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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

Table 1
Comparison of CCSD results and triples-corrected CCSD(T) results with exact calculations for the ground states of helium isotopes. The energies E are given in MeV, and the results are displayed for different basis sets as described in the text

Method	^{3}He	^{4}He	^{5}He	^{6}He
CCSD (OSC)	−6.21	−26.19	−21.53	−20.96
CCSD (RHF)	−6.10	−26.06	−21.55	−20.99
CCSD (SC-RHF)	−6.11	−26.06	−21.55	−21.04
CCSD(T) (OSC)	−6.40	−26.30	−21.91	−22.83
CCSD(T) (RHF)	−6.35	−26.24	−21.90	−22.56
CCSD(T) (SC-RHF)	−6.34	−26.24	−21.91	−22.62
Exact	−6.45	−26.3	−22.1	−22.7

complex k-plane. This combination of complex Woods–Saxon states for low values of angular momentum and harmonic oscillator states for higher values of angular momentum captures the relevant physics and keeps the total size of the single-particle basis manageable. We find good convergence of the HF energy with respect to the number of integration points and size of our single-particle model space.

Accuracy of the coupled-cluster method. Weakly bound and resonant nuclei present a double challenge to the coupled-cluster method. First, some of the considered helium isotopes have open-shell character. Such systems are more difficult to describe within single-reference coupled-cluster methods. Second, particle-unstable nuclei like ^{5,7}He have resonant ground states. Here, the physical ground state is not the ground state of the model space we employ since scattering states might have lower energies. We develop a procedure which allows one to identify the physical state on the many-particle energy surface. Both problems are addressed in what follows.

To study the accuracy for open-shell nuclei, we compare the CCSD energies of $^{3-6}$He with exact results obtained through diagonalization. For this purpose we use a finite oscillator space, and thereby separate open-shell aspects from properties related to open systems. The exact diagonalization is only possible in a relatively small model space consisting of s, p, and d states up to the $4s3p1d$ oscillator states. The results are presented in Table 1. The CCSD calculations use a reference Slater determinant built from a spherical oscillator (OSC) basis, from a spherical spin-restricted HF basis (RHF), and from a semi-canonical HF basis in which the Fock-matrix is diagonal in the hole/hole and particle/particle subspaces (SC-RHF) [38]. The basis sets are spherically symmetric, and there is a freedom in defining a reference Slater determinant for open-shell nuclei. For a nucleus with known spin J, we define our reference state such that its total spin projection is maximal. Furthermore, the orbits with largest absolute value of the spin projection m_j are filled first. For example, for ^{6}He we place the two outermost neutrons in the $m_j = 3/2, -3/2$ orbitals for the ground state calculation. In Table 1 we compare the results from diagonalization with the CCSD results and with triples-corrected results (CCSD(T)). The perturbative triples corrections are calculated using converged T_1 and T_2 amplitudes. For $^{3-5}$He the CCSD results differ by not more than 500 keV from the exact results. Triples corrections improve this deviation to 200 keV (or less). For the open-shell nucleus ^{6}He, the CCSD results differ by 1.7 MeV from the exact result, including triples correction the error decreases to 200 keV.

Using different basis sets, the CCSD(T) results for $^{3-5}$He do not vary by more than ~ 60 keV, indicating improved convergence with CCSD(T). However, for ^{6}He the CCSD(T) results vary by ~ 300 keV for the different basis sets used. This indicates that the perturbative triples correction CCSD(T) is less suitable for the nucleus ^{6}He, and that the triples clusters have to be treated more accurately for truly open-shell nuclei [39,40], for which a state with definite spin cannot be constructed from a single Slater determinant.

To study the accuracy of CCSD for particle-unstable nuclei, we consider the problem of ^{7}He (using a ^{4}He core) and compare with exact diagonalizations. Recall that the resonant state is embedded in a (quasi)continuum of scattering states. Thus, one must construct a procedure to identify it. Within CCSD, we use a reference state built from bound and resonant single-particle orbitals. Therefore, the reference state is a localized state in the Gamow-HF basis and the CCSD correlations are built upon it. Our model space for ^{7}He consists of one $p_{3/2}$ resonance and eight non-resonant $p_{3/2}$ continuum states above the ^{4}He core. The exact diagonalization yields a resonant state at energy $E = 2.37$ MeV and width $\Gamma = 0.23$ MeV, our CCSD result deviates from this result by less than 10 keV. We also checked that the results in this Letter show good convergence with respect to the number of discretization points of the contour, with respect to changes of the oscillator frequency of the basis states, and the center of mass. We estimate the error due to the limited discretization, to be within 100 keV for the real part and 20 keV for the imaginary part of the energy. The results presented in the last three paragraphs demonstrate that the CCSD calculations are very accurate and meet benchmarks from exact diagonalizations.

