Coupled-Cluster calculation of the $^{3-5}$He isotopes with Gamow-Hartree-Fock basis

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We present *ab-initio* CCSD calculations of the $^{3-5}$He ground states. We perform these calculations using a mixed basis of oscillator- and complex Woods-Saxon states for chosen partial waves. From this starting point we build a spherical Gamow-Hartree-Fock basis from a renormalized interaction of the low-momentum type generated from the N^{3}LO two-body potential. The Gamow-Hartree-Fock basis, which is a Berggren basis, treats bound, resonant and continuum states on an equal footing, and is therefore optimal for the description of nuclear states which may be embedded in the continuum. Within this *ab-initio* approach we are able to calculate that $^{3-4}$He are stable against particle decay, while ^{5}He has a non-neglible width and is therefore unstable with respect to one neutron emission, as is the case experimentally. We illustrate from these calculations that the CCSD approach is as accurate for closed shell nuclei as for open shell nuclei with ± 1 nucleon outside a closed shell. Finally, we perform various tests on the convergence of our CCSD results. We find that our results are well converged with respect to basis size and discretization of the continuum integral defining our Berggren basis.

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I. INTRODUCTION

In nuclear physics one would ideally like to start from nucleon degrees of freedom. The dominant philosophy within the nuclear theory community is that the nucleus (at low energies) as a whole may be fully described in terms of the the interactions between these constituents. *ab-initio* methods such as the Green's Function Monte Carlo (GFMC) approach [1–6], and the large-basis no-core Shell Model (NCSM) approach [7–10] have been successfully applied to the description of light nuclei. However, both approaches have limitations with respect to basis size and the number of active nucleons in the systems. More importantly, these methods have not been utilized to investigate nuclear widths in unstable nuclei.

It is well known that quantum systems with a tendency to decay by emission of fragments can not be described as closed quantum systems, in which particles are trapped in an infinite well such as a harmonic oscillator. In exotic nuclei near the driplines the outermost nucleons are mainly occupying loosely bound or unbound single-particle orbitals, resulting in matter densities with halo characteristics. Such matter densities can not easily be described by the use oscillator functions which do not display the correct asymptotic behaviour. A proper description of loosely bound and unbound nuclei should take into account the coupling of the internal with the external environment. The coupling of the 'external' continuum of positive energy states, with the 'internal' nuclear states has for a long time been a basic ingredient in nuclear reaction theory. Feshbach was the first to formulate a unified description of direct and compound nuclear reactions within the projection operator method [11, 12]. He showed that the coupling of the internal with the external environments could give rise to compound nuclear states, such as multi-channel resonances. Also, in atomic physics Feshbach resonances are of great importance. In the early 60's, at the same time as Feshbach's work, Fano [13] discussed how the mixing of a configuration belonging to a discrete spectrum with configurations belonging to a continuous spectrum gives rise to the phenomena of *autoionization*, which is considered a multi-channel resonance.

In nuclear physics, the Gamow shell model [14–23] has proven to be a reliable tool in the description of nuclei where continuum aspects play a dominant role. The basic idea in the Gamow shell model approach is to construct a many-body basis from a generalized single-particle basis which treats bound, resonant and continuum states on equal footing. Berggren was the first to rigorously derive such a basis [24]. The Berggren basis is an analytic continuation of the usual completeness relation in the complex energy plane. Recently, we reported the first results on loosely bound and resonant states in nuclei, starting from a realistic interaction and a Gamow - Hartree - Fock basis [25]. However, an *ab-initio* description of such nuclei within the Gamow shell model approach might presently not be feasible since the computational cost scales combinatorially with the number orbitals, and one typically needs large number of orbitals for each partial wave in order to discretize the continuum integral accurately.

In order to be able to provide an *ab-initio* description of nuclei with loosely bound and unbound characteristics we may need to depart from standard matrix diagonaliztion methods. In this work we discuss the *coupled-cluster* method [26–33] as a starting point for description of exotic nuclei. Computational scaling of the coupled-cluster method enables one to reach accurate reasults in extremely large model spaces. At the coupled-clusters in singles and

doubles (CCSD) level, floating-point operation counts scale as $n_o^2 n_u^4$, where n_0 is the number of occupied orbitals and n_u is the number of unoccupied orbitals in the single-particle basis. Such soft scaling when compared to the nearly combinatorial scaling of diagonalization procedures (as a function of basis size and/or particle number) allows one to build an extension of *ab-initio* description of nuclei to the medium mass region starting with nucleon degrees of freedom. The coupled-cluster method is also capable of systematic improvements and amenable to parallel computing.

The outline of this paper is the following. In Sec. II we give a brief outline of the coupled-cluster theory. In Sec. III it is discussed how one may derive a renormalized interaction of the low-momentum type (V_{low-k}) from similarity transformation techniques. In Sec. IV it is outlined how a Gamow-Hartree-Fock basis may be derived from the bare nucleon-nucleon interaction, and in Sec. V we present CCSD results of the ground states of the $^{3-5}$He isotopes using a Gamow-Hartree-Fock basis. Convergence with respect to basis size and number of discretization points is also analysed. Finally, in Sec. VI we conclude and mention future perspectives for this work.

