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Investigation on the deformation of Ne and Mg isotope chains within relativistic mean-field model*

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Ne and Mg isotope chains are investigated based on constrained calculations in the framework of a deformed relativistic mean-field (RMF) model with the NL075 parameter set. The calculated quadrupole deformation and binding energy are compared with other theoretical results as well as the available experimental data. It shows that the calculated deformations of Ne and Mg with the NL075 are more accurate than those obtained with the NL-SH. It is predicted that ^{19,29,32}Ne and ^{20,31}Mg maybe have a triaxial deformation and $^{25-28}$Ne and $^{27-30}$Mg exhibit a shape coexistence probably. The closure effect of neutron number N=8 for ^{20}Mg is predicted to be very weak.

Keywords: deformation, shape coexistence, binding energy, RMF model, constraint calculation
PACC: 2110F, 2110D, 2160J

1. Introduction

The development of unstable nuclear beam technique has opened a new field of the study of properties of unstable nuclei far from the stability line.[1−12] Up to now, most experimental studies are focused on the light nuclei due to the limitation of the technical condition. The study of properties of these nuclei is of great interest for it provides us the opportunities to understand the processes responsible for the synthesis of heavy elements. In addition, an interesting phenomenon is that these nuclei maybe experience large deformations. For example, some nuclei in Ne, Mg, Si and S chains have been experimentally confirmed to exhibit large or even super deformations.[13,14] The deformation effect may play an important role in the formation of exotic structure such as halo or skin, because the deformation may lead to an intrusion of orbits and therefore a change in the array of nucleons. Moreover, many of nuclei in this mass region have prolate and oblate shapes competing with the deformation of ground state changing with the addition of only a few nucleons, i.e. shape coexistence. Exotic properties of these nuclei provide a challenge to various theoretical models.

In the present work, the lighter Ne and Mg isotope chains from proton drip line to neutron drip line are calculated in the frame of an axially deformed rel-

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ativistic mean-field (RMF) model based on constraint calculations. It is known that Lalazissis *et al* have used the standard RMF force set NL-SH[15] or NL3[16] without inclusion of constraint calculations, to study bulk properties of the even–even Ne, Mg, Si, S, Ti, Cr and Ar nuclei.[17,18] Binding energy systematics were reproduced nicely, but the quadrupole deformation was underestimated in all cases. In addition, Mitra and Gangopadhyay studied even–even nuclei with Z=10–16 by using a generalized hybrid derivative coupling model (GHDCM) and obtained more accurate deformations[19] than those from Refs.[17,18] However, they provided too small a binding energy.

In order to improve the accuracy of calculated deformation values of these nuclei in the frame of the RMF model, we use another parameter set NL075[20] firstly, to investigate the doubly even Ne and Mg. Then we extend the calculation to the odd-A Ne and Mg, which have not been calculated systematically in the RMF model so far. The relevant results for the heavier isotope chains will be reported in the later paper.

2. Calculation

In the past decades, the RMF theory has been extensively used in the quantitative description of bulk properties in the ground states over the whole periodic table.[15,21–34] In particular, Lalazissis *et al* have used the RMF theory with constraint calculations to predict the excitation energy of nuclei with large or super deformations in the wide mass regions and achieved satisfactory results.[35]

Here, we just give a brief introduction for the RMF model. More details can be found in Refs.[15,21–34]. One should start from the local Lagrangian density for interacting nucleons, mesons and photons. The relativistic equation of motion is derived by means of the variational principle. Then the resulting Dirac equation for the baryons and the Klein-Gordon equation for the mesons are solved using the basis expansion method. Finally, Dirac spinor and meson fields are expanded in terms of the axially symmetric potential basis. In RMF calculations, we use the term $0.75 \times 41A^{1/3}$ to evaluate the correction of the additional energy due to the motion of the center of mass.[26]

The pairing correlations are considered in terms of the Bardeen–Cooper–Schrieffer (BCS) theory. For corresponding energy gap parameters, we choose the isospin dependence form proposed by Möller and Nix, $\Delta_{p(n)} = 4.8/Z(N)^{1/3}$.[36] In the present work, we use the parameter set NL075 to perform all calculations since the frequently used force sets, e.g. NL3 and NL-SH produce very small deformations.

