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Ground-State Properties of C, O, and Ne Isotopes in Hartree–Fock–Bogoliubov Calculation with Gogny Interaction*

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Abstract *Ground-state properties of C, O, and Ne isotopes are described in the framework of Hartree–Fock–Bogoliubov theory with density-dependent finite-range Gogny interaction D1S. We include all the contributions to the Hartree–Fock and pairing field arising from Gogny and Coulomb interaction as well as the center of mass correction in the numerical calculations. These ground-state properties of C, O, and Ne isotopes are compared with available experimental results, Hartree–Fock plus BCS, shell model and relativistic Hartree–Bogoliubov calculations. The agreement between experiments and our theoretical results is pretty well. The predicted drip-line is dependent strongly on the model and effective interaction due to their sensitivity to various theoretical details. The calculations predict no evidence for halo structure predicted for C, O, and Ne isotopes in a previous RHB study.*

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One of the most important concepts in the many-body theory of finite Fermi system is the mean-field approach. The self-consistent mean-field theories, both conventional mean-field (Hartree–Fock–Bogoliubov) and relativistic one (relativistic Hartree–Bogoliubov), are the backbone of many-body calculation in nuclear physics and have been proven successful. For decades, the microscopic description of mean-field theory has been widely applied to various nuclear structures, such as the band termination, band crossing, shape coexistence, rotational coexistence with axial symmetry or with triaxial shapes, and highly deformed molecular resonances.

Recent experimental developments in radioactive beam, high-efficiency new gamma-ray, and charged particle detector systems[1−3] allow us to extend our research toward exotic nuclei with extreme isospin, e.g., the measurements of r.m.s radii in weakly bound nuclei give evidence for a new phenomenon — the halo structure. The ground states of exotic nuclei display many interesting properties and phenomena. For example, a fascinating result of the modification of the effective single nucleon potential in neutron rich nuclei is the observed suppression of shell effects, the disappearance of spherical magic numbers, and the resulting onset of deformation and shape coexistence. The description of experimentally observed phenomena, as well as the prediction of new and unexpected properties for these nuclei, presents an exciting challenge for modern nuclear theory.

But these weakly bound nuclei are much difficult to be treated theoretically than the well bound systems.[4] A variety of theoretical methods and techniques, such as relativistic Hartree–Bogoliubov (RHB),[5−7] Hartree–Fock plus BCS (HF+BCS)[8] and extended shell model (SM),[9,10] have been used to investigate the properties of drip-line nuclei in different mass region. The problem is, in addition to the self-consistent mean-field potential, that pairing correlations have to be included in order to describe ground state properties of drip-line nuclei. Moreover, drip-line nuclei require a careful treatment of the asymptotic part of nucleonic densities, and therefore a unified description of mean field (particle-hole) and pairing (particle-particle) correlations. For strongly bound systems pairing can be included in the simple BCS scheme in the valence shell. But this kind treatment is inappropriate for drip-line nuclei due to a leakage of nucleons into the continuum.[11] Although the mean-field theory with Skyrme interaction describes major features of nuclei quite well, the zero-range Skyrme force does not take the pairing correlations into account well. The more complicated but theoretically more satisfactory way is to include pairing self-consistently via a Hartree–Fock–Bogoliubov (HFB) calculation.

The HFB theory with finite-range Gogny force has been used to treat the Hartree–Fock mean field and pairing correlation self-consistently, although the numerical complexity is involved due to its finite range.[12] In spite of the relative simplicity of mean-field approach, some additional approximations have been commonly used to make the problem more tractable. The complication in calculations usually arise from the exchange terms, either from the Coulomb force or from some components of the effective two-body interaction itself. In most

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HFB calculation with Gogny force, however, the following approximations[13−15] have been used in the past.

(i) In HF field the Fock term of Coulomb force is neglected because the Fock Coulomb term requires a large CPU time.

(ii) Contributions to the pairing field coming from the center of mass correction, Coulomb and spin-orbit terms are neglected. Only the pairing field from Brink–Boeker term is considered.

