Charge radii of exotic neon and magnesium isotopes

S. J. Novario⁽¹⁾, ^{1,2} G. Hagen⁽¹⁾, ^{2,1} G. R. Jansen, ^{3,2} and T. Papenbrock⁽¹⁾, ²

¹Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA ²Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA ³National Center for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA

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We compute the charge radii and ground-state energies of even-mass neon and magnesium isotopes from neutron number N = 8 to the dripline. Our calculations are based on nucleon-nucleon and three-nucleon potentials from chiral effective field theory that include Δ isobars. These potentials yield an accurate saturation point and symmetry energy of nuclear matter. We use the coupled-cluster method and start from an axially symmetric reference state. Binding energies and two-neutron separation energies largely agree with data, and the dripline in neon is accurate. The computed charge radii are accurate for many isotopes where data exist. Finer details, such as isotope shifts, however, are not accurately reproduced. These chiral potentials indicate a subshell closure at N = 14 for the radii (but not for two-neutron separation energies) and a decrease in charge radii at N = 8 (observed in neon and predicted for magnesium). They yield a continued increase of charge radii as neutrons are added beyond N = 14 yet underestimate the large increase at N = 20 in magnesium.

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Introduction. The radii of atomic nuclei carry information about their structure as isotopic trends reflect changes in nuclear deformation, shell structure, superconductivity (pairing), and weak binding. The difference between the radii of the neutron and proton distributions of an atomic nucleus also impact the structure of neutron stars. Matter radii are usually extracted from reactions with strongly interacting probes, which requires a model-dependent analysis [1,2]. In contrast, electric charge radii (and more recently also weak charge radii) can be determined using the precisely known electroweak interaction [3,4]. Precision measurements of nuclear charge radii have contributed much to our understanding of stable nuclei and rare isotopes, and they continue to challenge nuclear structure theory [5–8].

In the past two decades we have seen a lot of progress in ab initio computations of nuclei, i.e., calculations that employ only controlled approximations and are based on Hamiltonians that link the nuclear many-body problem to the nucleon-nucleon and few-nucleon systems. Virtually exact methods [9–12] scale exponentially with increasing mass number and depend on the exponential increase of available computational cycles for progress. A game changer has been combining ideas and soft interactions from effective field theory (EFT) [13–18] and the renormalization group [19–21] with approximate (but systematically improvable) approaches that scale polynomially with mass number. Examples of such methods are coupled-cluster (CC) theory [22-24], in-medium similarity renormalization group [25,26], nuclear lattice EFT [27,28], symmetry-adapted shell model [29], and self-consistent Green's function approaches [30,31].

Nuclei as heavy as 100 Sn have now been computed within this *ab initio* approach [32,33], and the first *ab initio* survey

of nuclei up to mass 50 or so has appeared [34]. Computing nuclei within this framework is much more costly than using, e.g., nuclear density-functional theory [35–37]. However, the ever-increasing availability of computational cycles makes these computations both feasible and increasingly affordable.

In this Rapid Communication, we compute the charge radii of neutron-rich isotopes of neon and magnesium. These nuclei are at the center of the island of inversion [39,40] and at the focus of current experimental interests. Charge radii are known for ^{17–28}Ne [41–43] and ^{21–32}Mg [38] leaving much to explore. The experimental situation for magnesium isotopes and our theoretical calculations (described in detail below) are shown in Fig. 1. Of particular interest is the impact (or lack thereof) of the "magic" neutron numbers N = 8, 14, and 20 on charge radii, the onset of deformation past N = 20, and the rotational structure of neutron-rich isotopes as the dripline is approached [44,45].

