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Is a trineutron resonance lower in energy than a tetraneutron resonance?

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We present quantum Monte Carlo calculations of few-neutron systems confined in external potentials based on local chiral interactions at next-to-next-to-leading order in chiral effective field theory. The energy and radial densities for these systems are calculated in different external Woods-Saxon potentials. We assume that their extrapolation to zero external-potential depth provides a quantitative estimate of three- and four-neutron resonances. The validity of this assumption is demonstrated by benchmarking with an exact diagonalization in the two-body case. We find that the extrapolated trineutron resonance — as well as the energy for shallow well depths — is lower than the tetraneutron resonance energy. This suggests that a three-neutron resonance exists below a four-neutron resonance in nature and is potentially measurable. To confirm that the relative ordering of three- and four-neutron resonances is not an artifact of the external confinement, we have tested that the odd-even staggering in the helium isotopic chain is reproduced within this approach. Finally, we discuss similarities between our results and ultra-cold Fermi gases.

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In recent years, there have been impressive theoretical and experimental investigations to determine properties of neutron-rich nuclei, including isotopic chains of oxygen, calcium, and others [1, 2]. However, understanding properties of nuclei beyond the drip-line is very challenging and intriguing. Pure neutron matter has also received much attention, as it provides a bridge between neutron-rich nuclei, through the symmetry energy, and neutron stars [3–6]. Therefore, understanding the interactions between neutrons is an important task.

This question has motivated experimental investigations of few-neutron systems. In 2002, an experimental claim for a bound tetraneutron emerged from the detection of neutron clusters from 14Be fragmentation [7]. However, this claim has not since been reproduced and it seems clear from several increasingly sophisticated studies [8–10] that a tetraneutron system must be unbound. The possibility of the existence of a tetraneutron resonance is still an open question. Recently, a candidate four-neutron resonance has been observed in the double-charge-exchange reaction 4He(5He,6Be) at an energy of (0.83 ± 0.65 ± 1.25) MeV, where the first error is statistical and the second error is systematic [11]. Several other experiments are approved to search for the tetraneutron resonance [12, 13], including a higher statistics run of the double-charge-exchange reaction [14].

On the theoretical side, regarding calculations of a possible tetraneutron resonance and their sensitivity to nuclear forces, the situation is inconclusive. Green’s Function Monte Carlo calculations [10] and No-Core-Shell-Model calculations [15] suggest that there might be a tetraneutron resonance with energy lower than about 2 MeV. Other calculations, however, suggest that in order to have a four-neutron resonance compatible with the experimental measurements above, the three-neutron interaction must be strongly modified [16], or even a four-neutron force needs to be invoked [17]. However, what still remains missing is an ab initio investigation based on two- and three-neutron interactions derived from chiral effective field theory (EFT). This Letter presents first results in this direction.

We investigate the properties of 2, 3, and 4 neutrons confined in an external potential. Our calculations provide evidence that i) nuclear Hamiltonians constructed within chiral EFT support a tetraneutron resonance at an energy of 2.1(2) MeV compatible with recent experiments, ii) because of the extreme diluteness of the system, the role of three-body (and higher-body) interactions as well as the effects of details of the regulators in the two-body systems are very small, iii) the energy of a three-neutron resonance at 1.1(2) MeV is lower than that of four neutrons, and iv) there are interesting analogies with systems made of ultra-cold fermions. These conclusions open the possibility for new experimental searches of a trineutron resonance, and that similar systems might be simulated by using ultra-cold Fermi gases.

We start our calculation from a many-body Hamiltonian that includes two- and three-nucleon interactions obtained within the framework of chiral EFT at next-to-next-to-leading-order (N2LO) recently developed in a local form [18–22]. Since the pure neutron system is unbound, we confine the neutrons in an external trap (called “neutron drops”). These systems can be very accurately solved by starting from microscopic nuclear Hamiltonians and have been extensively studied with the goal of improving energy-density functionals in extrapolating to large isospin asymmetries [23]. We model the system
starting from the Hamiltonian
\[ H = -\sum_i \frac{\hbar^2}{2m} \nabla_i^2 + \sum_i V_{WS}(r_i) + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk}, \]
where \( V_{WS}(r) = -V_0/[1 + e^{(r-R_{WS})/a}] \) is a Woods-Saxon potential with depth \( V_0 \), radius \( R_{WS} \) and diffuseness \( a = 0.65 \) fm [24], and \( V_{ij} \) and \( V_{ijk} \) are two- and three-body interactions constructed at \( N^2\)LO in Refs. [19, 21, 22]. We have checked that our results are insensitive to the precise value of the diffuseness parameter \( a \). Changing \( a \) by 20\% in either direction changes the energy by less than 1\% in the two-neutron case.

