Journey to Superheavy Valley

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An extensive theoretical search for the proton magic number in the superheavy valley beyond Z =82 and corresponding neutron magic number after N =126 is carried out. For this we scanned a wide range of elements $Z = 112 - 130$ and their isotopes. The well established non-relativistic Skryme-Hartree-Fock and Relativistic Mean Field formalisms with various force parameters are used. Based on the calculated systematics of pairing gap, two neutron separation energy and the shell correction energy for these nuclei, we find Z =120 as the next proton magic and N=172, 182/184, 208 and 258 the subsequent neutron magic numbers.

1. Introduction

After the discovery of artificial transmutation of elements by Sir Ernest Rutherford in 1919 [1], the search for new elements is an important issue in nuclear science. The existence of elements beyond the last heaviest naturally occurring ^{238}U, i.e., the discovery of Neptunium, Plutonium and other 14 elements (transuranium elements), which make a separate block in Mendeleev′s periodic table was a revolution in the Nuclear Chemistry. This enhancement in the periodic table raises a few questions in our mind:

- Whether there is a limited number of elements that can co-exist either in nature or can be produced from artificial synthesis by using modern technique ?
- What is the maximum number of protons and neutrons that of a nucleus ?
- What is the next double shell closure nucleus beyond ^{208}Pb ?

To answer these questions, first we have to understand the agent which is responsible to rescue the nucleus against Coulomb repulsion. The obvious reply is the shell energy, which stabilises the nucleus against Coulomb disintegration [2]. Many theoretical models, like the macroscopic−microscopic (MM) calculations to explain involve some prior knowledge of densities, single-particle potentials and other bulk properties which may accumulate serious error in the largely extrapolated mass region of interest. They predict the magic shells at Z=114 and N=184 [3–6] which could have surprisingly long life time even of the order of a million years [5, 7–10]. Some other such predictions of shell-closure for the superheavy region within the relativistic and non-relativistic theories depend mostly on the force parameters [11, 12].

Experimentally, till now, the quest for superheavy nuclei has been dramatically rejuvenated in recent years owing to the emergence of hot and cold fusion reactions. In cold fusion reactions involving a doubly magic spherical target and a deformed projectile were used by GSI [13–17] to produce heavy elements upto Z = 110−112. In hot fusion evaporation reactions with a deformed transuranium target and a doubly magic spherical projectile were used in the synthesis of superheavy nuclei Z = 112−118 at Dubna [18–24]. At the production time of Z = 112 nucleus at GSI the fusion cross section was extremely small ($1pb$), which led to the conclusion that reaching still heavier elements will be very difficult. At this time, the emergence of hot fusion reactions using ^{48}Ca projectiles at Dubna has dramatically changed the situation and nuclei with Z = 114−118 were synthesized and also observed their α-decay as well as terminating spontaneous fission events. It is observed that Z = 115−117 nuclei have long α-decay chains contrast to the short chains of Z = 114−118. Moreover, the life times of the superheavy nuclei with Z = 110−112 are in milliseconds and microseconds whereas the life time of Z = 114−118 up to 30 s. This pronounced increase in life times for these heavier nu-

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clei has provided great encouragement to search the magic number somewhere beyond Z =114. Moreover, it is also an interesting and important question for the recent experimental discovery [25–27] say chemical method of $Z = 122$ from the natural ^{211,213,217,218}Th which have long lived superdeformed (SD) and/ or hyperdeformed (HD) isomeric states 16 to 22 orders of magnitude longer than their corresponding ground-state (half-life of ^{292}122 is $t_{1/2} \geq 10^8$ years).

2. Theoretical framework

A. The Skyrme Hartree-Fock (SHF) method

The general form of the Skyrme effective interaction, used in the mean-field models, can be expressed as an energy density functional $\mathcal{H}$ [28, 29], as

$$\mathcal{H} = \mathcal{K} + \mathcal{H}_0 + \mathcal{H}_3 + \mathcal{H}_{eff} + \cdots \tag{1}$$

where $\mathcal{K} = \frac{\hbar^2}{2m}\tau$ is the kinetic energy term with m as the nucleon mass, $\mathcal{H}_0$ the zero range, $\mathcal{H}_3$ the density dependent and $\mathcal{H}_{eff}$ the effective-mass dependent terms, relevant for calculating the properties of nuclear matter, are functions of 9 parameters t_i, x_i $(i = 0, 1, 2, 3)$ and η, given as

