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A relativistic mean-field study of magic numbers in light nuclei from neutron to proton drip-lines

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Abstract. In an axially deformed relativistic mean-field calculation of single-particle energy spectra of $N = 8$ (Li–Mg) and $N = 14, 16$ (C–Mg) isotonic chain and the one- and two-neutron separation energies of various isotopes of Li–Mg, new magic numbers are found to exist at $N = 6$ and $N = 16$ and/or $N = 14$, which are in addition to the $N = 8$ and $N = 20$ magic numbers. In neutron-rich nuclei, the shell gap at $N = 6$ is larger than at $N = 8$ and a large gap is observed for $N = 16$ or 14 for the neutron-rich and $N = 14$ for proton-rich nuclei. Large shell gaps are also found to exist at $N = 14$ and 16 or $N = 16$ alone for nuclei near the β-stability line. The above results are independent of the parameter sets TM2, NL3 and NL–SH used here. Similarly, new large shell gaps are predicted at $Z = 6, 16$ and/or 14 for protons.

Keywords. Relativistic mean field theory; magic number; shell structures; drip-line.

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We know that magic numbers are the backbone of nuclear structure physics. For exotic nuclei near the drip-lines, recently the question of appearance of new magic numbers and/or disappearance of known magic numbers has been of much interest empirically, theoretically as well as experimentally. Theoretical calculations have predicted very different magic numbers for neutron-rich nuclei at the drip-line than are known for nuclei near the β-stability line [1–6]. Most of these calculations are based on the mean-field models, namely the Skyrme Hartree–Fock, the Skyrme Hartree–Fock–Bogoliubov or the relativistic mean-field approximation. Experimentally, the vanishing of the $N = 20$ magic shell due to the observed large deformation of ^{32}Mg was shown in the early β-decay and Coulomb excitation studies [7,8]. Similarly, the extinction of $N = 28$ as a magic number was first questioned theoretically for ^{40}Mg, ^{42}Si and ^{44}S nuclei [2,4,5] and then a large quadrupole deformation was measured experimentally [9]. Also, the observed mixing of $1s_{1/2}$ and $0p_{1/2}$ orbitals in the ground-state wave function of each of the neutron-rich ^{11}Li and ^{12}Be nuclei eliminates the magic character of $N = 8$ [10,11]. A significant contribution of $0d_{5/2}$ component is also expected for ^{12}Be [11].

Very recently, some new magic numbers have also been predicted for the exotic neutron- and proton-rich nuclei near the drip-lines. Empirically, the analyses by Ozawa *et al* [12] and Gupta *et al* [13] of the measured binding energy data suggest $N = 6$ and 16 as the new magic numbers, respectively, for the proton- and neutron-rich drip-line regions. Also, theoretical calculations based on the spin–isospin properties of nucleon–nucleon interaction show that the whole set of $N = 8$, 20,..., etc., can disappear and a new set of $N = 6$, 16,..., etc., could arise for neutron-rich exotic nuclei [14]. Furthermore, as already mentioned in the paragraph above, the relativistic mean-field (RMF) calculations show that the traditional magic numbers may not be valid when one discusses the shell structure of neutron drip-line nuclei [5,6]. However, as yet, there are no experimental signatures for the *appearance* of new magic numbers for nuclei near the neutron or proton drip-line, though, as stated above, the *disappearance* of magic numbers is already shown experimentally. In a recent experiment, Kanungo *et al* [15] have found some new magic numbers at $Z = 16$ and $N = 30$ in neutron-rich region. They have also observed shell closure at $N = 32$. The reported magic number at $N = 16$ [12] has been reconfirmed in the same ref. [15].

In this paper, we choose to analyse within the axially deformed relativistic mean-field (RMF) formalism, the $N = 8$ isotones with a view to see if this magic number is still valid and/or new magic numbers appear. Specifically, we have studied the $N = 8$, Li to Mg nuclei, which cover from the neutron-rich ^{11}Li, ^{12}Be and ^{13}B to proton-rich ^{17}F, ^{18}Ne, ^{19}Na and ^{20}Mg nuclei of the recently explored regions of neutron and proton drip-lines. The $N = 16$, C–Mg is also analysed extensively to examine the role of $N = 14$ and 16 neutron numbers. Note that ^{11}Li and ^{17}F are the known $2n$- and $1p$-halo nuclei, respectively. Also, nuclei like ^{14}C, ^{15}N and ^{16}O, lying near or at the β-stability line, are included. In other words, the chosen $N = 8$ isotonic chain has nuclei from all the three regions of neutron-rich, proton-rich and β-stability.

