Nuclear short-range correlations and the zero-energy eigenstates of the Schrödinger equation

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We present a systematic analysis of the nuclear two- and three-body short-range correlations and their relations to the zero-energy eigenstates of the Schrödinger equation. To this end we analyze the doublet and triplet coupled-cluster amplitudes in the high momentum limit, and show that they obey universal equations independent of the number of nucleons and their state. Furthermore, we find that these coupled-cluster amplitudes coincide with the zero-energy Bloch-Horowitz operator. These results illuminate the relations between the nuclear many-body theory and the generalized contact formalism, introduced to describe the nuclear two-body short range correlations, and they might also be helpful for general coupled-cluster computations as the asymptotic part of the amplitudes is given and shown to be universal.

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I. INTRODUCTION

Nuclear short-range correlations (SRCs) have been studied extensively over the last few decades (see Refs. [1,2] for recent reviews). Large momentum-transfer quasielastic electron and proton scattering reactions are the main experimental tools facilitating these studies [3,4]. In such reactions, interpreted in a high resolution picture, back-to-back SRC nucleon pairs were clearly identified [5–10], with a significant dominance of neutron-proton pairs [9,11–14]. Inclusive reactions where used to study the abundance of such SRC pairs [15–19]. Currently, *ab initio* approaches are unable to directly calculate the cross sections of these reactions, in all but the lightest nuclei. Nevertheless, qualitatively similar conclusions were obtained in structure studies, that focused mainly on the high momentum tail of the nuclear momentum distribution [20–28]. The study of nuclear three-body SRCs, i.e., three nucleons at close proximity, is still very preliminary at this stage [29,30] and their impact on nuclear quantities is still mostly unknown.

Following Tan's work on ultracold atoms [31–34], the generalized contact formalism (GCF) was introduced and utilized to analyze SRC effects in nuclei [35–38]. It is based on the scale separation ansatz, assuming a factorization of the nuclear wave function when two nucleons are close to each other. The GCF provides a framework to study both nuclear structure and nuclear reactions, and was successfully tested against *ab initio* studies, providing a good description of both two-body densities at short distance and high-momentum tails of different momentum distributions [36,39,40]. In addition, the GCF is found to be in good agreement with exclusive electron scattering experiments and other reactions sensitive to SRC pairs [12–14,37,41–45]. As such, the GCF allows for a quantitative comparison between *ab initio* calculations and experimental results, with direct connection to the underlying nuclear interaction. The GCF results lead to a comprehensive and consistent picture of nuclear SRCs, where the only tension is with respect to the analysis of inclusive reactions [46]. Recently, shell-model calculations were combined with the GCF to calculate nuclear matrix elements for neutrinoless double beta decay [47], taking into account both short-range and long-range contributions consistently.

As pointed out, the GCF is based on the asymptotic factorization ansatz for the many-body nuclear wave function Ψ, when nucleon i is close to nucleon j [36]:

$$\Psi \xrightarrow[r_{ij}\to 0]{} \sum_\alpha \varphi_{ij}^\alpha(\boldsymbol{r}_{ij}) A_{ij}^\alpha(\boldsymbol{R}_{ij}, \{\boldsymbol{r}_k\}_{k\neq i,j}). \tag{1}$$

In this picture, particles i and j are strongly interacting, and therefore are described by a two-body function φ_{ij}^α, decoupled from the rest of the system, which is described by the function A_{ij}^α. In the GCF, φ_{ij}^α is assumed to be universal, i.e., independent of the nucleus or its many-body state, and is defined to be the zero-energy solution of the two-body Schrödinger equation with quantum numbers α, obtained with the same nucleon-nucleon interaction model used for the many-body wave function. A similar factorization should hold in momentum space, for pairs with high relative momentum $\boldsymbol{k}_{ij}$:

$$\tilde{\Psi}(\boldsymbol{k}_1, \boldsymbol{k}_2, \dots, \boldsymbol{k}_A) \xrightarrow[k_{ij}\to \infty]{} \sum_\alpha \tilde{\varphi}_{ij}^\alpha(\boldsymbol{k}_{ij}) \tilde{A}_{ij}^\alpha(\boldsymbol{K}_{ij}, \{\boldsymbol{k}_n\}_{n\neq i,j}), \tag{2}$$

where $\tilde{\varphi}_{ij}^\alpha$ and $\tilde{A}_{ij}^\alpha$ are respectively the Fourier transforms of φ_{ij}^α and A_{ij}^α. Based on these asymptotic factorizations, nuclear contact matrices are defined as

$$C_{ij}^{\alpha\beta} = N_{ij}\langle A_{ij}^\alpha | A_{ij}^\beta\rangle. \tag{3}$$

Here, ij stands for one of the pairs: proton-proton, neutron-neutron or neutron-proton, and N_{ij} is the total number of ij pairs in the nucleus. The diagonal contact elements $C_{ij}^{\alpha\alpha}$ are proportional to the number of SRC pairs with quantum number α in a given nuclear state.

The asymptotic factorization, including the definition of the universal two-body functions, is the underlying assumption for the GCF predictions, and was verified numerically using ab-initio calculations [36,39,40]. It is also supported by the work of Refs. [48–50], based on renormalization group arguments. In view of its success, the two-body GCF is expected to be the leading order term of a short-range (or a high-momentum) expansion of the nuclear wave function. However, next order corrections are currently not well understood, especially the role of the elusive SRC triplets.

In this work we study the asymptotic form of the nuclear wave-function using the coupled-cluster (CC) expansion [51,52], aiming to put the GCF on a more solid theoretical grounds. In addition, the CC expansion provides a systematic way to include higher order corrections, e.g., three-body SRCs, beyond the leading two-body SRC term of the asymptotic expansion of the many-body wave function. Here, we limit our attention to Hamiltonians containing only two-body interaction, postponing the discussion of three-body forces to future works.

The paper is organized as follows. In Sec. II we provide a short introduction to the CC expansion method. Then, in Sec. III we discuss the momentum basis and its merits. The derivation of the high-momentum asymptotic equations governing the behavior of two-body and three-body SRCs is presented in Sec. IV. In Sec. V we focus on two-body correlations and analyze their universal behavior. Three-body effects are then analyzed in Sec. VI, where we derive the appropriate universal equation and show its relation to the solution of the zero-energy three-body problem. For the sake of brevity some more technical details are presented in the Appendixes.