$$\mathcal{H}_0 = \frac{1}{4}t_0\left[(2 + x_0)\rho^2 - (2x_0 + 1)\left(\rho_p^2 + \rho_n^2\right)\right] \tag{2}$$

$$\mathcal{H}_3 = \frac{1}{24}t_3\rho^\eta\left[(2 + x_3)\rho^2 - (2x_3 + 1)\left(\rho_p^2 + \rho_n^2\right)\right] \tag{3}$$

$$\begin{aligned}\mathcal{H}_{\text{eff}} &= \frac{1}{8}\left[t_1(2 + x_1) + t_2(2 + x_2)\right]\tau\rho \\ &+ \frac{1}{8}\left[t_2(2x_2 + 1) - t_1(2x_1 + 1)\right](\tau_p\rho_n + \tau_n\rho_p).\end{aligned} \tag{4}$$

The other terms, representing the surface contributions of a finite nucleus with b_4 and b'_4 as additional parameters, are

$$\begin{aligned}\mathcal{H}_{S\rho} &= \frac{1}{16}\left[3t_1(1 + \frac{1}{2}x_1) - t_2(1 + \frac{1}{2}x_2)\right](\vec{\nabla}\rho)^2 \\ &- \frac{1}{16}\left[3t_1(x_1 + \frac{1}{2}) + t_2(x_2 + \frac{1}{2})\right] \\ &\times\left[(\vec{\nabla}\rho_n)^2 + (\vec{\nabla}\rho_p)^2\right], \text{ and}\end{aligned} \tag{5}$$

$$\mathcal{H}_{S\vec{J}} = -\frac{1}{2}\left[b_4\rho\vec{\nabla}\cdot\vec{J} + b'_4(\rho_n\vec{\nabla}\cdot\vec{J_n} + \rho_p\vec{\nabla}\cdot\vec{J_p})\right]. \tag{6}$$

Here, the total nucleon number density $\rho = \rho_n + \rho_p$, the kinetic energy density $\tau = \tau_n + \tau_p$, and the spin-orbit density $\vec{J} = \vec{J_n} + \vec{J_p}$; n and p referring to neutron and proton, respectively. The $\vec{J_q} = 0$, $q = n$ or p, for spin-saturated nuclei, i.e., for nuclei with major oscillator shells completely filled. The total binding energy (BE) of a nucleus is the integral of the energy density functional $\mathcal{H}$. We have used here the Skyrme SkI4 set with $b_4 \neq b'_4$ [**?**], designed for considerations of proper spin-orbit interaction in finite nuclei, related to the isotope shifts in Pb region.

B. The relativistic mean-field (RMF) method

The relativistic Lagrangian density for a nucleon-meson many-body system [30, 31],

$$\begin{aligned}\mathcal{L} &= \overline{\psi_i}\{i\gamma^\mu\partial_\mu - M\}\psi_i + \frac{1}{2}\partial^\mu\sigma\partial_\mu\sigma - \frac{1}{2}m_\sigma^2\sigma^2 \\ &- \frac{1}{3}g_2\sigma^3 - \frac{1}{4}g_3\sigma^4 - g_s\overline{\psi_i}\psi_i\sigma - \frac{1}{4}\Omega^{\mu\nu}\Omega_{\mu\nu} \\ &+ \frac{1}{2}m_w^2V^\mu V_\mu + \frac{1}{4}c_3(V_\mu V^\mu)^2 - g_w\overline{\psi}_i\gamma^\mu\psi_i V_\mu \\ &- \frac{1}{4}\vec{B}^{\mu\nu}.\vec{B}_{\mu\nu} + \frac{1}{2}m_\rho^2\vec{R}^\mu.\vec{R}_\mu - g_\rho\overline{\psi}_i\gamma^\mu\vec{\tau}\psi_i.\vec{R}^\mu \\ &- \frac{1}{4}F^{\mu\nu}F_{\mu\nu} - e\overline{\psi}_i\gamma^\mu\frac{(1 - \tau_{3i})}{2}\psi_i A_\mu.\end{aligned} \tag{7}$$