The RMF approach is well-known and, its theory being well-documented, we skip all the details which can be found in refs [16–20]. Here we begin with the relativistic Lagrangian density for a nucleon–meson many-body system,

$$\begin{aligned}\mathscr{L} = {} & \overline{\psi_i}\{i\gamma^\mu\partial_\mu - M\}\psi_i + \frac{1}{2}\partial^\mu\sigma\partial_\mu\sigma - \frac{1}{2}m_\sigma^2\sigma^2 - \frac{1}{3}g_2\sigma^3 \\ & - \frac{1}{4}g_3\sigma^4 - g_s\overline{\psi_i}\psi_i\sigma - \frac{1}{4}\Omega^{\mu\nu}\Omega_{\mu\nu} + \frac{1}{2}m_w^2V^\mu V_\mu \\ & + \frac{1}{4}c_3(V_\mu V^\mu)^2 - g_w\overline{\psi}_i\gamma^\mu\psi_iV_\mu - \frac{1}{4}\vec{B}^{\mu\nu}\cdot\vec{B}_{\mu\nu} \\ & + \frac{1}{2}m_\rho^2\vec{R}^\mu\cdot\vec{R}_\mu - g_\rho\overline{\psi}_i\gamma^\mu\vec{\tau}\psi_i\cdot\vec{R^\mu} - \frac{1}{4}F^{\mu\nu}F_{\mu\nu} \\ & - e\overline{\psi}_i\gamma^\mu\frac{(1-\tau_{3i})}{2}\psi_iA_\mu, \end{aligned} \tag{1}$$

where the σ-meson field is denoted by σ, that of the ω-meson by V_μ and of the isovector ρ-meson by $\vec{R}_\mu$. A^μ denotes the electromagnetic field and ψ_i are the Dirac spinors for the nucleons whose third component of isospin is denoted by τ_{3i}. The g_s, g_w, g_ρ and $(e^2/4\pi)(=1/137)$ are the coupling constants for σ, ω, ρ mesons and photon, respectively, with g_2, g_3 and c_3 as the parameters for the non-linear terms of sigma and omega mesons. M is the mass of the nucleon and m_σ, m_ω and m_ρ are the masses of the σ, ω and ρ mesons, respectively. $\Omega^{\mu\nu}$, $\vec{B}^{\mu\nu}$ and $F^{\mu\nu}$ are the field tensors for the V^μ, $\vec{R}^\mu$ and the photon fields, respectively.

From the Lagrangian we get the field equations for nucleons and mesons which are solved by expanding the upper and lower components of the Dirac spinors and the boson fields in a deformed harmonic oscillator basis for an initial deformation. The number of oscillator shells, used as the expansion basis for the fermion and boson fields, is $N_{\mathrm{F}} = N_{\mathrm{B}} = 12$. The set of coupled equations is solved numerically by a self-consistent iteration procedure. The center-of-mass motion is estimated by the usual harmonic oscillator formula $E_{\mathrm{C.M.}} = \frac{3}{4}(41A^{-1/3})$. The total binding energy (BE) and other observables are obtained by using the standard relations (see [17]).

We have made our calculations using the parameter sets TM2, NL3 and NL–SH [20,21]. The predictive power of these forces is well-known and some examples can be found, e.g., in ref. [22] and the references quoted therein. The NL–SH parameter set is designed for the drip-line nuclei. The relatively new parameter set NL3 is considered to be very successful and it could be used with confidence for the investigations of new regions of nuclear stability. On the other hand, an interesting feature of the TM2 parametrization is that the sign of the quartic scalar self-coupling is positive in this set, contrary to the other standard non-linear sets where this sign is negative. In TM2, this is achieved by introducing a quartic self-interaction of the vector field in the effective force. Though TM2 is not yet used much, the quality of results reproduced by it is, in general, quite comparable to the other standard non-linear sets for light nuclei. This parameter set is meant for light nuclei. Due to the positive sign of g_3 in the σ-non-linear coupling, the TM2 parameter set is able to give a convergent solution even for a light nucleus which has a high central density, like the ^{12}C nucleus where there is no convergent solution for NL1 or NL3 parameter set [18]. It may be noted that the RMF parameter sets are determined by least squares fits to ground-state properties, like radii, binding energies and spin–orbit splittings of a few spherical nuclei, with no further adjustment to be made in the parameters so obtained.

