Mixture of composite-boson molecules and the Pauli exclusion principle

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Molecules made of two fermionic atoms are "cobosons"—a contraction for "composite bosons." These molecules "feel" each other not only through interactions between atoms, but also through the Pauli exclusion between their fermionic components. In order to point out the importance of this Pauli exclusion in cold atom physics, we have calculated here the energy change of N identical cobosonic molecules when a similar molecule, made of atoms having possibly different spin states, is added. Due to the difference in the number of fermion exchanges with a molecule having zero, one, or two atoms identical to the ones already present in the system, we may think that this energy change can take three different values, even for spin-independent interatomic interactions. We actually find that the energy change, in the Born approximation, is exactly the same at all orders in density, when the added molecule has two or just one atom identical to the ones already there. In other words, the scattering length is predicted to be the same if the added molecule can have exchanges with one set of fermionic components or with two sets. This unexpected equality, which of course holds for spin-independent interactions only, results from a subtle balance in the fermion exchanges. To prove it, we make use of a recent extension of the composite-exciton many-body theory we have constructed, to any type of cobosons, the physical understanding of the various exchange processes being enlightened by the Shiva diagram representation (so named because of the multiarm structure reminiscent of the Hindu god Shiva) of this many-body theory.

A few years ago, a significant breakthrough was made in the many-body physics of quantum particles: Through the study of interacting excitons, which are composite bosons with an electron and a hole for fermionic components, a formalism [1], free from any mapping to an ideal boson subspace, was constructed, and a simple visualization of the physical processes taking place between excitons was proposed through the so-called "Shiva diagrams," in reference to the multiarm Hindu god Shiva, as they have a multiarm structure [2].

Very recently [3], this exciton many-body theory was extended to include any type of "cobosons"—a contraction for "composite bosons"—made of two different fermions. The purpose of this extention is to possibly study the many-body physics of cold atoms or molecules, using the same concepts.

This coboson many-body theory relies on two sets of 2 ×2 scatterings [4,5]: The "interaction scatterings" and the "Pauli scatterings" [see Figs. 1(a) and 1(b)]. The first ones correspond to interactions between the fermionic components of the cobosons, the "in" and "out" cobosons being made with the same fermion pairs. The Pauli scatterings correspond to fermion exchange between cobosons, without any fermion interaction. These Pauli scatterings between *two* cobosons allow us to generate all possible fermion exchanges between any number of cobosons, these multiple exchanges being represented by Shiva diagrams like the one of Fig. 1(c). Note that, as the Pauli exclusion principle is N-body by essence, it is reasonable for the theory to make fermion exchanges between more than just two cobosons appear.

It is commonly thought that atomic cobosons should behave very differently from excitons because of the large mass

difference which exists between the fermionic components of these cobosons. While a large center-of-mass mass tends to support the representation of atoms or molecules as localized objects (all the components of the associated wave packets essentially having the same energy at the temperature scale), this is no more true for ultracold quantum particles: Their center of mass, now having a plane wave as
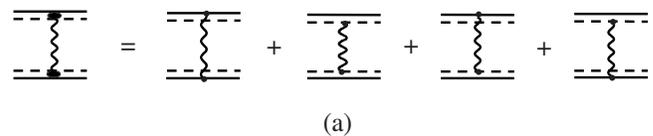
(a)

(b)   (c)

FIG. 1. (a) Direct interaction scattering ξ^{dir} between two cobosons, resulting from interactions between their fermions. (b) Pauli scattering λ_2 between two cobosons. (c) Shiva diagram for fermion exchange between three cobosons. This Shiva diagram represents the coefficient λ_3 appearing in the recursion relation (3.2) between the F_N's. In all diagrams, the fermionic atoms α are represented by a solid line, while the fermionic atoms β are represented by a dashed line.

wave function, is delocalized over the whole sample just as in the case for excitons, so that fermion exchanges between atomic cobosons are now possible, even in the very dilute limit.

The importance of fermion exchanges between excitons in the absence of Coulomb interaction between carriers, appears very clearly in semiconductor optical nonlinearities [6,7] as they provide the dominant terms for all effects at large photon detuning: Indeed, unabsorbed photons interact with a semiconductor through virtual excitons to which they are coupled. These virtual excitons are felt by the excitons present in the sample through both Coulomb interactions *and* the Pauli exclusion principle. While Coulomb scatterings are energylike quantities, Pauli scatterings are dimensionless. This makes them dominate the semiconductor response to a photon field at large detuning, due to a bare dimensional argument, since the relevant energy denominators are detuned energies.

In other physical effects [8–10], the Pauli exclusion principle generates Coulomb exchange terms as large as the Coulomb direct terms—or even larger when the direct terms can cel [8] such as for Coulomb processes in which one coboson stays unchanged.

In order to show that fermion exchanges are also of importance for ultracold atomic cobosons, we study here the energy change of N identical molecules made of two fermionic atoms, α and β, when a similar molecule made with atoms in possibly different spin states, α' and β', is added.

(i) For $\alpha' \neq \alpha$ and $\beta' \neq \beta$, the added molecule "feels" the previous ones through the interactions between its atoms (α', β') and any of the atoms (α, β) of the N molecules already present in the sample.

(ii) For $\alpha' = \alpha$ and $\beta' = \beta$, very many exchanges with the fermionic components of the molecules present in the sample can take place in addition to these interatomic interactions, since there is no way to know with which atoms the added molecule is really made of.

(iii) In the intermediate case, $\alpha' = \alpha$ and $\beta' \neq \beta$ (or $\alpha' \neq \alpha$ and $\beta' = \beta$), the number of possible exchanges is strongly reduced compared to (ii), but a certain amount still remains since there is no way to know which one of the $(N+1)$ atoms α is bound to the added atom β'.

In order to focus on the effects of the Pauli exclusion principle, we, in the following, consider that the interactions between fermionic atoms do not depend on their spin states. This makes the difference between the energy changes in the cases (i), (ii), and (iii) entirely due to fermion exchanges associated to the Pauli exclusion principle. For interatomic interactions depending on spin, a part of the energy-change difference—the naïve one—would come from a difference in the interactions. This would partly shade the subtle balance in fermion exchanges which makes the energy changes for (ii) and (iii) *exactly* equal when these changes are only due to the Pauli exclusion principle.

To show this effect in the case of excitons, we must start with N excitons made of one type of electrons and one type of holes. Such a state is easy to produce by the absorption of N circularly polarized photons in a quantum well. The resulting bright excitons, with a total spin ($S=1$) in the case of σ_+ photons, are made of heavy holes with a spin ($+3/2$) and conduction electrons with a spin ($-1/2$). By absorbing a σ_+ or a σ_- photon, it is quite simple to add to these bright excitons ($S=1$), either the same bright exciton, or a bright exciton with opposite spin ($S=-1$), its two carriers being then different from the ones already present in the sample. It is less trivial to add an exciton having one different carrier only. Indeed, excitons made of heavy holes ($+3/2$) and electrons ($+1/2$) have a total spin $S=2$ so that they are not coupled to light. We can think of adding a light-hole exciton, the one made of electrons ($+1/2$) and light holes ($+1/2$) being coupled to σ_+ photons. However, these excitons have a very short lifetime since, in quantum wells, light holes spontaneously decay towards heavy holes which have a lower energy. Consequently, it seems to be not easy to experimentally show that the energy changes are exactly equal when the added exciton has two or just one of its carriers identical to the ones present in the sample. The situation seems more favourable with atomic cobosons.