It is possible that there are several solutions for different equilibrium deformations with almost similar energies in a nucleus. Therefore, if one calculates a nucleus only with the non-constrained RMF, to some extent, different input deformations will lead to different results although this discrepancy is not large.[37] To smooth away this problem, we should carry out the constrained calculation of the quadrupole moment for a nucleus and find out the reasonable deformation parameters. The constrained calculation is briefly introduced as follows. The new Hamiltonian $\langle H' \rangle$ instead of the previous one $\langle H \rangle$ is minimized, where $H' = H - \lambda Q$ with $Q = r^2 Y_{20}(\theta, \phi)$. Here λ is the Lagrange multiplier and it is fixed by the constraint on the quadrupole moments: $\langle Q \rangle_\lambda = Q_0$ where Q_0 is proportional to the quadrupole deformation parameter β_2: $Q_0 = (9/5\pi)^{1/2} A R_0^2 \beta_2$ with $R_0 = 1.2A^{1/3}$ fm. Then the $\langle H \rangle_\lambda$ as a function of β_2 can be obtained, which provides the concave part of the energy surface curve.

3. Results and discussion

Binding energy (E) surface curves of even–even Ne and Mg isotope chains as a function of the quadrupole deformation parameter (β_2) are shown in Figs.1 and 2, respectively. It is clearly seen that all curves for Ne and Mg, except those of ^{18,30,32}Ne and ^{20,32}Mg have two pronounced minima corresponding to the large positive (prolate shape) and negative (oblate shape) deformations, respectively. The deformation with the lower binding energy should correspond to the ground state. It is evident that most nuclei in even–even Ne and Mg chains exhibit prolate shapes. Among the above five nuclei, ^{18,30}Ne and ^{20,32}Mg have the magic-number of neutron. One should note that, although the minima of ^{32}Ne and ^{20}Mg are both near to the zero deformation, the bottoms of the curves are very flat, unlike those for ^{18,30}Ne and ^{32}Mg. In other words, within a limited scope, ^{32}Ne and ^{20}Mg can manifest different deformations with similar binding energies. This implies that they display a large number of deformations with continuous values within our axially deformed RMF model. So it suggests that they might have a structure of triaxial deformation. If this is true, the neutron number N=8 is no longer a magic-number for

^{20}Mg. Since our calculations are based on the condition of axially symmetrical deformation, the triaxial deformation effect cannot be represented directly. The conclusion can be confirmed by the future triaxial calculation. For ^{26,28}Ne and ^{28,30}Mg, the prolate and the oblate quadrupole deformations correspond to two close-lying energy minima with a difference of a few hundred keV. This indicates that their ground states may have two competing configurations, i.e. shape coexistence.

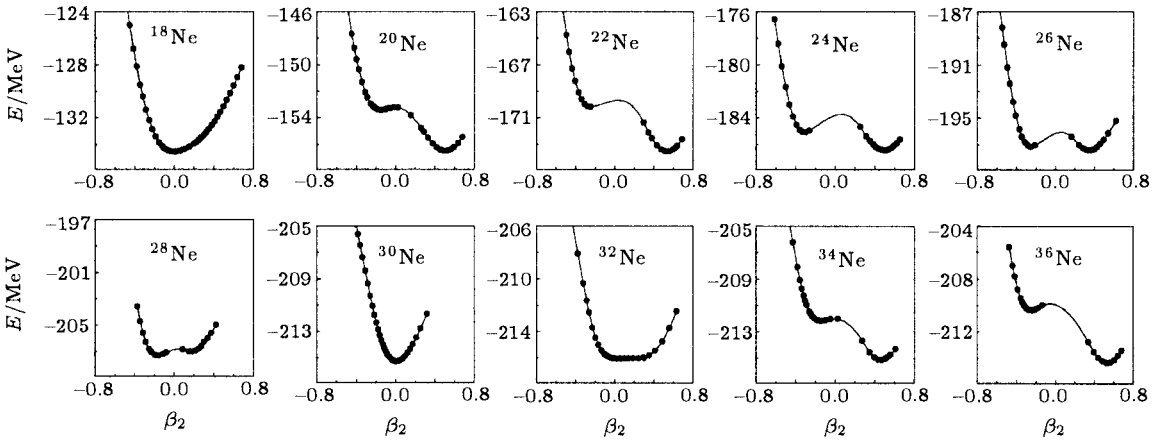


Fig.1. Binding energy as a function of quadrupole deformation parameter for even–even Ne isotopes, obtained by the constrained RMF+BCS calculation with the NL075 force. The black points are connected by a solid curve correspondingly.