For the pairing strength, the BCS approach provides a reasonably good description of nuclei close to or not too far from the stability line. For nuclei in the vicinity of the drip-lines, the coupling to the continuum becomes important. However, it has been shown that the self-consistent treatment of the BCS approximation breaks down when coupling between the bound states and the states in the continuum take place [23]. For most of the very neutron-rich/or deficient nuclei, like the ones studied here, the odd–even mass differences are not yet measured and little is known about the precise effect of the pairing interaction. On the other hand, a constant pairing strength, taken from experiments or from a standard formula, failed to reproduce the quadrupole deformation of light nuclei, like that of ^{20}Ne, and favors a very weak pairing strength [6]. Therefore, in the present investigation we have chosen to use the BCS formalism with a small constant pairing strength, namely $\Delta_{\mathrm{n}} = \Delta_{\mathrm{p}} = 0.5$ MeV. This type of prescription has already been adopted in the past and contributes very little to the total binding energy [2,24].

The calculations for odd–even and odd–odd nuclei in an axially deformed basis is a tough task in the RMF model. To take care of the lone odd nucleon, one has to violate the time-reversal symmetry in the mean field. In the present study only the time-like components V_0, b_0 and A_0 of the ω, ρ and photon fields are retained. The space components of these fields (which are odd under time reversal and parity) are neglected. They are important in the determination of properties like magnetic moments [25], but have a very small effect on the bulk properties, like the binding energies and quadrupole deformations, and can be neglected to a good approximation [26]. Thus we have adopted a simple average *m*-scheme in our present calculations.

We have calculated the single-particle energy spectra for the chosen $N = 8$ (Li–Mg), $N = 14$, 16 (C–Mg) isotonic chains and the binding energies for various isotopes of Li–Mg nuclei. From the calculated binding energies, we evaluate the one- and two-neutron separation energy (S_{1n} and S_{2n}) and the one-proton separation energy S_{1p} by using the relations $S_{1n}(N,Z) = \mathrm{BE}(N,Z) - \mathrm{BE}(N-1,Z)$, $S_{2n}(N,Z) = \mathrm{BE}(N,Z) - \mathrm{BE}(N-2,Z)$ and $S_{1p}(N,Z) = \mathrm{BE}(N,Z) - \mathrm{BE}(N,Z-1)$, respectively, where $\mathrm{BE}(N,Z)$ is the binding energy of a nucleus with N neutrons and Z protons.

Figures 1 and 2 show the neutron single-particle energy levels for the selected $N = 8, 14$ and 16 nuclei, using the TM2 and NL3 parameter sets. Each state occupies a maximum of two nucleons (each for protons and neutrons) due to the two-fold degeneracy along the z-axis (in m quantum number). Note that for the BCS pairing scheme, the conditions of quasi-particle come in to picture where a state is not purely a two-fold degenerate but may be a partially filled orbit. In the figures, both the filled and some of the empty states are shown. The dotted line shows the Fermi surface above which the states are empty. The single-particle energy spectrum of a nucleus gives significant information about its shell structure and thus provides a useful physical observable to analyse the magic number characteristics (the large shell gaps). Since we are working with the $N = 8$ and 16 isotonic chains of both the exotic nuclei at drip-lines and nuclei at the β-stability line, apparently we are concerned here with the appearance and/or disappearance of magic number $N = 8$, and any new magic number(s) that might arise.

We notice in figures 1a or 1b for neutrons that, in addition to a large gap at $N = 8$, there is a large shell gap at $N = 6$ in all the nuclei. In some nuclei, particularly in the neutron-rich side, the shell gap at $N = 6$ is even larger than at $N = 8$, for both the parameter sets. This means that for exotic neutron-rich nuclei the new magicity at $N = 6$ competes with the known $N = 8$ magicity, or, in other words, for neutron-rich nuclei near the drip-line, the $N = 8$ magicity is broken. Exactly, the same result is obtained for the NL–SH parameter set (not shown here). The large shell gap at $N = 6$ is apparently due to the sub-shell closure of $0p$ orbit (discussed in the next paragraph for the illustrative ^{12}Be nucleus). However, the $N = 2$ is still a distinct magic number for all the three parameter sets (TM2, NL3 and NL–SH).

From the analysis of the single-particle orbitals, we noticed that the Nilsson orbits for the lowest four neutron states in ^{12}Be, using TM2 parameter set, are $[000]\frac{1}{2}^+$, $[110]\frac{1}{2}^-$, $[101]\frac{3}{2}^-$ and $[101]\frac{1}{2}^-$ (the index is defined as $[Nn_3\Lambda]\Omega^\pi$). Note that these states for neutrons are occupied in this nucleus. Comparing this deformed single particle spectrum with the Nilsson diagram, we find that the $m = +3/2, +1/2$ levels of $p_{3/2}$ split strongly and create a large gap at $N = 6$, larger than the one at $N = 8$. A similar situation is presented for NL3 and NL–SH parameter sets. The creation of a larger gap at $N = 6$ for neutron-rich nuclei means the diminishing of the importance of magic number $N = 8$ for this region. The shell gap at $N = 6$ for other nuclei (the proton-rich and stable nuclei) is also large to term it as a magic number, but relatively smaller than at $N = 8$.

