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The 2- and 3-body wave-function factorization with a 2-body potential

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The 4'th workshop on SRCs and EMC effect in Paris-Saclay

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Generalized contact formalism

The 2-body short range correlations (SRCs) are successfully described by the generalized contact formalism (GCF)[1]

The GCF is based on the factorization ansatz

$$\lim_{r_{ij}\to 0} \quad = \sum_{c} \varphi^{c}_{ij}(\boldsymbol{r}_{ij})\, A^{c}_{ij}\left(\boldsymbol{R}^{\text{C.M.}}_{ij}, \{\boldsymbol{r}_k\}_{k\neq i,j}\right) \qquad ij \in \{pp, np, nn\}$$

- φ is a universal *zero-energy* two-body wave-function and obeys $\hat{H}\varphi = 0$
- A is the regular part, the "wave-function" of rest of the spectators

[1] Ronen Weiss, Betzalel Bazak, and Nir Barnea. In: *Phys. Rev.* C92.5 (2015).

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The contact is defined by $C^{cc'}_{ij} = \frac{N_{ij}}{2J+1} \sum_m \langle A^{c}_{ij} | A^{c'}_{ij} \rangle$

[1] Ronen Weiss, Betzalel Bazak, and Nir Barnea. In: *Phys. Rev.* C92.5 (2015).

Research goals & motivation

Present a systematic approach for:

- The factorization ansatz
- Higher-body SRCs
- Derive the universal function $'$
- Calculation of the contacts

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To achieve these goals we use the coupled-cluster (CC) method

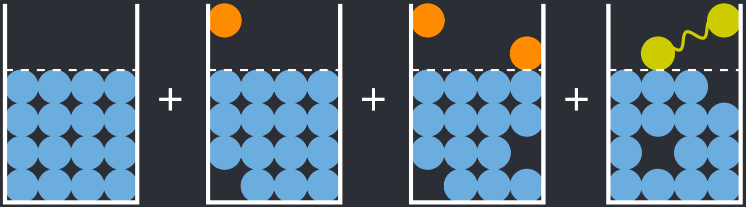
The CC method describes correlations naturally

Coupled cluster[2]

The wave-function is expanded in **clusters**

$$= e^{\hat{T}} \qquad \hat{T} = \hat{T}_1 + \hat{T}_2 + \hat{T}_3 +$$

$\hat{T}_n$ operator excites n particles from the Slater determinant

$j \quad i =$ 

$j \quad i \qquad \hat{T}_1 j \quad i \qquad \hat{T}_1 \hat{T}_1 j \quad i \qquad \hat{T}_2 j \quad i$

[2] Rodney J. Bartlett and Monika Musiał. In: *Rev. Mod. Phys.* 79 (1 2007).

A bit of notations

From now on

- The subscripts $i; j; k; l$ and the momentum $\boldsymbol{k}$ will denote a *hole state* $(k \quad k_f)$ which is contained in $j \quad i$
- The superscripts $a; b; c; d; e$ and the momentum $\boldsymbol{p}$ will denote a *particle state* $(p > k_f)$ which is an excitation from $j \quad i$
- $\hat{T}_1 = 0$ due to momentum conservation
- $\sum_i \boldsymbol{p}_i \quad \mathbf{0}$ for the pair or triplet

The wave-function in coupled cluster

The cluster operator is

$$\hat{T}_n = \frac{1}{(n!)^2} \sum_{ab \quad ;ij} t_{ij}^{ab} \quad \hat{a}^\dagger \hat{b}^\dagger \quad \hat{j}\hat{i}$$

and t_{ij}^{ab} is the corresponding cluster amplitude

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Define

$$\big|{}_{ij}^{ab}\big\rangle \quad \hat{a}^{\dagger}\hat{b}^{\dagger} \quad \hat{j}\hat{i} \, | \quad \rangle$$

Then, is written as ($= e^{\hat{T}} \ = \ \left[1 + \hat{T} + \quad \right]$)

$$| \ \rangle = | \ \rangle + \sum t_{ij}^{ab} \ \big|{}_{ij}^{ab}\big\rangle + \sum t_{ijk}^{abc} \ \big|{}_{ijk}^{abc}\big\rangle + \frac{1}{2} \sum t_{ij}^{ab} t_{kl}^{cd} \ \big|{}_{ijkl}^{abcd}\big\rangle +$$