Among the many available interactions from chiral EFT [15–17,46–50], the next-to-next-to leading order potentials NNLO_{sat} [18] and Δ NNLO_{GO} [51–53] stand out through their quality in describing nuclear radii. These interactions contain pion physics, three-nucleon forces, and—in the case of Δ NNLO_{GO}—effects of the Δ isobars. Both interactions have been constrained by data on the nucleon-nucleon interaction, and nuclei with mass numbers A = 3, 4. Although NNLO_{sat} also was constrained by binding energies and radii of nuclei as heavy as oxygen, Δ NNLO_{GO} was constrained by the binding energy, density and symmetry energy of nuclear matter at its saturation point. These potentials use the leading-order three-body forces from chiral EFT [54]. In this Rapid Communication we will employ two Δ NNLO_{GO} inter-





FIG. 1. Charge radii for magnesium isotopes with even mass numbers computed with the potentials $\Delta NNLO_{GO}(394)$ (red) and $\Delta NNLO_{GO}(450)$ (blue) compared to data (black points) [38]. The model spaces consist of 13 oscillator shells with oscillator frequencies $\hbar \omega = 12$ and 16 MeV as indicated by the bands.

actions which differ by their respective momentum cutoffs of 394 and 450 MeV c^{-1} . The interaction Δ NNLO_{GO}(394) is as soft as the 1.8/2.0(EM) interaction of Ref. [17], while Δ NNLO_{GO}(450) is as hard as NNLO_{sat} [18]. Nuclei as heavy as ¹⁰⁰Sn have been converged with the former [32,33,55], whereas the latter has been used for somewhat lighter nuclei [4,50,56–58].

Theoretical approach. Our coupled-cluster calculations start from an axially deformed product state built from natural orbitals. To construct the natural orbitals we start from a spherical harmonic-oscillator basis and perform a Hartree-Fock calculation that keeps axial, parity, and time-reversal symmetries. To obtain the axially symmetric deformed reference state we fill the partially occupied neutron and proton shells at the Fermi surface from low to high values of $|j_z|$. This creates a Hartree-Fock reference state with prolate deformation, and we checked that this state gives a lower energy than starting from an oblate reference (i.e., filling the high values of $|i_{\tau}|$ first). The self-consistent solution of the Hartree-Fock equations then yields a prolate deformed product state with the lowest energy. Following Ref. [59] we then compute the density matrix in second-order perturbation theory and diagonalize it to obtain the natural orbitals. As shown in Fig. 2 and discussed below, natural orbitals improve the convergence of the ground-state energies with respect to the number of threeparticle-three-hole (3p-3h) amplitudes in the coupled-cluster wave function.

The natural orbital basis is spanned by up to 13 spherical harmonic-oscillator shells. We present results for two different oscillator frequencies ($\hbar \omega = 12$ and 16 MeV) to gauge the model-space dependence. These values are close to the simple estimate $\omega \approx \frac{\hbar \Lambda}{2mR}$ that relates the optimal oscillator frequency to the cutoff Λ of the interaction and the radius R of the nucleus [60]. The three-nucleon interaction had the additional energy cut of $E_{3 \max} = N_1 + N_2 + N_3 \leq 16\hbar\omega$, where $N_i = 2n_i + l_i$ are single-particle energies. This cut is



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FIG. 2. Ground-state energy of ²⁰Ne with respect to the number of included 3*p*-3*h* amplitudes, computed from the Hartree-Fock basis (blue circles connected by a dashed line), and natural orbitals (red diamonds connected by a full line). For the Hartree-Fock basis we limited the number of 3*p*-3*h* excitations by the energy cut $\vec{E}_{pqr} = \tilde{e}_p + \tilde{e}_q + \tilde{e}_r < \tilde{E}_{3 \text{ max}}$, where $\tilde{e}_p = |N_p - N_F|$ is the energy difference between the single-particle energies and the Fermi surface N_F . The cut in the natural orbital basis is described in the main text. We used the $\Delta \text{NNLO}_{\text{GO}}(394)$ potential and a model space of 11 major spherical oscillator shells with the frequency $\hbar\omega = 16$ MeV. The black solid line is the experimental value, whereas the gray dashed line includes the energy gain from projection after variation of the Hartree-Fock result.

sufficient to converge the energies and radii reported in this Rapid Communication.

