General Many-Body Formalism for Composite Quantum Particles

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This Letter provides a formalism capable of exactly treating Pauli blocking between n-fermion particles. This formalism is based on an operator algebra made of commutators and anticommutators which contrasts with the usual scalar formalism of Green functions developed half a century ago for elementary quantum particles. We also provide the diagrams which visualize the very specific many-body physics induced by fermion exchanges between composite quantum particles.

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Although most physical effects deal with composite quantum particles, textbook many-body procedures [1,2] consider elementary fermions or bosons only. This comes from the lack of exact procedures able to handle the Pauli exclusion principle between the particle fermionic components. This Letter proposes a formalism capable of exactly treating this exclusion and provides diagrams to visualize the very specific many-body physics induced by fermion exchanges between composite quantum objects.

Various procedures [3–5] have been proposed to deal with composite particle many-body effects. These end by mapping the fermion space onto a subspace of effective particles taken as elementary fermions or bosons, depending on the fermionic component number. These particles interact through effective scatterings built from the ones of their elementary fermions dressed by a ‘‘certain amount’’ of fermion exchanges [6,7].

Such mappings are neither fully satisfactory nor, sometimes, consistent—the one commonly used for excitons [6] produces an effective Hamiltonian which is not Hermitian. Rather than working out a better mapping, we preferred to face the particle composite nature, fermion exchanges appearing explicitly in the theory. This was a challenge because, for five decades, no significant step has been taken in producing a many-body formalism appropriate to composite quantum particles. It implies to generate fermion exchanges between a large number of composite particles in a systematic way. It also implies to refresh the concept of particle interaction because we here deal with objects which are basically undefined since they keep exchanging their fermions. Since all known many-body procedures rely on interactions between well-defined objects, a conceptually new formalism is required.

A few years ago [8,9], we tackled the simplest of these composite objects by considering two fermions, having excitons in mind. These are bosonlike and indeed, were commonly treated as such up to now. Since boson operators commute, a natural approach appeared to us to calculate commutators of exciton creation operators and to see what could be extracted from them. It turned out that with two commutators, we can pick the 2×2 scatterings which describe interactions between the fermions of two excitons in the absence of fermion exchanges. Through two other commutators, we reach the 2×2 scatterings for fermion exchanges in the absence of fermion interaction. Exchanges between N excitons then follow from combining these 2×2 exchanges. We visualized these fermion exchanges through new diagrams [9,10] named for the Hindu god Shiva, due to their multiarm structure. Like Feynman diagrams [1,2], Shiva diagrams allow us to calculate the physical effect at hand through rather intuitive rules. They also provide a visual understanding for the many-body physics induced by Pauli blocking on composite bosons: whereas it is known that Pauli blocking produces the free electron Fermi sea, very little is understood on Pauli blocking with bound electron pairs, as exemplified by our latest work on Cooper pairs [11].

This composite exciton many-body theory allowed us to solve problems open for decades, such as the exact cancellation of volume-linear terms for nonlinear susceptibilities [12] or the analytical resolution of semiconductor Bloch equations in nonlinear optics [13]. Its major success, however, lies in providing a direct way to understand and better predict physical effects, such as the exciton Bose-Einstein condensation occurring in dark states [14,15]. We can also cite effects induced by unabsorbed photons through exchanges with virtual excitons: spin precession [16] and teleportation [17], Faraday rotation [18] and ‘‘oscillation’’ [19], Hadamard and phase gates for quantum computing [20].

These previous works on composite-boson excitons just constitute a ‘‘hors d'oeuvre’’ for a far more formidable task: the construction of a general many-body formalism for any quantum object. The challenge is to generate in a fully systematic way exchanges between particles made of an arbitrary number of fermions. If this number is odd, particles are fermionlike; their creation operators anticommute. Why then to consider commutators only, as we did for excitons?

The goal of this Letter is to present the general structure of a many-body formalism allowing an exact treatment of n-fermion particles. We show that scatterings which result from fermion interactions without fermion exchanges, are still generated by two commutation relations, Eqs. (7) and (8). These are two commutators for cobosons—a contraction for composite bosons—while the second commutator transforms into an anticommutator for cofermions—a contraction for composite fermions. Fermion exchanges without fermion interactions are far more demanding: n commutation relations are necessary to fully control fermion exchanges between n-fermion particles. For cobosons, these are just commutators while, for cofermions, they also contain anticommutators: to fully control fermion exchanges between 3-fermion particles, two anticommutators plus one commutator are required, see Eqs. (10), (12), and (14). We also show that other diagrams, called "Kali," are necessary in addition to Shiva-like diagrams, to visualize all possible fermion exchanges between n-fermion particles.

