expression of $F_N$

Let us introduce [14]

$$|\Psi_{\varphi}\rangle = \sum_{N=0}^{+\infty} \frac{1}{N!} e^{iN\varphi} \left(B_0^{\dagger}\right)^N |v\rangle.$$
 (24)

Using equation (2), this state also reads

$$\begin{split} |\Psi_{\varphi}\rangle &= \exp\left(\mathrm{e}^{\mathrm{i}\varphi}\sum_{\mathbf{k}}\phi_{\mathbf{k}}\,a_{\mathbf{k}}^{\dagger}\,b_{-\mathbf{k}}^{\dagger}\right)|v\rangle \\ &= \prod_{\mathbf{k}}\exp\left(\mathrm{e}^{\mathrm{i}\varphi}\,\phi_{\mathbf{k}}\,a_{\mathbf{k}}^{\dagger}\,b_{-\mathbf{k}}^{\dagger}\right)|v\rangle, \end{split}$$
(25)

since the operators  $(a_{\mathbf{k}}^{\dagger} b_{-\mathbf{k}}^{\dagger})$  with different **k**'s commute. By using  $(a_{\mathbf{k}}^{\dagger})^{N} | v \rangle = 0$  for  $N \geq 2$ ,  $| \Psi_{\varphi} \rangle$  can be rewritten as

$$|\Psi_{\varphi}\rangle = \prod_{\mathbf{k}} \left( 1 + e^{\mathbf{i}\varphi} \,\phi_{\mathbf{k}} \,a_{\mathbf{k}}^{\dagger} \,b_{-\mathbf{k}}^{\dagger} \right) |v\rangle \,\cdot \tag{26}$$

We now introduce  $A_{\varphi} = \langle \Psi_{\varphi=0} | \Psi_{\varphi} \rangle$ . By using  $\left[ a_{\mathbf{k}}, a_{\mathbf{k}'}^{\dagger} \right]_{+} = \delta_{\mathbf{k},\mathbf{k}'}$  and  $\langle v | a_{\mathbf{k}}^{\dagger} | v \rangle = 0$ ,  $A_{\varphi}$  is simply

$$A_{\varphi} = \prod_{\mathbf{k}} \left( 1 + e^{i\varphi} |\phi_{\mathbf{k}}|^2 \right) = \Xi(e^{i\varphi}).$$
 (27)

Since  $\langle v|B_0^N B_0^{\dagger M}|v\rangle = 0$  for  $N \neq M$ , we also have from equation (24)

$$A_{\varphi} = \sum_{M=0}^{+\infty} \frac{1}{(M!)^2} e^{iM\varphi} \langle v | B_0^M B_0^{\dagger M} | v \rangle \cdot$$
 (28)

It is then easy to check that the quantity we are interested in, can be obtained from  $A_{\varphi}$  through

$$\langle v|B_0^N B_0^{\dagger N}|v\rangle = (N!)^2 \int_0^{2\pi} \frac{\mathrm{d}\varphi}{2\pi} \,\mathrm{e}^{-\mathrm{i}N\varphi} \,A_\varphi. \tag{29}$$

By setting  $z = e^{i\varphi}$ , equation (29) leads to

$$F_N = N! \oint_C \frac{\mathrm{d}z}{2\mathrm{i}\pi} \frac{1}{z^{N+1}} \Xi(z), \qquad (30)$$

the contour C being the circle of unit radius around the origin. As  $\Xi(z)$  is analytic inside this circle, the residue theorem finally gives

$$F_N = \left[\frac{\mathrm{d}^N}{\mathrm{d}z^N}\,\Xi(z)\right]_{z=0} \,, \tag{31}$$

which is exactly equation (10) of reference [4].

#### 3.2 Recursion relation between the $F_N$ 's

Starting from equation (30), we can recover the recursion relation (12) of reference [4]. Indeed, the integration by part of the r.h.s. of equation (30) leads to

$$F_N = (N-1)! \oint_C \frac{\mathrm{d}z}{2\mathrm{i}\pi} \frac{1}{z^N} \frac{\mathrm{d}\Xi(z)}{\mathrm{d}z} \cdot \tag{32}$$