All the quantities have their usual well known meanings. From the above Lagrangian we obtain the field equations for the nucleons and mesons. These equations are solved by expanding the upper and lower components of the Dirac spinors and the boson fields in an axially deformed harmonic oscillator basis with an initial deformation β_0. The set of coupled equations is solved numerically by a self-consistent iteration method. The centre-of-mass motion energy correction is estimated by the usual harmonic oscillator formula $E_{c.m.} = \frac{3}{4}(41A^{-1/3})$. The quadrupole deformation parameter β_2 is evaluated from the resulting proton and neutron quadrupole moments, as $Q = Q_n + Q_p = \sqrt{\frac{16\pi}{5}}(\frac{3}{4\pi}AR^2\beta_2)$. The root mean square (rms) matter radius is defined as $\langle r_m^2 \rangle = \frac{1}{A}\int \rho(r_\perp, z)r^2 d\tau$, where A is the mass number, and $\rho(r_\perp, z)$ is the deformed density. The total binding energy and other observables are also obtained by using the standard relations, given in [31]. This set not only reproduces the properties of stable nuclei but also well predicts for those far from the β-stability valley. As outputs, we obtain different potentials, densities, single-particle energy levels, radii, deformations and the binding energies. For a given nucleus, the maximum binding energy corresponds to the ground state and other solutions are obtained as various excited intrinsic states.

3. Method of Calculation and results

In this letter, our aim is to look for the next double closed nucleus beyond ^{208}Pb which may be a possible candidate for the experimentalists to look for. For this, we have used two well-defined but distinct approaches (i) non-relativistic Skryme-Hartree-Fock (SHF) with FITZ, SIII, SkMP and SLy4 interactions [28, 29] (ii) Relativistic Mean Field (RMF) formalism [30, 31] with NL3, G1, G2 and NL-Z2 parameter sets. These models have been successfully applied in the description of nuclear structure phenomena both in $\beta-$stable and $\beta-$unstable regions throughout the periodic chart. The constant strength scheme is adopted to take care of pairing correlation [32] and evaluated the pairing gaps $\triangle_n$ and $\triangle_p$ for neutron and proton respectively from the celebrity BCS equations [33].

We scanned a wide range of nuclei starting from the proton-rich to the neutron-rich region in the superheavy valley (Z=112 to Z=130). It is well understood and settled that the properties of a magic number for a nuclear system has the following characteristics:

- The average pairing gap for proton Δ_p and neutron Δ_n at the magic number is minimum.
- The binding energy per particle is maximum compared to the neighboring one, i.e.there must be a sudden decrease (jump) in two neutron (or two proton) separation energy S_{2n} just after the magic number in an isotopic or isotonic chain.
- At the magic number, the shell correction energy E_{shell} is maximum negative. In other words, a pronounced energy gap in the single-particle levels $\epsilon_{n,p}$ appears at the magic number.

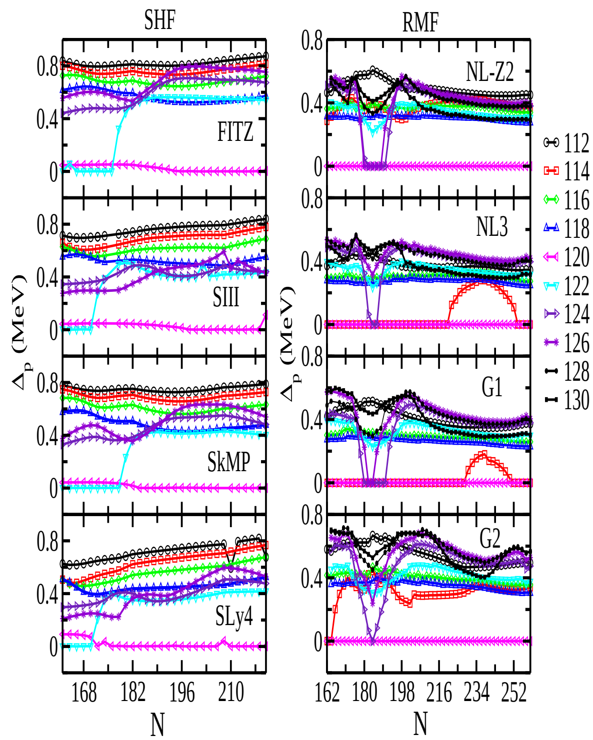

FIG. 1: The proton average pairing gap Δ_p for Z=112-126 with N=162-220 and Z=112-130 with N=162-260.