II. COUPLED CLUSTER THEORY

The general form of a Hamiltonian describing a many-particle system interacting via two-body potential $\hat{V}$ is given by

$$\begin{aligned}\hat{H} &\equiv \hat{H}_0 + \hat{U} + \hat{V}\\ &= \sum_r \epsilon_r \boldsymbol{r}^\dagger \boldsymbol{r} + \sum_{rr'} U^r_{r'} \boldsymbol{r}^\dagger \boldsymbol{r}' + \frac{1}{4}\sum_{rsr's'} V^{rs}_{r's'} \boldsymbol{r}^\dagger \boldsymbol{s}^\dagger \boldsymbol{s}' \boldsymbol{r}',\end{aligned} \tag{4}$$

where $\hat{H}_0$ is the "zero-order" or unperturbed Hamiltonian (not necessarily the free Hamiltonian), and $\hat{U}$ is the residual one-body interaction. The operators $\boldsymbol{r}, \boldsymbol{s}, \dots$ are the usual fermionic ladder operators corresponding to the single particle eigenstates $|r\rangle, |s\rangle, \dots$ of $\hat{H}_0$, i.e., $\hat{H}_0|r\rangle = \epsilon_r|r\rangle$, or equivalently

$$[\hat{H}_0, \boldsymbol{r}^\dagger] = \epsilon_r \boldsymbol{r}^\dagger \quad [\hat{H}_0, \boldsymbol{r}] = -\epsilon_r \boldsymbol{r}, \tag{5}$$

where $[\hat{A}, \hat{B}]$ is the regular commutator. They obey the anti-commutation relations

$$\{\boldsymbol{r}, \boldsymbol{s}\} = 0, \quad \{\boldsymbol{r}^\dagger, \boldsymbol{s}^\dagger\} = 0, \quad \{\boldsymbol{r}^\dagger, \boldsymbol{s}\} = \delta_{rs}. \tag{6}$$

In the following we will use the notation $|r_1 r_2 \cdots r_A\rangle$ to denote normalized antisymmetrized A-body states and $|r_1 r_2 \cdots r_A)$ to denote the simple, nonsymmetrized, many-body states, e.g., $|rs\rangle = \frac{1}{\sqrt{2}}[|rs) - |sr)]$. The matrix elements of the two-body potential $\hat{V}$ are then given by

$$V^{rs}_{r's'} = \langle rs|\hat{V}|r's'\rangle = (rs|\hat{V}|r's') - (rs|\hat{V}|s'r'). \tag{7}$$

The starting point of the CC method is a reference Slater-determinant state $|\Phi_0\rangle$, composed of A single particle states. In general, a wave function $|\Psi\rangle$ is a linear combination of all such Slater determinants. These determinants can be organized in a systematic way, by considering first the determinants obtained replacing a state occupied in $|\Phi_0\rangle$ with a state not occupied in $|\Phi_0\rangle$, then replacing two such states, and so on. Following the convention of Shavitt and Bartlett [53], we use the letters $i, j, \dots, n$ to denote "hole" states, i.e., single-particle states that are occupied in $|\Phi_0\rangle$, and the letters $a, b, \dots, f$ to denote "particle" states, i.e., single-particle states that are not occupied in $|\Phi_0\rangle$. $r, s, \dots, w$ will be used to denote both states. Therefore,

$$\boldsymbol{i}^\dagger|\Phi_0\rangle = 0 \quad \text{and} \quad \boldsymbol{a}|\Phi_0\rangle = 0. \tag{8}$$

The interacting many-body state $|\Psi\rangle$, an eigenstate of $\hat{H}$, is written in the CC formulation as

$$|\Psi\rangle = e^{\hat{T}}|\Phi_0\rangle, \quad \text{where } \hat{T} = \sum_n \hat{T}_n, \tag{9}$$

and

$$\hat{T}_n = \frac{1}{n!^2}\sum_{a_1\dots a_n, i_1\dots i_n} t^{a_1 a_2\dots a_n}_{i_1 i_2\dots i_n} \boldsymbol{a}_1^\dagger \boldsymbol{a}_2^\dagger \cdots \boldsymbol{i}_2 \boldsymbol{i}_1 \tag{10}$$

is the n-particle, n-hole (npnh) cluster operator.

To determine the amplitudes $t^{a_1 a_2\cdots a_n}_{i_1 i_2\cdots i_n}$, a set of nonlinear equations, the CC equations, can be obtained by projecting the Schrödinger equation on an npnh state $|\Phi^{ab\cdots}_{ij\dots}\rangle \equiv \boldsymbol{a}^\dagger \boldsymbol{b}^\dagger \cdots \boldsymbol{j}\boldsymbol{i}|\Phi_0\rangle$. The full derivation of the CC equations is given, e.g., in Ref. [53]. Omitting the one-body potential term $\hat{U}$ and the 1p1h cluster operator $\hat{T}_1$, the two- and three-body CC equations are given by

$$\begin{aligned}0 &= \big\langle \Phi^{ab}_{ij}\big|\hat{V} + [\hat{H}_0, \hat{T}_2] + [\hat{V}, \hat{T}_2] + \tfrac{1}{2}[[\hat{V}, \hat{T}_2], \hat{T}_2]\\ &\quad + [\hat{V}, \hat{T}_3] + [\hat{V}, \hat{T}_4]|\Phi_0\rangle, \end{aligned}\tag{11}$$

$$\begin{aligned}0 &= \big\langle \Phi^{abc}_{ijk}\big|[\hat{H}_0, \hat{T}_3] + [\hat{V}, \hat{T}_2] + \tfrac{1}{2}[[\hat{V}, \hat{T}_2], \hat{T}_2] + [\hat{V}, \hat{T}_3]\\ &\quad + [[\hat{V}, \hat{T}_2], \hat{T}_3] + [\hat{V}, \hat{T}_4] + [\hat{V}, \hat{T}_5]|\Phi_0\rangle.\end{aligned} \tag{12}$$

III. MOMENTUM BASIS STATES

To study SRCs it is most convenient to work with single-particle basis states, i.e., the eigenstates of $\hat{H}_0$ that have well defined momentum. This choice is natural for an infinite system like nuclear matter—see, e.g., [54,55]—but it might seem rather odd for describing a bound nucleus which is a compact object. However, large nuclei have relatively constant density and far from the surface behave like an infinite nuclear system. Thus, we set the problem in a box of size L with periodic boundary conditions. For L larger than the nucleus size, the wave function and the binding energy approach very fast the free space ($L \to \infty$) values and we need not worry about the impact of the boundary conditions on the nuclear SRCs.

Assuming $\boldsymbol{p} = (p_1, p_2, p_3)$ to be a triad of integers, the basis states $\{|\boldsymbol{p}\rangle\}$

$$\langle \boldsymbol{x}||\boldsymbol{p}\rangle = \frac{1}{\sqrt{\Omega}} e^{i\frac{2\pi}{L}\boldsymbol{x}\cdot\boldsymbol{p}}, \quad \langle \boldsymbol{p}||\boldsymbol{p}'\rangle = \delta_{\boldsymbol{p},\boldsymbol{p}'}, \tag{13}$$

with $\Omega = L^3$, are a complete set of orthonormal states, which combined with the spin and isospin degrees of freedom form our single-particle basis. A natural choice for $|\Phi_0\rangle$, the starting point of the CC expansion, is a Slater determinant composed of the A lowest kinetic energy single-particle states.

If there is a well defined Fermi momentum p_F, such that all the hole states are momentum states with momentum smaller than p_F, while particle states have momentum larger than p_F, then the system is called a *closed shell* system. To simplify matters, in the following we shall restrict our the discussion to such closed shell systems only.