II. COUPLED-CLUSTER THEORY

In coupled cluster theory we make an exponential ansatz for the exact correlated ground-state expressed through,

$$\hat{H}|\Psi\rangle = \hat{H}\exp(T)|\Phi_0\rangle = E\exp(T)|\Phi_0\rangle, \tag{1}$$

here $|\Phi_0\rangle$ is a chosen non-correlated reference Slater-determinant such as for example the Hartree-Fock state. The fully correlated many-body state $|\ \Psi\rangle$ is constructed by letting the correlation operator $\exp(T)$ operate on Φ_0. The operator T is a linear combination of n-particle-$n$hole excitation operators $T = T_1 + T_2 + ...$ of the form,

$$T_n = \sum_{ab\ldots,ij\ldots} t_{ij\ldots}^{ab\cdots} a_a^\dagger a_b^\dagger \cdots a_j a_i. \tag{2}$$

In order to derive the coupled-cluster equations we start by rewriting the Hamiltonian in normal-ordered form,

$$H = \sum_{pq} f_{pq}\left\{a_p^\dagger a_q\right\} + \frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle\left\{a_p^\dagger a_q^\dagger a_s a_r\right\} + \langle\Phi_0|H|\Phi_0\rangle = H_N + E_0, \tag{3}$$

here H_N is the normal ordered part of H and E_0 is just the vacuum expectation value of H. The Fock matrix element f_{pq} is given by,

$$f_{pq} = \langle p|t|q\rangle + \sum_i \langle pi||ri\rangle. \tag{4}$$

Using the normal ordered Hamiltonian and projecting Eq. 1 from the left with $\langle\Phi_0|\exp(-T)$ gives an equation for the coupled cluster correlation energy,

$$E_{\rm CC} = \langle\Phi_0|\exp(-T)\hat{H}_N\exp(T)|\Phi_0\rangle. \tag{5}$$

This equation may be simplified by using the Hausdorff commutator expansion of the similarity transformed Hamiltonian $\exp(-T)\hat{H}_N\exp(T)$, which truncates exactly at quadruply nested commutators for a two-body Hamiltonian. Using Wick's theorem for the commutators it may be shown that the only nonzero terms in the Hausdorff expansion are those in which H_N has at least one contraction with every cluster operator on its right, which is expressed through,

$$\exp(-T)\hat{H}_N\exp(T)|\Phi_0\rangle = \left[H_N\exp(T)\right]_C|\Phi_0\rangle. \tag{6}$$

here C indicates terms in which the Hamiltonian is connected to every cluster operator on its right. The equation for the Coupled-Cluser energy is then simply given by,

$$E_{\rm CC} = \langle\Phi_0|\left[H_N T_1 + \frac{1}{2}H_N T_2 + \frac{1}{2}H_N T_1^2\right]_C|\Phi_0\rangle = \sum_{ia} f_{ia}t_i^a + \frac{1}{4}\sum_{abij}\langle ij||ab\rangle t_{ij}^{ab} + \frac{1}{2}\sum_{ijab}\langle ij||ab\rangle t_i^a t_j^b. \tag{7}$$

This equation for the coupled-cluster correlation energy is an exact result which holds for two-body Hamiltonians and is independent of any truncations of the correlation operator T. In order to evaluate the coupled-cluster correlation energy it is obvious that we need to determine the $1p-1h$ and $2p-2h$ excitation amplitudes, t_i^a and t_{ij}^{ab}, appearing in Eq. 7. Although only t_i^a and t_{ij}^{ab} amplitudes appear in the energy expression in Eq. 7, the higher order cluster equations will modify the equations for t_i^a and t_{ij}^{ab} and therefore indirectly the coupled cluster energy equation. The algebraic

equation for the excitation amplitudes $t_{ij\ldots}^{ab\cdots}$ are obtained by left-projecting the similiarity transformed Hamiltonian with an n-particle-$n$hole excited Slater determinant giving

$$\langle \Phi_{ij\ldots}^{ab\cdots} | \left[H_N \exp(T) \right]_C | \Phi_0 \rangle = 0, \tag{8}$$

When written in its full glory one ends up with a non-linear set of equations for the excitation amplitudes. The derivation of the amplitude equations is a tedious task using Wick's theorem, but using a diagrammatic technique the amplitude and energy equations may be written down much more easily. The amplitude equations are nonlinear, and may be solved iteratively using convergence accelerators such as the direct inversion in the iterative subspace (DIIS) [34] technique or Krylov subspace accelerated inexact Newton (KAIN) techniques [35]. In our coupled-cluster calculations of open-shell nuclei we have found that convergence is considerably much more difficult to obtain than for closed shell nuclei. However, combining the iterative convergence accelerators with step-restriction and line-search in each iteration, convergence can be obtained within a reasonable number of iterations. Approximations in coupled-cluster theory appear only when the linear series is truncated at a level T_n, where n is smaller than the number of particles in the systemm, and in this work we report results for the $^{3-5}$He isotopes truncating the correlation operator T at the CCSD level. We note that even though the T-operator is truncated at $2p-2h$, the exponential ansatz indirectly induces higher excitations since we have products of T_1 and T_2 operators, when expanding the exponential.