Formalism.—To better grasp how the general structure of this many-body formalism transforms from bosonlike to fermionlike particles, let us concentrate on the simplest of these composite objects, namely, cobosons made of two fermions (α, β) and cofermions made of three fermions (α, β, γ). The reason for choosing commutator or anticommutator, crucial for building up a consistent theory, is easy to extend to $n > 3$. These fermions, which can be up or down spin electrons, valence band holes, protons, neutrons, or even quarks, are assumed to be different. Identical fermions, $\alpha \equiv \beta$, like in semiconductor triplet trions, will be considered elsewhere. Different fermion creation operators obey $[a^\dagger_{\mathbf{k}_\alpha}, b^\dagger_{\mathbf{k}_\beta}]_{\eta_{ab}} = 0 = [a_{\mathbf{k}_\alpha}, b^\dagger_{\mathbf{k}_\beta}]_{\eta_{ab}}$, with $[A, B]_\eta = AB + \eta BA$. For fermions belonging to the same species, $\eta_{ab} = 1$, while for different species, $\eta_{ab} = -1$. However, since η_{ab} ultimately appears as η_{ab}^2, we can, for simplicity, consider that all elementary fermion operators anticommute.

We take the n-fermion particles as being Hamiltonian eigenstates in order to form a complete orthogonal basis for n-fermion states: $\langle i|j\rangle = \delta_{ij}$ with $|i\rangle = C^\dagger_i|v\rangle$ where $C^\dagger_i$ is the i particle creation operator. For 2-fermion particles, $C^\dagger_i$, written as $B^\dagger_i$, is related to free fermion pairs:

$$B^\dagger_i = \sum_{\mathbf{k}_\alpha, \mathbf{k}_\beta} a^\dagger_{\mathbf{k}_\alpha} b^\dagger_{\mathbf{k}_\beta} \langle \mathbf{k}_\beta, \mathbf{k}_\alpha | i\rangle, \tag{1}$$

$$a^\dagger_{\mathbf{k}_\alpha} b^\dagger_{\mathbf{k}_\beta} = \sum_i B^\dagger_i \langle i|\mathbf{k}_\alpha, \mathbf{k}_\beta\rangle, \tag{2}$$

while for 3-fermion particles with creation operator $F^\dagger_i$,

$$F^\dagger_i = \sum_{\mathbf{k}_\alpha, \mathbf{k}_\beta, \mathbf{k}_\gamma} a^\dagger_{\mathbf{k}_\alpha} b^\dagger_{\mathbf{k}_\beta} c^\dagger_{\mathbf{k}_\gamma} \langle \mathbf{k}_\gamma, \mathbf{k}_\beta, \mathbf{k}_\alpha | i\rangle, \tag{3}$$

$$a^\dagger_{\mathbf{k}_\alpha} b^\dagger_{\mathbf{k}_\beta} c^\dagger_{\mathbf{k}_\gamma} = \sum_i F^\dagger_i \langle i|\mathbf{k}_\alpha, \mathbf{k}_\beta, \mathbf{k}_\gamma\rangle. \tag{4}$$

and so on.... These creation operators are such that

$$[C^\dagger_m, C^\dagger_i]_\eta = 0, \tag{5}$$

with $\eta = -1$ for cobosons like $B^\dagger_i$ while $\eta = +1$ for cofermions like $F^\dagger_i$. Composite particles can change states, i.e., interact in the most general sense, through either fermion interactions or just fermion exchanges. Let us now derive the set of commutation relations which controls these two types of processes.

(i) *Fermion interactions.*—The choice between commutator and anticommutator follows from $(H - E_i)C^\dagger_i|v\rangle = 0$ which, for arbitrary $|\psi\rangle$, gives

$$HC^\dagger_i|\psi\rangle = E_i C^\dagger_i|\psi\rangle + C^\dagger_i H|\psi\rangle + |\ldots\rangle. \tag{6}$$

$|\ldots\rangle$ comes from interactions between particle i and $|\psi\rangle$. Equation (6) thus always leads to a commutator:

$$[H, C^\dagger_i]_{-1} = E_i C^\dagger_i + V^\dagger_i. \tag{7}$$

The "creation potential" $V^\dagger_i$ describes all interactions with the fermions of particle i. Because of homogeneity, $V^\dagger_i$ reads as $\sum_m C^\dagger_m V^{(1)}_{mi}$ where, for two-fermion interaction, $V^{(1)}_{mi}$ contains products like $a^\dagger a$.