The next new neutron shell gaps in the studied $N = 14$ for ^{20}C and $N = 16$ isotonic series are found to occur at $N = 16$ and/or $N = 14$ for all the nuclei and all the parameter sets used (see figures 2a and 2b). The shell gaps at $N = 14$ and 16 are more pronounced for TM2 (figure 2a) than for the NL3 parameter set (figure 2b). In general, the pattern is similar in both the forces used in the present calculations. For neutron-rich isotones (^{22}C, ^{24}O and ^{25}F) the shell gap at $N = 16$ or 14 is relatively larger. As the isotonic mass increases the shell gap at $N = 16$ first decreases till ^{26}Ne and again increases from ^{27}Na. For the heavier

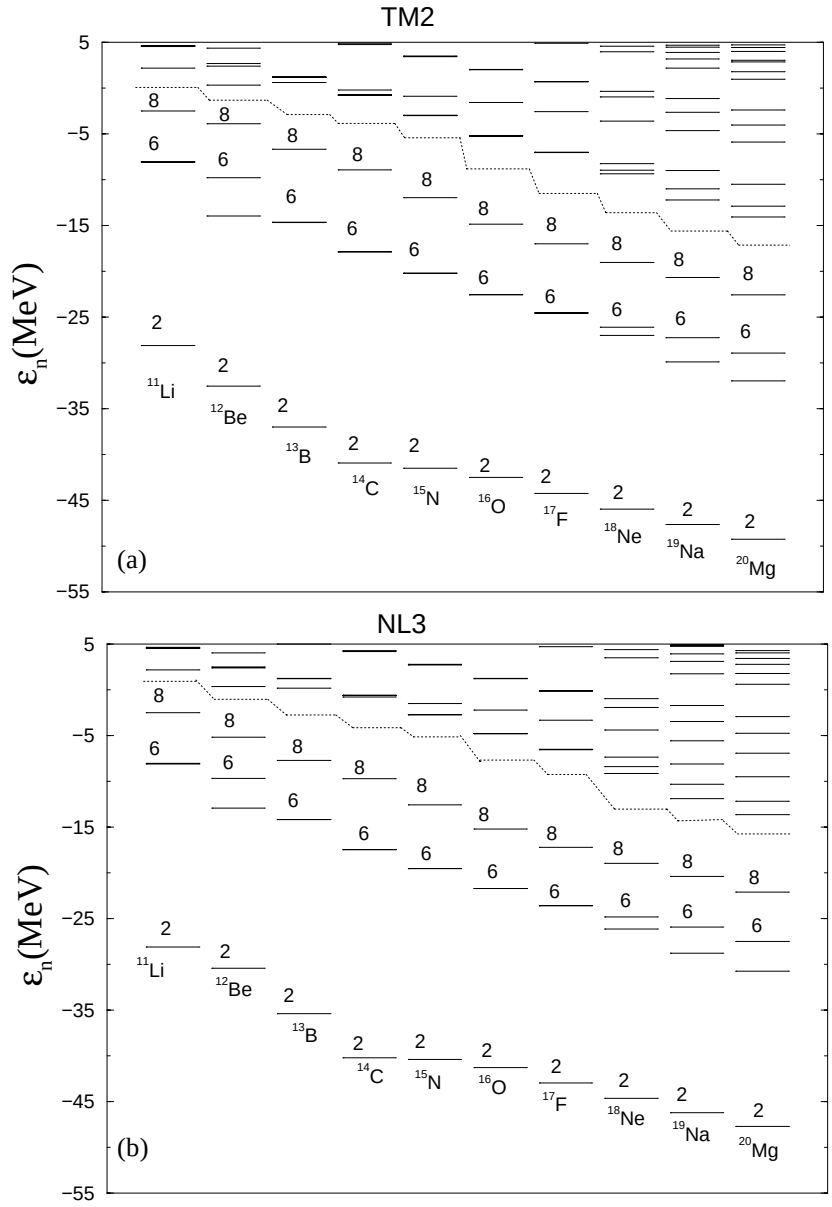

Figure 1. Single-particle energy spectra for neutrons in $N = 8$, Li–Mg nuclei using (**a**) TM2 and (**b**) NL3 parameter set. The Fermi surface is denoted by the dotted line.

nuclei, in particular for ^{24}O, ^{25}F and ^{26}Ne, the shell gap at $N = 14$ becomes much bigger than at $N = 16$. In general, the shell gaps at $N = 16$ and/or $N = 14$ for the exotic neutron- and proton-rich nuclei are large enough to classify them as magic numbers, like the one for $N = 6$.