Coupled cluster as a natural formalism to factorization

Consider $_A(\boldsymbol{p}_a\boldsymbol{p}_b\boldsymbol{k}_k)$, there are only 2 excited particles and therefore only $\hat{T}_2$ will contribute ($= e^{\hat{T}} = 1 + \hat{T} + $)

$$_A(\boldsymbol{p}_a\boldsymbol{p}_b\boldsymbol{k}_k) = (t_A)^{ab}_{ij} \; _A(\boldsymbol{k}_i\boldsymbol{k}_j\boldsymbol{k}_k)$$

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If $(t_A)^{ab}_{ij} \ / \ (t_A)^{ab}_{00}$, then we would get factorization

Let $\ _2(\boldsymbol{p}_a\boldsymbol{p}_b) = (t_2)^{ab}_{ij} \ _2(\boldsymbol{k}_i\boldsymbol{k}_j)$,

if $(t_A)^{ab}_{ij} \ / \ (t_2)^{ab}_{ij} \ / \ (t^{\ 1})^{ab}_{00}$ then

$$_A(\boldsymbol{p}_a\boldsymbol{p}_b\boldsymbol{k}_k \quad) \ / \quad _2(\boldsymbol{p}_a\boldsymbol{p}_b)$$

The complete 2- and 3-body CC equations

2-body:

$$0 = \Big\langle {}^{ab}_{ij} \Big| \hat{V} + [\hat{H}_0; \hat{T}_2] + [\hat{V}; \hat{T}_2] + \frac{1}{2}[[\hat{V}; \hat{T}_2]; \hat{T}_2] + [\hat{V}; \hat{T}_3] + [\hat{V}; \hat{T}_4] \Big| \Big\rangle$$

3-body:

$$0 = \Big\langle {}^{abc}_{ijk} \Big| [\hat{H}_0; \hat{T}_3] + [\hat{V}; \hat{T}_2] + \frac{1}{2}[[\hat{V}; \hat{T}_2]; \hat{T}_2] + [\hat{V}; \hat{T}_3] + [[\hat{V}; \hat{T}_2]; \hat{T}_3] + [\hat{V}; \hat{T}_4] + [\hat{V}; \hat{T}_5] \Big| \Big\rangle$$

The equations are coupled and non-linear

High-momentum approximations

The approximations follow after 2 principals

- can be normalized, hence $\hat{t}_n \; ! \;\; 0$ for high energy excitations
- Momentum conservation, e.g. $t_{ij}^{ab} \; / \;\; ^3(p_a + p_b \;\; k_i \;\; k_j)$

High-momentum approximations

The approximations follow after 2 principals

- can be normalized, hence $\hat{t}_n \to 0$ for high energy excitations
- Momentum conservation, e.g. $t_{ij}^{ab} / \;{}^3(p_a + p_b \;\; k_i \;\; k_j)$

$$0 = \left\langle {}^{ab}_{ij} \right| \hat{V} + [\hat{H}_0; \hat{T}_2] + [\hat{V}; \hat{T}_2] + \frac{1}{2}[[\hat{V}; \hat{T}_2]; \hat{T}_2] + [\hat{V}; \hat{T}_3] + [\hat{V}; \hat{T}_4] \left| \;\; \right\rangle$$

The e ects on the 2-body eq. ($p_a \;\; k_f$; $E_{ij}^{ab} \;\; E_a + E_b \;\; E_i \;\; E_j$)

$E_{ij}^{ab} t_{ij}^{ab} \quad V_{id}^{ak} t_{jk}^{bd} \quad \Rightarrow \quad [\hat{V}; \hat{T}_2] \to \frac{1}{2} V_{de}^{ab} t_{ij}^{de}$

$E_{ij}^{ab} t_{ij}^{ab} \quad V_{de}^{kl} t_{jl}^{de} t_{ik}^{ab} \quad \Rightarrow \quad [\hat{H}_0; \hat{T}_2] \quad \frac{1}{2}[[\hat{V}; \hat{T}_2]; \hat{T}_2]$

$t_{ikl}^{abd}; t_{ijkl}^{abde} \quad t_{00}^{ab} \quad \Rightarrow \quad [\hat{H}_0; \hat{T}_2] \quad [\hat{V}; \hat{T}_3]; \; [\hat{V}; \hat{T}_4]$

$E^{ab} \quad E^{ij} \quad \Rightarrow \quad E_{ij}^{ab} \to E^{ab}$

Solution of the asymptotic eq.