The breaking of rotational symmetry by the reference state is consistent with the emergent symmetry breaking and captures the correct structure of the nontrivial vacuum [61]. However, our approach lacks possible triaxial deformation and symmetry restoration for which several proposals exist [62–65]. Overcoming these limitations is, thus, possible but comes at a significant increase in computational cost: The loss of symmetries (either by permitting triaxiality or by rotating the Hamiltonian during projection) significantly increases the number of nonzero Hamiltonian matrix elements and coupled-cluster amplitudes. To estimate the impact of symmetry restoration we performed projection after variation of the deformed Hartree-Fock states for all nuclei considered in this Rapid Communication and found an energy gain from 3 to 6 MeV. This provides us with an upper limit on the energy that can be gained through symmetry restoration as we would expect that correlations beyond the mean-field partially restore broken symmetries. We note that triaxial deformations in the ground state are not expected to be significant for the nuclei we study in this Rapid Communication [66]. We finally note that the axially symmetric coupled-cluster computations are an order of magnitude more expensive than those that keep rotational invariance. Fortunately, the availability of leadership-class computing facilities and the use of graphics processor units (GPUs) now make such computations possible.

Our calculations start from the "bare" Hamiltonian,

$$H = T_{\rm kin} - T_{\rm CoM} + V_{NN} + V_{NNN} \tag{1}$$

based on the Δ NNLO_{GO} nucleon-nucleon and three-nucleon potentials V_{NN} and V_{NNN} , respectively. Here, T_{kin} denotes the kinetic energy, and we subtract the kinetic energy of the center-of-mass (CoM) T_{CoM} to remove the center of mass from the Hamiltonian. We express this Hamiltonian in terms of operators \hat{a}_p^{\dagger} and \hat{a}_q that create and annihilate a nucleon with quantum numbers p and q, respectively, in the natural orbital basis. The Hamiltonian H_N is normal ordered with respect to the reference state, and we only retain up to normalordered two-body forces; we have $H_N = F_N + V_N$ where the Fock term F_N denotes the normal-ordered one-body part and V_N the normal-ordered two-body terms [67]. We note that the normal-ordered two-body approximation breaks rotational invariance. In the case of particle-number-breaking methods a solution has been proposed in Ref. [68].

The coupled-cluster method [22–24,69–73] generates a similarity-transformed Hamiltonian,

$$\overline{H}_N \equiv e^{-\hat{T}} H_N e^{\hat{T}},\tag{2}$$

using the cluster-excitation operator,

$$\hat{T} = \hat{T}_1 + \hat{T}_2 + \hat{T}_3 \cdots$$

$$= \sum_{ia} t_i^a \hat{a}_a^\dagger \hat{a}_i + \frac{1}{4} \sum_{ijab} t_{ij}^{ab} \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i$$

$$+ \frac{1}{36} \sum_{ijkabc} t_{ijk}^{abc} \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_c^\dagger \hat{a}_k \hat{a}_j \hat{a}_i + \cdots .$$
(3)

The operator \hat{T}_n creates *n*-particle–*n*-hole excitations of the reference state $|\psi\rangle \equiv \prod_{i=1}^{A} \hat{a}_i^{\dagger} |0\rangle$. Here and in what follows, labels *i*, *j*, *k* refer to single-particle states occupied in the reference state, whereas *a*, *b*, *c* are for unoccupied states.

We truncate the expansion (3) at the 3p-3h level and include leading-order triples using the CC singles, doubles, and linearized triples (CCSDT-1) approximation [74,75]. In this approximation $e^T \approx e^{T_1+T_2} + T_3$, and the amplitudes t_i^a , t_{ij}^{abc} , and t_{ijk}^{abc} fulfill

$$\left|\psi_{ijk}^{abc}\right|(F_N\tilde{T}_3+V_N\tilde{T}_2)_{\rm con}||\psi\rangle=0.$$

In the first two lines $\hat{T} = \hat{T}_1 + \hat{T}_2$ enters the similarity transformation, which gives the commonly used CCSD approximation when $T_3 = 0$. In the last line only the connected terms enter. The correlation energy is then $E_0 = \langle \psi | \overline{H}_N | \psi \rangle$.