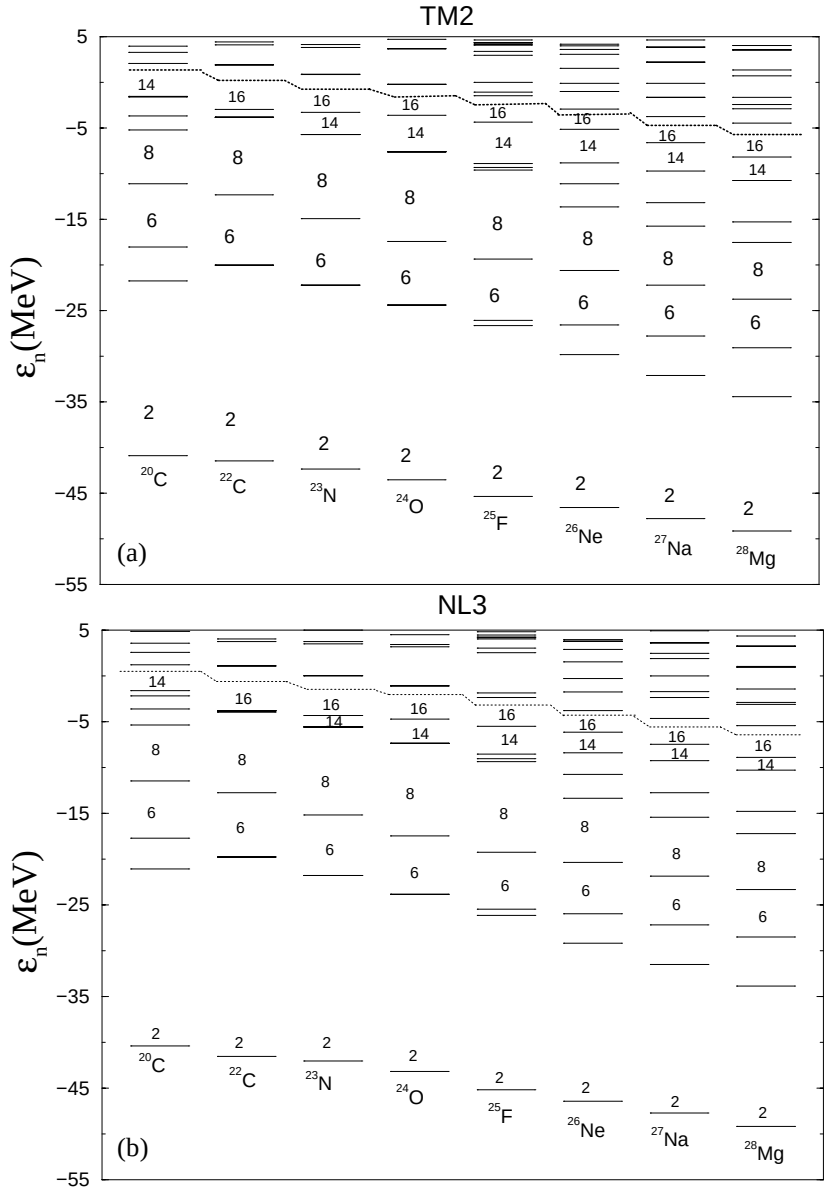

Figure 2. Single-particle energy spectra for neutrons in $N = 14$ for ^{20}C and in $N = 16$, C–Mg nuclei using (**a**) TM2 and (**b**) NL3 parameter sets. The Fermi surface is denoted by the dotted line.

We have also calculated the proton single-particle energy spectra for all the $N = 8$ isotones. This is illustrated in figures 3a and 3b for the TM2 and NL3 parameter sets alone, since the pattern of single-particle energies is the same for other parameter sets and we

have not shown those in the figures. Here again we find large shell gaps at $Z = 2$, 6 and 8 for all the nuclei. The new shell gaps at $Z = 6$ are comparable to the ones at $Z = 8$.