From the explicit form of  $\Xi(z)$  given in equation (27), we get

$$\frac{\mathrm{d}\ln\Xi(z)}{\mathrm{d}z} = \sum_{\mathbf{k}} \frac{|\phi_{\mathbf{k}}|^2}{1+z|\phi_{\mathbf{k}}|^2} = \sum_{n\geq 1} (-1)^{n-1} z^{n-1} \sum_{\mathbf{k}} |\phi_{\mathbf{k}}|^{2n},$$
(33)

which is valid for  $|z||\phi_{\bf k}|^2 < 1$ . Because |z| = 1 and  $\sum_{\bf k} |\phi_{\bf k}|^2 = 1$ , we can rewrite equation (32) as

$$F_N = (N-1)! \sum_{n=1}^{N} (-1)^{n-1} \sum_{\mathbf{k}} |\phi_{\mathbf{k}}|^{2n} \oint_C \frac{\mathrm{d}z}{2\mathrm{i}\pi} \frac{1}{z^{N+1-n}} \Xi(z),$$
(34)

since the integral for n > N gives 0, the function  $\Xi(z)$  being analytical inside C. Using the expression of  $F_N$  given in equation (30), we can thus rewrite equation (34) as

$$F_N = \sum_{p=1}^{N} (-1)^{p-1} \sigma_p \frac{(N-1)!}{(N-p)!} F_{N-p}, \qquad (35)$$

which is nothing but the recursion relation between the  $F_N$ 's given in equation (12) of reference [4].

#### 3.3 Explicit expression of $F_N$ in terms of the $\sigma_p$ 's

Starting from equation (30), we can also recover the expression of  $F_N$  given in equation (9) of reference [4]. For that, we rewrite  $\Xi(z)$  given in equation (27) as

$$\Xi(z) = \exp\left(\sum_{\mathbf{k}} \ln(1+z|\phi_{\mathbf{k}}|^2)\right)$$
$$= \exp\left(\sum_{n\geq 1} (-1)^{n+1} \frac{z^n}{n} \sum_{\mathbf{k}} |\phi_{\mathbf{k}}|^{2n}\right) , \qquad (36)$$

which is again valid for  $|z| |\phi_{\mathbf{k}}|^2 < 1$ . This leads to

$$\Xi(z) = \prod_{n \ge 1} \exp\left((-1)^{n+1} \frac{\sigma_n}{n} z^n\right) = \prod_{n \ge 1} \sum_{p \ge 0} \frac{1}{p!} \left((-1)^{n+1} \frac{\sigma_n}{n} z^n\right)^p .$$
(37)

Since  $\sigma_n$  is very small for macroscopic sample, being in  $(a_x^3/\mathcal{V})^{n-1}$ , we can insert this expansion of  $\Xi(z)$  into equation (30). We get

$$F_N = N! \oint_C \frac{\mathrm{d}z}{2\mathrm{i}\pi} \prod_{n \ge 1} \sum_{p \ge 0} \frac{1}{p!} \left( (-1)^{n+1} \frac{\sigma_n}{n} \right)^p \frac{z^{np}}{z^{N+1}} ,$$
(38)

in which the product and the sum can be commuted. The integral over z differs from 0 for  $\Sigma np = N$  only. For a given n, let us call  $p_n$  the corresponding p. Equation (38) thus leads to

$$F_N = N! \sum_{\{p_n\}} \prod_{n=1}^N \frac{1}{p_n!} \left( (-1)^{n+1} \frac{\sigma_n}{n} \right)^{p_n} , \qquad (39)$$

where the  $\{p_n\}$  are positive numbers such that  $\Sigma np_n = N$ . This expression of  $F_N$  is exactly the one given in equation (9) of reference [4].

#### 3.4 $\eta$ expansion of $F_{N+1}/F_N$

We can derive the  $\eta$  expansion of  $F_{N+1}/F_N$  from equation (30) by using a saddle point method. Equations (27, 29, 30) allow to rewrite  $F_N$  as

$$F_N = N! \oint_C \frac{\mathrm{d}z}{2\,\mathrm{i}\,\pi\,z} \,\mathrm{e}^{N\,g(z)},\tag{40}$$

$$g(z) = -\ln(z) + \frac{1}{N} \sum_{\mathbf{k}} \ln(1 + z \, |\phi_{\mathbf{k}}|^2) \,. \tag{41}$$

For a given N, g(z) is extremum for  $z_0$  such that

$$-\frac{1}{z_0} + \frac{1}{N} \sum_{\mathbf{k}} \frac{|\phi_{\mathbf{k}}|^2}{1 + z_0 \, |\phi_{\mathbf{k}}|^2} = 0 \,, \tag{42}$$

which also reads

$$\sum_{\mathbf{k}} \frac{|\phi_{\mathbf{k}}|^2}{N/z_0 + N \, |\phi_{\mathbf{k}}|^2} = 1 \, . \tag{43}$$

 $N |\phi_{\mathbf{k}}|^2$ , being of the order of  $\tilde{\eta}$ , is small, while  $\sigma_1 = 1$ . Equation (43) thus leads to  $N/z_0 = 1 + O(\tilde{\eta})$ . Consequently,  $z_0$  is positive (and real). Since

$$g''(z_0) = \frac{1}{z_0^2} - \frac{1}{N} \sum_{\mathbf{k}} \frac{|\phi_{\mathbf{k}}|^4}{(1+z_0 |\phi_{\mathbf{k}}|^2)^2}$$
$$= \frac{1}{N z_0} \sum_{\mathbf{k}} \frac{|\phi_{\mathbf{k}}|^2}{(1+z_0 |\phi_{\mathbf{k}}|^2)^2} , \qquad (44)$$