The CCSD approximation costs $o^2 u^4$ compute cycles for each iteration with o = A and u being the number of occupied and unoccupied states, respectively. The cost of CCSDT-1 is $o^3 u^4$ and, thus, an order of magnitude more expensive.

Both CCSD and CCSDT-1 are too expensive without further optimizations. To overcome this challenge we first take advantage of the block-diagonal structure of the Hamiltonian imposed by axial symmetry, isospin, and parity and only store and process matrix elements that obey these symmetries. Second, we impose a truncation on the allowed number of 3p-3hamplitudes by a cut on the product occupation probabilities n_p for three particles above the Fermi surface and for three holes below the Fermi surface, i.e., we require $n_a n_b n_c \leq \varepsilon$ and $(1 - n_i)(1 - n_i)(1 - n_k) \leq \varepsilon$. This cut favors configurations with large occupation probabilities near the Fermi surface and—as shown in Fig. 2—requires only a manageable number of 3p-3h amplitudes to be included. Third, we exploit the internal structure of the three-body symmetry blocks, which can be expressed as the tensor product of two- and one-body symmetry blocks, to formulate the equations as a series of matrix multiplications. This allows us to efficiently utilize the supercomputer Summit at the Oak Ridge Leadership Computing Facility, whose computational power mainly comes from GPUs.

For the computation of observables other than the energy (the radius in our case), we also need to solve the left eigenvalue problem as the similarity transformed Hamiltonian is non-Hermitian. This is performed using the equation-of-motion coupled-cluster method (EOM), see Refs. [24,72,75,76] for details. In this Rapid Communication we limit the computations of radii to the EOM-CCSD approximation level. For ³²Mg the inclusion of (computationally expensive) triples via the EOM-CCSDT-1 approximation [75] increases the radius by less than 1%, consistent with the findings of Refs. [57,77].

In EOM-CCSDT-1 the left ground-state eigenvalue problem is

$$\langle \psi | (1 + \hat{\Lambda}) \overline{H}_N = E_0 \langle \psi | (1 + \hat{\Lambda}).$$
(5)

Here $\hat{\Lambda}$ is a deexcitation operator with amplitudes Λ_a^i , Λ_{ab}^{ij} , and Λ_{abc}^{ijk} . We need to solve for

$$\begin{split} \hat{\Lambda} &= \hat{\Lambda}_1 + \hat{\Lambda}_2 + \hat{\Lambda}_3 \\ &= \sum_{ia} \Lambda_a^i \hat{a}_i^{\dagger} \hat{a}_a + \frac{1}{4} \sum_{ijab} \Lambda_{ab}^{ij} \hat{a}_i^{\dagger} \hat{a}_j^{\dagger} \hat{a}_b \hat{a}_a \\ &+ \frac{1}{36} \sum_{ijkabc} \Lambda_{abc}^{ijk} \hat{a}_i^{\dagger} \hat{a}_j^{\dagger} \hat{a}_k^{\dagger} \hat{a}_c \hat{a}_b \hat{a}_a. \end{split}$$
(6)

Given \overline{H}_N , Eq. (5) is an eigenvalue problem, and we are only interested in its ground-state solution $E = E_0$. In the EOM-CCSDT-1 approximation, the triples deexcitation part $\hat{\Lambda}_3$ only contributes to the doubles deexcitation part of the matrix-vector product via $\langle \psi | \hat{\Lambda}_3 V_N | \psi_{ab}^{ij} \rangle$, while the triples deexcitation part of the matrix-vector product is $\langle \psi | (\hat{\Lambda}_1 + \hat{\Lambda}_2)V_N + (\hat{\Lambda}_2 + \hat{\Lambda}_3)F_N | \psi_{abc}^{ijk} \rangle$. To compute the left ground state we can either solve a large-scale linear problem (because we know the ground-state energy E_0), or we use an iterative Arnoldi algorithm for general nonsymmetric eigenvalue problems to compute the ground state of \overline{H}_N . In our experience the latter approach is more stable and requires fewer iterations. The ground-state expectation value of an operator \hat{O} is

$$\langle \hat{O} \rangle \equiv \langle \psi | (1 + \hat{\Lambda}) \overline{O} | \psi \rangle. \tag{7}$$