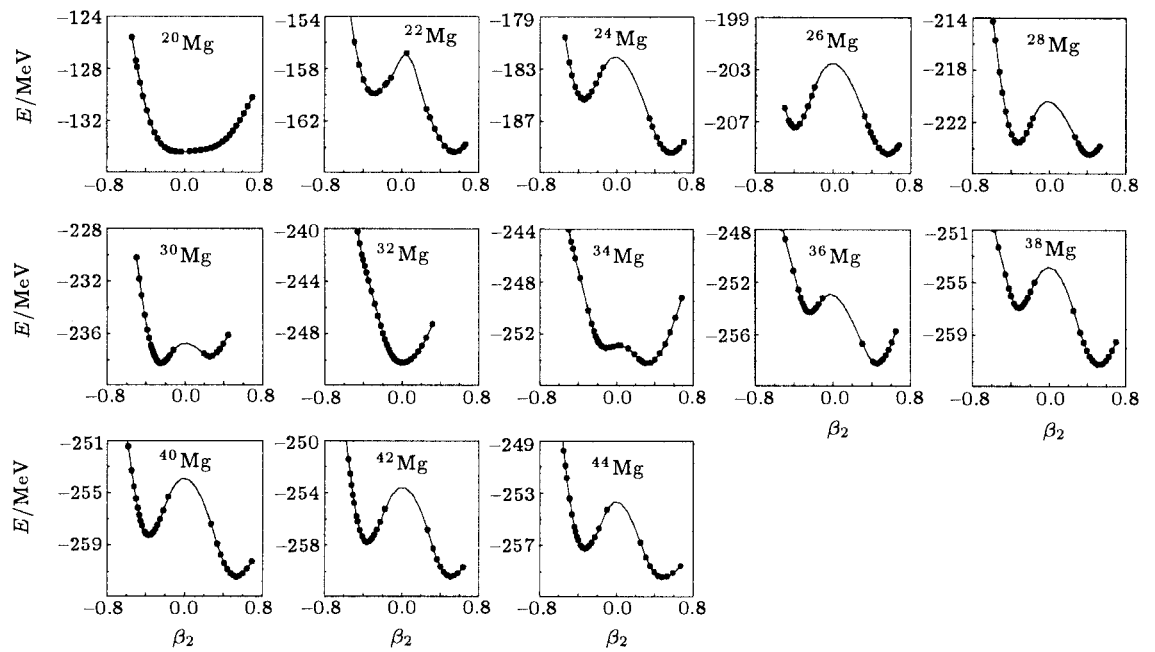


Fig.2. As Fig.1 but for the even–even Mg isotopes.

In order to verify the reliability of the above calculations for Ne and Mg chains, we plot in Figs.3 and 4 the quadrupole deformation β_2 for the even–even Ne and Mg obtained with the NL075, respectively. Those obtained with the GHDCM, NL-SH and the finite-range droplet model (FRDM),[38] and the available experimental data[13,14] are also displayed in these figures for comparison. The quadrupole deformations of even–even Ne and Mg isotopes are described well by the NL075 in the RMF model compared with experimental data available, except those of ^{18,28}Ne and ^{32}Mg, where the deformations are underestimated too

much. (For ^{28}Ne and ^{32}Mg, all models underestimate the deformation values.) Therefore, the experimentally defined disappearance of shell closure of neutron numbers N=8 for ^{18}Ne and N=20 for ^{32}Mg unfortunately fails to be predicted by the NL075. We know that all force parameter sets (such as NL075, NL-SH and NL3, etc) in the RMF model are determined by fitting the experimental properties of several standard spherical nuclei, such as ^{16}O and ^{40}Ca, etc.[15,16,20] In the fitting, the attention is mainly paid to the magic-number shells which overpower the spherical shape but the other possible contributions are neglected. Therefore, to some extent, some discrepancy between calculation and measurement occurs inevitably when these parameter sets are applied to the approach for some exotic nuclei. This can also be demonstrated explicitly by the results with the NL-SH.

