Multipolar exchange in a many-body homonuclear mixture of atoms in different internal states

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ABSTRACT

We develop a general method for constructing the many-body Hamiltonian of pairwise interactions describing homonuclear mixtures of atoms occupying states with different total angular momenta or other quantum numbers. The advantage of the irreducible spherical tensor operator formalism is demonstrated: these operators give the Hamiltonian an explicit physical structure, account for all scattering channels, and include multipolar exchange interactions. The latter correspond to the exchange of both angular-momentum projections and the total angular momentum. Particular realizations of the general Hamiltonian, widely used in the physics of ultracold gases, are also analyzed. The resulting Hamiltonian provides a universal framework for investigating a broad range of quantum many-body phenomena in bosonic and fermionic atomic gases.

HAMILTONIAN FOR A HOMONUCLEAR ATOMIC MIXTURE

Let us consider a pairwise interactions in a many-body system of atoms in different internal quantum states $i = \{f_i, \lambda_i\}$, where f_i is a total atomic angular momentum; $\lambda_i = \{l_i, s_i, \dots\}$ denotes the set of the remaining atomic quantum numbers.

$$H_{12}^{\rm int} = \frac{1}{2(1+\delta_{12})} \int d\mathbf{x} d\mathbf{x}' \sum_{m_1,m_2,m_1',m_2'} \left[\psi^*_{m_1}(\mathbf{x}) \psi^*_{m_2}(\mathbf{x}') \Phi^{\rm Proj}_{m_1 m_2 m_1' m_2'}(\mathbf{x}-\mathbf{x}') \psi_{m_2'}(\mathbf{x}') \psi_{m_1'}(\mathbf{x}) + \psi^*_{m_1}(\mathbf{x}) \psi^*_{m_2}(\mathbf{x}') \Phi^{\rm Mom}_{m_1 m_2 m_2' m_1'}(\mathbf{x}-\mathbf{x}') \psi_{m_1'}(\mathbf{x}') \psi_{m_2'}(\mathbf{x}) \right],$$

The interaction function $\Phi^{\rm Proj}_{m_1 m_2 m_1' m_2'}$ describes the exchange of angular-momentum projections, whereas $\Phi^{\rm Mom}_{m_1 m_2 m_2' m_1'}$ accounts for the exchange of the total angular momenta themselves.

$$\Phi^{\rm Proj}_{m_1 m_2 m_1' m_2'}(\mathbf{x}-\mathbf{x}') = \sum_F U^F_{12}(\mathbf{x}-\mathbf{x}')(2F+1)(-1)^{f_1+f_2+F} \sum_{K,\kappa} \begin{Bmatrix} f_1 & f_1 & K \\ f_2 & f_2 & F \end{Bmatrix} (-1)^\kappa (T^K_\kappa)_{m_1 m_1'} (T^K_{-\kappa})_{m_2 m_2'}. \quad (1)$$

$$\Phi^{\rm Mom}_{m_1 m_2 m_2' m_1'}(\mathbf{x}-\mathbf{x}') = \sum_F U^F_{12}(\mathbf{x}-\mathbf{x}')(2F+1)(-1)^{2f_1-F} \sum_{K,\kappa} \begin{Bmatrix} f_1 & f_2 & K \\ f_1 & f_2 & F \end{Bmatrix} (-1)^\kappa (T^K_\kappa)_{m_1 m_2'} (T^K_{-\kappa})_{m_2 m_1'}, \quad (2)$$

Here the 2×3 matrix specifies the Wigner $6j$ symbol and T^K_κ are irreducible spherical tensor operators acting in the spaces with angular momenta f_1 and f_2, respectively; $|f_1 - f_2| \le F \le f_1 + f_2$ is the total angular momentum of interacting atoms; $U^F_{12}(\mathbf{x}-\mathbf{x}')$ is the interaction amplitude of two atoms in the channel characterized by F.

GAS OF ATOMS IN EQUAL INTERNAL STATE, $f_1 = f_2$ AND $\lambda_1 = \lambda_2$

For s-wave scattering, the general interaction functions derived above reproduce the well-known results for atoms with equal total angular momenta.

Fermionic gas of atoms with $f_1 = f_2 = 1/2$

$$\Phi^{\rm Proj}_{v_1 v_2 v_1' v_2'}(\mathbf{x}-\mathbf{x}') = U^0_{1/2,1/2}(\mathbf{x}-\mathbf{x}') \delta_{v_1 v_1'} \delta_{v_2 v_2'}.$$

Thus, upon substituting the obtained result into Hamiltonian, one finds that only atoms with opposite spin projections participate in the scattering process.