Here the similarity-transformation $\overline{O} \equiv e^{-\hat{T}} \hat{O} e^{\hat{T}}$ of \hat{O} enters.

$$R_{\rm ch}^2 = R_p^2 + \langle r_p^2 \rangle + \frac{N}{Z} \langle r_n^2 \rangle + \langle r_{\rm DF}^2 \rangle + \langle r_{\rm SO}^2 \rangle.$$
(8)

Here, R_p^2 is the mean radius squared of the intrinsic pointproton distribution, and $\langle r_{SO}^2 \rangle$ is the spin-orbit corrections. These two quantities are actually computed with the coupledcluster method [4]. The corrections $\langle r_p^2 \rangle = 0.709 \text{ fm}^2$, $\langle r_n^2 \rangle = -0.106 \text{ fm}^2$, and $\langle r_{DF}^2 \rangle = 3/(4m^2) = 0.033 \text{ fm}^2$ (with *m* denoting the nucleon mass) are the charge radius squared of the proton (updated according to Refs. [78,79]), the neutron (updated value from Ref. [80]), and the Darwin-Foldy term, respectively.

Results. Our results for the charge radii of magnesium isotopes are shown in Fig. 1. Here, each band reflects modelspace uncertainties from using two oscillator frequencies of 12 and 16 MeV. This choice of frequencies is based on Ref. [57] where the convergence of the ⁶⁸Ni charge radius was studied in detail for similar interactions. The results for the softer interaction with a cutoff of 394 $MeVc^{-1}$ are shown in red and exhibit less model-space dependence than those for the harder interaction with 450 MeV c^{-1} shown in blue. Based on these results and our expert judgment we estimate that the uncertainties for the radii, both from the model space and the two interactions are about 2 to 3%, i.e., the full area covered by (and between) both bands. This uncertainty estimate is in line with theory error bars from similar calculations [50,52,57,58]. The experimental uncertainties are smaller than the marker size [38].

Overall, the $\Delta NNLO_{GO}$ potentials reproduce the prominent pattern of a minimum radius at the subshell closure N = 14, and they agree with data within uncertainties for mass numbers $22 \leq A \leq 30$. The computed radii continue to increase beyond N = 14, and they reflect the absence of the N = 20 shell closure in magnesium. This is, of course, the beginning of the island of inversion. However, the theory results do not reproduce the very steep increase from A = 30to 32. Thus, they seem to reflect remnants of a shell closure at N = 20 that are not seen in the data. Theory predicts increasing charge radii as the dripline is approached. This is consistent with an increase in nuclear deformation as neutrons are added [44]. We also note that theory predicts a marked shell closure at N = 8 for neutron-deficient magnesium. This is in contrast to the trend projected in Ref. [38]. The excited 2⁺ state in ¹⁸Mg at 1.6 MeV is somewhat higher that the 1.2 MeV observed in ²⁰Mg, and the question regarding a subshell closure at N = 8 is thus, undecided. It will be interesting to compare the theoretical results with upcoming laser spectroscopy experiments that are at the proposal stage [45].

The plot of isotopic variations in the charge radii, shown in Fig. 3, is interesting. Theory is not accurate regarding most isotopes shifts and overemphasizes shell closures at N = 14and N = 20 that are not in the data. This is perhaps a most important result of this study: Whereas state-of-the-art potentials and many-body methods can now describe trends of charge radii, finer details, such as isotope shifts, still escape the computations.



FIG. 3. As in Fig. 1 but for the isotope shift, i.e., the charge radii squared relative to 26 Mg. Data taken from Ref. [38].

Α

28 30 32 34 36 38 40

26

24

20 22

We show the results for binding energies in Fig. 4. Our calculations yield the dripline at 40 Mg with 42 Mg being about 1.8 MeV less bound for the Δ NNLO_{GO}(394) potential. However, computational limitations prevented us from including continuum effects, which can easily yield an additional binding energy of the order of 1 MeV [81]. This prevents us from predicting the unknown dripline in magnesium more precisely [82].

