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Complex coupled-cluster approach to an *ab-initio* description of open quantum systems

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Abstract

We develop *ab-initio* coupled-cluster theory to describe resonant and weakly bound states along the neutron drip line. We compute the ground states of the helium chain $^{3-10}$He within coupled-cluster theory in singles and doubles (CCSD) approximation. We employ a spherical Gamow–Hartree–Fock basis generated from the low-momentum N^{3}LO nucleon–nucleon interaction. This basis treats bound, resonant, and continuum states on an equal footing, and is therefore optimal for the description of properties of drip line nuclei where continuum features play an essential role. Within this formalism, we present an *ab-initio* calculation of energies and decay widths of unstable nuclei starting from realistic interactions. Published by Elsevier B.V.

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Exotic phenomena emerge in weakly bound and resonant many-body quantum systems. These phenomena include ground states that are embedded in the continuum, melting and reorganizing of shell structures, extreme matter clusterizations and halo densities. These unusual features occur in many branches of physics; as examples, we mention Fano resonances [1] in quantum dots [2], ultracold atom gases [3], auto-ionizing atoms [4] or molecules [5], and exotic nuclei. In nuclear physics we find such exotic systems moving away from the valley of nuclear stability towards the drip lines, where the outermost nucleons literally start to drip from the nuclei.

The theoretical description of weakly bound and unbound quantum many-body systems is a challenging undertaking. The proximity of the scattering continuum in these systems implies that they should be treated as open quantum systems where coupling with the scattering continuum can take place. Recent work with Gamow states employed in Hamiltonian diagonalization methods [6–10] have shown that these basis states correctly depict properties associated with open quantum systems. This Berggren basis is composed of bound, resonant, and (continuum) scattering single-particle states [11]. This basis significantly improves and facilitates the description of loosely bound systems and is essential in the description of unbound systems. In addition, several groups have worked on alternative methods, such as the so-called continuum shell model [12–16] and the recently developed shell model embedded in the continuum [17–20]. For the latter method, two subspaces of bound/quasi-bound states and scattering states are introduced and their coupling taken into account following the techniques discussed in for example Refs. [15,16]. However, the typically large number of discretized continuum states limits these approaches to traditional shell-model calculations where an inert core is employed with phenomenological interactions.

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In this Letter, we present an *ab-initio* approach to open quantum systems using a Gamow–Hartree–Fock basis and realistic interactions [8]. We employ coupled-cluster theory [21–29] to solve the quantum many-body problem for the helium chain in this basis. Coupled-cluster techniques computationally scale much more gently with increasing system size, than exact diagonalization methods, and are therefore very well suited for open quantum systems where the number of orbitals are typically orders of magnitude larger than for closed quantum systems. Its application with Gamow basis states is based on a non-Hermitian representation of the many-body Hamiltonian. This is a rather new direction in coupled-cluster theory [30], and we report its first successful application in nuclear theory. Other *ab-initio* methods like the Green's function Monte Carlo [31] (GFMC) or the no-core shell model [32] have been employed to compute the structure of helium isotopes. Recently, ^{5}He widths were computed using GFMC [33].

This Letter is organized as follows. We first introduce coupled-cluster theory, the interaction and the model space. Second, we provide several checks to gauge the accuracy of our approach by comparison with exact diagonalization methods. Third, we perform large-scale calculations of the ground states of helium isotopes.

Method and model space. In coupled-cluster theory we make the exponential ansatz for the exact correlated ground state,

$$|\Psi\rangle = \exp(T)|\Phi_0\rangle. \tag{1}$$

Here $|\Phi_0\rangle$ is an uncorrelated reference Slater determinant which might be either the Hartree–Fock (HF) state or a naive filling of the oscillator single-particle basis. Correlations are introduced through the exponential $\exp(T)$ operating on $|\Phi_0\rangle$. The operator T is a sum of n-particle–n-hole excitation operators $T = T_1 + T_2 + \cdots$ of the form,

$$T_n = \sum_{a_1\ldots a_n,\ i_1\ldots i_n} t_{i_1\ldots i_n}^{a_1\ldots a_n} a_{a_1}^\dagger \cdots a_{a_n}^\dagger a_{i_n} \cdots a_{i_1}, \tag{2}$$