Working with this single-particle momentum basis, $\hat{H}_0$ coincides with the kinetic energy operator and therefore $\hat{U} = 0$. The Slater determinant $|\Phi_0\rangle$, as well as the npnh states $|\Phi^{ab\ldots}_{ij\ldots}\rangle$, are products of single-particle momentum states, hence they are eigenstates of the total center-of-mass (CM) momentum operator $\hat{\boldsymbol{P}}_{\text{CM}}$. The two-body potential is translationally invariant, hence the CM momentum is a good quantum number, and the wave function $|\Psi\rangle$ is also an eigenstate of $\hat{\boldsymbol{P}}_{\text{CM}}$,

$$\hat{\boldsymbol{P}}_{\text{CM}}|\Psi\rangle = \hat{\boldsymbol{P}}_{\text{CM}} e^{\hat{T}}|\Phi_0\rangle = \boldsymbol{P}_{\text{CM}}|\Psi\rangle. \tag{14}$$

Closing the last equation with $\langle\Phi_0|$ and acting with $\hat{\boldsymbol{P}}_{\text{CM}}$ once to the left and once to the right, and noting that $\langle\Phi_0||\Psi\rangle \neq 0$, we must conclude that $|\Phi_0\rangle$ and $|\Psi\rangle$ share the same eigenvalue of the total momentum $\boldsymbol{P}_{\text{CM}}$.

We may now repeat the same argument for the 1p1h states. Closing Eq. (14) with $\langle\Phi^a_i|$ and using $\langle\Phi^a_i|\Psi\rangle = t^a_i$ we get

$$(\boldsymbol{p}_a - \boldsymbol{p}_i)t^a_i = \boldsymbol{0}, \tag{15}$$

which for all closed shell systems implies [54,56]

$$t^a_i = 0, \tag{16}$$

because $(\boldsymbol{p}_a - \boldsymbol{p}_i) \neq \boldsymbol{0}$, as $\boldsymbol{p}_a$ corresponds to a particle state while $\boldsymbol{p}_i$ to a hole state. Thus, with this choice of basis states, $\hat{T}_1$ is eliminated from the CC expansion, as was assumed in Eqs. (11) and (12).

Considering now the 2p2h states, multiplying Eq. (14) by $\langle\Phi^{ab}_{ij}|$ one gets [55]

$$(\boldsymbol{p}_a + \boldsymbol{p}_b - \boldsymbol{p}_i - \boldsymbol{p}_j)t^{ab}_{ij} = \boldsymbol{0}. \tag{17}$$

This implies that $\hat{T}_2$ conserves momentum, i.e., $t^{ab}_{ij} = 0$ if $\boldsymbol{p}_a + \boldsymbol{p}_b - \boldsymbol{p}_i - \boldsymbol{p}_j \neq \boldsymbol{0}$. It can be similarly shown that for a closed shell system all amplitude operators $\hat{T}_n$ must conserve momentum.

IV. COUPLED CLUSTER AMPLITUDES IN THE HIGH-MOMENTUM LIMIT

SRCs are associated with high-momentum particles. To understand their role in the many-body wave-function we need to study the high-momentum behavior of the CC amplitudes $\hat{T}_n$ as dictated by Eqs. (11) and (12). In the following we will assume a, b, and c to be highly excited states corresponding to momenta $p_a, p_b, p_c \gg p_{\text{F}}$. We note that in order for the wave function to be properly normalized the CC amplitudes $\hat{T}_n$ must vanish in this limit, e.g., $t^{abc}_{ijk} \to 0$ when $a, b, c \to \infty$.

For a system of fermions, we expect the CC amplitudes to admit the natural hierarchy, where double excitations are much more significant than three-body excitations which on their part are more important than the four-body excitations, etc. It follows that the contributions of $[\hat{V}, \hat{T}_3]$ and $[\hat{V}, \hat{T}_4]$ to the two-body equation can be neglected. Similarly, the terms $[\hat{V}, \hat{T}_4]$ and $[\hat{V}, \hat{T}_5]$ can be neglected in the three-body CC equation.

In order to understand the behavior of the CC amplitudes in the high-momentum limit, let us inspect the $\hat{T}_2$ equation, Eq. (11), in the limit $p_a, p_b \to \infty$. In this case, the leading terms are the source term V^{ab}_{ij} and the kinetic energy term $[\hat{H}_0, \hat{T}_2]$. Retaining only these terms leads to the well known asymptotic result

$$t^{ab}_{ij} \to -\frac{1}{E^{ab}_{ij}} V^{ab}_{ij}, \tag{18}$$

where E^{ab}_{ij} is the excitation energy given by the relation

$$E^{a_1a_2\ldots a_n}_{i_1i_2\ldots i_n} \equiv (\epsilon_{a_1} + \epsilon_{a_2} + \cdots \epsilon_{a_n}) - (\epsilon_{i_1} + \cdots + \epsilon_{i_n}). \tag{19}$$

If, for $p_a, p_b \to \infty$, the potential matrix elements V^{ab}_{ij} are independent of the exact holes states, i.e., $V^{ab}_{ij} \approx V^{ab}_{0_i0_j}$, with 0_i being a zero-momentum state (used loosely to indicate the lowest momentum state with the same quantum numbers as the state i), the asymptotic two-body amplitude presented in Eq. (18) is universal in the limited sense. That is, $t^{ab}_{ij} \approx -\frac{1}{E^{ab}_{00}} V^{ab}_{00}$ is independent of the number of nucleons A and the specifics of the nuclear state. On the other hand, it depends on the potential, therefore its universality is limited. This form of asymptotic behavior was first suggested by Amado [57] exploring the asymptotic form of the nuclear momentum distribution. It turns out, however, that although Eq. (18) is asymptotically correct, it is valid only at extremely high momentum, larger than 10 fm^{-1}, making it impractical for actual calculations [58]. Consequently, in order to get a reasonable description of the asymptotic nuclear wave function, we must retain more terms besides the source term and the $[\hat{H}_0, \hat{T}_n]$ terms in the CC equations.

With the three- and four-body amplitudes neglected, the CC $\hat{T}_2$ equation, Eq. (11), takes the form

$$0 = \langle\Phi^{ab}_{ij}|\hat{V} + [\hat{H}_0, \hat{T}_2] + [\hat{V}, \hat{T}_2] + \tfrac{1}{2}[[\hat{V}, \hat{T}_2], \hat{T}_2]|\Phi_0\rangle. \tag{20}$$

Comparing now the terms $[\hat{V}, \hat{T}_2]$ and $[[\hat{V}, \hat{T}_2], \hat{T}_2]$ we note that for the latter we get the following matrix elements, ignoring combinatorical factors:

$$V^{kl}_{de}t^{ab}_{ik}t^{de}_{jl}, \quad V^{kl}_{de}t^{ab}_{kl}t^{de}_{ij}, \quad V^{kl}_{de}t^{ad}_{ik}t^{be}_{jl}, \quad V^{kl}_{de}t^{ad}_{ij}t^{be}_{kl}. \tag{21}$$

Here, for brevity, we use the Einstein convention assuming implicit summation on repeated lower and upper indices. To inspect these terms in the high-momentum $p_a, p_b \to \infty$ limit it would be insightful to address them in the low density $i, j, k, l \to 0$ limit, in which case these terms take the form

$$2V_{de}^{00}t_{00}^{de}t_{00}^{ab} \quad \text{and} \quad 2V_{de}^{00}t_{00}^{ad}t_{00}^{be}. \tag{22}$$

The first of these terms is nothing but an energy shift, a correction to the excitation energy E_{ij}^{ab}, which we can neglect in the high-momentum limit. We note that the term is zero unless $\boldsymbol{p}_d = -\boldsymbol{p}_a$, $\boldsymbol{p}_e = -\boldsymbol{p}_b$, and $\boldsymbol{p}_b = -\boldsymbol{p}_a$. This term is clearly suppressed by a factor of t_{00}^{ab} with respect to $[\hat{V}, \hat{T}_2]$, and thus can be neglected as well.