III. RENORMALIZED NUCLEON-NUCLEON INTERACTION OF THE LOW-MOMENTUM TYPE.

The nuclear many-body Hamiltonian we work with is given by,

$$H = T - T_{\rm CoM} = \left(1 - \frac{1}{A}\right) \sum_{i=1}^{A} \frac{\mathbf{k}_i^2}{2m} + \sum_{i<j}^{A} \left(V(i,j) - \frac{\mathbf{k}_i \cdot \mathbf{k}_j}{mA} \right), \tag{9}$$

here V is the nucleon-nucleon interaction given by the N^{3}LO effective field theory expansion [36], based on chiral perturbation theory next-to-next-to-next-to-leading order. One would need huge basis sets in order to capture the high momentum modes of the interaction and achieve convergence for energies and wave functions. In order to make calculation feasible, the nucleon-nucleon interaction has to be renormalized in order to soften the core of the interaction. In this work we construct a renormalized interaction following the scheme outlined in [37–41]. We construct an effective interaction where the high momentum modes of the full two-body interaction have been integrated out. This interaction has become known as $V_{\rm low-k}$. $V_{\rm low-k}$ is energy and nucleus independent, and reproduces exactly nucleon-nucleon data below a cutoff Λ determining the border between low and high momentum modes.

In the following we briefly outline how to obtain a Hermitian interaction $V_{\rm low-k}$ based on the similarity transformation discussed in Refs. [38, 39, 42, 43]. A unitary transformation can be parametrized in terms of the model space P and the excluded space Q via

$$U = \begin{pmatrix} P(1+\omega^\dagger\omega)^{-1/2}P & -P\omega^\dagger(1+\omega\omega^\dagger)^{-1/2}Q \\ Q\omega(1+\omega^\dagger\omega)^{-1/2}P & Q(1+\omega\omega^\dagger)^{-1/2}Q \end{pmatrix}, \tag{10}$$

where the wave operator ω is defined to satisfy the condition

$$\omega = Q\omega P, \tag{11}$$

the so-called decoupling condition [44]. Note that the unitary transformation is by no means unique. In fact, one can construct infinitely many different unitary transformations which decouple the P and the Q subspaces, as discussed by Kuo *et al* [45]. The above transformation depends only on the operator ω which mixes the P and Q subspaces and is in some sense "the minimal possible" unitary transformation. Following the method of Ref. [38], one obtains

$$U = (1 + \omega - \omega^\dagger)(1 + \omega\omega^\dagger + \omega^\dagger\omega)^{-1/2}. \tag{12}$$

The operator U leads to the effective interaction $\tilde{V}$ using the definition

$$\tilde{V} = U^{-1}(T+V)U - T, \tag{13}$$

where T is the kinetic energy of the nucleons and V is the free nucleon-nucleon interaction. If we can determine the wave operator ω the spectrum of the effective Hamiltonian will correspond to exactly N_P eigenvalues of the full

problem. In order to derive the renormalized interaction in momentum space, one starts with the following definitions of the $P-$ and $Q-$space,

$$P = \left\{ |\bar{k}\rangle,\ |k| \leq \Lambda \right\},\ Q = \left\{ |\bar{k}\rangle,\ \Lambda < |k| < \infty \right\}. \tag{14}$$

The model space P here defines all the low-momenutm modes determined by the cutoff λ, while the complement $Q-$ space consists of the high-momentum modes. Solving the momentum space Schrödinger equation in the full space, one may obtain the solution of the wave-operator ω in a plane-wave basis and finally obtain the effective low-momentum interaction $V_{\mathrm{low-k}}$,

$$\begin{aligned} \langle \bar{k}|PV_{\mathrm{low-k}}P|\bar{k}'\rangle &= \sum_{k''}\sum_{k'''}\langle \bar{k}|P(P+\omega^{\mathrm{T}}\omega)^{1/2}P|\bar{k}''\rangle\langle \bar{k}''|P(T+V)P|\bar{k}'''\rangle\langle \bar{k}'''|P(P+\omega^{\mathrm{T}}\omega)^{-1/2}P|\bar{k}'\rangle \\ &- \frac{k^2}{m}\delta_{kk'}, \end{aligned} \tag{15}$$

where $|\bar{k}\rangle = k\sqrt{w}|k\rangle$. See Ref. [38] for further details. Typically Λ is chosen around 2 fm^{-1}, in order to capture the physics of elastic nucleon-nucleon scattering for energies < 350 MeV. However, the construction of an effective two-body interaction in a model-space for the $A-$body problem will necessarily generate three- and many-body forces. At the two-body level it has been shown that all low-momentum interactions collapse onto the same curve for a cutoff ~ 2 fm^{-1}, and therefore displays a model-independence. This is only true at the two-body level. Many-body calculations starting with a two-body low-momentum interaction display a considerable dependence on the particular interaction model from which it was derived. Further, many-body calculations starting with a two-body low-momentum interaction typically gives rise to considerable cutoff dependence and over-binding, especially in the medium mass regimes. The model-independence can only be restored at the A-body level by introducing all $A-$ body effective interactions generated through a similarity transformation of the A-body problem. The hope is that three-body effective interactions are sufficient to restore model-independence, and that they can be treated perturbatively. Preliminary CCSD results for the ground state of ^{16}O indicates that the low-momentum three-body force is indeed repulsive and can be treated perturbatively [46]. However, in this work we have truncated the Hamiltonian at the two-body level and neglect the effect of three-body forces. For all results reported in this work we constructed our low-momentum interaction from the N^{3}LO potential at a cotoff of $\Lambda = 2$ fm^{-1}.