To get rid of $V^{(1)}_{mi}$ and end with scalar scatterings only, we need a second commutation relation. Commutator or anticommutator follows from (i, j) symmetry [see Eq. (A1)]. Homogeneity then gives

$$[V^\dagger_i, C^\dagger_j]_\eta = \sum_{m,n} C^\dagger_m C^\dagger_n \xi\begin{pmatrix} n & j \\ m & i \end{pmatrix}. \tag{8}$$

The $\xi(\begin{smallmatrix} n & j \\ m & i \end{smallmatrix})$ scattering is represented by the diagram of Fig. 1. It comes from interactions between the elementary fermions of the composite particles (i, j), in the absence of fermion exchange, m and i being made with the same fermions. This "direct" scattering follows from two commutators in the case of cobosons but a commutator and an anticommutator in the case of cofermions.

(ii) *Fermion exchanges.*—Generating fermion exchanges between composite quantum particles is far more demanding. It is the difficult part of the problem. No progress has been made from the Green function formalism for elementary fermion or boson many-body effects. The exact handling of fermion exchanges between n-fermion particles is the original part of the present Letter.

$C^\dagger_i|v\rangle$ being H eigenstate, $[C_m, C^\dagger_i]_\eta|v\rangle$ gives $\delta_{m,i}|v\rangle$ whatever η. It, however, is natural to take the same com-

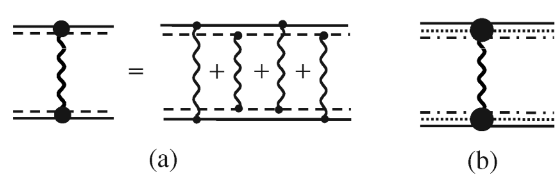

FIG. 1. (a) Interaction scattering $\xi(\begin{smallmatrix} n & j \\ m & i \end{smallmatrix})$ for cobosons made of 2 fermions, resulting from interactions between their fermionic components. (b) Same for 3-fermion cofermions.

mutation relation for $[C_m^\dagger, C_i^\dagger]$ and $[C_m, C_i^\dagger]$. This leads to [8–10]

$$[C_m, C_i^\dagger]_\eta = \delta_{m,i} - D_{mi}. \tag{9}$$

D_{mi} is a $(n-1)$-body operator: for fermion pairs, it reads in terms of products like $a^\dagger a$, while D_{mi} also contains products like $a^\dagger b^\dagger ba$ for fermion triplets, and so on.

To eliminate this operator, we need $(n-1)$ commutation relations. The choice between commutator and anticommutator again follows from particle symmetry [see Eq. (A2)]. Homogeneity then always leads to

$$[D_{mi}, C_j^\dagger]_{-1} = \sum_n C_n^\dagger D_{nmij}. \tag{10}$$

D_{nmij} reduces to a scalar $D_{nmij}^{(0)}$ for fermion pairs. For 3-fermion particles, it also contains a one-body operator $D_{nmij}^{(1)}$ in $(a^\dagger a,\ b^\dagger b,\ c^\dagger c)$, i.e., $D_{nmij} = D_{nmij}^{(0)} + D_{nmij}^{(1)}$, and so on.

Since $D_{nmij}|v\rangle$ reduces to $D_{nmij}^{(0)}|v\rangle$, Eq. (10) acting on vacuum gives this scalar part as

$$D_{nmij}^{(0)} = (\delta_{m,i}\delta_{n,j} - \eta\delta_{m,j}\delta_{n,i}) - \langle v|C_n C_m C_i^\dagger C_j^\dagger|v\rangle, \tag{11}$$

The two terms in the right-hand side would be equal if the particles were elementary: $D_{nmij}^{(0)}$ physically corresponds to all possible fermion exchanges between two n-fermion particles from initial states (i, j) to final states (m, n).

For fermion pairs, Eq. (10) then gives

$$[D_{mi}, B_j^\dagger]_{-1} = \sum_n B_n^\dagger \sum_{\rho=(\alpha,\beta)} \lambda_\rho\begin{pmatrix} n & j \\ m & i \end{pmatrix}, \tag{12}$$

where the scalar $\lambda_\rho\left(\begin{smallmatrix} n & j \\ m & i \end{smallmatrix}\right)$ corresponds to the Shiva diagram of Fig. 2(a): coboson i exchanges its fermion $\rho = \alpha$ or β with coboson j, to end in state m.