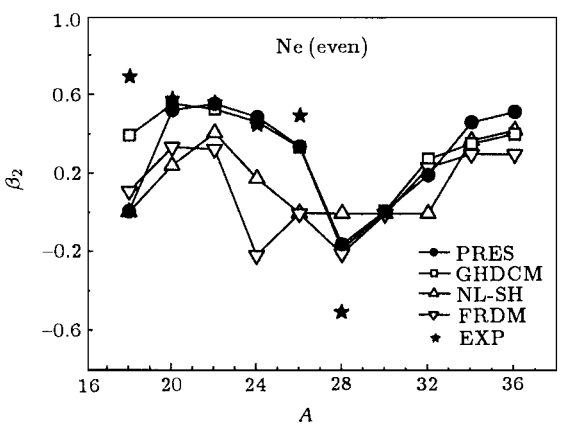


Fig.3. The quadrupole deformation parameter for even–even Ne isotopes with the NL075 (solid circles). A comparison is made with the results from the GHDCM (empty squares), the NL-SH (empty triangles), the FRDM (empty inverted triangles) and experiments (full stars). The experimental deformation data from ^{18}Ne to ^{28}Ne are available.

It is very interesting that the NL075 and the GHDCM give almost similar quadrupole deformation values for the even–even Na and Mg on a whole, except ^{18}Ne and ^{20}Mg. When comparing the theoretical results with the corresponding experimental data, one finds that except ^{18}Ne, the NL075 can provide a prediction for the deformation of even–even Na and Mg isotopes so well as the GHDCM does. The deformation values predicted by the NL-SH are extremely smaller than those obtained by the NL075 and the GHDCM in almost all cases. Specifically, the deformation values obtained with the NL-SH are much smaller than measurements. Therefore, the parameter set NL075 can produce more accurate deformation than the NL-SH. It also implies that the largely deformed nuclei can be described properly in the RMF model if a parameter set is chosen appropriately. The FRDM gives deformation values large enough for ^{24,28}Ne and ^{26,40}Mg, but underestimates too much in other cases, which is similar to the NL-SH.

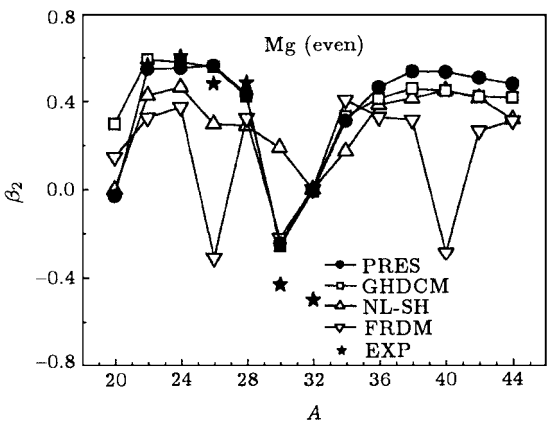


Fig.4. The same caption as that of Fig.3 but for even–even Mg isotopes. The experimental deformation data from ^{22}Mg to ^{32}Mg are available.

Binding energy (E) surface curves for odd-A Ne and Mg isotope chains as a function of the quadrupole deformation parameter (β_2) are displayed in Figs.5 and 6, respectively. The general trend of deformation transition of the odd-A Ne and Mg is very similar to that of the respective even–even nuclei, namely, most of them have a large deformation corresponding to prolate shape. With the similar discussion to the above, it seems that ^{19,29}Ne and ^{31}Mg may have a triaxial deformation. Besides, there may exist a shape coexistence in ^{25,27}Ne and ^{21,29}Mg. The deformation value for an odd-A (or even–even) nucleus flattens the transition for two adjacent even–even (odd-A) nuclei. For example, if one observes only the curves from ^{28}Mg to ^{30}Mg in Fig.2, there is a direct transition from prolate shape to oblate shape. But if the surface curve of ^{29}Mg is added, it will be found that there is a transition from a prolate shape through a shape coexistence to an oblate shape.