IV. GAMOW-HARTREE-FOCK SINGLE-PARTICLE BASIS

In our study of ^{5}He which is an unbound nucleus, the single-particle basis has to be constructed in such a way that correlation effects between nucleons in the scattering continuum can take place. To account for this non-neglible coupling with the continuum, we construct our basis using the Berggren formalism [24] in which bound, resonant and continuum states are treated on an equal footing. This single-particle basis is therefore optimal for construction of a many-body basis in which loosely bound and unbound nuclear states may be expanded. For our study of the $^{3-4}$He ground states a Berggren representation is not necessary since they are stable nuclei. However, we use the same Berggren basis for all nuclei studied here, so that we may be able to confirm the stability of $^{3-4}$He and the resonant character of ^{5}He.

Further, we would like to construct our single-particle basis from the self-energy of the nucleon-nucleon interaction so that our basis is optimal for the particular nucleus under study. At lowest order in perturbation theory, the self-energy is just the Hartree-Fock basis. In order to construct the Hartree-Fock basis one needs to transform the the nucleon-nucleon interaction from the relative and center of mass frame to the laboratory frame. In the case of an oscillator basis this procedes through the well-known Moshinsky transformation, for general bases the transformation is carried out with the so-called vector brackets [47–50]. If our basis is defined in the complex energy plane, the vector-bracket transformation coefficients have to be analytically continued in the complex plane. However, the vector-bracket transformation coefficients are not easily continued in the complex k-plane, and we therefore procede via the numerically and mathematically simpler route outlined in Ref. [25]. In Ref. [25] it was also illustrated how matrix elements of the nucleon-nucleon interaction may be obtained in a Berggren basis by expanding the interaction in a finite oscillator basis, i.e.

$$\langle ab|V_{\mathrm{osc}}|cd\rangle \approx \sum_{\alpha\leq\beta}^{N}\sum_{\gamma\leq\delta}^{N}\langle ab|\alpha\beta\rangle\langle\alpha\beta|V_{\mathrm{low-k}}|\gamma\delta\rangle\langle\gamma\delta|cd\rangle, \tag{16}$$

where the two-body oscillator completeness has been truncated at N for numerical purposes. Using a renormalized interaction of the low-momentum type, energies and wave functions of loosely bound and resonant systems were shown

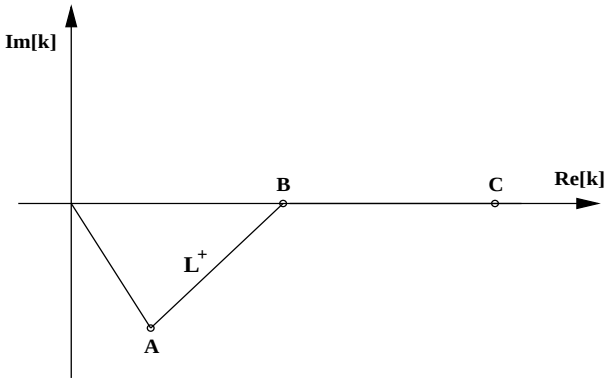

FIG. 1: Contour L_1^+ in the complex k-plane used in construction of the single-particle Berggren basis. The contour in specified by the points A, B and C discussed in the text.

to converge quickly with respect to the oscillator basis size. The fast convergence is just another illustration that renormalized interactions reduces infinite spaces to smaller model spaces, making calculations practical. From the matrix elements in Eq. 16, we may construct our Gamow-Hartree-Fock basis from

$$\langle a|h_{\rm HF}|c\rangle = \langle a|t|c\rangle + \frac{1}{\hat{j_a}^2}\sum_J\sum_h \hat{J}^2\langle ah|V_{\rm osc}|ch\rangle, \tag{17}$$

where h labels all quantum number of the proton and neutron hole states, and $\hat{J}^2 = J(J+1)$. The Hartree-Fock equation is iterated until self-consistency is obtained. One typically needs $f-g$ shells in no-core calculations in addition to including the continuum for each partial wave l the. Therefore we are calculating in an enormous many-body configuration space due to the dense discretization of the continuum integral, and even CCSD calculations become extremely computationally memory and time consuming.

To make calculations numerically feasible at present we therefore initialize our Hartree-Fock calculations with a mixed basis consisting of a finite set of Complex Woods-Saxon bound, resonant and non-resonant continuum states and a finite set of Harmonic Oscillator basis states for chosen partial waves. For protons we strictly define the space by a finite set of oscillators, while for the neutron space we use a complex Woods-Saxon basis for the $s-p$ partial waves and oscillators for the higher partial waves $d-g$. This choice of mixed basis may be justified since we are dealing with the ground states of the $^{3-5}$He isotopes. For these nuclei the proton separation energy is typically at the order of $20-30$ MeV and they are mainly occupying deeply bound s-orbits. On the other hand it is well known that the ^{5}He ground state is a resonance with width ~ 0.65MeV and with spin and parity $J^\pi = 3/2^-$, implying that the outermost neutron in ^{5}He is mainly in the $p_{3/2}$ shell.

We construct the complex Woods-Saxon basis by employing the Contour Deformation Method in momentum space, as outlined in Ref. [22]. In order to check the validity and convergence of our results, we construct our single-particle Berggren basis on two very different contours in the complex k-plane. In Figs. 1 and 2 we sketch how the two different contours L_1^+ and L_2^+ are defined respectively. The contour 1 is of triangular shape and defined by three line segments joined by the points A and B in the complex k-plane. The contour L_2^+ consists of a rotated and a translated line segment joined at the point A in the complex k-plane. Utilizing a contour of the type L_2^+, it was shown in Ref. [22] that both resonant and anti-bound states converge quickly with respect to number of integration points. Further it was shown that for the contour L_2^+, stable solutions of all physical scattering amplitudes, such as the t-matrix, may be obtained by a spectral representation of the Green's function. We discretize the contours L_1^+ and L_2^+ by Gauss-Legendre quadrature.