We focus on the shell closure properties in the superheavy valley based on the above three important observables and identify the magic proton and neutron numbers.

The average pairing gap for proton Δ_p and for neutron Δ_n are the representative of strength of the pairing correlations. The curves for Δ_p are displayed in FIG. 1 obtained by SHF and RMF with

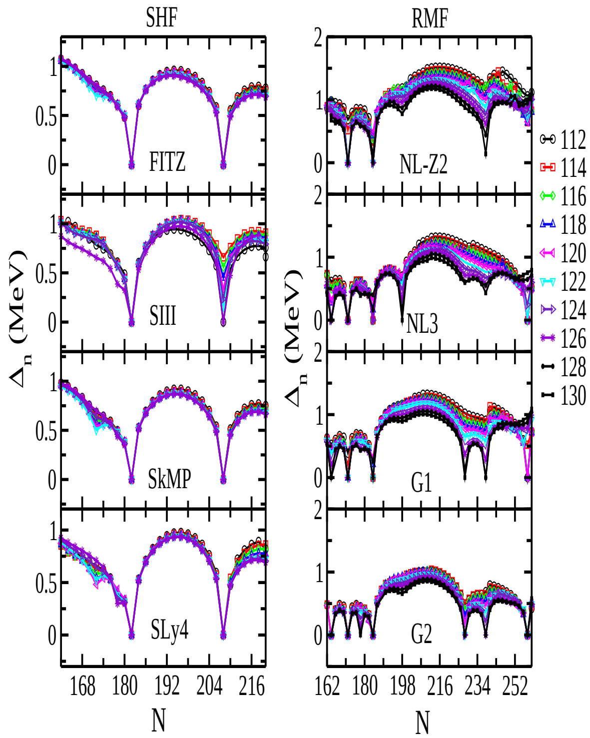

FIG. 2: Same as FIG.1 but for neutron average pairing gap Δ_n.

FITZ, SIII, SLy4, SkMP and NL3,NL-Z2, G1, G2 force parameterizations. If we investigate the figure carefully, it is clear that the value of Δ_p almost zero for the whole Z=120 isotopic chain in both the theorical approaches. A similar Δ_p is observed for few cases of Z=124 and Z=114 isotopes.

To predict the corresponding neutron shell closure of the magic Z=120, we have estimated the neutron pairing gap Δ_n for all elements Z=112−130 with their corresponding isotopic chain. As a result of this, the calculated Δ_n for the whole atomic nuclei in the isotopic chains are displayed in FIG. 2. We obtained an arc like structure with vanishing Δ_n at N= 182, 208 and N=172, 184, 258 respectively for SHF and RMF of the considered parameter sets. Further, the neutron pairing gap is found to be minimum among the isotopic chains pointing towards the magic nature of Z =120. Therefore, all of these force parameters are directing Z = 120 as the next magic number after Z =82.

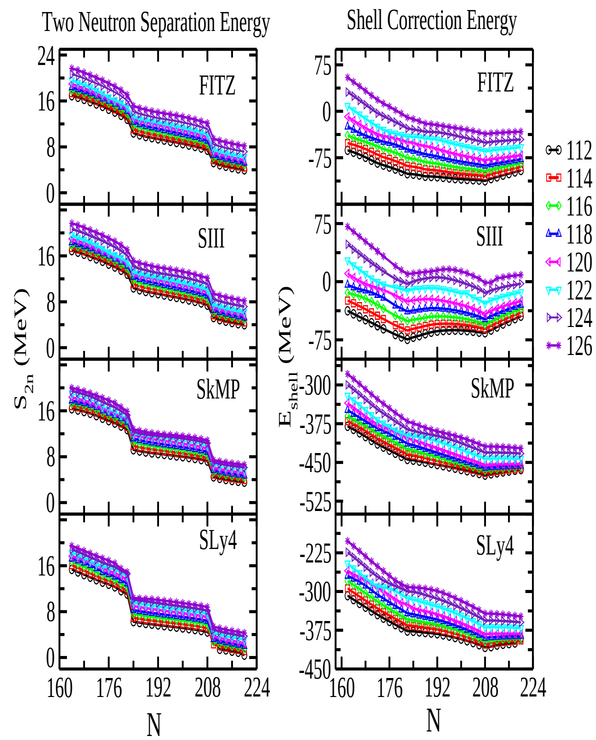

FIG. 3: The two neutron separation energy S_{2n} and the shell correction energy E_{shell} for Z=112-126 and N=162-220 in the framework of SHF theory