The definition of high momentum can now take shape. A momentum will be *high momentum* if (*i*) The kinetic energy is much higher than the potential matrix elements, and (*ii*) the momentum is much higher than the Fermi momentum p_{F}.

Note, however, that although the second point can always exist by considering higher p_a, p_b, the existence of the first point depends also on the chosen potential.

Considering now the $\hat{T}_3$ equation, Eq. (12). After neglecting the $\hat{T}_4, \hat{T}_5$ as well as the $[[\hat{V}, \hat{T}_2], \hat{T}_3] \ll [[\hat{V}, \hat{T}_2], \hat{T}_2]$ terms, we remain with

$$\begin{aligned} 0 =& \langle \Phi_{ijk}^{abc} | [\hat{H}_0, \hat{T}_3] + [\hat{V}, \hat{T}_2] \\ &+ \tfrac{1}{2}[[\hat{V}, \hat{T}_2], \hat{T}_2] + [\hat{V}, \hat{T}_3] | \Phi_0 \rangle. \end{aligned} \tag{23}$$

Comparing again the $[\hat{V}, \hat{T}_2]$ and $[[\hat{V}, \hat{T}_2], \hat{T}_2]$ terms, we see that the only terms that survive in the high-momentum/low-density limit are respectively $V_{e0}^{ab}t_{00}^{ce}$, and $V_{ef}^{a0}t_{00}^{be}t_{00}^{cf}$. Thus as before, the double commutator term is suppressed by a factor of t_{00}^{ab} and can be neglected.

Summing up, in the limit of high momenta, we expect the two- and three-body CC amplitudes to obey the equations

$$0 = \langle \Phi_{ij}^{ab} | [\hat{H}_0, \hat{T}_2] + [\hat{V}, \hat{T}_2] + \hat{V} | \Phi_0 \rangle, \tag{24}$$

$$0 = \langle \Phi_{ijk}^{abc} | [\hat{H}_0, \hat{T}_3] + [\hat{V}, \hat{T}_3] + [\hat{V}, \hat{T}_2] | \Phi_0 \rangle. \tag{25}$$

In the following sections we will analyze these equations.

V. THE TWO-BODY AMPLITUDE

In Sec. IV we argued that asymptotically the two-body CC equation takes the form of Eq. (24). In order to evaluate this equation, we note that there can be no contractions between the operators $\boldsymbol{a}^\dagger \boldsymbol{b}^\dagger \boldsymbol{j} \boldsymbol{i}$ that appear in the bra state, hence all the labels a, b, i, and j have to appear on the amplitude and potential operators. Therefore $\langle \Phi_{ij}^{ab} | \hat{V} | \Phi_0 \rangle = V_{ij}^{ab}$, and $\langle \Phi_{ij}^{ab} | [\hat{H}_0, \hat{T}_2] | \Phi_0 \rangle = E_{ij}^{ab} t_{ij}^{ab}$. To evaluate the commutator $[\hat{V}, \hat{T}_2] = \hat{V}\hat{T}_2 - \hat{T}_2\hat{V}$, we note that all the operators of $\hat{V}$ in $\hat{V}\hat{T}_2$ can be moved to the right of $\hat{T}_2$ and then the term will cancel with $\hat{T}_2\hat{V}$. In the process, all possible contractions between $\hat{V}$ and $\hat{T}_2$ will arise, i.e., at least one contraction should be made between them. This commutators yield five distinct terms, that combined with the potential and the $\hat{H}_0$ terms result in the linear coupled-cluster doublets (CCD) equation

$$\begin{aligned} 0 =& V_{ij}^{ab} + E_{ij}^{ab} t_{ij}^{ab} + \tfrac{1}{2} V_{de}^{ab} t_{ij}^{de} \\ &+ \tfrac{1}{2} V_{ij}^{kl} t_{kl}^{ab} + V_{id}^{ak} t_{jk}^{bd} + V_{kd}^{ak} t_{ij}^{bd} + V_{ik}^{lk} t_{jl}^{ab} \\ &+ \text{permutations}. \end{aligned} \tag{26}$$

The term "permutations" stands for antisymmetrization with respect to the indices ab or ij when not placed on the same matrix elements. The summation V_{kw}^{kv} is performed only on hole states because the string $\boldsymbol{r}^\dagger \boldsymbol{s}$ of $\hat{V}$, where both $\boldsymbol{r}, \boldsymbol{s}$ are particle operators, is already normal ordered and therefore its contraction is zero.

In the limit of high momentum/low density, the second line of (26) takes the form of either $V_{00}^{00} t_{00}^{ab}$ or $V_{a0}^{a0} t_{00}^{ab}$. In both cases these terms enter as small corrections to the excitation energy. It follows that these terms can be neglected for large p_a, p_b with respect to the terms appearing on the first line.

Refining this argument, due to momentum conservation we expect that in the limit $p_a, p_b \to \infty$ all the $\hat{T}_2$ terms on the second and third lines of Eq. (26) will be either exactly or at least approximately equal to t_{ij}^{ab} since the hole states carry only low momentum of the order of p_{F} and we assume weak momenta dependance on the hole states' quantum numbers. For example, in $V_{id}^{ak} t_{jk}^{bd}$ the momentum $\boldsymbol{p}_d$ associated with the state d must be of the order $\boldsymbol{p}_d = \boldsymbol{p}_a + \mathcal{O} p_{\mathrm{F}}$, implying that $t_{jk}^{bd} \approx t_{ij}^{ba}$. Comparing these terms to the term $E_{ij}^{ab} t_{ij}^{ab}$, we see that for large enough excitations

$$E_{ij}^{ab} \gg \sum_{kl} V_{ij}^{kl}, \ \sum_{kd} V_{id}^{ak}, \ \sum_{kd} V_{kd}^{ak}, \ \sum_{kl} V_{ik}^{lk},$$

and these terms can be neglected. It is important to observe that the neglected terms are all intensive and do not scale with the size of the system.

The resulting two-body amplitude equation is then

$$0 = t_{ij}^{ab} + \frac{1}{E_{ij}^{ab}} V_{ij}^{ab} + \frac{1}{2E_{ij}^{ab}} V_{de}^{ab} t_{ij}^{de}, \tag{27}$$

which is nothing but the particle-particle ladder approximation of the CCD equation, applied for example in Ref. [54] to estimate the nuclear matter equation of state. In the following we will use the notation $\hat{T}_2^\infty$ to denote the solution of Eq. (27) in the nonsymmetrized basis with $E^{ij} \equiv \epsilon_i + \epsilon_j \to 0$. As it is a linear equation, $\hat{T}_2^\infty$ is unique. We will show in Appendix A that indeed $\langle \boldsymbol{ab} | \hat{T}_2 | \boldsymbol{ij} \rangle \to \langle \boldsymbol{ab} | \hat{T}_2^\infty | \boldsymbol{ij} \rangle$ as $p_a, p_b \to \infty$.