2-body:

$$0 = \langle \Phi_{ij}^{ab} | \hat{V} + [\hat{H}_0, \hat{T}_2] + [\hat{V}, \hat{T}_2] + \frac{1}{2}[[\hat{V}, \hat{T}_2], \hat{T}_2] + [\hat{V}, \hat{T}_3] + [\hat{V}, \hat{T}_4] | \Phi \rangle$$

$$0 = E^{ab} t_{ij}^{ab} + V_{ij}^{ab} + \frac{1}{2} V_{de}^{ab} t_{ij}^{de}$$

In the CC jargon the equation is called

"The particle-particle ladder approximation"

Solution of the asymptotic eq.

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$$0 = E^{ab} t_{ij}^{ab} + V_{ij}^{ab} + \frac{1}{2} V_{de}^{ab} t_{ij}^{de}$$

The solution, $\hat{T}_2^1$, of the asymptotic equation takes the form

$$\hat{T}_2^1 = \frac{1}{1 - \hat{Q}_2 \hat{G}_0 \hat{V}} \hat{Q}_2 \hat{G}_0 \hat{V} \hat{P}_2 \qquad (t^1)_{ij}^{ab} \quad t_{ij}^{ab}$$

$\hat{G}_0$ is the zero-energy Green's function $\hat{G}_0 = \frac{1}{\epsilon - \hat{H}_0}$

$\hat{Q}$ is the projection operator into the particle subspace

$\hat{P}$ is the projection operator into the hole subspace

Relation to the zero-energy Schrödinger equation

2-body:

The $\hat{T}_2^{-1}$ is the Bloch-Horowitz operator in disguise![3]

$$\hat{T}_2^{-1} = \frac{1}{\hat{Q}_2(0 + i\epsilon - \hat{H})\hat{Q}_2}\hat{Q}_2\hat{H}\hat{P}_2$$

i.e.

$$\hat{Q}_2 |\psi_2\rangle = \hat{T}_2^{-1} |\psi_2\rangle \quad \Leftrightarrow \quad \hat{H} |\psi_2\rangle = 0$$

[3] Claude Bloch and Jules Horowitz. In: Nuclear Physics 8 (1958).

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The $\hat{T}_2^{1}$ is the Bloch-Horowitz operator in disguise![3]

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i.e.

$$\hat{Q}_2 |\;_2\rangle = \hat{T}_2^{1} \; |\;_2\rangle \qquad\qquad \hat{H} |\;_2\rangle = 0$$

Implications at high energies:

- $\hat{T}_2$ is related to $|\;_2\rangle$
- $\hat{T}_2$ depends only on the potential - universality

[3] Claude Bloch and Jules Horowitz. In: Nuclear Physics 8 (1958).

Relation to the zero-energy Schrödinger equat

3-body:

The asymptotic equation is

$$0 = E^{abc} t^{abc}_{ijk} + V^{ab}_{id} t^{dc}_{jk} + \frac{1}{2} V^{ab}_{de} t^{cde}_{ijk} + \text{permutations}$$

The solution of the asymptotic equation is

$$\hat{T}^1_3 = \frac{1}{1 \quad \hat{Q}_3 \hat{G}_0 \hat{V}} \hat{Q}_3 \hat{G}_0 \hat{V} \hat{T}^1_2 \hat{P}_3 \qquad (t^1)^{abc}_{ijk} \qquad t^{abc}_{ijk}$$

The 3-body relation to $|\;_3\rangle$ is more complicated but $\hat{T}^1_3$ admits*

$$\hat{T}^1_3 |\;_3\rangle \qquad \hat{Q}_3 |\;_3\rangle \qquad \hat{H} |\;_3\rangle = 0 \qquad \hat{P}_3 |\;_3\rangle = |\;_3\rangle$$

*For $k_F \to 0$; k_F large and any k_F when considering the asymptotic high-momentum contribution

The requirement for factorization

Recall that

$$(\; p_a p_b k_k \quad) = t_{ij}^{ab} \; (\; k_i k_j k_k \quad)$$

For factorization to occur we must demand:

$$t_{ij}^{ab} \; / \;\; (t^{1} \;)_{00}^{ab}$$

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This must be seen as a demand on the potential! i.e.