Next, in order to be able to get a little more information about the magic numbers between $N = 6$ and 8, and $N = 14$ and/or 16, following our own earlier work [6] and that

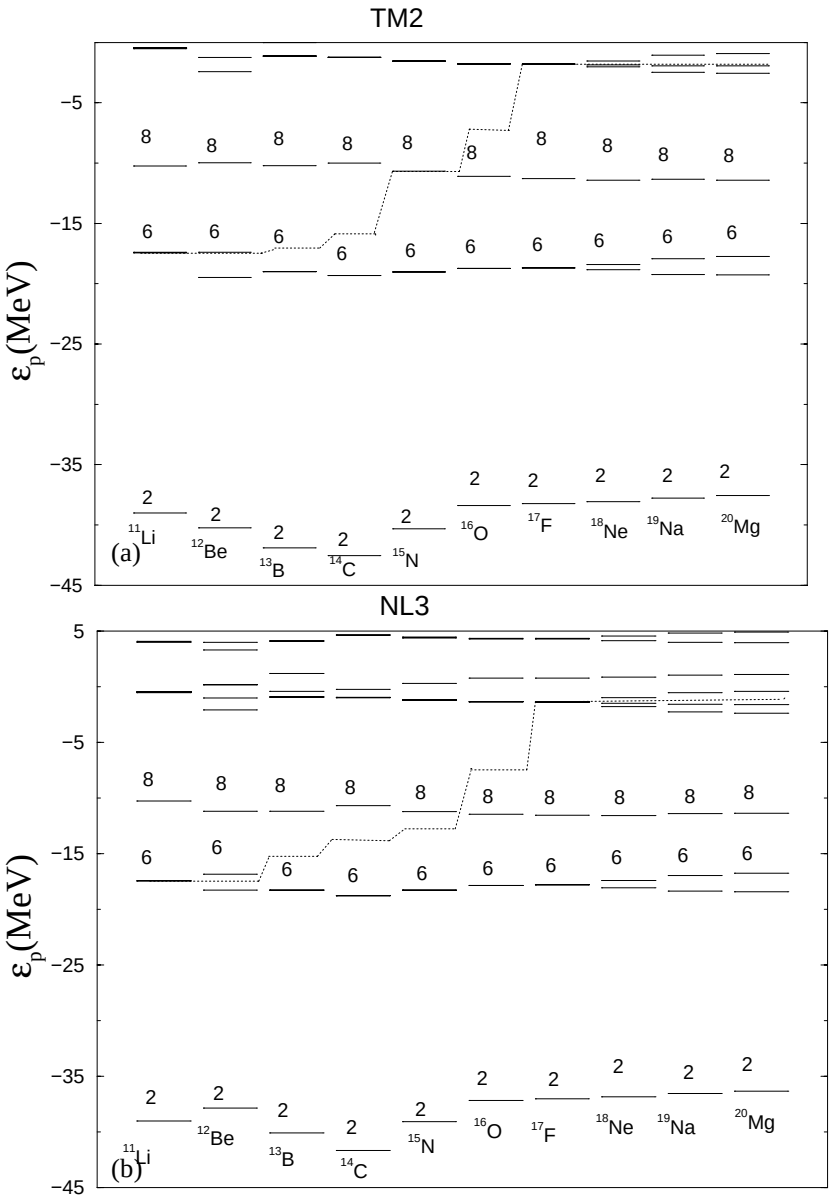

Figure 3. Same as figures 1a and 1b, but for proton in $N = 8$, Li–Mg nuclei using (**a**) TM2 and (**b**) NL3 parameter set.