Ideally we would like to construct our many-body Berggren basis utilizing as few continuum states as possible. In Tabs. I and II we study the convergence of the $s_{1/2}$ hole and $p_{3/2}$ particle states in ^{4}He at the Hartree-Fock level with respect to number of integration points, using the two contours given in Figs.1and 2. The total number of integration points is given by n, while n_i gives the number of points used to discretize a given line segment on the contour. The L_1^+ contour is defined by the points $A = 1.5 - 2i$MeV and $B = 3$MeV, and the contour L_2^+ by the point $A = -2i$MeV in the complex energy plane. The corresponding points in the complex k-plane are proportional to the square root of the points in the energy plane. We see that the hole and particle energies converge to the same values for the two different contours; this is expected since the location of bound- and resonant poles in the complex k-plane is given by the pole structure of the S-matrix and not by the particular choice of contour. Further, we see that satisfactory convergence is obtained with a total number of points given by $n \sim 20$. For the proton space we used $5s5p$ oscillators

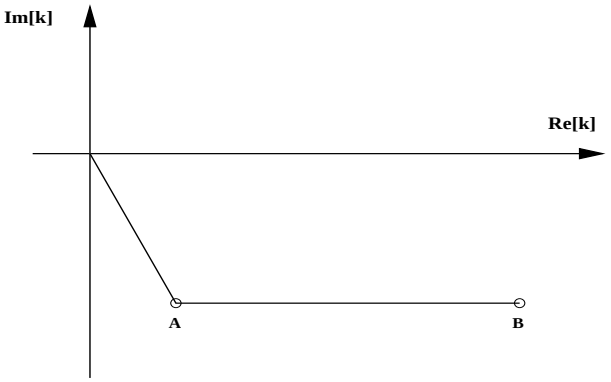

FIG. 2: Contour L_2^+ in the complex k-plane used in construction of the single-particle Berggren basis. The contour in specified by the points A and B discussed in the text.

with $\hbar\omega = 20$MeV. The $p_{3/2}$ proton state does not have a width, this is a consequence of using oscillator functions for our proton-space.

TABLE I: Convergence of the $s_{1/2}$ hole and the $p_{3/2}$ particle states in ^{4}He with increasing number of discretization points along the triangular contour L_1^+. The initial proton space was given by $5s5p$ oscillator states.

				Neutrons				Protons			
				$s_{1/2}$		$p_{3/2}$		$s_{1/2}$		$p_{3/2}$	
n	n_1	n_2	n_3	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]
15	3	3	9	-24.323	0.000	1.027	-0.536	-23.350	0.000	2.933	0.000
20	5	4	11	-24.323	0.000	1.000	-0.546	-23.350	0.000	2.930	0.000
25	7	5	13	-24.323	0.000	1.002	-0.548	-23.350	0.000	2.930	0.000
30	8	6	16	-24.323	0.000	1.002	-0.548	-23.350	0.000	2.930	0.000

TABLE II: Convergence of the $s_{1/2}$ hole and the $p_{3/2}$ particle states in ^{4}He with increasing number of discretization points along the contour L_2^+. The initial proton space was given by $5s5p$ oscillator states.

			Neutrons				Protons			
			$s_{1/2}$		$p_{3/2}$		$s_{1/2}$		$p_{3/2}$	
n	n_1	n_2	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]
15	3	12	-24.324	-0.001	1.003	-0.547	-23.352	0.001	2.926	0.001
20	4	16	-24.323	0.000	1.002	-0.547	-23.350	0.000	2.930	0.000
25	7	18	-24.323	0.000	1.002	-0.548	-23.350	0.000	2.930	0.000
30	8	16	-24.323	0.000	1.002	-0.548	-23.350	0.000	2.930	0.000

From the above numerical analysis on convergence, we choose to discretize our contour with 20 points, consequently our Gamow-Hartree-Fock basis for each of the $s-p$ partial waves are given by 20 states including bound, resonant and non-resonant continuum states. From this mixed Gamow-Hartree-Fock basis we may go ahead and construct our reference state Φ_0 which initializes our CCSD calculations.

V. CCSD RESULTS FOR $^{3-5}$HE GROUND STATES

We turn to a description of our CCSD calculations of the $^{3-5}$He isotopes. For all results reported here our renormalized low-momentum interaction was derived for a cutoff $\Lambda = 1.9$ fm^{-1} using the N^{3}LO potential. For the oscillator expansion and basis states, we used $\hbar\omega = 20$MeV.

In this paper, we present results concerning various convergence criterion and we compare to exact diagonalization of the many-body Hamiltonian using small basis sets. This will help us assess the accuracy of our CCSD results.