We use the auxiliary-field diffusion Monte Carlo method (AFDMC) [25] to project out the ground state from a variational trial wave function whose form is:
\[ \langle RS|\Psi_V\rangle = \langle RS|\prod_{i<j} f^c(r_{ij})\left[1 + \sum_{i<j} F_{ij} + \sum_{i<j<k} F_{ijk}\right]|\Phi_{JM}\rangle, \]
where \( |RS\rangle \) represent a collection of sampled 3A spatial coordinates and the 2A spinors of the 4 neutrons with an amplitude for the up and down spin, and \( f^c(r_{ij}) \), \( F_{ij} \), and \( F_{ijk} \) are two- and three-body spin-dependent functions that account for the short-range correlations among nucleons, see Ref. [26] for more details. \( |\Phi\rangle \) is an antisymmetric uncorrelated mean-field part that describes the correct quantum numbers and asymptotic behavior of the system. In our case, it is given by a linear combination of Slater determinants:
\[ \langle RS|\Phi_{JM}\rangle = \sum_n k_n \left[\prod_{i} D\{\phi_{\alpha}(r_i, s_i)\}\right]_{JM}, \]
\[ \phi_{\alpha}(r_i, s_i) = \Phi_{nlj}(r_i) [Y_{lm}(\hat{r}_i)\xi_{sm}(s_i)]_{jm}, \]
where \( \ldots ]_{JM} \) means a linear combination of Slater determinants coupled with Clebsch-Gordan coefficients to have the quantum numbers \( JM \). The radial components \( \Phi_{nlj} \) are obtained by solving the Hartree-Fock equations with the Skyrme force SKM [27], \( Y_{lm} \) are spherical harmonics, and \( \xi_{sm} \) are spinors in the usual up-down basis. For each \( (JM) \) set of quantum numbers there are several combinations of single-particle orbitals. In particular, we included orbitals in 1S1/2, 1P3/2, 1P1/2, 1D5/2, 2S1/2, and 1D3/2. Since for shallow external potentials the Hartree-Fock solution is unbound, we tuned the depth of the external trap (imposed on the orbitals, which is distinct from the external potential) to generate the orbitals in such a way that they are bound, and then we added an additional variational parameter to vary their width. The two- and three-body correlations as well as the coefficients \( k_n \) are obtained by minimizing the variational energy as described in Ref. [28]. The ground state of the system is finally obtained with a projection in imaginary time as \( \Psi(\tau) = \exp[-(H-E_T)\tau]|\Psi_V\rangle \), where \( E_T \) is a parameter that controls the normalization (the results are independent of the choice of \( E_T \)). In the limit of \( \tau \rightarrow \infty \) the lowest energy state with the symmetry of \( \Psi_V \) is found (for more details see Ref. [26]). One important point worth emphasizing is that the AFDMC method does not rely on a basis-set expansion. Therefore, in the infinite-volume limit, continuum states are automatically included.

We have calculated the energy of three and four neutrons for different depths \( V_0 \) and radii \( R_{WS} \). The results are summarized in Fig. 1, and they have been obtained using the local chiral potential of Ref. [22] with a cutoff of \( R_0 = 1.0 \) fm. The plot shows the energy as a function of \( V_0 \) for three (squares) and four (circles) neutrons. The blue (upper curves for various neutron numbers), green (middle curves), and red (lower curves) are the results obtained for different radii \( R_{WS} \) as indicated in the figure. The lines are quadratic fits to the energies of four (solid lines) and three (dashed lines) neutrons. The extrapolations to \( V_0 \rightarrow 0 \) obtained for the different values of \( R_{WS} \) converge to the same point, indicating that the results at zero well depth are independent of the geometry of the external potential (provided that it goes to zero at large distances, and its range is larger than the nucleon-nucleon effective range). Since we are simulating
a system that is naturally unbound, we enforce the center of mass to have no motion in order to calculate internal energies only, as is commonly done in quantum Monte Carlo calculations for nuclei, i.e., given the translationally invariant Hamiltonian, the Monte Carlo evolution is performed so that the center of mass of the system does not move.