The situation gets considerably more complicated when turning to 3-fermion particles. Cofermion i can exchange one or two of its three fermions with one cofermion j, but it can also exchange its three fermions with two cofermions j and k. Since, as seen from Fig. 2(b), $\lambda_\gamma\left(\begin{smallmatrix} n & j \\ m & i \end{smallmatrix}\right) = \lambda_{\alpha\beta}\left(\begin{smallmatrix} n & j \\ m & i \end{smallmatrix}\right)$, Eq. (10) then gives

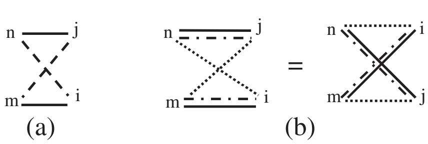

FIG. 2. (a) Shiva diagram for fermion exchanges between two cobosons made of fermions α and β (solid and dashed lines). (b) Shiva-like diagrams for fermion exchanges between two cofermions made of three fermions (α, β, γ).

$$[D_{mi}, F_j^\dagger]_{-1} = \sum_n F_n^\dagger \sum_\rho \left\{\lambda_\rho\begin{pmatrix} n & j \\ m & i \end{pmatrix} - (i \leftrightarrow j)\right\} + D_{mij}^\dagger, \tag{13}$$

where we have set $D_{mij}^\dagger = \sum_n F_n^\dagger D_{nmij}^{(1)}$, the sign change in $(i \leftrightarrow j)$ coming from double exchange.

To get rid of the operator $D_{mij}^\dagger$ and end with scalar scatterings only, we need a third commutation relation. The choice is again made from symmetry [see Eq. (A3)]. After some algebra, we end with

$$[D_{mij}^\dagger, F_k^\dagger]_{+1} = \sum_{p,n} F_p^\dagger F_n^\dagger \left\{\chi\begin{pmatrix} p & k \\ n & j \\ m & i \end{pmatrix} + \text{perm}\right\}, \tag{14}$$

where the permutations include (i, j, k) circular permutations as well as noncircular permutations with a minus sign. The scalar χ, represented by the Kali diagram of Fig. 3, describes fermion exchanges between three particles—instead of two as in Shiva diagrams. Its mathematical expression follows from trivial rules to calculate diagrams [9,10]: we take the "in" state wave functions, the complex conjugate of the "out" state wave functions, with the fermion coordinates read from the diagrams, and we sum over these coordinates:

$$\chi\begin{pmatrix} p & k \\ n & j \\ m & i \end{pmatrix} = \int\{d\mathbf{r}\}\phi_m^*(\mathbf{r}_{\alpha_1}, \mathbf{r}_{\beta_2}, \mathbf{r}_{\gamma_3})\phi_n^*(\mathbf{r}_{\alpha_2}, \mathbf{r}_{\beta_3}, \mathbf{r}_{\gamma_1})$$
$$\times\, \phi_p^*(\mathbf{r}_{\alpha_3}, \mathbf{r}_{\beta_1}, \mathbf{r}_{\gamma_2})\phi_k(\mathbf{r}_{\alpha_3}, \mathbf{r}_{\beta_3}, \mathbf{r}_{\gamma_3})$$
$$\times\, \phi_j(\mathbf{r}_{\alpha_2}, \mathbf{r}_{\beta_2}, \mathbf{r}_{\gamma_2})\phi_i(\mathbf{r}_{\alpha_1}, \mathbf{r}_{\beta_1}, \mathbf{r}_{\gamma_1}). \tag{15}$$

(iv) *How to use this formalism.*—We first rewrite the quantity at hand in terms of composite particle operators using equations similar to Eqs. (2) and (4). Next, we eliminate the Hamiltonian H by pushing it to the right through commutator constructed upon Eq. (7). The $V_i^\dagger$'s are eliminated through Eq. (8). This generates interaction scatterings $\xi\left(\begin{smallmatrix} n & j \\ m & i \end{smallmatrix}\right)$ and leaves composite particle scalar products. These are calculated by pushing the C_i's to the right according to Eq. (9), the D_{mi}'s being eliminated through equations like Eqs. (12) or (13) and (14). Previous works using this formalism for excitons [9] can

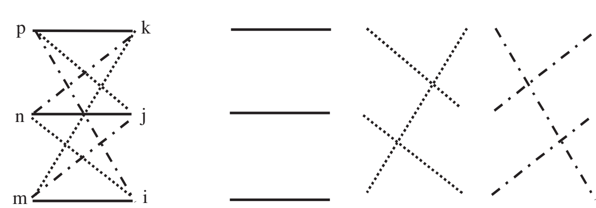

FIG. 3. Kali diagram for fermion exchanges between three cofermions. The (α, β, γ) lines are shown separately, to make the diagram topology clearer.

be used as exercises. This Letter demonstrates that calculations for n-fermion particles are conceptually similar.