In the present work, the ground state properties of C, O, and Ne isotopes are still discussed in the framework of Hartree–Fock–Bogoliubov with finite-range Gogny D1S interaction but with some improvements. For these elements, isotopes near the neutron drip should soon become accessible in experiments with radioactive beams[16] and will provide a test to our predictions. Our main improvements are that no approximation has been made in our numerical calculations, and that all the contributions to the Hartree–Fock and pairing field arising from Gogny and Coulomb interaction as well as the center of mass correction are included.

In our treatment, the self-consistent HFB equation is solved using three-dimensional harmonic oscillator basis with the Gogny D1S interaction,[17−19] which means that the axial and signature symmetries are simultaneously broken. To save the CPU time in the numerical calculation, we impose the $\hat{P}\,\mathrm{e}^{-\mathrm{i}\pi\hat{J}_z}$ (z-simplex) and $\hat{P}\,\mathrm{e}^{-\mathrm{i}\pi\hat{J}_y}\hat{\tau}$ ($\hat{S}_y^{\mathrm{T}}$) symmetries,[20,21] where $\hat{P}$ is the parity operator, $\mathrm{e}^{-\mathrm{i}\pi\hat{J}_i}$ the rotation operator around i axis by angle π, and $\hat{\tau}$ the time reversal operator. Due to the z-simplex and $\hat{S}_y^{\mathrm{T}}$ symmetries, the mass asymmetry of a nucleus is allowed only along the x axis.

The HFB equation to be solved is thus given as

$$\delta\langle\phi|\hat{H}-\lambda_p\hat{Z}-\lambda_n\hat{N}+\mu_x\langle\phi|\hat{x}|\phi\rangle\hat{x}|\phi\rangle=0\,, \tag{1}$$

$$\langle\phi|\hat{Z}|\phi\rangle=Z\,, \tag{2}$$

$$\langle\phi|\hat{N}|\phi\rangle=N\,, \tag{3}$$

$$\langle\phi|\hat{x}|\phi\rangle=0\,. \tag{4}$$

The chemical potentials λ_p and λ_n have to be determined by the particle number subsidiary condition in order that the expectation value of particle number operators in the ground state equals the number of nucleons. To keep the center of mass motion fixed, we impose the quadratic constrained operator $\mu_x\langle\phi|\hat{x}|\phi\rangle\hat{x}$[22] in the x-direction, where we take parameter $\mu_x=1.0\times10^{-4}[\ \mathrm{MeV}/\mathrm{fm}^2]$.

The self-consistency in mean-field theory emphasizes the potential well for nucleons computed from the nucleonic wave function. The nucleonic wave function is obtained by

$$\begin{pmatrix} h-\lambda & \Delta \\ -\Delta^* & -h^*+\lambda \end{pmatrix}\begin{pmatrix} U_k \\ V_k \end{pmatrix}=\epsilon_k\begin{pmatrix} U_k \\ V_k \end{pmatrix}, \tag{5}$$

where ϵ_k is quasi-particle energy. The Hartree–Fock mean-field Γ that encloses all the long-range particle-hole (ph) correlations, and a pairing field Δ that sums up the particle-particle (pp) correlations are defined as

$$\Gamma_{k_1k_3}=\sum_{k_2k_4}\bar{v}_{k_1k_2k_3k_4}\rho_{k_4k_2}\,, \tag{6}$$

$$\Delta_{k_1k_2}=\frac{1}{2}\sum_{k_3k_4}\bar{v}_{k_1k_2k_3k_4}\kappa_{k_3k_4}\,, \tag{7}$$

where the two-body interaction $\bar{v}_{k_1k_2k_3k_4}$ is antisymmetried, and density matrix ρ and pairing tensor κ are expressed as

$$\rho=V^*V^{\mathrm{T}}\,,\qquad \kappa=V^*U^{\mathrm{T}}\,. \tag{8}$$

With the aid of these quantities, we can express the expectation value of the nuclear Hamiltonian as

$$E=\langle\hat{H}F\rangle=\mathrm{Tr}(t\rho)+\frac{1}{2}\,\mathrm{Tr}\,(\Gamma\rho)-\frac{1}{2}\,\mathrm{Tr}\,(\Delta\kappa^*)\,. \tag{9}$$