We first compare the CCSD energy calculations of $^{3-5}$He with results obtained through diagonalization. In order to allow for an exact solution without particle-hole truncations in the wave function we define a small model space given $4s3p1d$ oscillator states for the proton and neutron side. Our CCSD results are given both for a reference Slater determinant built from a spherical oscillator and a spherical hartree-fock basis. Since we are working with a spherical single particle basis each partial wave lj is degenerate with respect to spin projection m_j, therefore there is an ambiguity in defining a unique reference Slater determinant for open-shell nuclei. For a particular nuclei with known spin J, we define our reference state such that $M = J$, further the orbits with largest spin projection m_j are filled first. Table III reports exact results versus results obtained at the CCSD level of approximation. For the cases considered, the CCSD results do not differ more than $\sim$ 500keV from the exact results, implying that higher order corrections such as triples corrections to the coupled-cluster wave function should be small. It is also quite encouraging that the single-reference CCSD works as well for open- as for closed shell nuclei, starting with a spherical basis. Table IV gives the converged CCSD ground state energies for the $^{3-5}$He isotopes for increasing number of

TABLE III: Comparison of CCSD and exact calculations of the $^{3-5}$He ground states using the low-momentum N^{3}LO nucleon-nucleon interaction. The single particle model space consisted of $4s3p1d$ oscillator states for the proton and neutron side. The energies E are given in MeV.

Method	^{3}He	^{4}He	^{5}He
CCSD (OSC)	-6.21	-26.19	-21.53
CCSD (HF)	-6.10	-26.05	-21.52
Exact	-6.45	-26.30	-22.01

partial waves in our single particle basis. $s-p$ refers to a $5s5p$ proton and $20s20p$ neutron space, $s-d$ refers to a $5s5p5d$ proton and $20s20p5d$ neutron space, $s-f$ refers to a $5s5p5d4f$ proton and $20s20p5d4f$, and finally $s-g$ refers to a $5s5p5d4f3g$ proton and $20s20p5d4f3g$ neutron space respectively. We see that the results are reasonable

TABLE IV: CCSD calculation of the $^{3-5}$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. [51].

	^{3}He		^{4}He		^{5}He	
lj	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]
$s-p$	-4.94	0.00	-24.97	0.00	-20.08	-0.54
$s-d$	-6.42	0.00	-26.58	0.00	-23.56	-0.22
$s-f$	-6.81	0.00	-27.27	0.00	-24.56	-0.17
$s-g$	-6.91	0.00	-27.35	0.00	-24.87	-0.16
Expt.	-7.72	0.00	-28.30	0.00	-27.41	-0.33

well converged with respect to number of partial waves in our basis. Going from the $s-f$ to the $s-g$ model space we only obtain 300keV more binding for ^{5}He, while the imaginary part only changes by 10keV. Further it is seen that the exerimental binding energy of ^{3}He and ^{4}He is well reproduced using $V_{\mathrm{low-k}}$ derived from N^{3}LO and a cutoff $\Lambda = 1.9\mathrm{fm}^{-1}$, also we confirm that their ground states are stable with respect to particle emission since the calculated width is neglegible. For the ^{5}He calculation we confirm that its ground-state is unstable with respect to one-neutron emission, however the width obtained is about half that of the experimental value, $\Gamma \sim 0.65$MeV. We are also missing $\sim$ 2.5MeV for the real part of the ^{5}He ground state energy, as seen from Tab. III this can hardly be assigned to triples correction in the coupled-cluster wave function. It is more likely that the extra binding comes from three-body forces. It is however interesting to observe that we get under-binding for ^{5}He using $V_{\mathrm{low-k}}$, while for heavier closed-shell nuclei such as ^{16}O a large over-binding is typically observed.

Although our results are reasonably well converged with respect to number of partial waves in our basis, there are still other convergence aspects which must be considered. First, we have the energy truncation of the single-particle oscillator basis ($2n + l \leq 10$) and a truncation of the expansion of the interaction in Eq. 16. If our basis is complete there will be no dependence on the particular choice of $\hbar\omega$ defining the oscillator basis functions. In order to check whether the basis is complete in this sense, we performed calculations of the ^{5}He ground state in the $s-d$ space for several different values of $\hbar\omega$. In Figs. 3 and 4 we plot the real and imaginary parts of the ^{5}He ground state energy as we varied $\hbar\omega$ in the energy interval $\hbar\omega \in (14, 28)$MeV. We observe that the dependence on $\hbar\omega$ is very weak. For the real part it varies no more than $\sim$ 100 keV and for the imaginary part $\sim$ 10 keV in range of $\hbar\omega$ values. This is an indication that our basis is approximately complete, and the error introduced throug our basis truncation is smaller

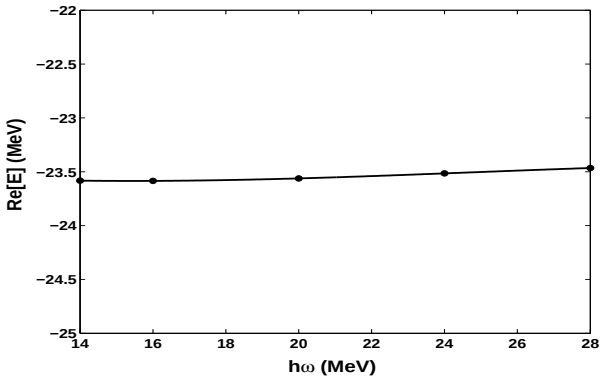

FIG. 3: $\hbar\omega$ dependence of the real part of the ^{5}He ground state energy.

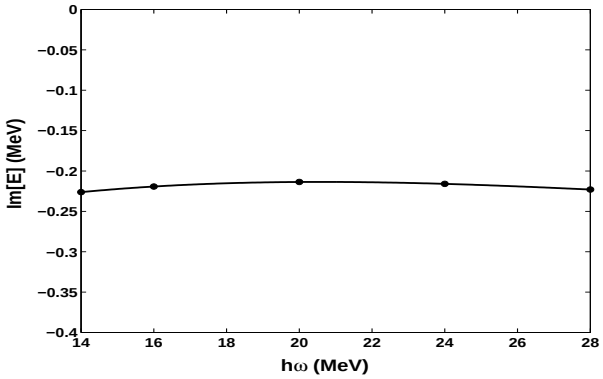

FIG. 4: $\hbar\omega$ dependence of the imaginary part of the ^{5}He ground state energy.

than the expected accuracy of the CCSD approximation.

