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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

February 1, 2023

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

$$\lim_{\boldsymbol{r}_{ij}\to 0} \Psi = \sum_c \varphi_{ij}^c(\boldsymbol{r}_{ij}) A_{ij}^c\left(\boldsymbol{R}_{ij}^{\text{C.M.}}, \{\boldsymbol{r}_k\}_{k\neq i,j}\right) \qquad ij \in pp,\ np,\ nn$$

- 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

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The contact is defined by $C_{ij}^{cc'} = \frac{N_{ij}}{2J+1}\sum_m \left\langle A_{ij}^c \middle| A_{ij}^{c'} \right\rangle$

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Research goals & motivation

Present a systematic approach for:

- The factorization ansatz
- Higher-body SRCs
- Derive the universal function φ
- 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

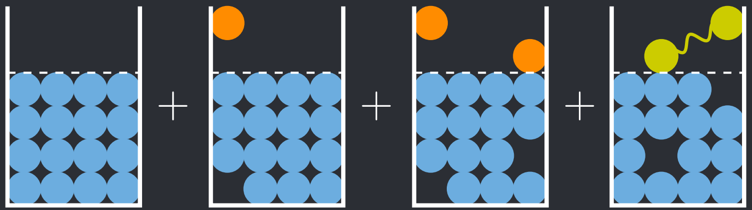
Coupled cluster[2]

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

$$\Psi = e^{\hat{\boldsymbol{T}}}\Phi \qquad \hat{\boldsymbol{T}} = \hat{T}_1 + \hat{T}_2 + \hat{T}_3 + \cdots$$

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

$|\Psi\rangle =$



$\cdots$

$$|\Phi\rangle \qquad \hat{T}_1 |\Phi\rangle \qquad \hat{T}_1 \hat{T}_1 |\Phi\rangle \qquad \hat{T}_2 |\Phi\rangle$$

[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* $(k \leq k_f)$ which is contained in $|\Phi\rangle$
- 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 $|\Phi\rangle$
- $\hat{T}_1 = 0$ due to momentum conservation
- $\sum_i \boldsymbol{p}_i \approx \mathbf{0}$ for the pair or triplet

The wave-function in coupled cluster

The cluster operator is

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

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Define

$$\left|\Phi_{ij\cdots}^{ab\cdots}\right\rangle \equiv \hat{\boldsymbol{a}}^\dagger \hat{\boldsymbol{b}}^\dagger \cdots \hat{\boldsymbol{j}} \hat{\boldsymbol{i}} \left|\Phi\right\rangle$$

Then, Ψ is written as ($\Psi = e^{\hat{\boldsymbol{T}}} \Phi = \left[1 + \hat{\boldsymbol{T}} + \cdots\right] \Phi$)

$$|\Psi\rangle = |\Phi\rangle + \sum t_{ij}^{ab} \left|\Phi_{ij}^{ab}\right\rangle + \sum t_{ijk}^{abc} \left|\Phi_{ijk}^{abc}\right\rangle + \frac{1}{2} \sum t_{ij}^{ab} t_{kl}^{cd} \left|\Phi_{ijkl}^{abcd}\right\rangle + \cdots$$

Coupled cluster as a natural formalism to factorization

Consider $\Psi_A\left(\boldsymbol{p}_a\boldsymbol{p}_b\boldsymbol{k}_k\cdots\right)$, there are only 2 excited particles and therefore only $\hat{T}_2$ will contribute ($\Psi = e^{\hat{\boldsymbol{T}}}\Phi = \left[1 + \hat{\boldsymbol{T}} + \cdots\right]\Phi$)

$$\Psi_A\left(\boldsymbol{p}_a\boldsymbol{p}_b\boldsymbol{k}_k\cdots\right) = \left(t_A\right)_{ij}^{ab}\Phi_A\left(\boldsymbol{k}_i\boldsymbol{k}_j\boldsymbol{k}_k\cdots\right)$$

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- If $(t_A)_{ij}^{ab} \propto (t_A)_{00}^{ab}$, then we would get factorization
- Let $\Psi_2\left(\boldsymbol{p}_a\boldsymbol{p}_b\right) = (t_2)_{ij}^{ab}\,\Phi_2\left(\boldsymbol{k}_i\boldsymbol{k}_j\right)$,