 $g''(z_0)$  is also positive. Using the principal branch cut of the logarithm, and writing g(z) as  $g(z_0) + \frac{1}{2} (z-z_0)^2 g''(z_0)$ , we are led to transform the integral of equation (40) into an integral along the imaginary axis. By setting  $z - z_0 = i y$ , we get

$$F_N \simeq N! \int_{-\infty}^{+\infty} \frac{\mathrm{i}\,\mathrm{d}y}{2\,\mathrm{i}\,\pi\,z_0} \exp\left(N(g(z_0) - \frac{1}{2}\,g''(z_0)\,y^2)\right)$$
$$= \frac{N!}{2\,\pi\,z_0} \,\mathrm{e}^{Ng(z_0)}\,\sqrt{\frac{2\,\pi}{N\,g''(z_0)}}.$$
(45)

The simplest way to obtain  $F_{N+1}/F_N$  is to note that equation (40) leads to

$$F_{N+1} = (N+1)! \oint_C \frac{\mathrm{d}z}{2\,\mathrm{i}\,\pi\,z^2} \,\mathrm{e}^{N\,g(z)},\tag{46}$$

so that, by calculating the integral as we did for  $F_N$ , we immediately obtain  $F_{N+1}/F_N = (N+1)/z_0$ . For large N's, this leads to a quite compact expression of this ratio, namely

$$\frac{F_{N+1}}{F_N} = \frac{(N+1)}{z_0} \simeq \frac{N}{z_0} \,. \tag{47}$$

In order to obtain the dependence of  $N/z_0$  with  $\tilde{\eta}$ , we set  $N/z_0 = 1 + \gamma_1 \tilde{\eta} + \gamma_2 \tilde{\eta}^2 \dots$ , and use this expansion in equation (43). We then get

$$1 = \sum_{\mathbf{k}} |\phi_{\mathbf{k}}|^{2} \left\{ 1 - (N |\phi_{\mathbf{k}}|^{2} + \gamma_{1} \tilde{\eta} + \gamma_{2} \tilde{\eta}^{2}) + (N |\phi_{\mathbf{k}}|^{2} + \gamma_{1} \tilde{\eta})^{2} + \mathcal{O}\left(\tilde{\eta}^{3}\right) \right\}, \quad (48)$$

from which we deduce

$$\gamma_1 = -N\sigma_2/\tilde{\eta} = -f(2) ,$$
  

$$\gamma_2 = \gamma_1^2 + 2\gamma_1 N \sigma_2/\tilde{\eta} + N^2\sigma_3/\tilde{\eta}^2 = f(3) - f^2(2)$$
(49)

and so on ... Using this procedure, we recover all the terms of  $F_{N+1}/F_N$  as obtained from the recursion relation (15).

Figure 1 shows the  $N/z_0$  dependence of  $F_{N+1}/F_N$ , as obtained from the numerical resolution of equation (43).



Fig. 1. Solid line:  $\eta = N a_x^3 / \mathcal{V}$  dependence of  $F_{N+1}/F_N$  as obtained from equation (47), using  $N/z_0$  as numerically calculated from equation (43). Dotted line: Asymptotic expansion of  $F_{N+1}/F_N$  obtained from the first two terms of equation (23).  $F_{N+1}/F_N$  stays close to its perfect boson value 1, for  $\eta$  extremely small only.

The insert shows its small  $\eta$  behavior for comparison with the first terms of the  $\eta$  expansion of  $F_{N+1}/F_N$ , as given in equation (23), namely  $1 - (33\pi/2)\eta + \cdots$ . Because of the very large prefactors of this expansion, we see that  $\eta$ has to be extremely small for  $F_{N+1}/F_N$  to be close to its perfect boson value 1.

# 4 Some numerical results on $F_{\text{N}}$ for N up to 200

Although the total number of excitons in a macroscopic sample is usually large, it is interesting to study  $F_N$  for not too large N's, since calculations of  $F_N$  are then numerically tractable. In order to perform such calculations, the recursion relation (35) between the  $F_N$ 's turns out to be much more convenient that the compact expression of  $F_N$  given in equation (31), or even the explicit expression of  $F_N$  in terms of  $\sigma_n$  as given in equation (39): Indeed the number of terms in this sum becomes rapidly extremely large.