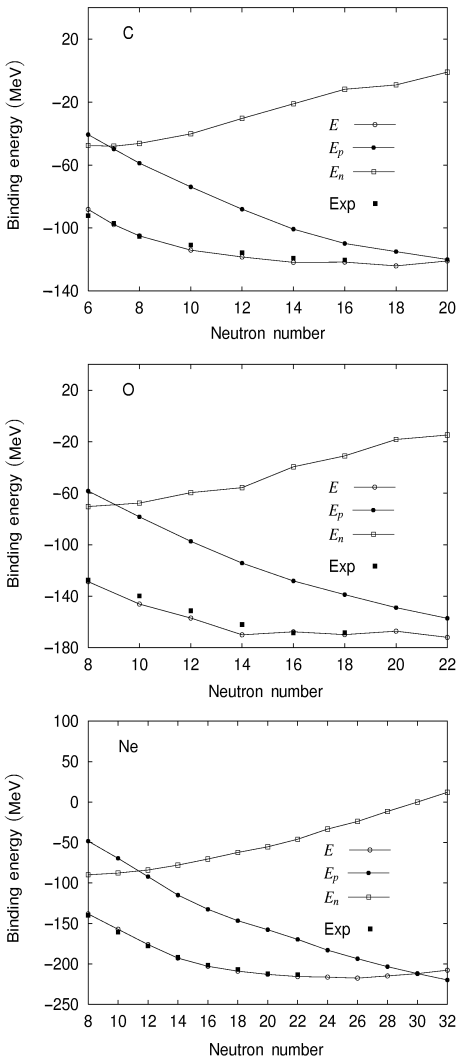

Fig. 1 Calculated total (open circle), proton (filled circle), and neutron (open square) binding energies and experimental results (filled square) for C, O, and Ne isotopes as a function of neutron number.

In our numerical calculations, the s.p. wave function has been expanded in a three-dimensional harmonic oscil-

lator basis up to the principal quantum number $N = 8$. A set of range parameters of the Hermite polynomials is optimized to produce the largest binding energy of ground HFB state. The optimized range parameters thus obtained include the effects of higher major shells. In the course of solving HFB equation, each iterative process is achieved by introducing a new density matrix and pairing tensor constructed by the former eigenvectors. A convergence is considered to be completed when the resultant density matrix and pairing tensor is equivalent to the preceding one within a given accuracy. The convergence condition is

$$\sum_{i=1}^{N} \left| \epsilon_i^{(n)} - \epsilon_i^{(n-1)} \right| \leq 0.1 \quad (\text{keV}) \,, \tag{10}$$

where $\epsilon_i^{(n)}$ is quasi-particle energy in the n-th iterations.

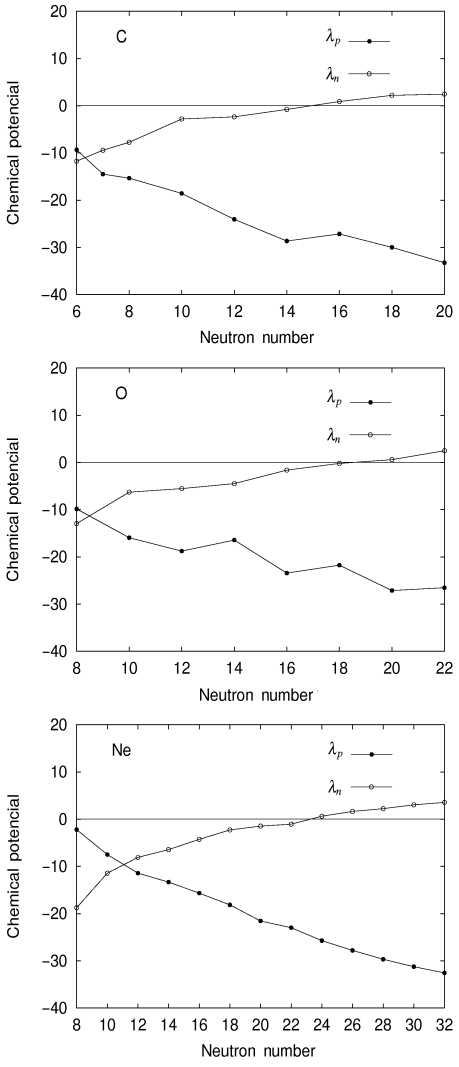

Fig. 2 Calculated proton and neutron chemical potentials for C, O, and Ne isotopes as a function of neutron number.