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

$$\Psi_A\left(\boldsymbol{p}_a\boldsymbol{p}_b\boldsymbol{k}_k\cdots\right) \propto \Psi_2\left(\boldsymbol{p}_a\boldsymbol{p}_b\right)$$

The complete 2- and 3-body CC equations

2-body:

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

3-body:

$$0 = \left\langle \Phi_{ijk}^{abc} \middle| [\hat{H}_0, \hat{T}_3] + [\hat{V}, \hat{T}_2] + \frac{1}{2}[[\hat{V}, \hat{T}_2], \hat{T}_2] + [\hat{V}, \hat{T}_3] + [[\hat{V}, \hat{T}_2], \hat{T}_3] + [\hat{V}, \hat{T}_4] + [\hat{V}, \hat{T}_5] \middle| \Phi \right\rangle$$

The equations are coupled and non-linear

High-momentum approximations

The approximations follow after 2 principals

- Ψ can be normalized, hence $\hat{T}_n \to 0$ for high energy excitations
- Momentum conservation, e.g. $t_{ij}^{ab} \propto \delta^3\left(\boldsymbol{p}_a + \boldsymbol{p}_b - \boldsymbol{k}_i - \boldsymbol{k}_j\right)$

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

The effects on the 2-body eq. $(p_a \gg k_\text{f},\ E_{ij}^{ab} \equiv E_a + E_b - E_i - E_j)$

- $E_{ij}^{ab} t_{ij}^{ab} \gg V_{id}^{ak} t_{jk}^{bd} \quad \Rightarrow \quad [\hat{V}, \hat{T}_2] \to \frac{1}{2} V_{de}^{ab} t_{ij}^{de}$
- $E_{ij}^{ab} t_{ij}^{ab} \gg V_{de}^{kl} t_{jl}^{de} t_{ik}^{ab} \quad \Rightarrow \quad [\hat{H}_0, \hat{T}_2] \gg \frac{1}{2}[[\hat{V}, \hat{T}_2], \hat{T}_2]$
- $t_{ikl}^{abd}, t_{ijkl}^{abde} \approx t_{00}^{ab} \quad \Rightarrow \quad [\hat{H}_0, \hat{T}_2] \gg [\hat{V}, \hat{T}_3],\ [\hat{V}, \hat{T}_4]$
- $E^{ab} \gg E^{ij} \quad \Rightarrow \quad E_{ij}^{ab} \to E^{ab}$

Solution of the asymptotic eq.

2-body:

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

$$\downarrow$$

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

In the CC jargon the equation is called

"The particle-particle ladder approximation"

Solution of the asymptotic eq.

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$$\downarrow$$

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

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

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

- $\hat{G}_0$ is the zero-energy Green's function $\hat{G}_0 = \frac{1}{i\varepsilon - \hat{H}_0}$
- $\hat{Q}$ 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 $\hat{T}_2^\infty$ is the Bloch-Horowitz operator in disguise![3]

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

i.e.

$$\hat{Q}_2 \left|\Psi_2\right\rangle = \hat{T}_2^\infty \left|\Psi_2\right\rangle \qquad\qquad \hat{H}\left|\Psi_2\right\rangle = 0$$

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

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Implications at high energies:

- $\hat{T}_2$ is related to $\left|\Psi_2\right\rangle$
- $\hat{T}_2$ depends only on the potential - **universality**

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

Relation to the zero-energy Schrödinger equation

3-body:

The asymptotic equation is

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

The solution of the asymptotic equation is

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

The 3-body relation to $|\Psi_3\rangle$ is more complicated but $\hat{T}_3^{\infty}$ admits *

$$\hat{T}_3^{\infty} |\alpha_3\rangle \approx \hat{Q}_3 |\Psi_3\rangle \qquad \hat{H} |\Psi_3\rangle = 0 \qquad \hat{P}_3 |\alpha_3\rangle = |\alpha_3\rangle$$

*For $k_\mathrm{F} \to 0, k_\mathrm{F}$ large and any k_F when considering the asymptotic high-momentum contribution