The experimental observation of Bose-Einstein condensation of molecules in ultracold trapped Fermi gases of ^{6}Li and ^{40}K [11] now offers a very unique route towards precise investigations of condensed matter problems. Two research directions have essentially been subsequently pursued. On the one side, degenerate spin polarized fermions are studied. These correspond to controlled amounts of two selected different spin states of a fermionic atom interacting via so-called tunable Feshbach resonances. Very recently, a phase separation has been demonstrated when imbalanced spin populations interact [12]. On the other hand, ultracold atomic mixtures are also generating a lot of interest and open new perspectives. Quantum degenerate atomic mixtures have been obtained very recently [13], first in the case of Bose-Fermi mixtures which should allow for efficient ways to investigate three-body collisions [14]. Ultracold heteronuclear fermionic molecules could also be used to probe spectacular effects related to the Pauli exclusion principle, as the one described here. Indeed, an appropriate choice of three distinct fermion species, with coincident or sufficiently close Feshbach resonances, would satisfy the previously mentioned cases (i), (ii) and (iii) at a fixed applied magnetic field.

The energy of N cobosonic molecules (α, β) plus one cobosonic molecule (α', β') is here calculated, in the Born approximation, as the mean value of the system Hamiltonian H in a state $|\psi_{N;g}\rangle$ made with N individual ground state molecules 0 constructed on (α, β) plus one ground state molecule 0_g constructed on (α', β'), with $g = (0, 1, 2)$ for molecule having $0, 1, 2$ atoms identical to the ones of 0 (this makes $0_2 \equiv 0$). Following Keldysh and Koslov [15], the state $|\psi_{N;g}\rangle$ is the ground state of these $(N+1)$ cobosonic molecules at zero order in interactions. Let us however stress that the concept of "zero order" here is somewhat tricky because, as there is no clean way [16] to write the interactions between composite quantum particles as a potential V—due to possible fermion exchanges between composite bosons—there is no clean way to define an unperturbed Hamiltonian, and thus a ground state at zero order in V. It is however reasonable to think that an order in the interactions has to be associated with an order in the coboson density. We are going to show that this $(N+1)$-molecule state indeed

leads to the expected ground state energy at zero order in density, namely, $(N+1)E_0$, with E_0 being the ground state energy of a molecule in any of the three states 0_g, independent of g for interatomic interactions independent of spin.

The Hamiltonian expectation value is easy to calculate using the four commutators on which the coboson many-body theory is based. It ultimately reads in terms of interaction and Pauli scatterings, the physics involved in the various terms being readily seen from their Shiva diagram representations.

For spin independent interactions between fermions, the difference between the energy changes can only come from the difference in the number of exchanges between the added cobosonic molecule and the ones already present. It turns out that, for $g=1$ or $g=2$, the increase in the number of exchanges appearing in the Hamiltonian matrix element calculated in the $|\psi_{N;g}\rangle$ state is exactly compensated by the increase in the number of exchanges appearing in the normalization factor of this $|\psi_{N;g}\rangle$ state; so that we end with two energy changes only: one when no exchange takes place, i.e., when the two added atoms are different from the ones of the N molecules present in the sample, and one when exchanges exist, i.e., when one *or* two atoms are identical to the ones already there.

To experimentally verify this somehow counterintuitive behavior, the investigated cobosonic molecules must have a high stability against inelastic collisional processes. In the present work, inelastic collisions have been neglected to emphasize the role played by the Pauli exclusion principle in the physics of ultracold heteronuclear molecules. In a two-component cold Fermi gas, our case (ii), dimers with a large positive scattering length are weakly bound, their spatial extension largely exceeding the extension of deep bound states. A relaxation in the latter, which limits the lifetime of the molecular gas, would require at least three fermionic atoms with interatomic distances of the order of the size of deep bound states. As two atoms are necessarily identical, cobosonic molecules are highly stable against collisional processes in the dilute limit [17]. The effective scattering length between identical dimers has been already calculated in this regime [18]. In the case (iii) that we consider here, the added molecule has only one fermion identical to the ones building the other molecules. Atom-dimer inelastic scatterings are therefore potentially efficient. However, for low enough densities, atomic hyperfine states can have a lifetime reaching a few tens or even a few hundreds of milliseconds [19]. This should allow to experimentally probe the role of the Pauli exclusion principle in these systems. Since our work predicts an identical energy change in the cases (ii) and (iii) in the Born approximation when inelastic collisions are neglected, interacting weakly bound dimers should exhibit identical effective scattering lengths when they have just one or two fermions in common.

The paper is organized as follows.

In Sec. I, we briefly recall the main results of the coboson many-body theory which are necessary to calculate the energy of $(N+1)$ composite molecules with intermolecular exchanges included in an exact way.

In Sec. II, we calculate the energy change when the cobosonic molecule 0_g is added to a system only having one

molecule 0. Although we expect the change induced by interactions to be extremely small in the large sample limit, since the probability for the two molecules to be close enough to significantly interact is vanishingly small, this very simple calculation allows us to grasp some important aspects of the problem.

In Sec. III, we calculate the same energy change when one cobosonic molecule 0_g is added not to one but to N molecules 0. For that, we first have to calculate the normalization factor of the $(N+1)$-molecule state $|\psi_{N;g}\rangle$. We show that it easily reads in terms of the one for N identical cobosonic molecules 0, for all three values of g. We then calculate the diagonal matrix element of the Hamiltonian in this state $|\psi_{N;g}\rangle$ and we visualize the obtained result in terms of Shiva diagrams, to grasp the physics involved. From this Hamiltonian matrix element and the state normalization factor, it is then straightforward to derive the Hamiltonian expectation value for N cobosonic molecules 0 plus one cobosonic molecule 0_g having zero, one, or two atoms identical to the ones of the molecules 0. This allows us to prove that these expectation values are indeed equal when one or two atoms are the same.

I. FORMALISM

We consider molecules made of two fermionic atoms α and β having a spin degree of freedom. It is convenient [3] to introduce two complete basis for these fermionic atoms, $a^\dagger_{\mathbf{K}_\alpha}|v\rangle$ and $b^\dagger_{\mathbf{K}_\beta}|v\rangle$, where $\mathbf{K}_\alpha$ stands for an orbital index $\mathbf{k}_\alpha$ and a spin index s_α for the fermion α, while $\mathbf{K}_\beta$ stands for an orbital index $\mathbf{k}_\beta$ and a spin index σ_β for the fermion β.

The expansion on this atomic basis of a molecular eigenstate $|I\rangle = B^\dagger_I|v\rangle$ allows us to write its creation operator as

$$B^\dagger_I = \sum_{\mathbf{K}_\alpha,\mathbf{K}_\beta} a^\dagger_{\mathbf{K}_\alpha} b^\dagger_{\mathbf{K}_\beta} \langle \mathbf{K}_\beta, \mathbf{K}_\alpha | I \rangle. \tag{1.1}$$

If the $|I\rangle$'s are eigenstates of the system Hamiltonian, they also form a complete set for one-atom-pair states; so that the atom-pair operators in the same way read in terms of the molecular operators as

$$a^\dagger_{\mathbf{K}_\alpha} b^\dagger_{\mathbf{K}_\beta} = \sum_I B^\dagger_I \langle I | \mathbf{K}_\alpha, \mathbf{K}_\beta \rangle. \tag{1.2}$$

A. Pauli scatterings

From Eqs. (1.1) and (1.2), it is easy to derive the first two key equations of the coboson many-body theory [3,5], namely,

$$[B_M, B^\dagger_I] = \delta_{M,I} - D_{MI}, \tag{1.3}$$

$$[D_{MI}, B^\dagger_J] = \sum_P \left[\Lambda \begin{pmatrix} P & J \\ M & I \end{pmatrix} + \Lambda \begin{pmatrix} M & J \\ P & I \end{pmatrix} \right] B^\dagger_P. \tag{1.4}$$