In Fig. 1 the total, proton and neutron binding energies are plotted as a function of neutron number for C, O, and Ne isotopes, respectively. The calculated binding energies are in good agreement with the experimental results[23] for C, O, and Ne isotopes. Proton binding energy increases smoothly as a function of neutron number, while neutron binding energy decreases although the neutron number increases. Thus, total binding energy increases first, then decreases after reaching the maximum as a function of neutron number. Since the position of two-neutron drip-line is defined by two-neutron separation energy $S_{2n}(Z,N) = E(Z,N) - E(Z,N-2) = 0$, the last stable isotopes against two-neutron emission are predicted to be ^{24}C, ^{26}O, and ^{36}Ne in our HFB calculation, as indicated by their maximal binding energy seen from Fig. 1. HF+BCS and SM calculations[8] give ^{28}O and ^{34}Ne, ^{26}O and ^{34}Ne as the last stable isotopes, respectively. Another SM calculations[10] show ^{24}O and ^{34}Ne as the last bound isotopes. Owing to their sensitivity on various theoretical details (e.g., approximations used, effective interaction, parameter values), the predicted drip-line is strongly dependent on the model and effective interaction.

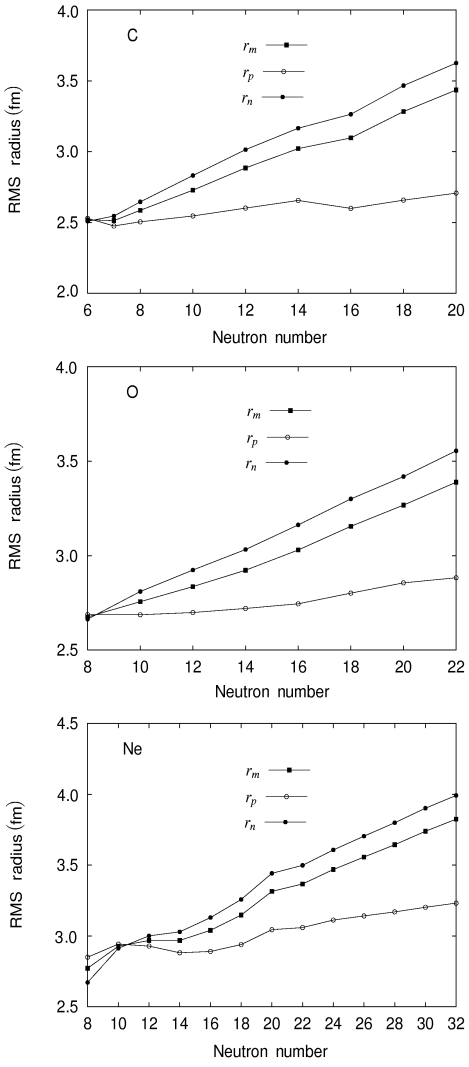

Fig. 3 Calculated RMS radius for C, O, and Ne isotopes.

Figure 2 shows the calculated proton and neutron chemical potential for C, O, and Ne isotopes. Proton chemical potential decreases as a function of neutron number, which show the proton cluster becomes tighter and tighter. The situation is just *vice versa* for neutron systems which are bound looser and looser as an increase of the neutron number. It is observed that for nuclei heavier than ^{20}C, ^{26}O, and ^{32}Ne the neutron chemical potential becomes positive. That is, for nuclei heavier than ^{20}C, ^{26}O, and ^{32}Ne, the neutron begins to escape from the potential well. For example, for the nucleus heavier than ^{32}Ne, one neutron is weakly bound and begins to freely escape from the potential well. But only for nucleus heavier than ^{34}Ne, do two neutrons start to escape from potential well, which can be seen from Fig. 1.