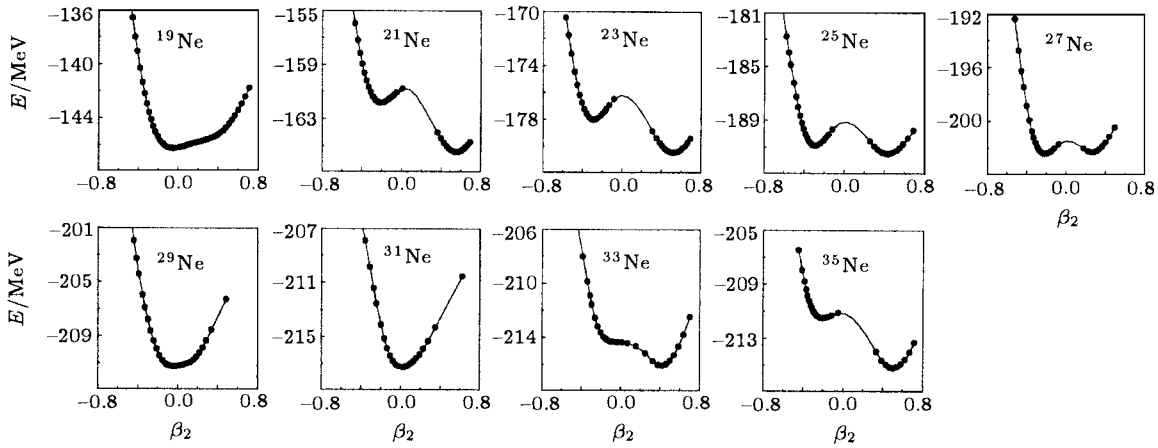


Fig.5. Binding energy as a function of quadrupole deformation parameter for odd-A Ne isotopes obtained by the constrained RMF+BCS calculation with the NL075 force. The black points are connected by solid curves correspondingly.