The Pauli scattering $\Lambda \begin{pmatrix} P & J \\ M & I \end{pmatrix}$ of two cobosonic molecules from the "in" states (I,J) to the "out" states (M,P), that emerges from these commutators, is shown in Fig. 2(a). For interatomic interactions independent of spins, the molecular
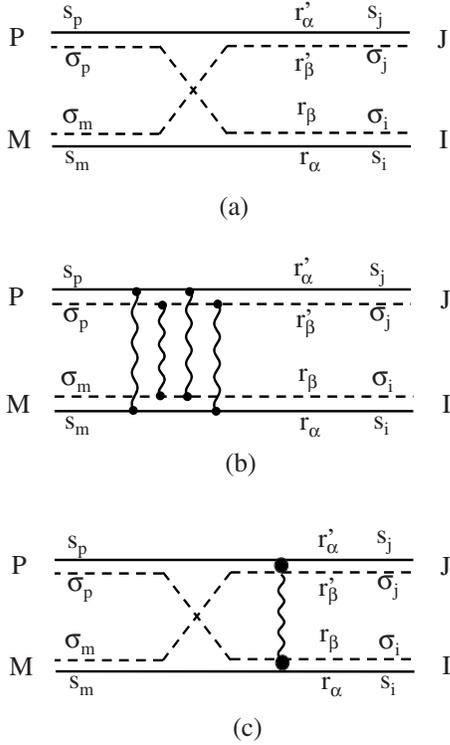
(a)

(b)

(c)

FIG. 2. (a): Diagram for the Pauli scattering $\Lambda\left(\begin{smallmatrix} P & M \\ J & I \end{smallmatrix}\right)$ defined in Eq. (1.5). (b) Diagram for the direct interaction scattering $\Xi^{\mathrm{dir}}\left(\begin{smallmatrix} P & M \\ J & I \end{smallmatrix}\right)$ defined in Eq. (1.10). (c) Diagram for the "in" exchange interaction scattering $\Xi^{\mathrm{in}}\left(\begin{smallmatrix} P & M \\ J & I \end{smallmatrix}\right)$ defined in Eq. (2.6).

wave functions are spin independent. The Pauli scattering then splits into a spin part and an orbital part. Let us set $I = (i, s_i, \sigma_i)$, where i stands for the orbital index of a molecule made of one atom α with spin s_i and one atom β with spin σ_i. As, in $\Lambda\left(\begin{smallmatrix} P & J \\ M & I \end{smallmatrix}\right)$ shown in Fig. 2(a), the molecule M has the same atom α as I and the same atom β as J, this scattering differs from zero for $s_m = s_i$ and $\sigma_m = \sigma_j$ only. In the same way, we must have $s_p = s_j$ and $\sigma_p = \sigma_i$ for $\Lambda\left(\begin{smallmatrix} P & J \\ M & I \end{smallmatrix}\right)$ to differ from zero. The orbital part of this scattering is readily obtained in a standard way from the diagram of Fig. 2(a), by taking the "in" wave functions and the complex conjugates of the "out" wave functions with their respective atomic variables. This leads to [5]

$$\Lambda\begin{pmatrix} P & J \\ M & I \end{pmatrix} = \delta_{s_m, s_i} \delta_{s_p, s_j} \delta_{\sigma_p, \sigma_i} \delta_{\sigma_m, \sigma_j} \lambda\begin{pmatrix} p & j \\ m & i \end{pmatrix},$$

$$\lambda\begin{pmatrix} p & j \\ m & i \end{pmatrix} = \int d\mathbf{r}_\alpha d\mathbf{r}_\beta d\mathbf{r}'_\alpha d\mathbf{r}'_\beta \phi_m^*(\mathbf{r}_\alpha, \mathbf{r}'_\beta) \phi_p^*(\mathbf{r}'_\alpha, \mathbf{r}_\beta) \phi_i(\mathbf{r}_\alpha, \mathbf{r}_\beta)$$
$$\times \phi_j(\mathbf{r}'_\alpha, \mathbf{r}'_\beta). \tag{1.5}$$

One important property of the deviation-from-boson operator D_{MI} is

$$D_{MI}|v\rangle = 0, \tag{1.6}$$

as readily found by making Eq. (1.3) act on vacuum $|v\rangle$.

B. Interaction scatterings

To get the two other key equations of this coboson many-body theory, we start with

$$(H - E_I)B_I^\dagger|v\rangle = 0, \tag{1.7}$$

for molecular states $|I\rangle$ eigenstates of the system Hamiltonian, and we introduce [3,5] the creation potential $V_I^\dagger$ of the cobosonic molecule I through

$$[H, B_I^\dagger] = E_I B_I^\dagger + V_I^\dagger. \tag{1.8}$$

The interaction scattering from two cobosons in the "in" states (I, J) to two cobosons in the "out" states (M, P) then follows from

$$[V_I^\dagger, B_J^\dagger] = \sum_{M,P} \Xi^{\mathrm{dir}}\begin{pmatrix} P & J \\ M & I \end{pmatrix} B_M^\dagger B_P^\dagger. \tag{1.9}$$

It is shown in Fig. 2(b). For interactions between fermions independent of their spins, $\Xi^{\mathrm{dir}}\left(\begin{smallmatrix} P & J \\ M & I \end{smallmatrix}\right)$ splits, as the Pauli scatterings, into a spin part and an orbital part. It is readily obtained from Fig. 2(b) as

$$\Xi^{\mathrm{dir}}\begin{pmatrix} P & J \\ M & I \end{pmatrix} = \delta_{s_m, s_i} \delta_{\sigma_m, \sigma_i} \delta_{s_p, s_j} \delta_{\sigma_p, \sigma_j} \xi^{\mathrm{dir}}\begin{pmatrix} p & j \\ m & i \end{pmatrix},$$

$$\xi^{\mathrm{dir}}\begin{pmatrix} p & j \\ m & i \end{pmatrix} = \int d\mathbf{r}_\alpha d\mathbf{r}_\beta d\mathbf{r}'_\alpha d\mathbf{r}'_\beta \phi_m^*(\mathbf{r}_\alpha, \mathbf{r}_\beta) \phi_p^*(\mathbf{r}'_\alpha, \mathbf{r}'_\beta)$$
$$\times \phi_i(\mathbf{r}_\alpha, \mathbf{r}_\beta) \phi_j(\mathbf{r}'_\alpha, \mathbf{r}'_\beta) \left[v_{\alpha\alpha}(\mathbf{r}_\alpha, \mathbf{r}'_\alpha) + v_{\beta\beta}(\mathbf{r}_\beta, \mathbf{r}'_\beta) \right.$$
$$\left. + v_{\alpha\beta}(\mathbf{r}_\alpha, \mathbf{r}'_\beta) + v_{\alpha\beta}(\mathbf{r}'_\alpha, \mathbf{r}_\beta) \right]. \tag{1.10}$$

The bracket of Eq. (1.10) just corresponds to the *direct* interactions between the fermions of the cobosons I and J, the "out" coboson M being made of the same fermion pair as the "in" coboson I.

One important property of the creation potential $V_I^\dagger$ is

$$V_I^\dagger|v\rangle = 0, \tag{1.11}$$

as readily found by making Eq. (1.8) act on vacuum.

C. Many-body effects

In order to calculate many-body effects between cobosons in an easy way, it is convenient to use similar commutators with N cobosons. They are obtained [1,8] by the iteration of Eqs. (1.3), (1.4), (1.8), and (1.9).