Results. We now turn to large-scale CCSD calculations for $^{3-10}$He isotopes. Table 2 presents CCSD ground state energies for the $^{3-10}$He isotopes for increasing number of partial waves. In our largest calculation (s–i) we include $5s5p5d4f4g4h4i$ proton orbitals and $20s20p5d4f4g4h4i$ neutron orbitals. The s and p orbitals are taken from the Berggren basis. Continuum d states do not contribute to the results. As a check we calculated the ground state energies of ^{5}He and ^{8}He using 20 continuum states for the $d_{5/2}$ and $d_{3/2}$ partial waves in the s–d model-space. For ^{5}He we obtained $E = -23.71 - 0.19i$ and for ^{8}He we obtained $E = -23.14 - 0.00i$ which should be compared to $E = -23.56 - 0.20i$ and $E = -23.07 - 0.00i$ respectively (see Table 2). It is seen that the effect of d-continuum states is negligible for the width and very small for the real part of the energy. The additional binding ~ 100 keV we obtain using d-continuum is an effect from having a more complete basis compared to our calculations using the limited oscillator basis with the energy truncation $N = 2n + l \leqslant 10$.

Our CCSD calculations show excellent convergence with respect to the single-particle basis size. Here, we report convergence within 10 keV for the real part and within 0.1 keV for

Table 2
CCSD calculation of the $^{3-10}$He ground states with the low-momentum N^{3}LO nucleon–nucleon interaction for increasing number partial waves. The energies E are given in MeV for both real and imaginary parts. Experimental data are from Ref. [42]. Our calculated width of ^{10}He is ≈ 0.002 MeV

lj	^{3}He		^{4}He		^{5}He		^{6}He		^{7}He		^{8}He		^{9}He		^{10}He	
	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]
s–p	−4.94	−0.00	−24.97	−0.00	−20.33	−0.56	−19.07	−0.18	−17.09	−0.25	−17.02	−0.01	−15.44	−0.28	−13.86	−0.14
s–d	−6.44	−0.00	−26.61	−0.00	−23.56	−0.20	−23.25	−0.07	−22.22	−0.09	−23.07	−0.00	−21.58	−0.13	−20.69	0.00
s–f	−6.82	−0.00	−27.27	−0.00	−24.53	−0.16	−24.69	−0.07	−24.19	−0.10	−25.44	−0.00	−24.16	−0.05	−23.67	−0.00
s–g	−6.91	−0.00	−27.35	−0.00	−24.84	−0.15	−25.17	−0.08	−24.90	−0.12	−26.25	−0.00	−25.10	−0.04	−24.77	−0.00
s–h	−6.92	−0.00	−27.37	−0.00	−24.90	−0.15	−25.28	−0.09	−25.08	−0.13	−26.45	−0.00	−25.34	−0.03	−25.05	−0.00
s–i	−6.92	−0.00	−27.37	−0.00	−24.91	−0.15	−25.31	−0.09	−25.11	−0.13	−26.49	−0.00	−25.38	−0.03	−25.10	−0.00
Expt.	−7.72	0.00	−28.30	0.00	−27.41	−0.33(2)	−29.27	0.00	−28.83	−0.08(2)	−31.41	0.00	−30.14	−0.05(3)	−30.34	−0.09(6)

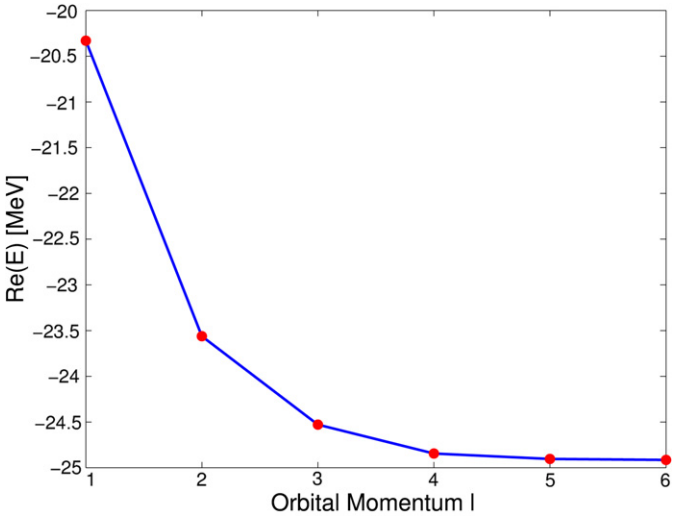

Fig. 1. Convergence of the real part of the ^{5}He ground state as function of the maximum orbital momentum that can be reached for a given model space. See text for further details.

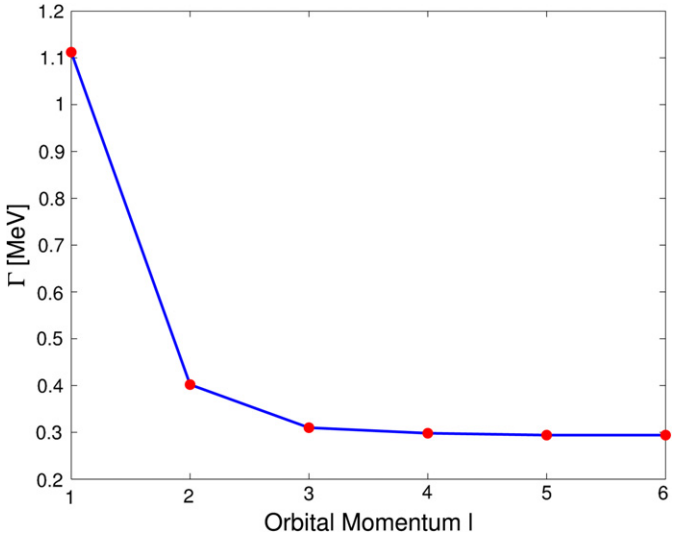

Fig. 2. Convergence of the imaginary part of the ^{5}He ground state as function of the maximum orbital momentum that can be reached for a given model space. See text for further details.