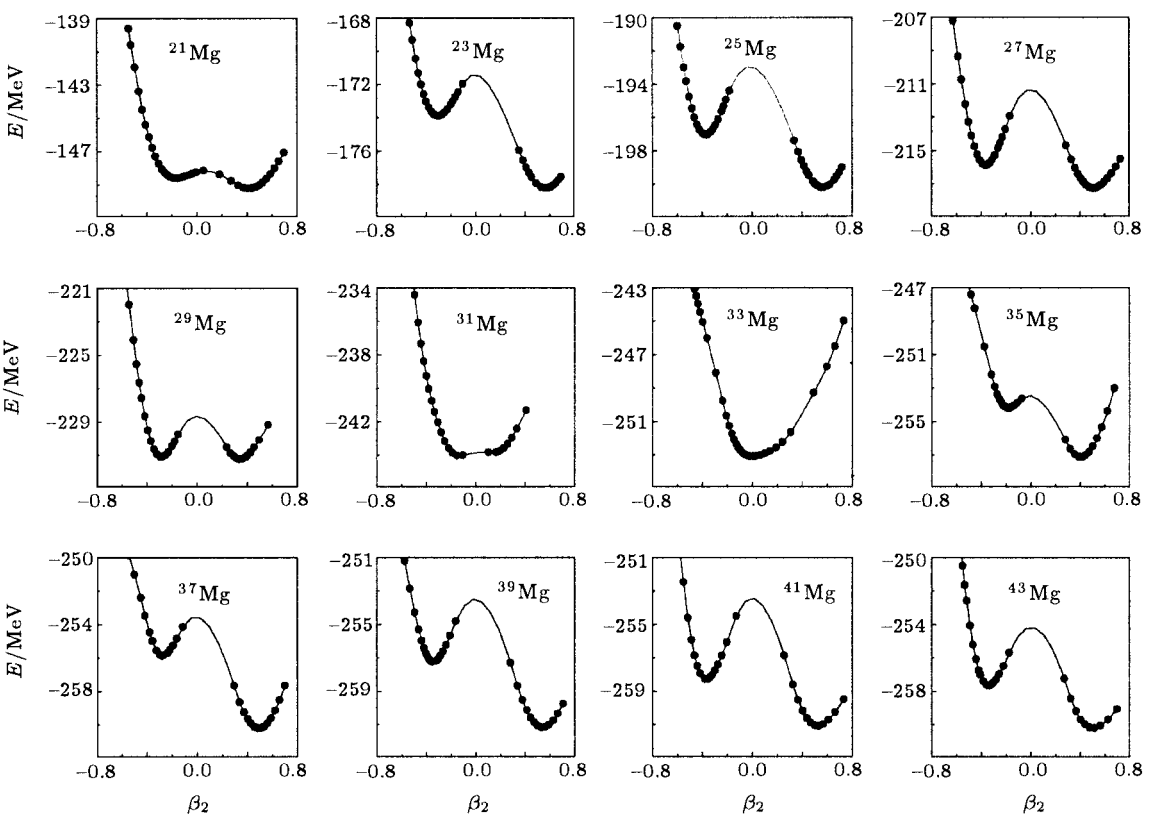


Fig.6. The same caption as that of Fig.5 but for odd-A Mg isotopes.

Since the NL075 force can give a good description for even–even Ne and Mg chains, it is suitable to apply it to the odd-A Ne and Mg. For odd-A nuclei, the last odd nucleon does not have a partner to occupy its time-reversed state. Therefore, in principle, time-reversal symmetry breaking as well as space-like components of meson fields should be considered in the mean field, which, however, causes the calculations for odd-A nuclei to be more difficult. It is well known that these contributions are very important to magnetic moment and moment of inertia which depend on only a few nucleons but influence hardly bulk properties such as binding energy, deformation and density distribution, etc. Based on this discussion, we did not employ violation of time-reversal symmetry in the calculations for odd-A nuclei.

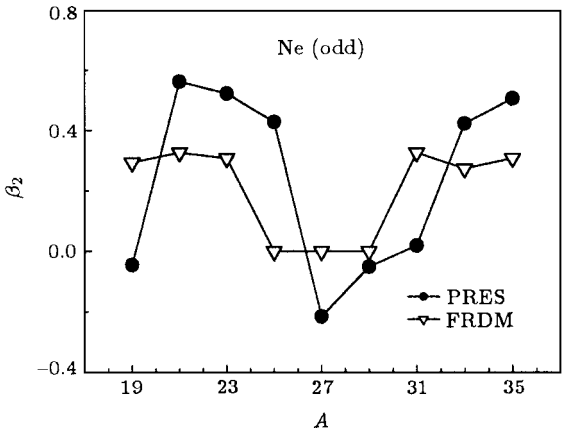


Fig.7. The quadrupole deformation parameter for odd-A Ne isotopes with the NL075 (solid circles) and comparison with the FRDM (empty inverted triangles).

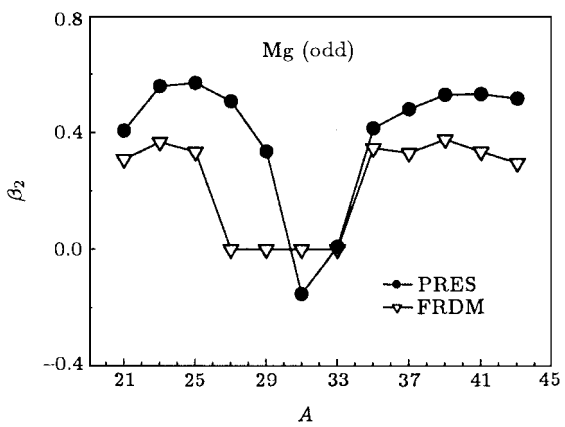


Fig.8. The same caption as that of Fig.7 but for the odd-A Mg isotopes.

The deformations of the odd-A Ne and Mg are shown in Figs.7 and 8, respectively. Only the results of the FRDM are shown for comparison since there are no results for odd-A nuclei from the NL-SH, the GHDCM and experiments. The general trend of the NL075 results seems to be in agreement with that of the FRDM, namely, most of these odd-A nuclei are shown to be prolate by the FRDM and NL075. However, there exist some differences between the two theoretical results. The deformation transitions evolve from a prolate shape through an oblate and spherical shape into a prolate shape for the NL075, and from a prolate shape through a spherical shape into a prolate shape for the FRDM. The main difference is the deformation value. The deformations from the NL075 are overwhelmingly larger than those from the FRDM, except^{19,31}Ne, in which the shell of neutron is close to the shell closure N=8 and N=20, respectively. In particular, ^{25,27}Ne and ^{27,29,31}Mg are predicted to be spherical by the FRDM but shown to be evidently prolate or oblate by the NL075. One should remember that the FRDM underestimated the quadrupole deformation for even–even nuclei too much compared with experimental data. We expect that the future experiments will confirm the conclusion.