Bosonic gas of atoms with $f_1 = f_2 = 1$

Introducing the spherical components of the total angular momentum operator, $f_0 = f_z$,, $f_\pm = \mp\frac{1}{\sqrt{2}}(f_x \pm i f_y)$, where f_x, f_y and f_z are its Cartesian components, we can represent the corresponding interaction function in familiar form

$$\Phi^{\rm Proj}_{n_1 n_2 n_1' n_2'}(\mathbf{x}-\mathbf{x}') = \left(\frac{1}{3} U^0_{1,1}(\mathbf{x}-\mathbf{x}') + \frac{2}{3} U^2_{1,1}(\mathbf{x}-\mathbf{x}') \right) \delta_{n_1 n_1'} \delta_{n_2 n_2'} + \left(\frac{1}{3} U^2_{1,1}(\mathbf{x}-\mathbf{x}') - \frac{1}{3} U^0_{1,1}(\mathbf{x}-\mathbf{x}') \right) \mathbf{f}_{n_1 n_1'} \mathbf{f}_{n_2 n_2'}.$$

Rem. Comparing Eqs. (1) and (2), we find that the two functions have identical forms up to a permutation of the last two indices, $m_1' \leftrightarrow m_2'$. Therefore, it is sufficient to determine the explicit form of only one of them. For definiteness, we choose the function $\Phi^{Proj}_{m_1 m_2 m_1' m_2'}(\mathbf{x}-\mathbf{x}')$.

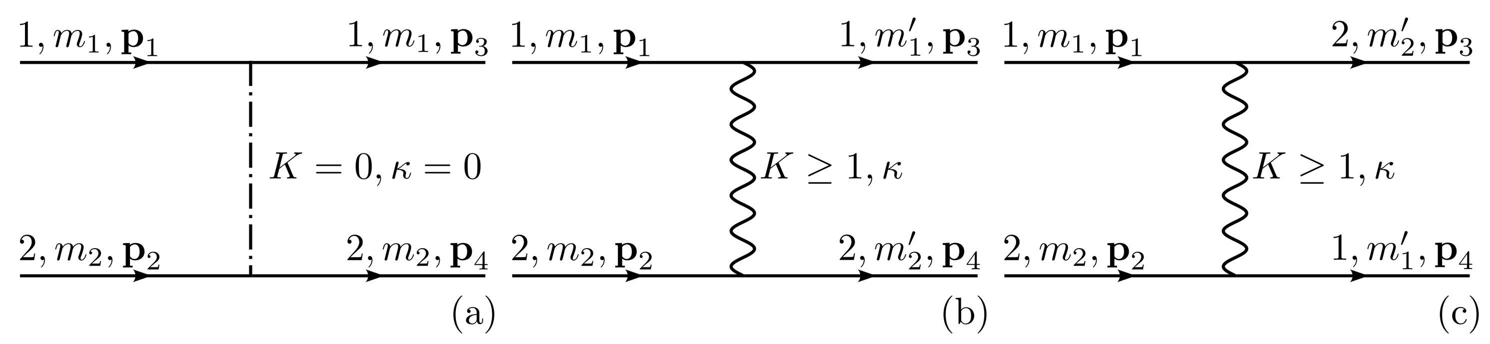

Fig. 1: Feynman diagrams of the interaction terms in the Hamiltonian, represented as an effective exchange of: (a) a virtual scalar particle, (b) a virtual photon without total angular momentum transfer, and (c) a virtual photon with total angular momentum transfer.

MIXTURE OF ATOMS IN DIFFERENT INTERNAL STATES $f_1 \neq f_2$

Bosonic mixture of atoms with $f_1 = 0,\ f_2 = 1$

$$\Phi^{\rm Proj}_{m_1 n_2 m_1' n_2'}(\mathbf{x}-\mathbf{x}') = \sqrt{3} U^1_{01}(\mathbf{x}-\mathbf{x}') (T^0_0)_{m_1 m_1'} (T^0_0)_{n_2 n_2'},$$
$$\Phi^{\rm Mom}_{m_1 n_2 n_2' m_1'}(\mathbf{x}-\mathbf{x}') = -U^1_{01}(\mathbf{x}-\mathbf{x}') \sum_\kappa (-1)^\kappa (T^1_\kappa)_{m_1 n_2'} (T^1_{-\kappa})_{n_2 m_1'}, \quad (3)$$

The spherical tensor operators appearing in Eq. (3) have the *rectangular* form

$$(T^1_{-1})_{m_1 n_2'} = \begin{pmatrix} 1 & 0 & 0 \end{pmatrix}, \quad (T^1_0)_{m_1 n_2'} = \begin{pmatrix} 0 & -1 & 0 \end{pmatrix}, \quad (T^1_1)_{m_1 n_2'} = \begin{pmatrix} 0 & 0 & 1 \end{pmatrix},$$
$$(T^1_{-1})_{n_2 m_1'} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad (T^1_0)_{n_2 m_1'} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad (T^1_1)_{n_2 m_1'} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}.$$