The ones for fermion exchanges read

$$[D_{MI}, B_J^{\dagger N}] = N B_J^{\dagger N-1} \sum_P \left[\Lambda\begin{pmatrix} P & J \\ M & I \end{pmatrix} + \Lambda\begin{pmatrix} M & J \\ P & I \end{pmatrix} \right] B_P^\dagger, \tag{1.12}$$

$$[B_M, B_I^{\dagger N}] = N B_I^{\dagger N-1}(\delta_{M,I} - D_{MI})$$
$$- N(N-1) B_I^{\dagger N-2} \sum_P \Lambda\begin{pmatrix} P & I \\ M & I \end{pmatrix} B_P^\dagger, \tag{1.13}$$

while the ones for fermion interactions are given by

$$[V_I^\dagger, B_J^{\dagger N}] = N B_J^{\dagger N-1} \sum_{MP} \Xi^{\mathrm{dir}}\begin{pmatrix} P & J \\ M & I \end{pmatrix} B_M^\dagger B_P^\dagger, \tag{1.14}$$

$$[H, B_I^{\dagger N}] = N B_I^{\dagger N-1}(E_I B_I^\dagger + V_I^\dagger)$$
$$+ \frac{N(N-1)}{2} B_I^{\dagger N-2} \sum_{MP} \Xi^{\mathrm{dir}}\begin{pmatrix} P & I \\ M & I \end{pmatrix} B_M^\dagger B_P^\dagger.$$
$$(1.15)$$

These four commutators of course reduce to the key ones for $N=1$. They actually constitute the basic equations from which all the many-body physics of composite bosons can be derived, with fermion exchanges included in an exact way.

D. The problem at hand

We consider N identical molecules 0 made of fermionic atoms α and β having a spin s and σ respectively, the creation operator of these molecules being $B_0^\dagger$. The Hamiltonian expectation value in such a state reads [8]

$$\langle H \rangle_N = \frac{\langle v | B_0^N H B_0^{\dagger N} | v \rangle}{\langle v | B_0^N B_0^{\dagger N} | v \rangle}. \qquad (1.16)$$

To these N molecules, we add a similar molecule 0_g having its atoms with spins s' and σ' possibly different from (s, σ). The Hamiltonian expectation value in this $(N+1)$-molecule state reads

$$\langle H \rangle_{N;g} = \frac{\langle \psi_{N;g} | H | \psi_{N;g} \rangle}{\langle \psi_{N;g} | \psi_{N;g} \rangle} = \frac{\langle v | B_0^N B_{0_g} H B_{0_g}^\dagger B_0^{\dagger N} | v \rangle}{\langle v | B_0^N B_{0_g} B_{0_g}^\dagger B_0^{\dagger N} | v \rangle}, \qquad (1.17)$$

with $\langle H \rangle_{N;2}$ reducing to $\langle H \rangle_{N+1}$ since $0_2 \equiv 0$.

In the Born approximation, the energy change induced by the added molecule is simply given by

$$\langle H \rangle_{N,g} - \langle H \rangle_N = E_0 + \mathcal{E}_{N;g} \qquad (1.18)$$

since, for spin independent interatomic interactions, the molecular energy does not depend on spin, so that $E_{0_g} = E_0$.

$\mathcal{E}_{N;g}$ comes from the interactions between the cobosonic molecule 0_g and the N cobosonic molecules 0 already present. For $g=0$, i.e., for $s' \neq s$ and $\sigma' \neq \sigma$, these interactions reduce to direct interactions between molecules, while for $g=2$, i.e., $s'=s$ and $\sigma'=\sigma$, and for $g=1$, i.e., $(s'=s, \sigma' \neq \sigma)$ or $(s' \neq s, \sigma'=\sigma)$, these interactions also include exchanges between the two sets of fermions, or between one set only. Consequently, $\mathcal{E}_{N;g}$ should *a priori* take three different values depending on the relative values of (s', σ') and (s, σ).

In order to have a simple understanding of the problem, let us start with $N=1$.

II. ENERGY CHANGE FOR $N=1$

For molecular states $B_I^\dagger | v \rangle$ being eigenstates of the Hamiltonian, we have, due to Eq. (1.7), $\langle v | B_0 B_0^\dagger | v \rangle = 1$ while $\langle v | B_0 H B_0^\dagger | v \rangle = E_0$, so that

$$\langle H \rangle_1 = E_0. \qquad (2.1)$$

For two molecules, we readily find [3,5], by pushing B_M to the right according to the commutators (1.3) and (1.4),

$$\langle v | B_P B_M B_I^\dagger B_J^\dagger | v \rangle = \delta_{M,I} \delta_{P,J} - \Lambda\begin{pmatrix} P & J \\ M & I \end{pmatrix} + (M \leftrightarrow P). \qquad (2.2)$$

Due to Eq. (1.5), the Pauli scattering $\Lambda\begin{pmatrix} 0_g & 0_g \\ 0 & 0 \end{pmatrix}$ reduces to $\delta_{\sigma',\sigma} \lambda\begin{pmatrix} o & o \\ o & o \end{pmatrix}$ while the Pauli scattering $\Lambda\begin{pmatrix} 0 & 0_g \\ 0_g & 0 \end{pmatrix}$ reduces to $\delta_{s',s} \lambda\begin{pmatrix} o & o \\ o & o \end{pmatrix}$. We then end with

$$\langle v | B_0 B_{0_g} B_{0_g}^\dagger B_0^\dagger | v \rangle = 1 + \delta_{s',s} \delta_{\sigma',\sigma} - (\delta_{s',s} + \delta_{\sigma',\sigma}) \lambda\begin{pmatrix} o & o \\ o & o \end{pmatrix}. \qquad (2.3)$$

Dimensional arguments show that $\lambda\begin{pmatrix} o & o \\ o & o \end{pmatrix}$ is a dimensionless parameter of the order of $(a/L)^3$, where a is the molecule extension and L the sample size. Consequently, $\lambda\begin{pmatrix} o & o \\ o & o \end{pmatrix}$ is a vanishingly small parameter in the large sample limit. For a cobosonic molecule having a relative-motion wave function equal to $(e^{-r/a}/\sqrt{\pi a^3})$, its precise value [5] is $\lambda\begin{pmatrix} o & o \\ o & o \end{pmatrix} = (33\pi/2)(a/L)^3$.

In the same way, the diagonal matrix element of the system Hamiltonian H in this two-molecule subspace is obtained by pushing H to the right according to the commutators (1.8) and (1.9). This leads to [8]

$$\langle v | B_0 B_{0_g} (H - 2E_0) B_{0_g}^\dagger B_0^\dagger | v \rangle = \sum_{MP} \Xi^{\mathrm{dir}}\begin{pmatrix} P & 0 \\ M & 0_g \end{pmatrix}$$
$$\times \langle v | B_0 B_{0_g} B_M^\dagger B_P^\dagger | v \rangle. \qquad (2.4)$$

So that, by using Eq. (2.2), we end with

$$\langle v | B_0 B_{0_g} (H - 2E_0) B_{0_g}^\dagger B_0^\dagger | v \rangle = \Xi^{\mathrm{dir}}\begin{pmatrix} 0 & 0 \\ 0_g & 0_g \end{pmatrix} + \Xi^{\mathrm{dir}}\begin{pmatrix} 0_g & 0 \\ 0 & 0_g \end{pmatrix}$$
$$- \Xi^{\mathrm{in}}\begin{pmatrix} 0 & 0 \\ 0_g & 0_g \end{pmatrix} - \Xi^{\mathrm{in}}\begin{pmatrix} 0_g & 0 \\ 0 & 0_g \end{pmatrix}. \qquad (2.5)$$