The requirement for factorization

Recall that

$$\Psi\left(\boldsymbol{p}_a \boldsymbol{p}_b \boldsymbol{k}_k \cdots\right) = t_{ij}^{ab} \Phi\left(\boldsymbol{k}_i \boldsymbol{k}_j \boldsymbol{k}_k \cdots\right)$$

For factorization to occur we must demand:

$$t_{ij}^{ab} \propto \left(t^{\infty}\right)_{00}^{ab}$$

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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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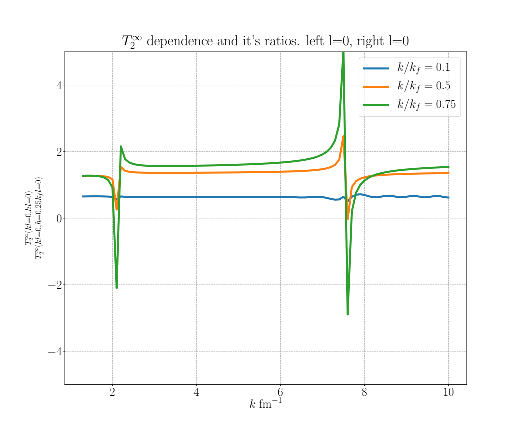
Not all potentials admit wave-function factorization!

The simplest counter example is a Gaussian potential (e.g. $\not\pi$EFT) for which

$$\left(t^{\infty}\right)^{ab}_{ij} \to -\frac{V^{ab}_{ij}}{E^{ab}} \propto -\frac{e^{-R^2\left(p_a^2-2\boldsymbol{p}_a\boldsymbol{k}_i+k_j^2\right)}}{E^{ab}} \propto \left(t^{\infty}\right)^{ab}_{00}\, e^{2R^2\boldsymbol{p}_a\boldsymbol{k}_i}$$

Factorization with AV18 potential[4]



For AV18, $(t^\infty)^{ab}_{ij} \propto (t^\infty)^{ab}_{00}$ **already from** ~ 2.5 **fm**$^{-1}$

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

Invert the relation, get $\hat{T}_2$ in terms of Ψ_2

To get the factorization in terms of Ψ_2, the relation

$$\Psi_2\left(\boldsymbol{p}_a\boldsymbol{p}_b\right) = \langle \boldsymbol{p}_a\boldsymbol{p}_b|\,\hat{T}_2^{\infty}\,|\Psi_2\rangle \propto \sum_{ij} \langle \boldsymbol{p}_a\boldsymbol{p}_b|\,\hat{T}_2^{\infty}\,|\mathbf{0}_i\mathbf{0}_j\rangle\,\Psi_2\left(\boldsymbol{k}_i\boldsymbol{k}_j\right)$$

must be inverted.

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must be inverted.

This can be done by considering all channels of Ψ_2 and then

$$\langle \boldsymbol{p}_a\boldsymbol{p}_b| \, \hat{T}_2^{\infty} \, |\mathbf{00}\rangle = \sum_{\alpha} c_\alpha \Psi_2^{\alpha}\left(\boldsymbol{p}_a\boldsymbol{p}_b\right)$$

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$$\langle\boldsymbol{p}_a\boldsymbol{p}_b|\,\hat{T}_2^{\infty}\,|\boldsymbol{00}\rangle = \sum_{\alpha} c_\alpha\Psi_2^\alpha\left(\boldsymbol{p}_a\boldsymbol{p}_b\right)$$

Thus

$$\Psi_A\left(\boldsymbol{p}_a\boldsymbol{p}_b\boldsymbol{k}_k\cdots\right) \approx \sum_{\alpha}\Psi_2^\alpha\left(\boldsymbol{p}_a\boldsymbol{p}_b\right)\mathcal{A}_2^\alpha\left(\boldsymbol{k}_k\cdots\right)$$

The contacts: $C_n^{\alpha\beta} = \binom{n}{2} \left\langle \mathcal{A}_n^{\alpha} \middle| \mathcal{A}_n^{\beta} \right\rangle$