Reference [4] gives the explicit expression of  $F_N$  for  $1 \leq N \leq 5$ . Further calculations show that the number of terms  $\Sigma_N$  contained in  $F_N$  increases very rapidly with N: We find  $\Sigma_{10} = 42$ ,  $\Sigma_{20} = 627$ ,  $\Sigma_{30} = 5604$ ,  $\Sigma_{40} = 37338$  and more than 10<sup>5</sup> for N = 50. Due to equation (39), this number of terms  $\Sigma_N$  is nothing but the number p(N) of partitions [15] of N: For large N, it increases as  $(1/4N\sqrt{3}) \exp(\pi\sqrt{2N/3})$ .

#### 4.1 Sample volume for $\mathsf{F}_{\mathsf{N}}$ to be close to 1

We could naïvely expect that  $F_N$  is close to 1 when the exciton density is such that excitons exist. Figure 2 shows the sample volume in  $a_x^3$  units for which  $F_N = 0.8$ , as a



Fig. 2. Sample volume in Bohr radius units for which  $F_N = 0.8$ , as a function of N for  $1 \le N \le 200$  in 3D systems. 100 excitons must occupy a volume as large as  $10^6$  exciton volumes to have a  $F_N$  factor rather close to its perfect boson value 1. The lower figure shows  $N^2 a_x^3 / \mathcal{V}$  for  $F_N$  to be equal to 0.8. For N > 50, the density  $n = N/\mathcal{V}$  to have  $F_N = 0.8$  decreases as 1/N.

function of N. We see that for only 100 excitons, this volume should be as large as  $10^6$  exciton volumes for  $F_N$  to deviate from its perfect boson value 1 by 0.2 only. Figure 2 also shows  $N^2 a_x^3/\mathcal{V}$  as a function of N for  $F_N$  to be equal to 0.8. We see that, for N > 50, this quantity stays constant, so that for large N, the exciton density to have  $F_N = 0.8$  varies as 1/N. As shown in Figure 3, it is interesting to note that, in 2D samples, the order of magnitude of these results are essentially the same. Actually these 2D results are of importance for the possible observation of Bose-Einstein condensation of excitons, as the present experiments on this subject are made on quantum wells.

Figure 4 shows  $F_N$  as a function of  $a_x^3/\mathcal{V}$  for various N between 50 and 100. We see that  $F_N$  deviates extremely rapidly from its boson value 1 when  $\mathcal{V}/a_x^3$  decreases slightly from infinity.

From all these figures, we conclude that, except for very large samples with volumes above  $10^6$  exciton volumes, the factor  $F_N$  appearing in the norm of the



Fig. 3. Same curves as Figure 2 for 2D systems. The orders of magnitude for 3D and 2D systems are essentially the same.



**Fig. 4.** Values of  $F_N$  for N = 50, 60, 70, 80, 90, 100 as a function of  $a_x^3/\mathcal{V}$ .  $F_N$  decreases extremely rapidly from its exact boson value 1, when the sample volume decreases.

N-ground-state-exciton state is extremely small even if we have only 100 excitons. Consequently, in most experimental conditions,  $F_N$ , which comes from the fact that excitons are not perfect bosons, cannot be replaced by its bosonic exciton value 1.



**Fig. 5.** Densities for which  $F_{N+1}/F_N$  remains equal to 0.95 and to 0.995, as a function of the exciton number N. We see that these densities reach their large N limit once N gets larger than 50.

#### 4.2 Exciton density for $\mathsf{F}_{\mathsf{N}+1}/\mathsf{F}_\mathsf{N}$ to be close to 1

As shown in equation (21),  $F_N$  contains an additional factor N in front of all  $N a_x^3/\mathcal{V}$  dependent terms which makes its value extremely small for macroscopic samples. The superextensivity of  $F_N$  explains why this quantity does not directly enter physical effects. On the opposite, ratios like  $F_{N+1}/F_N$  depending only on the density can reasonably appear in physical quantities. They are linked to "purely Pauli" effects, *i.e.*, many-body effects which exist quite independently from any Coulomb process, so that these ratios are crucial for the understanding of these novel manybody effects between close-to-boson particles.

Figure 5 shows the exciton density  $Na_x^3/\mathcal{V}$  for which  $F_{N+1}/F_N$  stays very close to 1, namely 0.95 and 0.995, as a function of the exciton number N. We note that this density stays constant once N gets larger than say, 50.

#### 5 Conclusion

We have rederived important relations verified by the quantity  $F_N$  which enters in the N-exciton normalization

factor and which differs from 1 because excitons are not true bosons. To do that, we have followed our new commutation technique for interacting close-to-bosons, and also a procedure inspired by the one used in the BCS theory of superconductivity.

We have given explicit expressions of  $F_N$  and  $F_{N+p}/F_N$  valid for  $N a_x^3/\mathcal{V}$  but  $N^2 a_x^3/\mathcal{V}$  large, as well as some exact results for  $N \leq 200$ .

It is important to stress that  $F_N$  is a quite crucial quantity in all many-body effects between excitons, because it is directly related to the "purely Pauli" part of these effects.

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