where $i_1, i_2, \ldots$ are summed over hole states and $a_1, a_2, \ldots$ are summed over particle states. One obtains the algebraic equation for the excitation amplitudes $t_{ij\ldots}^{ab\cdots}$ by left-projecting the similarity-transformed Hamiltonian with an n-particle–n-hole excited Slater determinant giving

$$\left\langle \Phi_{ij\ldots}^{ab\cdots} \right| \left(H_N \exp(T)\right)_C \left|\Phi_0\right\rangle = 0, \tag{3}$$

where the Hamiltonian (H_N) is normal-ordered with respect to the reference state Φ_0. The subscript C indicates that only connected diagrams enter. We iteratively solve the non-linear set of coupled equations (3) for the excitation amplitudes. The solutions determine the coupled-cluster correlation energy

$$E_{\mathrm{CC}} = \langle \Phi_0 | \left(H_N \exp(T)\right)_C | \Phi_0 \rangle. \tag{4}$$

In this work, we truncate the cluster operator T at the two-particle–two-hole level (CCSD), i.e. we approximate $T = T_1 + T_2$. We also investigate whether the perturbative triples correction CCSD(T) [34] improve on the CCSD results.

We construct our basis using the Berggren formalism [11] in which bound, resonant and continuum states are treated on equal footing. The Berggren basis is an analytic continuation of the usual completeness relation in the complex energy plane. The representation of the Hamiltonian in a finite Berggren basis is no longer Hermitian but rather complex symmetric, and renders the coupled-cluster equations (3) and (4) complex.

The nuclear Hamiltonian is given by

$$H = t - t_{\mathrm{CoM}} + V. \tag{5}$$

Here, t denotes the operator of the kinetic energy, and t_{CoM} is the kinetic energy of the center of mass. The nucleon–nucleon interaction V is based on chiral effective field theory within the N^{3}LO expansion [35]. This potential is a systematic momentum-space expansion to fourth order of a Lagrangian that obeys QCD symmetries. It contains high-momentum components and is therefore not suitable for the limited basis sets we employ. In order to make the calculation feasible, we construct a low-momentum interaction $V = V_{\text{low-}k}$ following the formalism outlined in [36]. We integrate out those high-momentum modes of the chiral potential that exceed the chosen momentum cutoff Λ. The construction of $V_{\text{low-}k}$ is a renormalization group transformation and therefore generates three-body forces and also forces of higher rank. These forces depend on the cutoff, and only the sum of all forces is cutoff-independent. In this work, we limit ourselves to two-body forces and use a cutoff $\Lambda = 1.9\ \mathrm{fm}^{-1}$. Below, we will see that the Helium isotopes are underbound for this value of the cutoff. This is in contrast to the Argonne Av-18 based $V_{\text{low-}k}$ which overbinds ^{3}H and ^{4}He at the same cutoff [37].

We build our coupled-cluster reference state from a single-particle basis obtained through a self-consistent Gamow-HF calculation [8]. For the helium isotopes considered in this work, the proton separation energy is typically of the order of 20–30 MeV, and protons mainly occupy deeply bound s-orbits. It is also known that in neutron-rich systems the protons become more correlated, and therefore gain additional binding compared to the case of symmetric nuclei. The situation is, however, quite different for the neutrons, where in neutron-rich systems near the dripline the separation energy is typically very small. Furthermore, neutrons in s- and p-orbits are known to build up the main part of halo densities in p-shell dripline nuclei such as in the cardinal cases of ^{6}He and ^{11}Li. Based on these observations we use harmonic oscillator wave functions (with $\hbar\omega = 20$ MeV) for the protons and for the higher partial waves ($dfghi$ partial waves) on the neutron side. For neutrons in s and p orbits, we use a complex Woods–Saxon basis where the non-resonant continuum is defined on a triangular contour in the complex k-plane (see Fig. 3 in Ref. [8] for details). Using Gauss–Legendre quadrature, the discretization of the contour has been carried out with 3 points in the interval $(0, A)$, 4 points in the interval (A, B), and 13 points in the interval (B, C). Consequently, for each of the s–p partial waves on the neutron side, we have a discretized basis built from bound, resonant, and non-resonant continuum states. For all other partial waves on the proton and neutron side, we use an oscillator basis with the energy truncation $N = 2n + l \leqslant 10$. The single-particle basis is (bi-)orthogonal for all partial waves since the Berggren basis is based on an analytical continuation of the radial functions in the