Finally, we asses whether we have convergence with respect to the number of discretization points ($n = 20$) of the countour L_1^+, definig our complex Woods-Saxon basis. We have already shown in the previous section that the Hartree-Fock energy for ^{4}He is well converged with only $n = 20$ points. In order to check whether the CCSD energy is converged we performed calculations of the ^{5}He ground state in the $s - d$ space using the two different contours given in Figs.1 and 2. If our discretization of the contours is dense enough the two calculations should give exactly the same results for both the real- and imaginary parts of the energy. In Figs.V and 6 we give a plot of the convergence of the real and imaginary parts of the coupled cluster energy for the two different contours. It is seen that the real part of the CCSD energy differs by 10keV and the imaginary part differs by only $\sim$ 3keV, indicating that our results are well converged with respect to the number of integration points used to derive the Berggren basis for the $s - p$ neutron space.

VI. CONCLUSION AND FUTURE PERSPECTIVES.

We presented CCSD calculations of the $^{3-5}$He isotopes. Using a Gamow-Hartree-Fock basis, we depart from Hermitian to non-Hermitian representations, and are therefore able to calculate resonant widths starting with the bare nucleon-nucleon interaction and nucleon degrees of freedom. The calculated ground state energies of $^{3-4}$He are very close to experimental values using a renormalized interaction of the low-momentum type ($V_{\mathrm{low-k}}$ derived from the N^{3}LO potential. For ^{5}He ground state we are able to confirm that it is unstable with respect to one-neutron emission, we get a width $\sim$ 0.35MeV compared to the experimental value $\sim$ 0.65MeV. We have shown that single-reference CCSD is an accurate approximation for closed shell nuclei and nuclei with ± 1 nucleon outside a closed shell ,by direct comparison with exact results in a small model-space. Convergence with respect to model-space size and discretization of the deformed contour L^+ defining our Berggren-basis has been checked, and we are quite confident that our results are well converged. Future work will involve implementation of triples corrections, three-body forces and study of matter densities in loosely bound and unbound nuclei such as ^{11}Li.

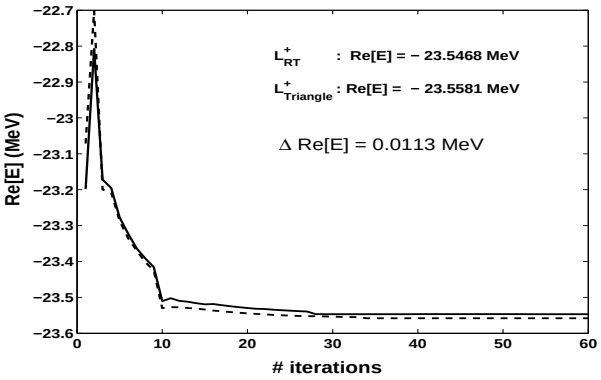

FIG. 5: Convergence of the real part of the ^{5}He ground state energy for two different contours L^+. The dashed line are represents convergence with a triangular contour and the solid for a rotated+translated contour.

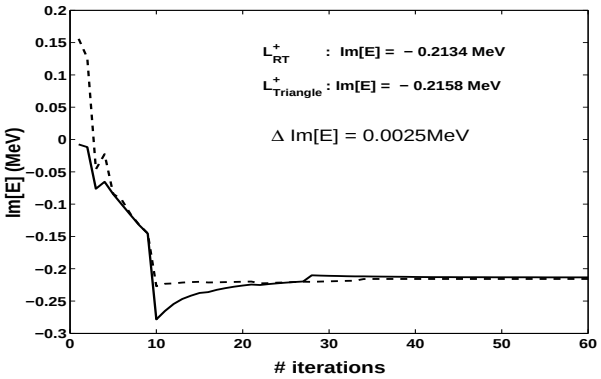

FIG. 6: Same caption as in Fig.V but for the imaginary part.

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[1] B. Pudlinger, V. Pandharipande, J. Carlson, and R. Wiringa, Phys. Rev. Lett. **74**, 4396 (1995).
[2] B. S. Pudlinger, V. R. Pandharipande, J. Carlson, S. C. Pieper, and R. B. Wiringa, Phys. Rev. C **56**, 1720 (1997).
[3] R. B. Wiringa, S. C. Pieper, J. Carlson, and V. R. Pandharipande, Phys. Rev. C **62**, 014001 (2000).
[4] S. C. Pieper and R. B. Wiringa, Ann. Rev. Nucl. Part. Sci. **51**, 53 (2001).
[5] S. C. Pieper, V. R. Pandharipande, R. B. Wiringa, and J. Carlson, Phys. Rev. C **64**, 014001 (2001).
[6] S. C. Pieper, K. Varga, and R. B. Wiringa, Phys. Rev. C **66**, 044310 (2002).
[7] P. Navrátil and B. R. Barrett, Phys. Rev. C **57**, 562 (1998).
[8] P. Navrátil, J. P. Vary, and B. R. Barrett, Phys. Rev. Lett. **84**, 5728 (2000).
[9] P. Navrátil, J. P. Vary, and B. R. Barrett, Phys. Rev. C **62**, 054311 (2000).
[10] P. Navrátil, G. P. Kamuntavicius, and B. R. Barrett, Phys. Rev. C **61**, 044001 (2000).
[11] H. Feshbach, Ann. Phys. **5**, 357 (1958).
[12] H. Feshbach, Ann. Phys. **19**, 287 (1962).
[13] U. Fano, Phys. Rev. **124**, 1866 (1961).
[14] N. Michel, W. Nazarewicz, and M. Płoszajczak, Phys. Rev. C **70**, 064313 (2004).
[15] N. Michel, W. Nazarewicz, M.Płoszajczak, and J. Rotureau, Rev. Mex. Fis. **50 Suppl. 2**, 74 (2004).
[16] J. Dobaczewski, N. Michel, W. Nazarewicz, M. Płoszajczak, and M. V. Stoitsov, nucl-th/0401034 (2004).
[17] N. Michel, W. Nazarewicz, M. Płoszajczak, and K. Bennaceur, Phys. Rev. Lett. **89**, 042502 (2002).