Not all potentials admit wave-function factorization!

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Not all potentials admit wave-function factorization!

The simplest counter example is a Gaussian potential (e.g. EFT) for which

$$(t^{1})^{ab}_{ij} \; ! \quad \frac{V^{ab}_{ij}}{E^{ab}} \; / \quad \frac{e^{\;R^2 \;\; p_a^2 \;\; 2p_a k_i + k_j^2}}{E^{ab}} \; / \; (t^{1})^{ab}_{00} \, e^{2R^2 p_a k_i}$$

Factorization with AV18 potential[4]

For AV18, $(t^{1})^{ab}_{ij} / (t^{1})^{ab}_{00}$ already from $2{:}5\ \mathrm{fm}^{1}$

[4] R. B. Wiringa, V. G. J. Stoks, and R. Schiavilla. In: Phys. Rev. C 51 (1 1995).

Invert the relation, get $\hat{f}_2$ in terms of $_2$

To get the factorization in terms of $_2$, the relation

$$_2(p_a p_b) = \langle p_a p_b | \hat{f}_2^{1} | _2 \rangle \propto \sum_{ij} \langle p_a p_b | \hat{f}_2^{1} | 0_i 0_j \rangle \, _2(k_i k_j)$$

must be inverted.

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To get the factorization in terms of $_2$, the relation

$$_2(p_a p_b) = \langle p_a p_b | \hat{f}_2^{1} | \;_2 \rangle / \sum_{ij} \langle p_a p_b | \hat{f}_2^{1} | 0_i 0_j \rangle \;_2(k_i k_j)$$

must be inverted.

This can be done by considering all channels of $_2$ and then

$$\langle p_a p_b | \hat{f}_2^{1} | 00 \rangle = \sum c \;_2(p_a p_b)$$

Invert the relation, get $\hat{T}_2$ in terms of $_2$

To get the factorization in terms of $_2$, the relation

$$_2(p_a p_b) = \langle p_a p_b | \hat{T}_2^{1} | \;_2\rangle \propto \sum_{ij} \langle p_a p_b | \hat{T}_2^{1} | 0_i 0_j \rangle \;_2(k_i k_j)$$

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$$\langle p_a p_b | \hat{T}_2^{1} | 00 \rangle = \sum c \;_2(p_a p_b)$$

Thus

$$_A(p_a p_b k_k \quad) \sum \;_2(p_a p_b) A_2 (k_k \quad)$$

The contacts: $C_n = \frac{n}{2} A_n A_n$

The regular functions and hence the contacts can be calculated from first principles

$$C_n = X$$

Factorization

The contacts: $C_n = \frac{n}{2} \; A_n \; A_n$

The regular functions and hence the contacts can be calculated from first principles

$$C_n = X$$

The contacts at *"zeroth-order approximation"* are as expected

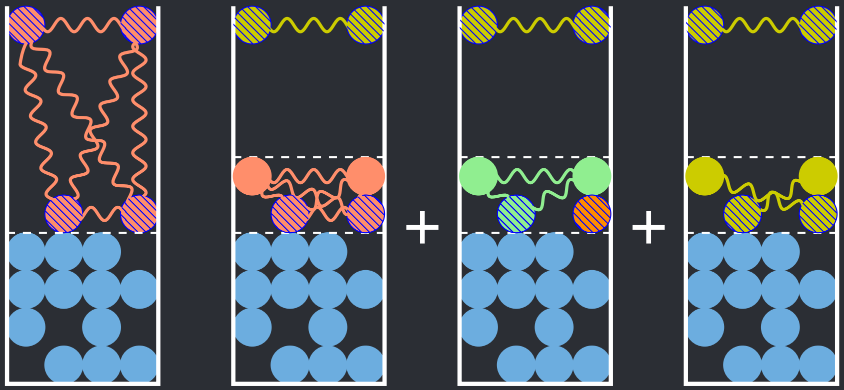
$$C_2 \quad \frac{n}{2} \; X \; c \; c \; Z \; \frac{k_3 \; k_A}{k_1^0 k_2^0 k_1^{00} k_2^{00}} \; A \; k_1^0 k_2^0 k_3 \quad A \; k_1^{00} k_2^{00} k_3$$