We can now discuss the properties of $\hat{T}_2^\infty$. As stated above, the cluster operator $\hat{T}_2^\infty$ is defined as the solution of the equation

$$0 = (t^\infty)_{ij}^{ab} + \frac{1}{E^{ab}} V_{ij}^{ab} + \frac{1}{2E^{ab}} V_{de}^{ab} (t^\infty)_{ij}^{de}, \tag{28}$$

where $E^{ab} = \epsilon_a + \epsilon_b$. A similar result was derived by Zabolitzky in Ref. [58]. To analyze this equation, it is convenient to introduce the particle-particle and hole-hole projection operators,

$$Q_2 = \sum_{de} |de)(de|, \quad P_2 = \sum_{lm} |lm)(lm|, \tag{29}$$

and the Green's function

$$\hat{G}_0(E) = \frac{1}{E - \hat{H}_0 + i\varepsilon}. \tag{30}$$

Eqaution (28) can then be written as

$$\hat{T}_2^\infty = Q_2 \hat{G}_0(0) \hat{V} \hat{T}_2^\infty + Q_2 \hat{G}_0(0) \hat{V} P_2, \tag{31}$$

and formally solved to yield

$$\hat{T}_2^{\infty} = \frac{1}{1 - Q_2 \hat{G}_0(0) \hat{V}} Q_2 \hat{G}_0(0) \hat{V} P_2. \tag{32}$$

Clearly, $P_2 \hat{T}_2^{\infty} = \hat{T}_2^{\infty} Q_2 = 0$ as expected from a cluster operator. Using the relation $Q_2 \hat{H}_0 P_2 = 0$ the solution (32) can be rewritten as (see Appendix B)

$$\hat{T}_2^{\infty} = \frac{1}{Q_2(0 + i\varepsilon - \hat{H}) Q_2} Q_2 \hat{H} P_2. \tag{33}$$

Before proceeding, we note that P_2 is not equivalent to $\bar{Q}_2 = 1 - Q_2$, the complement of Q_2, as $\bar{Q}_2$ must include not only hole-hole states but also particle-hole states. For infinite nuclear matter we expect, however, that $\hat{T}_2^{\infty}$ is translationally invariant and therefore we can consider only pairs with zero CM momentum. For such pairs, there are no particle-hole contributions and we can replace P_2 by $\bar{Q}_2$. In this subspace

$$\hat{T}_2^{\infty} = \frac{1}{Q_2(0 + i\varepsilon - \hat{H}) Q_2} Q_2 \hat{H} \bar{Q}_2. \tag{34}$$

Comparing now Eq. (34) with the Bloch-Horowitz equations [59],

$$\bar{Q}_2 |\Psi\rangle = \frac{1}{\bar{Q}_2(E + i\varepsilon - \hat{H}) \bar{Q}_2} \bar{Q}_2 \hat{H} Q_2 |\Psi\rangle \tag{35}$$

$$Q_2 |\Psi\rangle = \frac{1}{Q_2(E + i\varepsilon - \hat{H}) Q_2} Q_2 \hat{H} \bar{Q}_2 |\Psi\rangle, \tag{36}$$

it is clear that $\hat{T}_2^{\infty}$ is nothing but the zero-energy two-body Bloch-Horowitz operator

$$\hat{O}_2^{\text{B.H.}} = \frac{1}{Q_2(0 + i\varepsilon - \hat{H}) Q_2} Q_2 \hat{H} \bar{Q}_2. \tag{37}$$

This operator fulfills the relation $\hat{O}_2^{\text{B.H.}} |\Psi_2\rangle = Q_2 |\Psi_2\rangle$ for any zero energy eigenstate $|\Psi_2\rangle$ that obeys $\hat{H}|\Psi_2\rangle = 0$. It follows that if $\hat{H}|\Psi_2\rangle = 0$ and $\hat{\boldsymbol{P}}_{\text{CM}} |\Psi_2\rangle = 0$, then

$$Q_2 |\Psi_2\rangle = \hat{T}_2^{\infty} |\Psi_2\rangle. \tag{38}$$

Inspecting Eqs. (33) and (38), we can conclude that (*i*) the asymptotic two-body behavior of $\hat{T}_2$, and therefore of the many-body wave function, is related to the zero-energy solutions of the two-body problem, and (*ii*) the relation to the zero-energy solutions at the high-momentum/low-density limit shows the universality of the asymptotic behavior in the limited sense, as system dependencies will enter as a small correction.

VI. THE THREE-BODY AMPLITUDE

As we have argued in Sec. IV, the behavior of the three-body amplitude $\hat{T}_3$ at high momentum is dictated by Eq. (25). Explicitly, this equation takes the form

$$\begin{aligned} 0 = {} & E_{ijk}^{abc} t_{ijk}^{abc} - V_{ij}^{la} t_{kl}^{bc} - V_{id}^{ab} t_{jk}^{cd} \\ & + \tfrac{1}{2} V_{de}^{ab} t_{ijk}^{cde} + \tfrac{1}{2} V_{ij}^{lm} t_{klm}^{abc} + V_{dl}^{al} t_{ijk}^{bcd} + V_{id}^{al} t_{jkl}^{bcd} + V_{il}^{lm} t_{jkm}^{abc} \\ & + \text{permutations}. \end{aligned} \tag{39}$$

Here, the first term on the right-hand side (rhs) is due to $[\hat{H}_0, \hat{T}_3]$, the next two terms come from the $[\hat{V}, \hat{T}_2]$ commutator, and the next five are due to the $[\hat{V}, \hat{T}_3]$ commutator. The term "permutations" stands for antisymmetrization with respect to the indices abc or ijk when not placed on the same matrix elements. Due to momentum conservation, for very large p_a the potential matrix elements V_{ij}^{la} must vanish, leaving $V_{id}^{ab} t_{jk}^{cd}$ as the only source term. In addition, all terms coming from the $[\hat{V}, \hat{T}_3]$ commutator, except for the first term in the second line (and its corresponding permutations), are approximately proportional to t_{ijk}^{abc}. Therefore, for excitation energy E_{ijk}^{abc} large enough

$$E_{ijk}^{abc} \gg \sum_{lm} V_{ij}^{lm}, \ \sum_{ld} V_{dl}^{al}, \ \sum_{ld} V_{id}^{al}, \ \sum_{ml} V_{il}^{lm}, \tag{40}$$

and the corresponding terms can be neglected in comparison to the free term $E_{ijk}^{abc} t_{ijk}^{abc}$. As a consequence only the terms $\frac{1}{2} V_{de}^{ab} t_{ijk}^{cde}$ remain. Utilizing these observations, and defining the symmetrization operator $\hat{\mathcal{S}}_{123} \equiv 1 + (123) + (132)$ where (123) is the permutation operator, Eq. (39) takes the form

$$0 = t_{ijk}^{abc} + \frac{\hat{\mathcal{S}}_{abc}\big(\hat{\mathcal{S}}_{ijk}\big(V_{id}^{ab} t_{jk}^{dc}\big)\big)}{E_{ijk}^{abc}} + \frac{\hat{\mathcal{S}}_{abc}\big(V_{de}^{ab} t_{ijk}^{cde}\big)}{2E_{ijk}^{abc}}. \tag{41}$$

As in the two-body case we define $\hat{T}_3^{\infty}$ to be the solution of Eq. (41) in the limit $E_{ijk}^{abc} \to E^{abc}$ and $t_{jk}^{dc} \to (t^{\infty})_{jk}^{dc}$. We show in Appendix C that $\langle \boldsymbol{abc} | \hat{T}_3 | \boldsymbol{ijk} \rangle \to \langle \boldsymbol{abc} | \hat{T}_3^{\infty} | \boldsymbol{ijk} \rangle$ as $p_a, p_b, p_c \to \infty$.