Another uncertainty stems from the lack of angular momentum projection. To estimate the corresponding energy correction, we performed a projection after variation within the Hartree-Fock computations. These projections lower the Hartree-Fock energy by about 3–5 MeV, see Fig. 2 for an example. We expect that a projection of the coupled-cluster results would yield slightly less energy gains (because these calculations already include some of the correlations that are associated with a projection). Overall, Fig. 4 shows that the $\Delta NNLO_{GO}$ potentials accurately describe nuclear binding energies also for open-shell nuclei.

Binding-energy differences, such as the two-neutron separation energy, is another observable sensitive to shell structure and dripline physics. Figure 5 shows that the overall pattern in the data is accurately reproduced within the uncertainties from the employed interactions and model spaces. Although our radii suggest a subshell closure at N = 14, neither theory



FIG. 4. As in Fig. 1 but for the ground-state energies.



FIG. 5. As in Fig. 1 but for the two-neutron separation energies.

nor data support this closure for the two-neutron separation energies.

We finally turn to neon isotopes. Here, our computations have been less extensive to manage the available computational cycles. We limited the computations of energies to the Δ NNLO_{GO}(394) potentials in a model space of 13 harmonicoscillator shells at $\hbar \omega = 16$ MeV. For the charge radii we also employed the Δ NNLO_{GO}(450) potential at $\hbar \omega = 12$ MeV. Figure 6 shows that the ground-state energies are close to the data. We estimate theoretical uncertainties to be a bit smaller than for the magnesium isotopes. We also note that about 3–5 MeV of energy gain is expected from a projection of angular momentum (see again Fig. 2). We find the dripline at ³⁴Ne, in agreement with data [83]. Our computations yield that ³⁶Ne is unbound by several MeV, too much to be changed by continuum effects.

The computed two-neutron separation energies, shown in Fig. 7, confirm this picture. Compared to magnesium, it is interesting that the addition of two protons shifts the drip line by about six neutrons. Again we estimate that theoretical uncertainties are a bit smaller than for the magnesium isotopes.

Finally, we show results for charge radii in Fig. 8 using the $\Delta NNLO_{GO}(394)$ and $\Delta NNLO_{GO}(450)$ potentials. We only



FIG. 6. Ground-state energies for neon isotopes with even mass numbers computed with the potentials $\Delta NNLO_{GO}(394)$ shown as a red line. The model spaces consist of 13 oscillator shells. Data [84] are shown as black bars.



FIG. 7. As in Fig. 6 but for the two-neutron separation energies.

employed one oscillator frequency for each interaction. Thus, the theoretical uncertainties are estimated to be somewhat larger than the area between the two lines (compare with Fig. 1 of the magnesium isotopes). Based on these estimates, theoretical results are not quite accurate below ²²Ne, although they qualitatively reproduce the overall trend. The results accurately reflect the known subshell closures at N = 14 and N = 8. We see no closure at N = 20, and it will be interesting to confront this prediction with data.

Conclusion. We computed ground-state energies, twoneutron separation energies, and charge radii for neon and magnesium isotopes. Our computations were based on nucleon-nucleon and three-nucleon potentials from chiral EFT, and we employed coupled-cluster methods that started from an axially symmetric reference state. The computed energies and radii are accurate when taking expected corrections from angular momentum projection into account. Trends in charge radii, and the minimum and neutron number N = 14are qualitatively reproduced. Within our estimated uncertainties of about 2 to 3%, however, quantitative accuracy is not



FIG. 8. Charge radii for neon isotopes with even mass numbers computed with the potentials $\Delta NNLO_{GO}(394)$ and $\Delta NNLO_{GO}(450)$ shown in red and blue, respectively. The model spaces consist of 13 oscillator shells. Data is shown as black squares with statistical and systematic uncertainties [41,42] and as gray circles with statistical uncertainties [43].

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achieved for all isotopes, and isotope shifts still challenge theory. Nevertheless, we predict a continuous increase as the neutron dripline is approached, and this is consistent with a considerable nuclear deformation. Proposed experiments will soon confront these predictions.

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