Fermionic mixture of atoms with $f_1 = 1/2,\ f_2 = 3/2$

$$\Phi^{\rm Proj}_{v_1 w_2 v_1' w_2'}(\mathbf{x}-\mathbf{x}') = \left(\frac{3}{2\sqrt{2}} U^1_{1/2,3/2}(\mathbf{x}-\mathbf{x}') + \frac{5}{2\sqrt{2}} U^2_{1/2,3/2}(\mathbf{x}-\mathbf{x}') \right) (T^0_0)_{v_1 v_1'} (T^0_0)_{w_2 w_2'}$$
$$+ \left(-\frac{5}{2\sqrt{10}} U^1_{1/2,3/2}(\mathbf{x}-\mathbf{x}') + \frac{5}{2\sqrt{10}} U^2_{1/2,3/2}(\mathbf{x}-\mathbf{x}') \right) \sum_\kappa (-1)^\kappa (T^1_\kappa)_{v_1 v_1'} (T^1_{-\kappa})_{w_2 w_2'},$$
$$\Phi^{\rm Mom}_{v_1 w_2 w_2' v_1'}(\mathbf{x}-\mathbf{x}') = \left(-\frac{1}{4} U^1_{1/2,3/2}(\mathbf{x}-\mathbf{x}') - \frac{5}{4} U^2_{1/2,3/2}(\mathbf{x}-\mathbf{x}') \right) \sum_\kappa (-1)^\kappa (T^1_\kappa)_{v_1 w_2'} (T^1_{-\kappa})_{w_2 v_1'}$$
$$+ \left(\frac{3}{4} U^1_{1/2,3/2}(\mathbf{x}-\mathbf{x}') - \frac{1}{4} U^2_{1/2,3/2}(\mathbf{x}-\mathbf{x}') \right) \sum_\kappa (-1)^\kappa (T^2_\kappa)_{v_1 w_2'} (T^2_{-\kappa})_{w_2 v_1'}. \quad (4)$$

Just as for the bosonic case, the interaction with momentum exchange is described by *rectangular* matrices:

$$(T^1_0)_{v_1 w_2'} = \begin{pmatrix} 0 & -\frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & -\frac{1}{\sqrt{2}} & 0 \end{pmatrix}, \quad (T^1_{-1})_{v_1 w_2'} = \begin{pmatrix} \frac{\sqrt{3}}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \end{pmatrix}, \quad (T^1_1)_{v_1 w_2'} = \begin{pmatrix} 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{3}}{2} \end{pmatrix},$$
$$(T^1_0)_{w_2 v_1'} = \begin{pmatrix} 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 \end{pmatrix}, \quad (T^1_{-1})_{w_2 v_1'} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ \frac{1}{2} & 0 \\ 0 & \frac{\sqrt{3}}{2} \end{pmatrix}, \quad (T^1_1)_{w_2 v_1'} = \begin{pmatrix} \frac{\sqrt{3}}{2} & 0 \\ 0 & \frac{1}{2} \\ 0 & 0 \\ 0 & 0 \end{pmatrix}.$$

CONCLUSION

- We propose a general method for constructing the many-body Hamiltonian of pairwise interactions in homonuclear mixtures of atoms occupying states with different values of the total angular momentum and other quantum numbers.
- Our approach is based on the formalism of spherical tensor operators, which provides the Hamiltonian with a transparent physical structure, naturally incorporates all scattering channels, and allows one to include all multipolar exchange interactions. The latter describe both the exchange of angular-momentum projections and the exchange of the angular momenta themselves.
- The obtained results for the interaction functions written in terms of tensor operators admit a clear physical interpretation. The exchange interaction can be viewed as an effective exchange mediated by a virtual particle (see Fig. 1). The rank K of the tensor operator determines the total angular momentum of the exchanged particle, while its component κ specifies the corresponding projection. The transfer of angular momentum or its projection by a virtual particle is, in general, a natural concept within quantum electrodynamics.
- We demonstrate the generality of the prososed Hamiltonian for ultracold gases with both equal and unequal total angular momenta. The latter case corresponds to the ground and the longest-lived metastable states of ^{4}He and ^{3}He atoms.
- The resulting Hamiltonian provides a convenient and universal framework for theoretical studies of a wide range of quantum many-body phenomena in bosonic and fermionic high-spin atomic gases, where multipolar exchange induced by angular momentum plays an essential role.

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