We plot the binding energy per particle of doubly even Ne and Mg with the NL075, the GHDCM and NL-SH in Figs.9 and 10, respectively, in which the results for odd-A nuclei with the NL075 are also summarized. The experimental data from Refs.[39, 40] are also shown for comparison. The NL075 can give a good description for even–even Ne and Mg isotopes on the sides of proton-rich and neutron-rich and the largest relative errors are about 2.0% for Ne and 2.7% for Mg. For the nuclei near to the β stable valley, the NL075 underestimates the binding energies for both Ne and Mg chains. The largest relative errors are about 2.8% for the even–even Na and 4.5% for the even–even Mg. The parameter set NL-SH provides a more excellent prediction for biding energy in all cases. This implies that it is a disadvantage for the

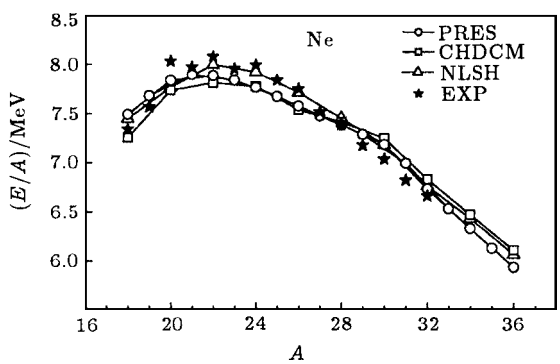


Fig.9. The binding energy per particle for Ne isotopes. The symbols are as follows: empty circles (NL075), empty squares (GHDCM), empty triangles (NL-SH) and full stars (experiments).

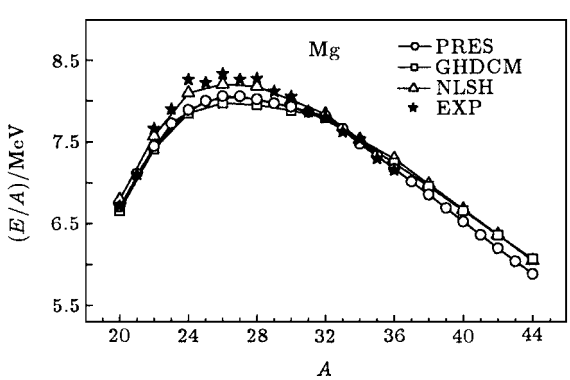


Fig.10. As Fig.9 but for Mg isotopes.

NL075 although it can give a better description for deformation than the NL-SH. However, the NL075 improves the accuracy of binding energy better than the GHDCM for both Ne and Mg chains.

As expected, although the effect of time-reversal symmetry breaking is not considered, the features of binding energy for odd-A Ne and Mg nuclei can still be predicted well. The largest relative errors between the theoretical and the experimental data are 2.1% for the odd-A Ne and 2.5% for the odd-A Mg, which are both less than those in the case of even–even nuclei. This might mainly be attributed to the odd–even staggering of nuclear mass. Whether or no, one can state that the RMF model can properly predict the bulk properties of odd-A nuclei without inclusion of the contribution of time-reversal symmetry breaking.

4. Summary

We have investigated features of the ground state for Ne and Mg isotope chains in the axially deformed RMF model with the NL075 parameter set. It is found that the deformation and binding energy can be predicted properly as a whole. The parameter set NL075 improves the accuracy of deformation for even–even Ne and Mg isotope chains compared with the NL-SH, although the former provides a little pooper description for binding energy than the latter. For odd-A Ne and Mg chains, the deformation values predicted in the present calculations are much bigger than those in the FRDM calculations in most cases. Comparing with the prediction for doubly even Ne and Mg chains, our descriptions are expected to be closer to a real nuclei. The theoretical binding energies of the odd-A Ne and Mg from the NL075 are more accurate than those of doubly even nuclei. It is also found that some of nuclei like ^{19,29,32}Ne and ^{20,31}Mg may show a triaxial deformation. In $^{25-28}$Ne and $^{27-30}$Mg, there may appear a shape coexistence. In addition, the shell closure of N=8 for ^{20}Mg is predicted to be very weak.

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