Summary

- Used the CC method to obtain the equations governing 2,3-body SRCs
- The relation to the zero-energy Schrödinger equation has been shown
- The AV18 potential admits factorization already from 2.5 fm^{1}
- Computation of the regular functions and the contacts can be done from first principals


THE
END

Decomposition of the cluster amplitudes



The factorization is true even if $k_j > k_F$

The recipe for obtaining the CC equations

1. Define $j \quad i \quad e^{\hat{T}^{y}} \quad {}_{ij}^{ab} \quad \mathrm{E}$ which is orthogonal to

$$h \quad j \quad i = \mathrm{D} \quad {}_{ij}^{ab} \quad e^{\hat{T}} e^{\hat{T}} \, j \quad i = \mathrm{D} \quad {}_{ij}^{ab} \quad \mathrm{E} = 0$$

The recipe for obtaining the CC equations

1. Define $\left|\ \right\rangle \ e^{\hat{T}^{\dagger}} \left|{}^{ab}_{ij}\right\rangle$ which is orthogonal to

$$\left\langle\ \middle|\ \right\rangle = \left\langle{}^{ab}_{ij}\right| e^{\hat{T}} e^{\hat{T}} \left|\ \right\rangle = \left\langle{}^{ab}_{ij}\ \middle|\ \right\rangle = 0$$

2. For any $\hat{H}\left|\ \right\rangle = E\left|\ \right\rangle$

$$0 = E\left\langle\ \middle|\ \right\rangle = \left\langle{}^{ab}_{ij}\right| e^{\hat{T}} \hat{H} e^{\hat{T}} \left|\ \right\rangle$$

The recipe for obtaining the CC equations

1. Define $|\tilde{\Psi}\rangle = e^{-\hat{T}^{\dagger}}|\Phi_{ij}^{ab}\rangle$ which is orthogonal to

$$\langle\tilde{\Psi}|\Psi\rangle = \langle\Phi_{ij}^{ab}|e^{-\hat{T}}e^{\hat{T}}|\Phi_0\rangle = \langle\Phi_{ij}^{ab}|\Phi_0\rangle = 0$$

2. For any $\hat{H}|\Psi\rangle = E|\Psi\rangle$

$$0 = E\langle\tilde{\Psi}|\Psi\rangle = \langle\Phi_{ij}^{ab}|e^{-\hat{T}}\hat{H}e^{\hat{T}}|\Phi_0\rangle$$

3. Use Baker-Campbell-Hausdorff formula ($\hat{H}$ is a 2-body operator)

$$0 = \langle\Phi_{ij}^{ab}|\hat{H} + [\hat{H},\hat{T}] + \frac{1}{2!}[[\hat{H},\hat{T}],\hat{T}] + \frac{1}{3!}[[[\hat{H},\hat{T}],\hat{T}],\hat{T}] + \frac{1}{4!}[[[[\hat{H},\hat{T}],\hat{T}],\hat{T}],\hat{T}]|\Phi_0\rangle$$

Factorization in a zero-range theory

For zero-range theory

$$R \;!\; 0 \qquad\qquad R \qquad p^{\;1}$$

R is the range of the interaction

p is the momentum transfer

Factorization in a zero-range theory

For zero-range theory

$$R \to 0 \qquad\qquad R \sim p^{-1}$$

R is the range of the interaction

p is the momentum transfer

In this limit

$$(t^{-1})^{ab}_{ij} \propto (t^{-1})^{ab}_{00}\, e^{2R^2 \mathbf{p}_a \mathbf{k}_i} \to (t^{-1})^{ab}_{00}$$

and factorization occurs

Generalized contact formalism - example[5]

$$\lim_{k \to \infty} n_p(k) = C^d_{pn} \left|\varphi^d_{pn}(k)\right|^2 + C^0_{pn} \left|\varphi^0_{pn}(k)\right|^2 + C^0_{pp} \left|\varphi^0_{pp}(k)\right|^2$$

The contacts were derived from the 2-body momentum distribution

$$\lim_{k \to \infty} n_{pn}(k_{\text{rel}}) = C^d_{pn} \left|\varphi^d_{pn}(k_{\text{rel}})\right|^2 + C^0_{pn} \left|\varphi^0_{pn}(k_{\text{rel}})\right|^2$$

$$\lim_{k \to \infty} n_{pp}(k_{\text{rel}}) = C^0_{pp} \left|\varphi^0_{pp}(k_{\text{rel}})\right|^2$$