Some exotic nuclei far from the β stability line show halo structure, such as the first experimentally observed neutron-halo nucleus ^{11}Li.[24] The root-mean-square (rms) radii can give evidence for halo structure. Proton, neutron, and matter root-mean-square radii are shown for C, O, and Ne isotopes in Fig. 3. Neutron rms radius changes smoothly as a function of neutron number. On the other hand, proton rms radius is almost constant, and only displays a slow constant increase. For C, O, and Ne isotopes, no evidence for halo structure is found in our HFB calculations, while RHB calculations[5] show some evidence for the occurrence of neutron halo in heavier Ne isotopes.

In summary, in this work we have applied Hartree–Fock–Bogoliubov theory with finite-range Gogny interaction in an analysis of ground-state properties of C, O, Ne isotopes. These properties are compared with available experimental results, and the results from Hartree–Fock plus BCS, shell model and relativistic Hartree–Bogoliubov calculations. There is a good agreement between experiments and our theoretical calculations. The calculations predict no evidence for halo structure found for C, O, Ne drip-line nuclei. The predicted drip-line is strongly dependent on the model and effective interaction due to their sensitivity to various theoretical details.

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References

[1] J. Simpson, Nucl. Phys. **A654** (1999) 178c.

[2] A.C. Mueller, Nucl. Phys. **A654** (1999) 215c.

[3] I. Tanihata, Nucl. Phys. **A654** (1999) 235c.

[4] J. Dobaczewski and W. Nazarewicz, Phil. Trans. R. Soc. Lond. **A356** (1998) 2007.

[5] W. Pöschl, D. Vretenar, G.A. Lalazissis, and P. Ring, Phys. Rev. Lett. **79** (1997) 3841.

[6] G.A. Lalazissis, D. Vretenar, and P. Ring, Phys. Rev. **C63** (2001) 034305.

[7] D. Vretenar, G.A. Lalazissis, and P. Ring, Phys. Rev. Lett. **82** (1999) 4595.

[8] T. Siiskonen and P.O. Lipas, Phys. Rev. **C60** (1999) 034312.

[9] B.A. Brown and P.G. Hansen, Phys. Lett. **B381** (1996) 391.

[10] E. Caurier, F. Nowacki, A. Poves, and J. Retamosa, Phys. Rev. **C58** (1998) 2033.

[11] G.A. Lalazissis, D. Vretenar, P. Ring, M. Stoitsov, and L.M. Robledo, Phys. Rev. **C60** (1999) 014310.

[12] M. Anguiano, J.L. Egido, and L.M. Robledo, Nucl. Phys. **A683** (2001) 227.

[13] M. Girod, J.P. Delaroche, and J.F. Berger, Phys. Lett. **B325** (1994) 1.

[14] M. Girod and B. Grammaticos, Phys. Rev. **C27** (1983) 2317.

[15] J.L. Egido and L.M. Robledo, Phys. Rev. Lett. **70** (1993) 2876.

[16] NSCL newsletter **N21** (2001).

[17] M. Girod, J.P. Delaroche, and J.F. Berger, Phys. Lett. **B325** (1994) 1.

[18] J. Dechargé and D. Gogny, Phys. Rev. **C21** (1980) 1568.

[19] M. Girod and B. Grammaticos, Phys. Rev. **C27** (1983) 2317.

[20] J.F. Berger, M. Girod, and D. Gogny, Nucl. Phys. **A428** (1983) 23c.

[21] J. Dobaczewski, J. Dudek, S.G. Rohozinski, and T.R. Werner, Phys. Rev. **C62** (2000) 014310.

[22] J. Dobaczewski, J. Dudek, S.G. Rohozinski, and T.R. Werner, Phys. Rev. **C62** (2000) 014311.

[23] H. Flocard, P. Quentin, A.K. Kerman, and D. Vautherin, Nucl. Phys. **A203** (1973) 433.

[24] G. Audi, O. Bersillon, J. Blachot, and A.H. Wapstra, Nucl. Phys. **A624** (1997) 1.

[25] I. Tanihata, *et al.*, Phys. Rev. Lett. **55** (1985) 2676.