$\Xi^{\mathrm{in}}\begin{pmatrix} P & J \\ M & I \end{pmatrix}$, shown in Fig. 2(c), corresponds to an interaction scattering between the "in" cobosons I and J followed by a fermion exchange, so that M ends by having the fermion α of I and the fermion β of J. Its orbital part is given by [3]

$$\xi^{\mathrm{in}}\begin{pmatrix} o & o \\ o & o \end{pmatrix} = \int d\mathbf{r}_\alpha d\mathbf{r}_\beta d\mathbf{r}'_\alpha d\mathbf{r}'_\beta \phi_o^*(\mathbf{r}_\alpha, \mathbf{r}'_\beta) \phi_o^*(\mathbf{r}'_\alpha, \mathbf{r}_\beta)$$
$$\times \phi_o(\mathbf{r}_\alpha, \mathbf{r}_\beta) \phi_o(\mathbf{r}'_\alpha, \mathbf{r}'_\beta) [v_{\alpha\alpha}(\mathbf{r}_\alpha, \mathbf{r}_{\alpha'}) + v_{\beta\beta}(\mathbf{r}_\beta, \mathbf{r}_{\beta'})$$
$$+ v_{\alpha\beta}(\mathbf{r}_\alpha, \mathbf{r}_{\beta'}) + v_{\alpha\beta}(\mathbf{r}_{\alpha'}, \mathbf{r}_\beta)]. \qquad (2.6)$$

This leads to rewriting Eq. (2.5) in terms of orbital scatterings as

$$\langle v | B_0 B_{0_g} (H - 2E_0) B_{0_g}^\dagger B_0^\dagger | v \rangle = (1 + \delta_{s',s} \delta_{\sigma'\sigma}) \xi^{\mathrm{dir}}\begin{pmatrix} o & o \\ o & o \end{pmatrix}$$
$$- (\delta_{s',s} + \delta_{\sigma',\sigma}) \xi^{\mathrm{in}}\begin{pmatrix} o & o \\ o & o \end{pmatrix}. \qquad (2.7)$$

Due to dimensional arguments, $\xi^{\mathrm{dir}}\begin{pmatrix} o & o \\ o & o \end{pmatrix}$ and $\xi^{\mathrm{in}}\begin{pmatrix} o & o \\ o & o \end{pmatrix}$ are energylike quantities of the order of $E_0(a/L)^3$. Let us note

that, as readily seen from Eq. (1.10), the direct scattering $\xi^{\text{dir}}\left(\begin{smallmatrix}o&o\\o&o\end{smallmatrix}\right)$ reduces to zero if the attraction between (α,β) is as large as the repulsion between (α,α) and (β,β)—as for the Coulomb interaction between the electrons and the protons of two hydrogen atoms, or between the electrons and the holes of two excitons. For hydrogen atoms or excitons having a relative motion wave function equal to $(e^{-r/a}/\sqrt{\pi a^3})$,

the exchange-interaction scattering is given [8] by $\xi^{\text{in}}\left(\begin{smallmatrix}o&o\\o&o\end{smallmatrix}\right)$ $=(-26\pi/3)(e^2/2a)(a/L)^3$.

The Hamiltonian expectation value in a state with one molecule 0 and one molecule 0_g having its fermions in the same orbital states as the ones of 0, but in a possibly different spin state, follows from Eqs. (2.3) and (2.7). It reads

$$\langle H \rangle_{1;g} = 2E_0 + \frac{(1 + \delta_{s',s}\delta_{\sigma',\sigma})\xi^{\text{dir}}\left(\begin{smallmatrix}o&o\\o&o\end{smallmatrix}\right) - (\delta_{s',s} + \delta_{\sigma',\sigma})\xi^{\text{in}}\left(\begin{smallmatrix}o&o\\o&o\end{smallmatrix}\right)}{1 + \delta_{s',s}\delta_{\sigma',\sigma} - (\delta_{s',s} + \delta_{\sigma',\sigma})\lambda\left(\begin{smallmatrix}o&o\\o&o\end{smallmatrix}\right)}$$

$$\equiv \langle H \rangle_1 + E_0 + \mathcal{E}_{1;g}. \tag{2.8}$$

This shows that the interacting part of the energy change when one cobosonic molecule 0_g is added to one cobosonic molecule 0, can take two values only, namely,

$$\mathcal{E}_{1;g} = \begin{cases} \xi^{\text{dir}}\left(\begin{smallmatrix}o&o\\o&o\end{smallmatrix}\right) & \text{for } g=0, \text{ i.e., for } (s'\neq s,\ \sigma'\neq\sigma), \\[2ex] \dfrac{\xi^{\text{dir}}\left(\begin{smallmatrix}o&o\\o&o\end{smallmatrix}\right) - \xi^{\text{in}}\left(\begin{smallmatrix}o&o\\o&o\end{smallmatrix}\right)}{1 - \lambda\left(\begin{smallmatrix}o&o\\o&o\end{smallmatrix}\right)} & \text{for } g=(1,2), \text{ i.e., for}(s'\neq s,\sigma'=\sigma),(s'=s,\sigma'\neq\sigma),(s'=s,\sigma'=\sigma). \end{cases} \tag{2.9}$$

The fact that the added molecule feels the two atoms of the molecule already present by the Pauli exclusion principle, or one atom only, has no effect on this energy change.

Note that since λ, ξ^{dir} and ξ^{in} go to zero as $(a/L)^3$ in the large sample limit, $\mathcal{E}_{1;g}$ also goes to zero in this limit: If we only have two molecules in an infinitely large sample, the energy change induced by their interactions is vanishingly small, as physically reasonable. We however expect that, if one molecule is now added to a set of N molecules, the terms in $(a/L)^3$ will appear with a N prefactor; so that the energy change induced by interactions has to depend on the molecule density through the dimensionless parameter

$$\eta = N(a/L)^3, \tag{2.10}$$

which is the relevant parameter of all many-body effects between composite quantum particles. Let us show it by calculating the energy change when one molecule 0_g is added to N identical molecules 0.

III. ENERGY CHANGE FOR LARGE N

To obtain this change, we have to calculate the normalization factors of the states with N and $N+1$ cobosonic molecules as well as the diagonal matrix elements of the Hamiltonian in these molecular states.

A. Normalization factor

In previous works [20,21], we have shown that the normalization factor of N identical cobosons reads

$$\langle v|B_0^N B_0^{\dagger N}|v \rangle = N!\, F_N, \tag{3.1}$$

where F_N, which differs from 1 due to fermion exchanges between cobosons, is exponentially small in macroscopic samples. Using Eqs. (1.12) and (1.13), it is possible to derive the recursion relation which exists between these F_N's. It reads [21]

$$F_N = \sum_{n=1}^{N} (-1)^{n-1} \frac{(N-1)!}{(N-n)!} \lambda_n F_{N-n}. \tag{3.2}$$

The coefficients λ_n in this recursion relation come from fermion exchanges between n cobosons 0. They just correspond to Shiva diagrams [2] like the one of Fig. 1(c), with n coboson lines instead of 3, all the "in" and "out" cobosons being cobosons 0. This leads to $\lambda_2 = \lambda\left(\begin{smallmatrix}o&o\\o&o\end{smallmatrix}\right)$, while 1 is replaced by λ_1 for convenience. Due to dimensional arguments, these λ_n's are of the order of $(a^3/L^3)^{n-1}$, making the prefactor of F_{N-n} in Eq. (3.2) of the order of η^{n-1}. Consequently, in the large N limit, the expansion of F_{N-1}/F_N, deduced from Eq. (3.2), appears as an η expansion [21]

$$f_N = \frac{F_{N-1}}{F_N} \simeq 1 + N\lambda_2 + N^2(2\lambda_2^2 - \lambda_3) + O(\eta^3) = \tilde{f}(\eta). \tag{3.3}$$

In order to calculate the normalization factor when one cobosonic molecule 0_g is added to these N molecules 0, we make use of Eq. (1.3) to get

$$\langle v|B_0^N B_{0_g} B_{M_g}^\dagger = \langle v|B_0^N (B_{M_g}^\dagger B_{0_g} + \delta_{0_g,M_g} - D_{0_g M_g}), \quad (3.4)$$

where $B_{M_g}^\dagger$ creates a cobosonic molecule in an orbital state m, its fermionic atoms having the spins of the molecule 0_g, so that δ_{0_g,M_g} reduces to $\delta_{o,m}$.