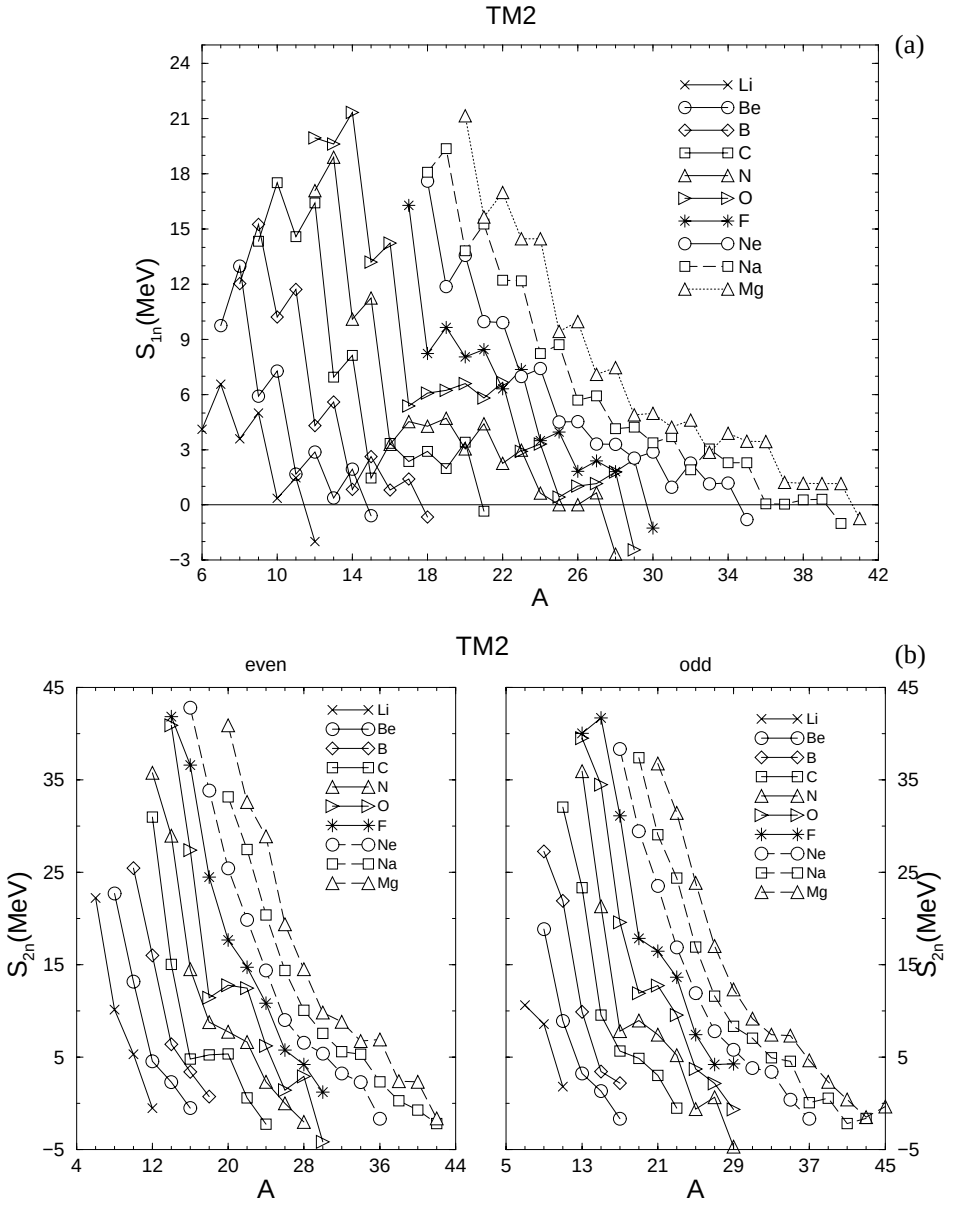

Figure 4. (**a**) One- and (**b**) two-neutron separation energy (S_{1n} and S_{2n}) as a function of mass number A for various isotopes of Li–Mg nuclei, using TM2 parameter set.

of Ozawa *et al* [12], we have plotted in figures 4 the one-neutron (S_{1n}) (figure 4a) and two-neutron (S_{2n}) (figure 4b) separation energies as a function of mass number A for various isotopes of Li–Mg nuclei, including the $N = 8$ isotones studied above, for the illustrative TM2 parameter set. We notice from figures 4, a sudden fall in one- and two-neutron separation energies from $N = 6$ to $N = 8$ for all the isotopic chains. For the lighter neutron-

rich nuclei ($Z = 3$–5), the rate of fall of S_{1n} and S_{2n} for $N = 4, 6, 8$ and 10 are almost equal, which means the breaking of $N = 8$ magic number or an appearance of a new $N = 6$ magic number, in addition to $N = 8$. For nuclei with $Z > 5$, in addition to the above noted fall of S_{1n} and S_{2n} values at $N = 6$ and $N = 8$, we notice a similar fall of S_{1n} at $N = 16$ and/or $N = 14$ which is as large as for $N = 20$. This gives an indication of the appearance of new magic numbers at $N = 16$ and/or $N = 14$, in addition to the $N = 20$ magic number. Interestingly, these results are consistent with the behavior of single-particle energy spectra in figures 1, 2 and 3 and also agree well with the empirical analysis of refs [12,13]. Then we analysed the one- and two-neutron separation energies for NL3 and NL–SH parameter sets. Except for the fact that NL3 set does not give convergent solutions for all the light nuclei (no convergent solution is obtained for ^{12}C), the behavior of S_{1n} and S_{2n} energies for both the NL3 and NL–SH parameter sets is similar to one discussed above for the TM2 parameter set.