As mentioned earlier, the binding energy per particle (BE/A) is maximum for double closed nucleus compared to the neighbouring one. For example, the BE/A with SHF (FITZ set) for $^{300,302,304}120$ are 7.046, 7.048 and 7.044 MeV corresponding to N=180, 182 and 184 respectively. Similarly with SLy4 these values are 6.950, 6.952 and 6.933 MeV. This is reflected in the sudden jump of S_{2n} from a higher value to a lower one at the magic number in an isotopic chain. This lowering in two neutron separation energy is an acid test for shell closure investigation. FIG. 3 shows the S_{2n} as a function of neutron number for all the isotopic chain of the considered elements for both SHF and RMF formalisms.

TABLE I: Single-particle levels $\epsilon_{n,p}$ (MeV) for ^{302} 120 in SHF(SLy4 and FITZ) and ^{304}120 in RMF (NL3 and G2).

Orbit	neutron (ϵ_n)				Orbit	proton (ϵ_p)			
	SLy4	FITZ	NL3	G2		SLy4	FITZ	NL3	G2
$s_{1/2}$	-58.0	-50.7	-55.4	-54.0	$s_{1/2}$	-38.6	-34.6	-39.8	-38.8
$p_{3/2}$	-53.7	-47.4	-51.8	-50.2	$p_{3/2}$	-34.8	-31.1	-36.3	-35.1
$p_{1/2}$	-53.4	-47.2	-51.6	-50.0	$p_{1/2}$	-34.6	-31.0	-36.1	-34.8
$d_{5/2}$	-48.0	-42.9	-46.7	-45.1	$d_{5/2}$	-29.9	-26.6	-31.4	-30.2
$d_{3/2}$	-47.2	-42.3	-46.0	-44.3	$d_{3/2}$	-29.2	-26.1	-30.7	-29.3
$s_{1/2}$	-43.8	-39.2	-41.0	-40.3	$s_{1/2}$	-26.2	-23.1	-26.3	-26.1
$f_{7/2}$	-41.5	-37.5	-40.6	-39.1	$f_{7/2}$	-24.2	-21.3	-25.7	-24.5
$f_{5/2}$	-39.9	-36.4	-39.3	-37.6	$f_{5/2}$	-22.7	-20.2	-24.2	-22.8
$p_{3/2}$	-36.0	-32.8	-34.6	-33.5	$p_{3/2}$	-19.1	-16.5	-19.8	-19.0
$p_{1/2}$	-35.8	-32.5	-34.5	-33.1	$p_{1/2}$	-18.9	-16.3	-19.7	-18.7
$g_{9/2}$	-34.2	-31.5	-33.9	-32.5	$g_{9/2}$	-17.9	-15.3	-19.3	-18.1
$g_{7/2}$	-31.7	-29.6	-31.8	-30.0	$g_{7/2}$	-15.3	-13.4	-17.0	-15.4
$d_{5/2}$	-28.0	-26.2	-27.8	-26.3	$d_{5/2}$	-11.9	-9.5	-12.9	-11.6
$d_{3/2}$	-26.8	-25.2	-27.2	-25.4	$h_{11/2}$	-11.1	-8.8	-12.5	-11.3
$h_{11/2}$	-26.5	-25.0	-26.9	-25.3	$d_{3/2}$	-10.9	-8.7	-12.3	-10.7
$s_{1/2}$	-25.1	-24.1	-24.8	-23.3	$s_{1/2}$	-9.8	-7.2	-10.2	-9.3
$h_{9/2}$	-22.7	-22.2	-23.8	-21.8	$h_{9/2}$	-7.3	-6.0	-9.3	-7.5
$f_{7/2}$	-19.8	-19.2	-20.5	-18.7	$f_{7/2}$	-4.5	-2.4	-5.8	-4.1
$i_{13/2}$	-18.5	-18.1	-19.6	-18.1	$i_{13/2}$	-4.0	-2.0	-5.5	-4.1
$f_{5/2}$	-17.7	-17.5	-19.4	-16.9	$f_{5/2}$	-2.6	-0.9	-4.7	-2.4
$p_{3/2}$	-16.5	-15.9	-16.9	-14.9	$p_{3/2}$	-1.4	0.4	-2.6	-0.8
$p_{1/2}$	-16.2	-15.7	-16.7	-14.4					
$i_{11/2}$	-13.3	-14.1	-15.6	-13.1					
$g_{9/2}$	-11.7	-11.9	-13.2	-11.0					
$j_{15/2}$	-10.3	-10.9	-12.1	-10.5					
$g_{7/2}$	-8.8	-9.6	-11.5	-8.6					
$d_{5/2}$	-8.0	-8.5	-9.5	-7.2					
$d_{3/2}$	-7.0	-7.7	-9.2	-6.6					
$s_{1/2}$	-3.6	-5.7	-8.2	-6.0					
$j_{13/2}$			-7.3	-4.3					