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

$$C_n^{\alpha\beta} = \cdots \checkmark$$

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

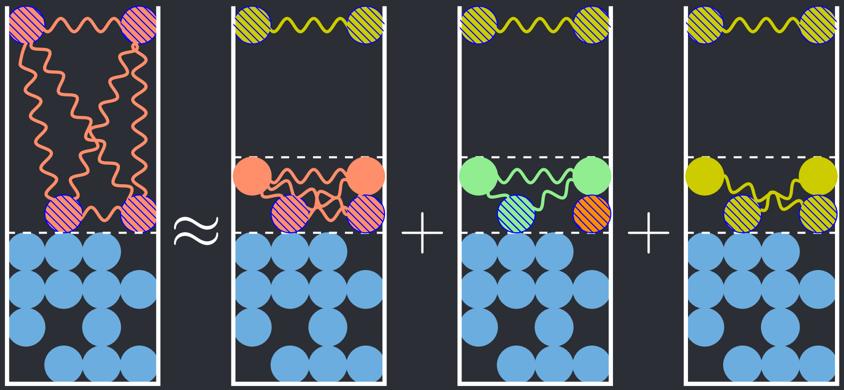
$$C_2^{\alpha\beta} \approx \binom{n}{2} \sum_{\alpha\beta} \bar{c}_\alpha c_\beta \int_{\substack{\boldsymbol{k}_3 \cdots \boldsymbol{k}_A \\ \boldsymbol{k}_1' \boldsymbol{k}_2' \boldsymbol{k}_1'' \boldsymbol{k}_2''}} \bar{\Psi}_A^{\alpha} \left(\boldsymbol{k}_1' \boldsymbol{k}_2' \boldsymbol{k}_3 \cdots \right) \Psi_A^{\beta} \left(\boldsymbol{k}_1'' \boldsymbol{k}_2'' \boldsymbol{k}_3 \cdots \right)$$

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 $\sim 2.5\ \mathrm{fm}^{-1}$
- 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 $|\delta\Psi\rangle \equiv e^{-\hat{T}^{\dagger}} \left|\Phi_{ij\cdots}^{ab\cdots}\right\rangle$ which is orthogonal to Ψ

$$\langle\delta\Psi|\Psi\rangle = \left\langle \phi_{ij\cdots}^{ab\cdots}\right| e^{-\hat{T}} e^{\hat{T}} |\phi\rangle = \left\langle \phi_{ij\cdots}^{ab\cdots}\middle|\phi\right\rangle = 0$$

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

$$0 = E\langle\delta\Psi|\Psi\rangle = \left\langle \Phi_{ij\cdots}^{ab\cdots}\right| e^{-\hat{T}} \hat{H} e^{\hat{T}} \left|\Phi\right\rangle$$

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

$$\begin{aligned} 0 = & \left\langle \Phi_{ij\cdots}^{ab\cdots} \right| \hat{H} + \left[\hat{H}, \hat{T}\right] + \frac{1}{2!}\left[\left[\hat{H}, \hat{T}\right], \hat{T}\right] + \\ & + \frac{1}{3!}\left[\left[\left[\hat{H}, \hat{T}\right], \hat{T}\right], \hat{T}\right] + \frac{1}{4!}\left[\left[\left[\left[\hat{H}, \hat{T}\right], \hat{T}\right], \hat{T}\right], \hat{T}\right] \left|\Phi\right\rangle \end{aligned}$$

Factorization in a zero-range theory

For zero-range theory

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

- R is the range of the interaction
- p is the momentum transfer

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In this limit

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

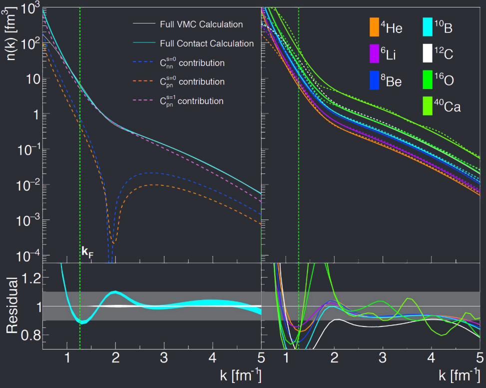
and factorization occurs

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

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



5 R. Weiss et al. In: *Phys. Lett. B* 780 (2018).