We have also estimated the neutron and proton drip-lines from the calculated S_{1n} and S_{1p} values for the three parameter sets. A nucleus is stable against neutron (or proton) decay when its S_{1n} (or S_{1p}) is positive and the last isotope (or isotone) in the series with positive one-nucleon separation energy defines the drip-line for neutron (or proton). The estimated neutron and proton drip-lines for Li–Mg nuclei, using TM2, NL3 and NL–SH parameter sets, are given in table 1. The proton drip-line for Li-nucleus displayed in the table is not actually the last isotope in the series. This undefined proton drip-line is due to the uncertainty in the calculated results for the H-isotopes in our RMF approach. It is clear from the table that the predictions of drip-lines are similar for the three parameter sets. The notable exceptions are nitrogen nucleus for neutron and N, F, Ne and Na for proton drip-line, the largest difference being two units. A comparison of these predictions with experiments or extrapolated data (derived from experimental binding energies [27]) indicate the importance of different parameter sets for different nuclei. Since for light nuclei, both one-nucleon and two-nucleon halo nuclei are observed, we have also added the condition of S_{2n} (or S_{2p})=0 in determining the drip-lines [28]. These results are also presented in table 1 which are of interest when $S_{2n} < S_{1n}$ (for halo-structure, not studied here) and S_{2n} (or S_{2p}) goes to zero earlier than S_{1n} (S_{1p}).

In summary, we have first calculated the single-particle energy spectra for $N = 8$, 14 and 16, Li–Mg isotonic series in an axially deformed relativistic mean-field theory, using TM2, NL3 and NL–SH parameter sets. These nuclei start from the neutron drip-line and go over to proton drip-line, including also the in between β-stable nuclei. The one- and two-neutron separation energies for all the isotopic chains of Li–Mg nuclei are also evaluated. The analysis of neutron single-particle energy spectra of the calculated $N = 8$, 14 and 16, Li–Mg isotonic chains shows the existence of new magic numbers at $N = 6$ and $N = 16$ and/or 14 for all the nuclei and independent of the choice of parameter set, which are in addition to $N = 8$ and 20 magic numbers. Particularly, for the exotic neutron-rich nuclei, the shell gap at $N = 6$ is larger than at $N = 8$ and we found large shell gap at $N = 16$ or 14. For proton-rich nuclei, the shell gap at $N = 14$ is also comparable to the shell gap of a magic orbit. The appearance of a larger shell gap at $N = 6$, or the breaking of $N = 8$ magic shell, in neutron-rich nuclei is due to the splitting of $0p_{3/2}$ sub-shell. This analysis is also supported by the one- and two-neutron separation energies, in terms of a large fall in the separation energy exactly at the above mentioned new neutron magic numbers. Also, large proton shell gaps are noted at $Z =$2, 6, 8 and 16 for all the nuclei studied here, along with a significant proton shell gap that appears at $Z = 14$ for the heavier $N = 8$, $Z \geq 8$ nuclei.

Table 1. The axially deformed RMF results for the neutron and proton drip-lines, using various parameter sets, compared with experimental numbers derived from the $S_{1n} \to 0$ and $S_{1p} \to 0$, using the experimental (or extrapolated) binding energies [27]. Also, the drip-lines are evaluated for the two-nucleons separation energies going to zero. These numbers are given in the parenthesis. Whenever there is no number in the parenthesis, then the drip-lines obtained by one-nucleon and two-nucleon separation energies are same. More than one number for a drip-line (in experimental data) means that the inbetween nucleus is unstable. The calculated proton drip-line for Li isotopes is not define, because the calculated data for H-isotopes are not clear in our calculations.

	p-drip line			Expt.	*n*-drip line			Expt.
Nucleus	NL3	TM2	NL-SH	$(S_{1p}(S_{2p})\to 0)$	NL3	TM2	NL-SH	$(S_{1n}(S_{2n})\to 0)$
	A	A	A	A	A	A	A	A
Li	6	6	6	6(4)	11(12)	11(10)	11(12)	9,11(11)
Be	7	7	7	6(7)	14(15)	14(15)	14(15)	12,14(14)
B	8	8	8	8	17(20,21)	17(18)	17(18)	15,17,19(19)
C	9	9	9	8(9)	20(22,23)	20(21,22)	20(21,22)	20,22(22)
N	11(10)	12(11)	12(10)	12(11)	25(26,27)	27(26)	27(26)	23(24)
O	12	12(13)	12(13)	12(13)	28(29)	28(27)	28(27)	24,26(26)
F	17(14)	17(15)	16(14)	17(15)	29(32)	29(30)	29(30)	27,29(29)
Ne	19(17)	18(17)	17(18)	16(17)	34(35)	34(35)	34(35)	30,32(32)
Na	19	18(19)	19(18)	20(19)	39(40)	39(38)	39(38)	34(35)
Mg	20	20(19)	20	20	40(41)	40(41)	40(41)	34,36(>37)

It is to be noted here that the present calculations have been done in a relativistic mean field approximation. Several important factors have been neglected, for example, we have taken a very rough value of the pairing gap of protons and neutrons in the BCS calculations to take pairing correlation into account. It is also known that the simple BCS approximation breaks down near the drip-line. To get better prediction, one should use an improved treatment of the pairing (beyond a simple BCS) for the drip-line nuclei.

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