In spite of the complexity about single-particle and collective properties of the nuclear interaction some simple phenomenological facts emerge from the bulk properties of the low-lying states in the even-even atomic nuclei. The S_{2n} energy is sensitive to this collective/single-particle inter play and provides sufficient information about the nuclear structure effects. From FIG. 3, we notice such effect, i.e., jump in two neutron separation energy at N=182 and 208 with SHF. However, such jumps are found at N=172, 184, 258 in RMF calculations confirming the shell closure properties of the neutron numbers.

The shell correction energy E_{shell} is a key quantity to determine the shell closure of nucleon. This concept was introduced by Strutinski [34] in liquid-drop model to take care of the shell effects. As a result, the whole scenario of liquid properties converted to shell structure which could explain the magic shell even in the frame-work of liquid-drop model. The magnitude of total (proton plus neutron) E_{shell} energy is dictated by the level density around the Fermi level. A positive E_{shell} reduces the binding energy and a negative shell correction energy increases the stability of the nucleus. As a representative case, we have depicted our SHF result of E_{shell} in FIG. 3. It is clear from the figure the extra stability of ^{302,328}120. We find similar results of large negative shell energy for RMF calculation at neutron number 172, 184, 258. Such calculations for few cases are reported in Ref. [35].

As a further confirmative test, the single-particle energy levels for neutrons and protons $\epsilon_{n,p}$ are analyzed. The calculated $\epsilon_{n,p}$ are presented in Table I for ^{302}120 SHF(SLy4 and FITZ) and for ^{304}120 RMF(NL3 and G2) as representative cases. From the Table, one can estimate the energy gaps $\triangle\epsilon_{n,p}$ for neutron and proton orbits. For example, in ^{302}120 (FITZ), the gap $\triangle\epsilon_n = \epsilon_n(3d_{3/2}) - \epsilon_n(4s_{1/2})$ at N=182 is 1.977 MeV which is comparable with 1.898 MeV of the known magic gap at N=50 for the same nucleus. For the proton case at Z=120, we get $\triangle\epsilon_p = \epsilon_p(2f_{5/2}) - \epsilon_p(3p_{3/2}) = 1.340$ MeV which is again a large gap of similar order ($\triangle\epsilon_p = \epsilon_p(1g_{9/2}) - \epsilon_p(1g_{7/2}) = 1.862$ MeV) for N=50. Almost identical behaviour is noticed with other SHF and RMF (at N=184) calculations, irrespective of parameter used, confirming Z=120 as a clear magic number.

4. Summary and Conclusion

In summary, we have analyzed the pairing gap Δ_p and Δ_n, two-neutron separation energy S_{2n}, shell correction energy E_{shell} and single-particle energy for the whole $Z = 112-130$ region covering the proton-rich to neutron-rich isotopes. To our knowledge, this is one of the first such extensive and rigorous calculation in both SHF and RMF models using a large number of parameter sets. The recently developed effective field theory motivated relativistic mean field forces G1 and G2 are also involved. Although the results depend slightly on the forces used, the general set of magic numbers beyond ^{208}Pb are Z=120 and N=172, 182/184, 208 and 258. The highly discussed proton magic number $Z = 114$ in the past (last four decades) is found to be feebly magic in nature.

Acknowledgments

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