To analyze $\hat{T}_3^{\infty}$ we write Eq. (41) in first quantization using the nonsymmetrized basis defined above. In the three-body case, the relation between the antisymmetrized matrix elements and the nonsymmetrized ones is

$$\langle rst | \hat{O} | uvw \rangle = \hat{\mathcal{S}}_{uvw} [(rst | \hat{O} | uvw) - (rst | \hat{O} | vuw)], \tag{42}$$

and for a two-body operator closed by three-particle states

$$(rst | \hat{O}_2 | uvw) \equiv \sum_{i=1}^{3} (rst | \hat{O}_2(i) | uvw), \tag{43}$$

where $\hat{O}_2(i)$ does not act on the ith particles, e.g., $(rst|\hat{O}_2(3)|uvw) = (rs|\hat{O}_2|uv)\delta_{t,w}$. With the projection operators

$$Q_3 = \sum_{def} |def)(def|, \quad P_3 = \sum_{lmn} |lmn)(lmn|, \tag{44}$$

the asymptotic equation for $\hat{T}_3^{\infty}$ can be written as

$$\begin{aligned} \hat{T}_3^{\infty} &= Q_3 \hat{G}_0(0) \hat{V} \hat{T}_3^{\infty} + Q_3 \hat{G}_0(0) \hat{V} \hat{T}_2^{\infty} P_3 \\ &= \frac{1}{1 - Q_3 \hat{G}_0(0) \hat{V}} Q_3 \hat{G}_0(0) \hat{V} \hat{T}_2^{\infty} P_3 \\ &= \frac{1}{Q_3(0 + i\varepsilon - \hat{H}) Q_3} Q_3 \hat{H} \hat{T}_2^{\infty} P_3. \end{aligned} \tag{45}$$

Comparing Eq. (45) with the three-body Bloch-Horowitz equations [59] and noting that for two-body interactions

$Q_3H\bar{Q}_3 = Q_3H(Q_1P_2 + Q_2P_1)$ with $\bar{Q}_3 = 1 - Q_3$

$$\bar{Q}_3|\Psi\rangle = \frac{1}{\bar{Q}_3(E + i\varepsilon - \hat{H})\bar{Q}_3}\bar{Q}_3\hat{H}Q_3|\Psi\rangle, \quad (46)$$

$$Q_3|\Psi\rangle = \frac{1}{Q_3(E + i\varepsilon - \hat{H})Q_3}Q_3\hat{H}\bar{Q}_3|\Psi\rangle, \quad (47)$$

we can connect $\hat{T}_3^\infty$ to the zero-energy Bloch-Horowitz operator. Specifically, if $|\Psi_3\rangle$ is a zero-energy three-body eigenstate of $\hat{H}$, and if there is a three-hole state $|\alpha_3\rangle$ such that

$$\hat{T}_2^\infty|\alpha_3\rangle \approx (Q_1P_2 + Q_2P_1)|\Psi_3\rangle, \quad (48)$$

then

$$\hat{T}_3^\infty|\alpha_3\rangle \approx Q_3|\Psi_3\rangle \quad (49)$$

and we can identify the matrix elements of $\hat{T}_3^\infty$ with the Q_3 components of the zero-energy solutions of the Schrödinger equation. In the next section we will argue that Eq. (49) approximately holds.

Here we wish to remark that if we would include a three-body potential into our formalism it would change the kernel and the source term of the asymptotic equation. Its importance to three-body correlations will be decided by its relative strength with respect to the two-body potential.

The three-body zero-energy eigenstate

We first note that a zero-energy three-body eigenstate of the Schrödinger equation, $\hat{H}|\Psi_3\rangle = 0$, can be formally expanded in the CC method as

$$|\Psi_3\rangle = \mathcal{N}_3^{-1}e^{\hat{\tilde{T}}}|\Phi_0\rangle = \mathcal{N}_3^{-1}(1 + \hat{\tilde{T}}_2 + \hat{\tilde{T}}_3)|\tilde{\Phi}_0\rangle, \quad (50)$$

where $\hat{\tilde{T}}_2$, $\hat{\tilde{T}}_3$ are the three-body cluster operators, and

$$\mathcal{N}_3^2 = 1 + \mathrm{Tr}(\hat{\tilde{T}}_2^\dagger\hat{\tilde{T}}_2) + \mathrm{Tr}(\hat{\tilde{T}}_3^\dagger\hat{\tilde{T}}_3) \quad (51)$$

is a normalization factor. Working with the momentum basis, we note that whereas the A-body operators $\hat{T}_k$ are defined with respect to the A-body Fermi level p_F, the three-body operators $\hat{\tilde{T}}_2$, $\hat{\tilde{T}}_3$ are defined with respect to a three-body reference state, which we denote as $|000\rangle$ to indicate that it corresponds to single-particle states with momentum which is either zero or very close to zero. We note that in this case the state $|000\rangle$ acts as a closed-shell state as the other possible Slater-determinants with zero momenta holes have different conserved quantum numbers, such as $\hat{J}_z$, and cannot contribute to $|\Psi_3\rangle$. It follows that

$$|\Psi_3\rangle = \mathcal{N}_3^{-1}\Bigg(|000\rangle + \frac{1}{2}\sum_{lm}\tilde{t}_{00}^{lm}|lm0\rangle + \frac{1}{2}\sum_{de}\tilde{t}_{00}^{de}|de0\rangle + \frac{1}{6}\sum_{lmn}\tilde{t}_{000}^{lmn}|lmn\rangle + \frac{1}{2}\sum_{dlm}\tilde{t}_{000}^{dlm}|dlm\rangle + \frac{1}{2}\sum_{del}\tilde{t}_{000}^{del}|del\rangle + \frac{1}{6}\sum_{def}\tilde{t}_{000}^{def}|def\rangle\Bigg). \quad (52)$$

Here, we keep labeling the states according to the A-body Fermi level, e.g., d, e, f correspond to particle states while l, m, n correspond to hole states. As a result, terms such as $|dl0\rangle$ cannot appear in the expansion, as momentum conservation implies that if the state d is above the Fermi level then so must be l.