In order to establish the role of the cutoff $R_0$ in the nucleon-nucleon interaction, and that of the three-body forces, we have repeated the calculation using $R_0 = 1.2$ fm, and turning off the three-neutron interaction. The results are indistinguishable from the cases shown in Fig. 1, within statistical errors (which are smaller than the points). Given the density of the system this is not totally unexpected, as we discuss below. Another source of systematic uncertainty comes from the truncation of the chiral expansion at $N^2$LO. To estimate this uncertainty, we have considered the case of four neutrons in the Woods-Saxon well with $R_{WS} = 6.0$ fm and repeated our calculations at leading order (LO) and next-to-leading order (NLO). Following Ref. [29], we estimate the uncertainty coming from the truncation of the chiral expansion at $N^2$LO. We add these in quadrature to the quantum Monte Carlo statistical uncertainties. These are displayed as the error bars in Fig. 1 for the case with $R_{WS} = 6.0$ fm. They are still smaller than the points, and within the uncertainties we have quoted, do not affect the extrapolated energy of the four-neutron system. The inset also shows the LO, NLO, and $N^2$LO results with uncertainties as described above. One can see that, especially near the limit where the system becomes unbound, the results are not very sensitive to the chiral order. The fits in Fig. 1 give an energy per particle of 0.37(7) MeV for three neutrons and 0.53(5) MeV for four neutrons. This suggests that there could be a trineutron resonance in nature at a lower energy than the four-neutron resonance. We have also considered the extrapolation from a different approach. We have multiplied the $N^2$LO interaction by an overall scale factor $\alpha$ and tuned $\alpha$ until the four neutrons were bound as in Ref. [30]. We find a scale factor of $\alpha \sim 1.3$ is sufficient to bind the four neutrons. We have varied $\alpha$ and performed an extrapolation similar to what is shown in Fig. 1 and found an energy for the unbound system at $\alpha = 1$ of $E = 2.0(1.0)$ MeV, which is consistent with our results coming from the trapped four neutrons.

Our results rely on the assumption that the extrapolation of the energy to the zero-depth external potential may be interpreted as a resonance energy, as suggested in Ref. [10]. To provide support for this interpretation we have designed a simple $S$-wave potential consisting of two Gaussians.

\[
V(r) = V_1 e^{-\left(\frac{r}{R_1}\right)^2} + V_2 e^{-\left(\frac{r-r_2}{R_2}\right)^2},
\]

with parameters $V_1 = -1000$ MeV, $V_2 = 865$ MeV, $R_1 = 0.4981$ fm, $R_2 = 0.2877$ fm, and $r_2 = 0.9972$ fm, such that we have an attractive well at the origin and a repulsive barrier at $\sim 1.0$ fm. This potential gives a resonance at $E_R = 1.84$ MeV with a width of $\Gamma = 0.282$ MeV.

In Fig. 2, we have diagonalized the two-body Hamiltonian with this simple $S$-wave potential plus Woods-Saxon wells of various widths and depths. Extrapolating the bound-state energies to zero well depth as in the realistic case, we have found an energy intercept $E_R = 1.83(5)$ MeV. Similarly, we have constructed a two-body interaction that does not have any resonance (a purely attractive Gaussian) and found that the Woods-Saxon depth required to bind the system is unnaturally large, and that the extrapolations for individual widths do not converge to the same energy at zero well depth. In addition, we have calculated the energy of two neutrons interacting via the chiral $N^2$LO interactions in a Woods-Saxon well, and found an extrapolation compatible with the virtual state energy of $\sim 0.1$ MeV. These exact calculations therefore provide evidence that our extrapolation method can provide meaningful resonance energies.