[18] N. Michel, W. Nazarewicz, M. Płoszajczak, and J. Okołowicz, Phys. Rev. C **67**, 054311 (2003).
[19] R. IdBetan, R. J. Liotta, N. Sandulescu, and T. Vertse, Phys. Rev. Lett. **89**, 042501 (2002).
[20] R. IdBetan, R. J. Liotta, N. Sandulescu, and T. Vertse, Phys. Rev. C **67**, 014322 (2003).
[21] R. IdBetan, R. J. Liotta, N. Sandulescu, and T. Vertse, Phys. Lett. B **584**, 48 (2004).
[22] G. Hagen, J. S. Vaagen, and M. Hjorth-Jensen, J. Phys. A: Math. Gen. **37**, 8991 (2004).
[23] G. Hagen, M. Hjorth-Jensen, and J. Vaagen, Phys. Rev. C **71**, 044314 (2005).
[24] T. Berggren, Nucl. Phys. A **109**, 265 (1968).
[25] G. Hagen, M. Hjorth-Jensen, and N. Michel, Phys. Rev. C **37**, 8991 (2006).
[26] F. Coester, Nucl. Phys. **7**, 421 (1958).
[27] F. Coester and H. Kümmel, Nucl. Phys. **17**, 477 (1960).
[28] J. Čížek, J. Chem. Phys. **45**, 4256 (1966).
[29] J. Čížek and J. Paldus, Int. J. Quantum Chem. **5**, 359 (1971).
[30] D. J. Dean and M. Hjorth-Jensen, Phys. Rev. C **69**, 054320 (2004).
[31] K. Kowalski, D. J. Dean, M. Hjorth-Jensen, T. Papenbrock, and P. Piecuch, Phys. Rev. Lett. **92**, 132501 (2004).
[32] M. Włoch, D.J.Dean, J. R. Gour, M. Hjorth-Jensen, K. Kowalski, T. Papenbrock, and P. Piecuch, Phys. Rev. Lett. **94**, 132501 (2005).
[33] J. Gour, P. Piecuch, M. Hjorth-Jensen, M. Włoch, and D.J.Dean, Phys. Rev. C **74**, 024310 (2006).
[34] P. Pulay, Chem. Phys. Lett. **73**, 393 (1980).
[35] R. J. Harrison, J. Comput. Chem. **25**, 328 (2004).
[36] D. R. Entem and R. Machleidt, Phys. Lett. B **524**, 93 (2002).
[37] S. K. Bogner, T. T. S. Kuo, and A. Schwenk, Phys. Rep. **386**, 1 (2003).
[38] S. Fujii, E. Epelbaum, H. Kamada, R. Okamoto, K. Suzuki, and W. Glöckle, Phys. Rev. C **70**, 024003 (2004).
[39] S. Fujii, R. Okamoto, and K. Suzuki, Phys. Rev. C **71**, 054301 (2004).
[40] S. Bogner, T. T. S. Kuo, L. Coraggio, A. Covello, and N. Itaco, Phys. Rev. C **65**, 051301 (2002).
[41] A. Nogga, S. K. Bogner, and A. Schwenk, Phys. Rev. C **70**, 061002 (2004).
[42] K. Suzuki, Progr.Theor.Phys. **68**, 246 (1982).
[43] K. Suzuki and R. Okamoto, Progr.Theor.Phys. **93**, 905 (1995).
[44] S. Okubo, Prog. Theor. Phys. **12**, 603 (1954).
[45] J. D. Holt, T. T. S. Kuo, and G. E. Brown, Phys. Rev. C **69**, 034329 (2004).
[46] T. Papenbrock, G. Hagen, D. Dean, and M. Hjorth-Jensen, To be published (2006).
[47] R. Balian and E.Brezin, Nuovo Cim. **61**, 403 (1969).
[48] C. W. Wong and D. M. Clement, Nucl. Phys. A **183**, 210 (1972).
[49] C. L. Kung, T. T. S. Kuo, and K. F. Ratcliff, Phys. Rev. C **19**, 1063 (1979).
[50] D. Bonatsos and H. Müther, Nucl. Phys. A **496**, 23 (1989).
[51] R. B. Firestone, V. S. Shirley, C. M. Baglin, S. Y. F. Chu, and J. Zipkin, Table of Isotopes, Eighth Edition (Wiley Interscience, New York) (1996).