the imaginary part of the ground state energy. Our results show that for s- and p-shell nuclei the number of partial waves in the basis can be truncated at $l = 5/6$, at least for the ground state. Our largest calculation of ^{10}He with ~ 850 active single particle orbitals, would correspond to a shell model dimension of $\sim 10^{22}$. In Figs. 1 and 2 we show the convergence of the real and imaginary parts of the ground state energy of ^{5}He, with increasing number of partial waves in the basis. The computed decay widths of the helium isotopes are in semi-quantitative agreement with experiment. The comparison of binding energies shows that ^{5}He and ^{7}He are unstable with respect to one-neutron emission, while ^{8}He is stable with respect to the emission of up to three neutrons. The Borromean nucleus ^{6}He is stable with respect to one-neutron emission but unstable with respect to two-neutron emission. It has a nonzero decay width. All helium isotopes are unstable with respect to ^{4}He plus residual neutrons in the continuum. (We recall that CCSD can only capture the emission of up to two nucleons.) The pattern of binding energies and the unstable ^{6}He is in qualitative agreement with GFMC results for helium isotopes obtained with the two-nucleon potential Argonne Av18 [41]. The underbinding should be overcome by the inclusion of three-nucleon forces (3NFs). In dilute and neutron-rich systems, the short-range contact terms of the 3NF play a minor role compared to the two-pion exchange terms. The latter are on average attractive for commonly employed nucleon–nucleon potentials (with cutoffs not too small) [37,41]. Since our results are essentially converged for a two-body Hamiltonian, the observed discrepancy between theory and experiment is most likely due to neglected three-body interactions.

We have also computed the ground state expectation value of J^2. In the case of exact or variationally determined wave functions, the expectation value of an operator O can be evaluated via the Hellmann–Feynman theorem, $\frac{dE}{d\lambda}|_{\lambda=0} = \langle\psi(0)|O|\psi(0)\rangle$ by adding the small perturbation λO to the Hamiltonian. Thus, we are using the Hellmann–Feynman theorem to compute the expectation value of J. This is somewhat problematic since the applicability of this theorem rests on a variational principle. Recall that coupled-cluster theory is neither variational nor exact whenever truncations are made to the particle-hole excitation operator T. However, the Hellmann–Feynman theorem is *effectively* fulfilled provided the ground state is determined with sufficient accuracy [43]. Thus, the expectation value of J is another indicator for the quality of our calculations. We find that the spins of all nuclei are well reproduced (to about one part in 1000) compared with experimental

values, except for ^{6}He where the CCSD result is $J = 0.6$. It seems that a full inclusion of three-particle–three-hole clusters would be needed to improve this expectation value. To validate this hypothesis we did a full CCSDT calculation for the ground state of ^{6}He with the oscillator basis used in the results reported in Table 1. A full CCSDT calculation is not yet possible for the model spaces employed in Table 2. In the full CCSDT calculation of ^{6}He the expectation value of J came down to $J \sim 0.04$. Since the inaccuracy of the CCSD ^{6}He ground state wave function is an effect coming from the open-shell character and not from the proximity of continuum, these findings should be basis independent. We also performed calculations using the iterative and self-consistent CCSDT-n ($n = 1, 2, 3$) [44] approaches, where the triples are treated in increasingly sophisticated ways. The CCSDT-n approaches yields the improved result $J \approx 0.3$. The perturbative triples correction CCSD(T) gives $J \approx 0.6$ and did not improve on the expectation value of J compared to CCSD. Thus, the CCSDT result for ^{6}He shows that this is a very accurate representation of the exact wave function.

In summary, we applied coupled-cluster theory for the *ab-initio* description of loosely bound and unbound nuclei. This is the first time that decay widths have been computed in an *ab-initio* way for an isotopic chain. The decay widths of unbound nuclei are in semi-quantitative agreement with experimental data, and the binding energies meet expectations for *ab-initio* calculations based on two-body Hamiltonians. The calculated masses follow the experimental pattern where ^{5,7,9}He are unstable with respect to one-neutron emission and ^{6,8}He stable with respect to one-neutron emission. For small model spaces we verified that the employed CCSD approximation agrees well with results from exact diagonalizations, and that CCSD(T) corrections improve our open-shell results. Our CCSD(T) results for ^{6}He indicate that nuclei with a truly open-shell character are more difficult to treat. The inclusion of three-nucleon clusters and three-nucleon forces is under way. With the inclusion of the latter we may hopefully be able to tell how much of the spectrum is driven by a coupling to resonances and the non-resonant continuum and how much is due to possible three-nucleon forces.

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