Using Eq. (1.13), we can rewrite the first term of Eq. (3.4) as

$$\langle v|B_0^N B_{M_g}^\dagger B_{0_g} = \langle v| \left\{ N\delta_{0,M_g} B_0^{N-1} \right.$$
$$\left. - N(N-1)B_0^{N-2}\sum_P \Lambda\begin{pmatrix} 0 & P \\ 0 & M_g \end{pmatrix} B_P \right\} B_{0_g}$$
$$= \delta_{g,2}\langle v| \left\{ N\delta_{o,m} B_0^N \right.$$
$$\left. - N(N-1)B_0^{N-1}\sum_p \lambda\begin{pmatrix} o & p \\ o & m \end{pmatrix} B_{P_2} \right\} B_{0_2},$$
$$(3.5)$$

since $\delta_{0,M_g} = \delta_{g,2}\delta_{o,m}$ while $\Lambda\begin{pmatrix} 0 & P \\ 0 & M_g \end{pmatrix}$ differs from zero for M_g

and P having their two fermionic atoms with the spins of 0.

The last term of Eq. (3.4) is calculated using Eq. (1.12),

$$\langle v|B_0^N D_{0_g M_g} = N\langle v|B_0^{N-1}\sum_P \left[\Lambda\begin{pmatrix} 0 & P \\ 0_g & M_g \end{pmatrix} + \Lambda\begin{pmatrix} 0_g & P \\ 0 & M_g \end{pmatrix} \right] B_P^\dagger,$$
$$(3.6)$$

the bracket being equal to zero for $g=0$, to $\lambda\begin{pmatrix} o & p \\ o & m \end{pmatrix}$ for $g=1$ and to $2\lambda\begin{pmatrix} o & p \\ o & m \end{pmatrix}$ for $g=2$.

If we now insert Eqs. (3.5) and (3.6) into Eq. (3.4), we find that, when the two atomic spins of the added molecule are different from the spins of 0,

$$\langle v|B_0^N B_{0_0} B_{M_0}^\dagger = \delta_{m,o}\langle v|B_0^N. \quad (3.7)$$

We also find that the states when exchanges exist between the two sets of atoms or between one set only, are linked by

$$\langle v|B_0^N B_{0_1} B_{M_1}^\dagger = \frac{1}{N+1}\langle v|B_0^{N+1} B_{M_2}^\dagger. \quad (3.8)$$

By setting $m=0$ in the above equations, we readily obtain the normalization factor of $(N+1)$ cobosonic molecules as

$$\langle v|B_0^N B_{0_g} B_{0_g}^\dagger B_0^{\dagger N}|v\rangle = \begin{cases} N!\,F_N & \text{for } g=0, \text{ i.e., } (s' \neq s, \sigma' \neq \sigma) \\ N!\,F_{N+1} & \text{for } g=1, \text{ i.e., } (s'=s, \sigma' \neq \sigma) \text{ or}(s' \neq s, \sigma'=\sigma) \\ (N+1)!\,F_{N+1} & \text{for } g=2, \text{ i.e.,} (s'=s, \sigma'=\sigma). \end{cases} \quad (3.9)$$

This, in particular, shows that the normalization factor for $(N+1)$ cobosonic molecules having exchanges between their $(N+1)$ fermionic atoms α *and* between their $(N+1)$ fermionic atoms β, is $(N+1)$ times larger than the normalization factor when exchanges exist between the $(N+1)$ fermionic atoms α only,

$$\langle v|B_0^{N+1} B_0^{\dagger N+1}|v\rangle = (N+1)\langle v|B_0^N B_{0_1} B_{0_1}^\dagger B_0^{\dagger N}|v\rangle. \quad (3.10)$$

Due to the same counting of atom exchanges, this relation can be generalized, according to Eq. (3.8), as

$$\langle v|B_0^{N+1} B_{M_2}^\dagger|\Phi_N\rangle = (N+1)\langle v|B_0^N B_{0_1} B_{M_1}^\dagger|\Phi_N\rangle, \quad (3.11)$$

for *any* state $|\Phi_N\rangle$ made of N pairs of atoms. The above relation is the key on which is based the main result of the present paper.

B. Matrix element of the Hamiltonian

We now turn to the matrix elements of the system Hamiltonian between cobosonic molecular states.

1. States with N cobosonic molecules 0

In a previous work [8], we have calculated the Hamiltonian matrix element when all the cobosons are in the same

state. Due to the commutator (1.15), we readily find

$$\langle v|B_0^N (H - NE_0)B_0^{\dagger N}|v\rangle = R_N/2,$$

$$R_N = \sum_{MP} \langle v|B_0^N B_0^{\dagger N-2} B_M^\dagger B_P^\dagger|v\rangle \Xi^{\text{dir}}\begin{pmatrix} P & 0 \\ M & 0 \end{pmatrix} N(N-1).$$
$$(3.12)$$

R_N is represented by the diagram of Fig. 3(a): Two cobosons 0 among the N cobosons 0 interact to give the cobosons M and P. These cobosons (M,P) can then exchange their fermions with the remaining $(N-2)$ cobosons 0 in all possible ways to give back N cobosons 0. The factor $N(N-1)$ appearing in Eq. (3.12) or in the diagram of Fig. 3(a) comes from the number of ways to choose the two cobosons 0 which interact, among N.

The density expansion of R_N, shown in Fig. 3(b), is obtained by passing $B_M^\dagger$, or $B_P^\dagger$, over B_0^N according to Eq. (1.13). This expansion readily leads to [8]

$$R_N = \langle v|B_0^{N-2} B_0^{\dagger N-2}|v\rangle \{N(N-1)\zeta_2 N(N-1)\}$$
$$+ \langle v|B_0^{N-3} B_0^{\dagger N-3}|v\rangle \{N(N-1)(N-2)\zeta_3 N(N-1)(N-2)\}$$
$$+ \cdots. \quad (3.13)$$
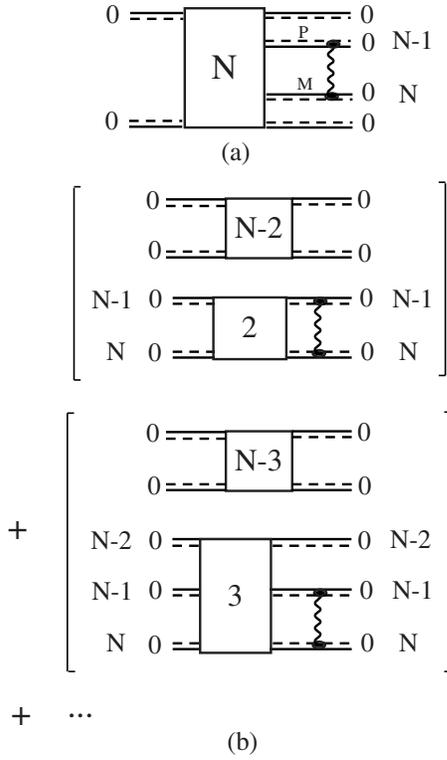
So that, using Eq. (3.1), we end with

(a)

(b)

FIG. 3. (a) Shiva diagram representing R_N, defined in Eq. (3.12). It corresponds to the interaction part of the Hamiltonian expectation value for N cobosonic molecules 0. (b) Density expansion of R_N, given in Eq. (3.13). As explained in Ref. [2], it is obtained from the diagram (a) by extracting the $(N-2)$, $(N-3)$,... cobosonic molecules 0 which are not involved in Pauli scatterings with the cobosonic molecules (M, P) resulting from the interactions of two molecules 0. According to Eq. (3.1), these extracted parts give $(N-n)!F_{N-n}$. The N factors appearing in these diagrams come from the number of ways to, among N, choose the cobosonic molecules 0 involved in the scatterings.