We have just used [21] the cofermion version of this formalism to calculate the time evolution of two semiconductor trions, made of opposite spin electrons and a hole. To get the effective scattering ruling their time evolution, we start with $e^{-iHt}F_i^\dagger F_j^\dagger|v\rangle$, replace e^{-iHt} by its integral representation [9] in terms of $(z-H)^{-1}$, and push H to the right using $(z-H)^{-1}F_i^\dagger = [F_i^\dagger + (z-H)^{-1}V_i^\dagger]\times[z-H-E_i]^{-1}$ which follows from Eq. (7). The second bracket acting on $F_j^\dagger|v\rangle$ gives $(z-E_j-E_i)^{-1}$. We are then left with $V_i^\dagger F_j^\dagger|v\rangle$ which reads in terms of $\xi\left(\begin{smallmatrix} n & j \\ m & i\end{smallmatrix}\right)$, using Eq. (8). The diagram of Fig. 1(b) gives it as

$$\xi\begin{pmatrix} n & j \\ m & i\end{pmatrix} = \delta_{\mathbf{Q}_m+\mathbf{Q}_n,\mathbf{Q}_i+\mathbf{Q}_j} V_{\mathbf{Q}_m-\mathbf{Q}_i}|\gamma_{\mathbf{Q}_m-\mathbf{Q}_i}|^2. \quad (16)$$

$\mathbf{Q}_i$ is the trion i center-of-mass momentum, $V_\mathbf{q}$ the free carrier Coulomb interaction. $\gamma_\mathbf{q}$ results from the trion composite nature. For transition within the relative motion ground state $\langle \mathbf{k},\mathbf{p}|\eta_0\rangle$ [22], it reads

$$\gamma_\mathbf{q} = \sum_{\mathbf{k},\mathbf{p}}[2\langle\eta_0|\mathbf{k}+\alpha_h\mathbf{q},\mathbf{p}\rangle - \langle\eta_0|\mathbf{k}-\alpha_e\mathbf{q},\mathbf{p}\rangle]\langle\mathbf{k},\mathbf{p}+\beta_e\mathbf{q}|\eta_0\rangle, \quad (17)$$

with $\alpha_e = 1-\alpha_h = m_e/(m_e+m_h)$ and $\beta_e = m_e/(2m_e+m_h)$. The trion composite nature shows up for large q only on the trion scale [22], $\gamma_\mathbf{q}$ reducing to 1 for $q=0$, as physically reasonable since trions for small q appear as elementary negative charges.

The effective scattering also contains exchange contributions. Obtained through $\langle v|F_mF_ne^{-iHt}F_i^\dagger F_j^\dagger|v\rangle$, they formally read as $\sum_{k,l}\lambda_\rho\left(\begin{smallmatrix} n & l \\ m & k\end{smallmatrix}\right)\xi\left(\begin{smallmatrix} l & j \\ k & i\end{smallmatrix}\right)$. They contain 27 physical processes, which reduce to 9 different quantities, due to internal symmetries. For more details, see Ref. [21].

Conclusion.—We here provide a general many-body formalism to deal with fermion exchanges between n-fermion particles in an exact way. This formalism is impressively compact in view of the initial complexity of the problem: it reduces to $(n+2)$ equations. These read in terms of commutators and anticommutators between the creation operators of these composite quantum objects. Fermion exchanges are efficiently visualized through multiarm diagrams called Shiva and Kali.

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Appendix: Symmetry requirements.—For readers willing to better grasp the deep reasons for choosing between commutators and anticommutators, we here list three useful identities: (i,j) symmetry in

$$[[H,C_i^\dagger]_{-1},C_j^\dagger]_{\eta_1} = -\eta[[H,C_j^\dagger]_{-\eta\eta_1},C_i^\dagger]_\eta, \quad (A1)$$

imposes $\eta_1=\eta$, while it imposes $\eta_2=-1$ in

$$[[C_m,C_i^\dagger]_\eta,C_j^\dagger]_{\eta_2} = -\eta[[C_m,C_j^\dagger]_{-\eta\eta_2},C_i^\dagger]_{-1}. \quad (A2)$$

(j,k) symmetry in

$$[[[F_m,F_i^\dagger]_{+1},F_j^\dagger]_{-1},F_k^\dagger]_{\eta_3} = -[[[F_m,F_i^\dagger]_{+1},F_k^\dagger]_{-\eta_3},F_j^\dagger]_{+1}, \quad (A3)$$

imposes $\eta_3=+1$, i.e., an anticommutator in Eq. (14).

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