Before substituting the three-body wave function (52) into the Q-space Bloch-Horowitz equation (47) we note that (*i*) the operator $\bar{Q}_3$ kills the 3p0h states $|def\rangle$, and (*ii*) for two-body interactions the term $Q_3\hat{H}\bar{Q}_3$ annihilates the 0p3h states, thus

$$Q_3\hat{H}\bar{Q}_3|\Psi_3\rangle = Q_3\hat{H}\bar{Q}_3\big|\Psi_3^{(1\mathrm{p},2\mathrm{p})}\big\rangle, \quad (53)$$

where

$$\big|\Psi_3^{(1\mathrm{p},2\mathrm{p})}\big\rangle \equiv (Q_1P_2 + Q_2P_1)|\Psi_3\rangle = \frac{\mathcal{N}_3^{-1}}{2}\Bigg(\sum_{de}\tilde{t}_{00}^{de}|de0\rangle + \sum_{del}\tilde{t}_{000}^{del}|del\rangle + \sum_{dlm}\tilde{t}_{000}^{dlm}|dlm\rangle\Bigg). \quad (54)$$

Inspecting Eq. (54), we note that the last term on the rhs is zero unless $p_d < 2p_\mathrm{F}$. It follows that this term must vanish if we consider a very dilute A-body system, i.e., the limit $p_\mathrm{F} \to 0$. Interestingly, in this limit also the first two terms coincide as $\tilde{t}_{000}^{del} \to \tilde{t}_{000}^{de0}$ with $l \to 0$. Hence, in the limit $p_\mathrm{F} \to 0$, $Q_3\hat{H}\bar{Q}_3|\Psi_3\rangle \approx 2\mathcal{N}_3^{-1}Q_3\hat{H}\hat{\tilde{T}}_2|000\rangle$. Recalling now that Eq. (41) is an asymptotic equation derived in the limit $p_a, p_b, p_c \to \infty$, and that in this limit $\hat{\tilde{T}}_2 \to \hat{T}_2^\infty$, we may conclude that for $i, j, k = 0$ the asymptotic three-body cluster operator $\hat{T}_3^\infty$, Eq. (45), can be redefined replacing $\hat{T}_2^\infty$ with $\hat{\tilde{T}}_2$. The resulting operator admits

$$\hat{T}_3^\infty|\alpha_3\rangle \approx Q_3|\Psi_3\rangle \quad (55)$$

with $|\alpha_3\rangle \equiv 2\mathcal{N}_3^{-1}|000\rangle$.

Considering now nuclear matter in the limit of dense matter (i.e., p_F very large compared to the Fermi momentum at saturation density), we have $\frac{1}{2}\sum_{de}\tilde{t}_{00}^{de}|de0\rangle \to \hat{T}_2^\infty|000\rangle$. Under this condition we also expect that the 2p1h terms $\frac{1}{2}\sum_{del}\tilde{t}_{000}^{del}|del\rangle$ are dominated by two-body rather than three-body correlations, i.e., most contributions will come from states with $p_l \ll p_d, p_e$. Therefore there is a three-hole state $|\alpha_3^{(2p)}\rangle$ such that $\frac{1}{2}\sum_{del}\tilde{t}_{000}^{del}|del\rangle \approx \hat{T}_2^\infty|\alpha_3^{(2p)}\rangle$. The 1p2h term $\frac{1}{2}\sum_{dlm}\tilde{t}_{000}^{dlm}|dlm\rangle$ is clearly zero if the momentum of state d, p_d, is larger than $2p_F$. We also expect that the main contribution of this term will appear when $p_d, p_l \approx p_F$ and the third momentum is approximately zero. Here again we can find a 0p3h state such that $\frac{1}{2}\sum_{dlm}\tilde{t}_{000}^{dlm}|dlm\rangle \approx \hat{T}_2^\infty|\alpha_3^{(1p)}\rangle$. This observation implies that there is a 0p3h state α_3 such that

$$\left|\Psi_3^{(1p,2p)}\right\rangle \approx \hat{T}_2^\infty|\alpha_3\rangle, \tag{56}$$

and hence also in this limit

$$\hat{T}_3^\infty|\alpha_3\rangle \approx Q_3|\Psi_3\rangle. \tag{57}$$

This relation holds also for any value of p_F if we consider the most asymptotic high-momentum contribution to $\hat{T}_3^\infty$, hence we expect it to approximately hold for finite nuclei as well.

Summarizing this discussion we conclude that, as in the two-body case, (*i*) the asymptotic high-momentum behavior of $\hat{T}_3$ is related to a three-body zero-energy eigenfunction of the Schrödinger equation, and (*ii*) at the high-momentum/low-density limit, the asymptotic behavior is universal in the limited sense.

VII. SUMMARY

The CC method was utilized to set a more rigorous foundation for the successful GCF. To this end we have computed the two- and three-body cluster operators in the high-momentum limit and showed that they act as the Bloch-Horowitz operators for the two- and three-body zero-energy eigenstates of the Schrödinger equation. We therefore concluded that the two- and trhee-body cluster operators in the high-momentum/low-density limit are universal in the limited sense, i.e., they do not depend on the system but do depend on the potential.

The presented method is systematic and opens up the path for including higher order corrections to the GCF. A more complete discussion regarding the asymptotic wave function factorization is postponed to a forthcoming article. We note that our results may be useful for general CC computations, as asymptotic expressions or approximations for the cluster operators.

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APPENDIX A: THE ASYMPTOTICS OF $\hat{T}_2$

To show that indeed the full two-body amplitude $\hat{T}_2$ coincides with $\hat{T}_2^\infty$ in the limit $p_a, p_b \to \infty$, we seek an iterative solution for Eq. (11) [53]. To this end we denote by $\hat{T}_2^{(k)}$ the approximate solution of $\hat{T}_2$ after k iterations. Taking the asymptotic solution to be our initial guess $\hat{T}_2^{(0)} = \hat{T}_2^\infty$, we can write

$$\hat{T}_2^{(k)} = \hat{T}_2^\infty + \Delta\hat{T}_2^{(1)} + \Delta\hat{T}_2^{(2)} + \cdots + \Delta\hat{T}_2^{(k)}, \tag{A1}$$

where the kth correction $\Delta\hat{T}_2^{(k)}$ is obtained by substituting $\hat{T}_2 = \hat{T}_2^{(k-1)} + \Delta\hat{T}_2^{(k)}$ in (11) and solving the linearized equation.

The equation for $\Delta\hat{T}_2^{(1)}$ reads

$$\begin{aligned} 0 = &\langle\Phi_{ij}^{ab}|\hat{V} + [\hat{H}_0, \hat{T}_2^\infty] + \left[\hat{H}_0, \Delta\hat{T}_2^{(1)}\right] + [\hat{V}, \hat{T}_2^\infty] \\ &+ \left[\hat{V}, \Delta\hat{T}_2^{(1)}\right] + \tfrac{1}{2}[[\hat{V}, \hat{T}_2^\infty], \hat{T}_2^\infty] + [\hat{V}, \hat{T}_3] + [\hat{V}, \hat{T}_4] \\ &+ \tfrac{1}{2}\left[[\hat{V}, \hat{T}_2^\infty], \Delta\hat{T}_2^{(1)}\right] + \tfrac{1}{2}\left[\left[\hat{V}, \Delta\hat{T}_2^{(1)}\right], \hat{T}_2^\infty\right]|\Phi_0\rangle \end{aligned} \tag{A2}$$