$$R_N = N! \left[F_{N-2}\zeta_2 N(N-1) + F_{N-3}\zeta_3 N(N-1)(N-2) + \cdots \right].$$
(3.14)

The ζ_n's correspond to the connected diagrams [2] between n cobosonic molecules 0, in which enters one interaction scattering Ξ^{dir}. The N-dependent factors in Eq. (3.13) again come from the number of ways to choose these n molecules 0, among N. Figure 4 shows the two first ζ_n's. From this figure we readily find

$$\zeta_2 = \xi^{\mathrm{dir}}\begin{pmatrix} o & o \\ o & o \end{pmatrix} - \xi^{\mathrm{in}}\begin{pmatrix} o & o \\ o & o \end{pmatrix}.$$
(3.15)

2. States with N cobosonic molecules 0 plus one cobosonic molecule 0_g

In order to calculate the H matrix element when a cobosonic molecule 0_g is added to N cobosonic molecules 0, we first use Eq. (1.8). This leads to
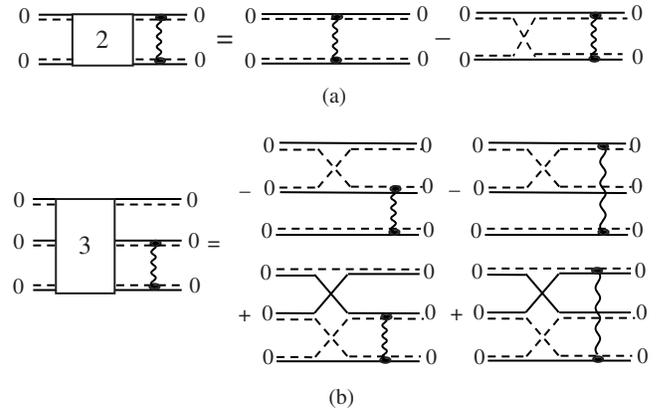

(a)

(b)

FIG. 4. (a) Shiva diagrams for ζ_2, appearing in Eq. (3.13). It corresponds to direct and exchange interactions between two cobosonic molecules 0 giving back these 0 states. (b) Shiva diagrams for ζ_3. We see that ζ_3 contains processes in which one of the three cobosonic molecules 0 conserves its fermionic atoms as well as processes in which all the three cobosonic molecules are involved in fermion exchanges.

$$\langle v|B_0^N B_{0_g}[H - (N+1)E_0]B_{0_g}^\dagger B_0^{\dagger N}|v\rangle$$
$$= \langle v|B_0^N B_{0_g}\{B_{0_g}^\dagger(H - NE_0) + V_{0_g}^\dagger\}B_0^{\dagger N}|v\rangle. \quad (3.16)$$

We then use Eq. (1.14) to calculate $V_{0_g}^\dagger B_0^{\dagger N}|v\rangle$. By noting that $\Xi^{\mathrm{dir}}\begin{pmatrix} P & 0 \\ M & 0_g \end{pmatrix}$ is a direct interaction scattering, we end with

$$\langle \psi_{N;g}|H - (N+1)E_0|\psi_{N;g}\rangle$$
$$= \langle v|B_0^N B_{0_g}\left\{ B_{0_g}^\dagger(H - NE_0)B_0^{\dagger N} \right.$$
$$\left. + N\sum_{m,p} \xi^{\mathrm{dir}}\begin{pmatrix} p & o \\ m & o \end{pmatrix}B_{M_g}^\dagger B_{P_2}^\dagger B_0^{\dagger N-1} \right\}|v\rangle. \quad (3.17)$$

To go further, it is necessary to differentiate the cases in which atom exchange can or cannot take place.

C. Energy change in the absence of atom exchange

When the added molecule is a molecule $0_{g=0}$, i.e., a molecule made of two atoms with spins different from the ones of the molecules 0, no exchange takes place between the added molecule and the molecules present in the system. Making use of Eq. (3.7), we then get the matrix element of the system Hamiltonian in this $|\psi_{N;g=0}\rangle$ state, given in Eq. (3.17), as

$$\langle \psi_{N;0}|H - (N+1)E_0|\psi_{N;0}\rangle$$
$$= \langle v|B_0^N(H - NE_0)B_0^{\dagger N}|v\rangle$$
$$+ N\sum_p \langle v|B_0^N B_{P_2}^\dagger B_0^{\dagger N-1}|v\rangle \xi^{\mathrm{dir}}\begin{pmatrix} p & o \\ o & o \end{pmatrix}. \quad (3.18)$$

The second term of the above equation is shown in Fig. 5(a). It corresponds to a direct interaction between the added molecule 0_0 and one of the N molecules 0 already present, the N in front of the sum of Eq. (3.18) coming from the number of ways to, among N, choose the molecule 0 which interacts
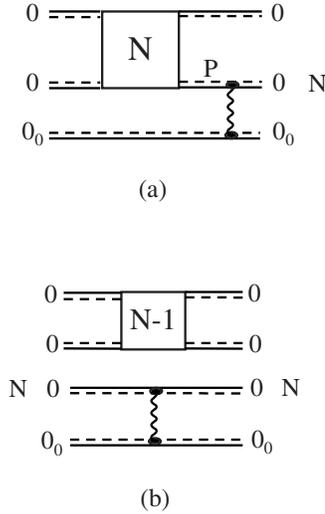
(a)

(b)

FIG. 5. (a) Shiva diagram representing the second term of Eq. (3.18), the added cobosonic molecule 0_0 having its two fermionic atoms with spins different from the ones of the cobosonic molecule 0. (b) Dominant term of the density expansion of the diagram (a), as obtained by extracting the $(N-1)$ cobosonic molecules 0 not involved in the exchange process with the cobosonic molecule 0 interacting with 0_0. The N factors are the number of ways to, among N, choose the cobosonic molecule 0 interacting with 0_0.

with 0_0: Since the two fermionic atoms of the molecule 0_0 are different from the ones of the molecules 0, the added molecule 0_0 can feel the molecules 0 by fermion interactions but not by the Pauli exclusion principle, i.e., fermion exchanges.

If we now use the normalization factor of the state $|\psi_{N;0}\rangle$ given in Eq. (3.9), we find

$$\langle H \rangle_{N;0} - \langle H \rangle_N = E_0 + \mathcal{E}_{N;0},$$

$$\mathcal{E}_{N;0} = \frac{\sum_p \langle v|B_0^N B_{P_2}^\dagger B_0^{\dagger N-1}|v\rangle \xi^{\text{dir}}\begin{pmatrix} p & o \\ o & o \end{pmatrix} N}{\langle v|B_0^N B_0^{\dagger N}|v\rangle}. \quad (3.19)$$

As for R_N in Eq. (3.12), we calculate the density expansion of the above sum by passing $B_{P_2}^\dagger$ over B_0^N according to Eq. (1.13). We find that the dominant term of this sum, shown in Fig. 5(b), is equal to $N^2 \xi^{\text{dir}}\begin{pmatrix} o & o \\ o & o \end{pmatrix}(N-1)! F_{N-1}$, the additional factor N coming from the number of ways to, among N, choose the molecule 0 which results from the scattering, by direct interactions, of the two molecules 0_0 and 0.

All this leads to a density expansion of the energy change when no atom exchange takes place given by

$$\mathcal{E}_{N;0} = \frac{N^2 \xi^{\text{dir}}\begin{pmatrix} o & o \\ o & o \end{pmatrix}(N-1)! F_{N-1} + \cdots}{N! F_N}$$

$$\simeq N \xi^{\text{dir}}\begin{pmatrix} o & o \\ o & o \end{pmatrix} + O(\eta^2). \quad (3.20)$$

Note that the leading term of this energy change, of the order of η, reduces to zero if the attraction between fermions

(α, β) is as large as the repulsion between (α, α) and (β, β)—as in the case of Coulomb interaction between fermions having opposite charges—since we then have $\xi^{\text{dir}}\begin{pmatrix} p & j \\ i & i \end{pmatrix}=0$, as seen from Eq. (1.10). It is possible to show that this cancellation in fact remains at any order in density. This result, not obvious at first, tells that there is no energy change, in the Born approximation, for systems having an (α, β) attraction as large as the (α, α), (β, β) repulsions, when fermion exchanges do not exist between the added molecule and the ones present in the sample.