We have also computed the density distribution of neutrons in the trap. In Fig. 3 we show the neutron distribution inside the trap for three and four neutrons in different Woods-Saxon wells with $R_{WS} = 6$ fm, normalized such that their integral is equal to the number of neutrons. As can be seen, the density of the systems never exceeds the value of $\sim 0.01$ fm$^{-3}$ suggesting that the system is very dilute. In the case of infinite neutron matter [19, 21, 22], at such low densities the energy per neutron is totally dominated by the $S$-wave part of the neutron-neutron interaction, and the results are almost
independent of the two-body cutoff $R_0$ and the three-neutron interaction. However, it is interesting to note that in the same well the three-neutron system is always denser near the center than the four-neutron system, and the latter shows a distribution with a peak around 3 fm, suggesting that the system is arranged on a “shell”. Notably, this difference in shape between the three- and four-neutron systems persists as the geometry of the trap is changed. One possible interpretation is that in the case of three neutrons one pair (up-down) of neutrons is sitting in the center of the trap, and one extra neutron is orbiting around in a $P$ state. In the case of four neutrons, instead the two pairs are orbiting around the center, making the system less dense in the center. It would be very interesting to measure these properties by tracking the position of the neutrons. The density of four neutrons in Woods-Saxon wells with different $V_0$ and $R_{WS}$ is shown in Fig. 4. Also in this case we can verify that the systems is very dilute.

Finally, we have performed additional calculations of two to six neutrons in different wells adapted to qualitatively mimic the helium isotopes. In this model, we replace the two protons with a Woods-Saxon potential, and calculate the energy of neutrons in such a well, interacting with the $N^3$LO interaction. This model has been successfully applied to describe the oxygen isotopic chain [31]. In Fig. 5, we show the energy of the helium isotopic chain as obtained from this simplified model. The results are normalized to the $^4$He energy, which corresponds to the energy of only two neutrons in the Woods-Saxon well. Again, we keep the center of mass of the system fixed. Considering different Woods-Saxon potentials, we find in this case the expected odd-even pairing effects, i.e., the systems with odd numbers of neutrons always have higher energies than the neighboring systems with an even number of neutrons. In this case $V_0$ is strongly attractive and compared to Fig. 1 the ordering of three versus four neutron energies is reversed. For the helium isotopes, we attribute this due to the additional pairing attraction generated from interacting with the $^4$He core. The ordering, with a lower trinucler energy, changes in the region of small $V_0$ with densities are much lower than for the helium isotopes.
Our results can be interpreted from the viewpoint of ultracold atom experiments. We observe that the extrapolated resonance energies of three- and four-neutron states in Fig. 1 scale with the number of pairs, which is $N(N-1)/2$. This behavior can be qualitatively understood by considering the diluteness of the system. For large particle number $N$, the scaling with the number of pairs is consistent with the scaling of the mean-field (MF) interaction energy of a dilute gas of spin-1/2 fermions [32],

$$E_{MF} = \frac{\pi a}{m} N^2 \frac{1}{V}, \quad (5)$$

which scales as $N^2$. Here, $a$ is the two-body scattering length and $V$ is the volume. Quantum degenerate Fermi gases can also be engineered in experiments with ultracold atoms [33]. The mean-field energy of a two-component Fermi gas in a harmonic trap was measured for both signs of the scattering length using radio-frequency spectroscopy [34]. This suggests that few-neutron resonances and the transition from few- to many-body physics could be simulated in experiments with ultracold atoms. Similar experiments have already been carried out for quasi-one-dimensional systems with an impurity where it was found that systems with $N \geq 4$ majority atoms already develop a Fermi sea [35]. Moreover, experiments with ultracold atoms could be used to investigate whether the properties of the density distributions in Figs. 3 and 4 are governed by universal large-scattering length physics or details of nuclear forces.

In this Letter, we have simulated two, three and four neutrons in external potentials and extrapolated to the zero well-depth limit. These extrapolations are independent of the trap geometry since different Woods-Saxon widths converge to the same energy at zero well depth. We found a tetraneutron resonance energy in agreement with recent measurements. Taken together with the results from the simple $S$-wave potential and the results mimicking the helium isotopic chain, our results suggest that a trinucleon resonance may be lower in energy than a four-neutron resonance and therefore possibly experimentally observable. We also conclude that the effects of three-neutron interactions are very small in these systems due to their diluteness. In addition, the diluteness of these systems offers the exciting possibility to shed more light on the properties of few-neutron systems with experiments with ultracold atomic Fermi gases.

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