Utilizing Eq. (28) we obtain

$$\begin{aligned} \Delta t^{(1)ab}_{\ \ ij} = &-\frac{(\hat{V}\hat{T}_2^\infty)_{\rm res}}{E_{ij}^{ab}} + \frac{E^{ij}}{E_{ij}^{ab}}(t^\infty)_{ij}^{ab} - \frac{1}{E_{ij}^{ab}}\langle\Phi_{ij}^{ab}|\left[\hat{V}, \Delta\hat{T}_2^{(1)}\right] + \frac{1}{2}[[\hat{V}, \hat{T}_2^\infty], \hat{T}_2^\infty] + [\hat{V}, \hat{T}_3] + [\hat{V}, \hat{T}_4] \\ &+ \frac{1}{2}\left[[\hat{V}, \hat{T}_2^\infty], \Delta\hat{T}_2^{(1)}\right] + \frac{1}{2}\left[\left[\hat{V}, \Delta\hat{T}_2^{(1)}\right], \hat{T}_2^\infty\right]|\Phi_0\rangle, \end{aligned} \tag{A3}$$

where $(\hat{V}\hat{T}_2^\infty)_{\rm res}$ stands for the terms that appear in (26) but are not included in (28). Asymptotically, as $p_a, p_b \to \infty$, the source terms should dominate:

$$\Delta t^{(1)ab}_{\ \ ij} \to -\frac{(\hat{V}\hat{T}_2^\infty)_{\rm res}}{E_{ij}^{ab}} + \frac{E^{ij}}{E_{ij}^{ab}}(t^\infty)_{ij}^{ab} - \frac{1}{E_{ij}^{ab}}\langle\Phi_{ij}^{ab}|\frac{1}{2}[[\hat{V}, \hat{T}_2^\infty], \hat{T}_2^\infty] + [\hat{V}, \hat{T}_3] + [\hat{V}, \hat{T}_4]|\Phi_0\rangle. \tag{A4}$$

Using the momentum arguments presented above and using the inherent hierarchy, the three- and four-body terms and $(\hat{V}\hat{T}_2^\infty)_{\rm res}$ are suppressed by a factor $\langle\hat{V}\rangle/E_{ij}^{ab}$ (or E^{ij}/E_{ij}^{ab}) compared to $\hat{T}_2^\infty$. Hence asymptotically $\Delta\hat{T}_2^{(1)} \ll \hat{T}_2^\infty$. By iterating the process one can see that asymptotically the higher order $k > 1$ corrections are suppressed by a factor of the order $(\langle\hat{V}\rangle/E_{ij}^{ab})^k$. This completes the iterative proof that $t_{ij}^{ab} \to (t^\infty)_{ij}^{ab}$, and therefore in the high-momentum limit we can replace the two-body cluster operator $\hat{T}_2$ with the operator $\hat{T}_2^\infty$.

APPENDIX B: $\hat{T}_2^\infty$ AS THE BLOCH-HOROWITZ OPERATOR

Recalling that $\hat{G}_0(E) = \frac{1}{E+i\varepsilon-\hat{H}_0}$ and that it commutes with the projection operators Q_2, P_2, we can write for the Q_2 subspace

$$\begin{aligned}\hat{T}_2^\infty &= \frac{1}{1-Q_2\hat{G}_0(E)\hat{V}}Q_2\hat{G}_0(E)\hat{H}P_2\\ &= \frac{1}{Q_2-\hat{G}_0(E)Q_2\hat{V}Q_2}\hat{G}_0(E)Q_2\hat{H}P_2\\ &= \frac{1}{Q_2(E+i\varepsilon-\hat{H}_0-\hat{V})Q_2}Q_2\hat{H}P_2\\ &= \frac{1}{Q_2(E+i\varepsilon-\hat{H})Q_2}Q_2\hat{H}P_2. \qquad \text{(B1)}\end{aligned}$$

Taking the value $E = 0$ it can be rewritten as

$$\hat{T}_2^\infty = \frac{1}{Q_2(0-\hat{H})Q_2}Q_2\hat{H}P_2. \qquad \text{(B2)}$$

APPENDIX C: THE ASYMPTOTICS OF $\hat{T}_3$

To show that $t_{ijk}^{abc} \to (t^\infty)_{ijk}^{abc}$ as $p_a, p_b, p_c \to \infty$, we substitute $\hat{T}_3 = \hat{T}_3^\infty + \Delta\hat{T}_3$ in Eq. (12) and solve for $\Delta\hat{T}_3$ after using the definition of $\hat{T}_3^\infty$ in Eq. (45). Moreover, as explained at Sec. IV, $\frac{1}{2}[[\hat{V},\hat{T}_2],\hat{T}_2] \ll [\hat{V},\hat{T}_2]$ in the limit $p_a, p_b, p_c \to \infty$, hence the equation for Δt_{ijk}^{abc} becomes

$$\begin{aligned}\Delta t_{ijk}^{abc} = &-\frac{(\hat{V}\hat{T}_3^\infty)_{\rm res}}{E_{ijk}^{abc}} + \frac{E^{ijk}}{E_{ijk}^{abc}}(t^\infty)_{ijk}^{abc}\\ &-\frac{1}{E_{ijk}^{abc}}\langle\Phi_{ijk}^{abc}|[\hat{H}_0,\Delta\hat{T}_3]+[\hat{V},\Delta\hat{T}_2]+[\hat{V},\Delta\hat{T}_3]\\ &+\frac{1}{2}[[\hat{V},\hat{T}_2],\Delta\hat{T}_3]+[\hat{V},\hat{T}_4]+[\hat{V},\hat{T}_5]|\Phi_0\rangle, \quad \text{(C1)}\end{aligned}$$

where $(\hat{V}\hat{T}_3^\infty)_{\rm res}$ stands for the terms that appear in (39) but are not included in (41) and $\Delta\hat{T}_2 = \hat{T}_2 - \hat{T}_2^\infty$. Asymptotically, the source terms should dominate, and thus

$$\begin{aligned}\Delta t_{ijk}^{abc} \to &-\frac{(\hat{V}\hat{T}_3^\infty)_{\rm res}}{E_{ijk}^{abc}} + \frac{E^{ijk}}{E_{ijk}^{abc}}(t^\infty)_{ijk}^{abc} - \frac{1}{E_{ijk}^{abc}}\\ &\times\langle\Phi_{ijk}^{abc}|[\hat{V},\Delta\hat{T}_2]+[\hat{V},\hat{T}_4]+[\hat{V},\hat{T}_5]|\Phi_0\rangle. \quad \text{(C2)}\end{aligned}$$

The terms in the first row are trivially much smaller than $(t^\infty)_{ijk}^{abc}$. Also, the four- and five-body terms are also much smaller than $(t^\infty)_{ijk}^{abc}$ due to hierarchy and the suppression of the factor $\frac{1}{E_{ijk}^{abc}}$. For the term $[\hat{V},\Delta\hat{T}_2]$ we can use the results of the previous section $(\Delta t)_{jk}^{cd} \ll (t^\infty)_{jk}^{cd}$ and note, from Eq. (45), that $(t^\infty)_{ijk}^{abc} \sim -\frac{1}{E_{ijk}^{abc}}\hat{\mathcal{S}}_{abc}[\hat{\mathcal{S}}_{ijk}[V_{id}^{ab}(t^\infty)_{jk}^{cd}]]$. Altogether we get the desired result $(\Delta t)_{ijk}^{abc} \ll (t^\infty)_{ijk}^{abc}$, i.e., $t_{ijk}^{abc} \to (t^\infty)_{ijk}^{abc}$.

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