D. Energy change in the presence of atom exchanges

1. Exchanges within the two sets of fermionic atoms or within one set only

Making use of Eq. (3.11) in Eq. (3.17), we readily find

$$\langle \psi_{N;1}|H - (N+1)E_0|\psi_{N;1}\rangle = \frac{1}{N+1}\langle \psi_{N;2}|H - (N+1)E_0|\psi_{N;2}\rangle. \quad (3.21)$$

So that, due to the link between the normalization factors given in Eq. (3.10), we simply have

$$\langle H \rangle_{N;1} = \langle H \rangle_{N;2}. \quad (3.22)$$

This proves that, within the Born approximation, the energy changes are equal *at any order in density* if exchanges exist between the two sets of fermionic atoms or between one set only: The increase of atom exchanges appearing in the Hamiltonian matrix element is exactly balanced by the same increase of atom exchanges appearing in the normalization factor, this balance existing at any order in density—a result far from intuitive.

2. Precise calculation of this energy change

Since $\langle H \rangle_{N;2} = \langle H \rangle_{N+1}$, we can calculate this energy change as $(\langle H \rangle_{N+1} - \langle H \rangle_N - E_0)$. Equations (1.16), (1.18), (3.1), and (3.12) allow us to write it as

$$\mathcal{E}_{N;1} = \mathcal{E}_{N;2} = \frac{R_{N+1}}{2(N+1)! F_{N+1}} - \frac{R_N}{2N! F_N}. \quad (3.23)$$

By using the density expansion of R_N given in Eq. (3.14), the energy change when exchanges between molecules take place thus appears as

$$\mathcal{E}_{N;1} = \mathcal{E}_{N;2} = [\zeta_2 A_2(N) + \zeta_3 A_3(N) + \cdots]/2, \quad (3.24)$$

where we have set

$$A_{n+1}(N) = \frac{F_{N-n}}{F_{N+1}}\frac{(N+1)!}{(N-n)!} - \frac{F_{N-1-n}}{F_N}\frac{N!}{(N-n-1)!}. \quad (3.25)$$

In order to calculate the density expansions of this quantity, it is convenient to note that it also reads

$$A_{n+1}(N) = \left[(n+1)\frac{F_{N-n-1}}{F_N} + (N+1)\left(\frac{F_{N-n}}{F_{N+1}} - \frac{F_{N-1-n}}{F_N} \right) \right]$$

$$\times \frac{N!}{(N-n)!}. \qquad (3.26)$$

The density expansion of the ratio F_{N-2}/F_N appearing in $A_2(N)$ is obtained by noting that

$$\frac{F_{N-2}}{F_N} = \frac{F_{N-1}}{F_N}\frac{F_{N-2}}{F_{N-1}} = f_N\left(f_N - \frac{\partial f_N}{\partial N} + \cdots \right). \qquad (3.27)$$

If we then use the density expansion of $f_N = \tilde{f}(\eta)$ given in Eq. (3.3), this ratio reads as

$$\frac{F_{N-2}}{F_N} \simeq \tilde{f}(\eta)\left[\tilde{f}(\eta) - \frac{\eta}{N}\tilde{f}'(\eta) + \cdots \right]. \qquad (3.28)$$

In the same way, the leading term of the ratio difference $(F_{N-1}/F_{N+1} - F_{N-2}/F_N)$ appearing in $A_2(N)$ reads as $2\eta\,\tilde{f}(\eta)\tilde{f}'(\eta)/N$, so that the second term of $A_2(N)$ is smaller than the first one by a factor of the order of η.

By using Eqs. (3.3) and (3.15), it is then easy to show that the leading term of the energy change given in Eq. (3.24) reduces to

$$\mathcal{E}_{N;1} = \mathcal{E}_{N;2} \simeq N\left[\xi^{\text{dir}}\begin{pmatrix} o & o \\ o & o \end{pmatrix} - \xi^{\text{in}}\begin{pmatrix} o & o \\ o & o \end{pmatrix} \right] + O(\eta^2),$$

$$(3.29)$$

the term in η^2 coming from the first factor of $A_3(N)$, the second factor of $A_2(N)$, and also the fact that $\tilde{f}(\eta) = 1 + O(\eta)$.

It is actually possible to recover the above result by noting that, for large N,

$$E_0 + \mathcal{E}_{N;2} = \langle H \rangle_{N+1} - \langle H \rangle_N = \frac{\partial \langle H \rangle_N}{\partial N}. \qquad (3.30)$$

The R_N expansion given in Eq. (3.14) then leads to

$$\langle H \rangle_N = N\left[E_0 + \frac{N}{2}\zeta_2 + O(\eta^2) \right]. \qquad (3.31)$$

The energy change of Eq. (3.29) readily follows from Eqs. (3.15), (3.30), and (3.31).

When comparing Eq. (3.29) to Eq. (3.20), we see that an additional contribution to the energy change, namely, $-N\xi^{\text{in}}\begin{pmatrix} o & o \\ o & o \end{pmatrix}$, appears when atom exchanges are possible between the added molecule and the molecules present in the sample, as physically expected. Less expected is the fact that this additional contribution is the same when exchanges exist between one set or between the two sets of fermionic atoms, due to an exact balance, at any order in density, between the

increase in the number of exchanges entering the H matrix element and the increase in the number of exchanges entering the state normalization factor. This leads us to predict that the scattering lengths for molecules having one or two atoms with the same spin are, in the Born approximation, equal.

It is of importance to recall that, by calculating the energy change through the expectation value of the Hamiltonian in the state $|\psi_{N,g}\rangle$, we, by construction, get this change at first order in fermion interactions, so that we calculate it in the Born approximation. To obtain this energy change at second order in fermion interactions, we would have to use the $(N+1)$ coboson state at first order in the interactions, this state differing from a bare coboson product $|\psi_{N;g}\rangle$, due to the interactions between cobosons which have then to be included at first order. The procedure to derive this first order state has not been found yet, due to major difficulties [12] in properly handling exchanges between composite quantum particles, which makes the system Hamiltonian not possible to write as $H_0 + V$, with V being a potential *between* composite quantum particles. We are going to address this difficult problem in the near future.

IV. CONCLUSION

We have studied the effect of the Pauli exclusion principle in a mixture of cobosonic molecules made of two fermionic atoms through the energy change of N identical molecules when a similar molecule made of fermionic atoms, with possibly different spins, is added. To focus on the consequences of the Pauli exclusion principle, the calculation presented here is restricted to interactions between atoms independent of their spins, inelastic scatterings being neglected. In spite of the larger number of atom exchanges when the two atoms of the added molecule are identical to the ones already present, we find that the energy change calculated in the Born approximation is exactly the same as the one when the added molecule only has one fermionic atom identical to the ones present in the sample. Such an exact balance in fermion exchanges, which exists at any order in density, is certainly not easy to guess. Its proof relies on a very careful calculation of this energy change, with the consequences of the Pauli exclusion principle included in an exact way. As a consequence, this work predicts the equality, within the Born approximation, of the scattering lengths for molecules made of one or two atoms having same spin.

The present work makes use of the recent extension [3] of the exciton many-body theory [1] to any type of composite bosons, the Shiva diagram representation [2] of this many-body theory allowing an easy understanding of the physics involved in the various terms.

[1] For a short review, see M. Combescot and O. Betbeder-Matibet, Solid State Commun. **134**, 11 (2005). and references therein.

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