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Symmetry-adapted No-core Shell-model Calculations for Probing the Structure of Atomic Nuclei

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Abstract: Exploiting special symmetries to unmask simplicity within complexity that remains the "holy grail" of nuclear theory is re-examined within the framework of its historical context and current *ab initio* no-core shell-model approaches that exploit high-performance computing resources and applied math methodologies. Examples using the symmetry-adapted no-core shell model (SA-NCSM) that clearly demonstrate the important role group theory plays in this evolving story will serve to elucidate current state-of-the-art developments in this arena, including comparisons of excitation spectra and transition rates with experimental results for light and medium-mass nuclei. An interesting extension of the SA-NCSM, an advanced method with a novel twist that enables one to incorporate deformation from the onset, will be proffered as a further way to manage the combinatorial growth of model-space dimensionalities that remains the nemesis of all theories that seek an *ab initio* understanding of nuclear collectivity, and in so doing extends applicability of the theory to heavier and more exotic nuclear species.

Key words: no-core shell-model; symmetry-adapted; *ab initio* calculation
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1 Introduction

Recent advances in the development of realistic inter-nucleon interactions[1–4] and the availability of massively parallel high performance computing (HPC) resources have placed *ab initio* nuclear structure models at the forefront of nuclear structure explorations. Building upon the success of the independent-particle model of Mayer and Jensen[5–6], particle-driven models, such as the no-core shell model (NCSM)[7–8] and its extensions (see, *e.g.*, Refs. [9–11]), have been very successful in describing low-lying states of *s*- and *p*-shell nuclei. The NCSM is a complete microscopic theory, usually utilizing symmetries such as time reversal, parity, and translational invariance. It uses a harmonic oscillator (HO) single-particle basis characterized by the $\hbar\Omega$ oscillator frequency, and organizes the complete space into "horizontal" slices. The model space is limited by the $N_{\max}$ cutoff, which describes the cutoff in total oscillator quanta above the lowest HO configuration for a given nucleus.

Predating the NCSM is a collective symplectic model[13–14], developed by Rowe and Rosensteel, with Sp$(3,\mathbb{R})$ the underpinning symmetry, which provides a theoretical framework for understanding deformation-dominated collective phenomena in nuclei[12, 14–15] (Fig. 1). Through partitioning the complete space into physically relevant subspaces, this model exposes important dynamical symmetries in nuclei. It is the microscopic realization to the Bohr-Mottelson theory[16], and reduces to the microscopic Elliott model[17–18] in the limit of a single shell. Indeed, the seminal work by Elliott identifies the importance of the $SU(3)$ symmetry, the subgroup of Sp$(3,\mathbb{R})$, in light and intermediate-mass nuclei. In heavier nuclei, pseudo-spin symmetry and its pseudo-$SU(3)$ complement have been shown to play an important role in accounting for deformation in the upper *pf* and lower *sdg* shells, and in particular, in strongly deformed nuclei of the rare-earth and actinide regions[19], as well as in many other studies (*e.g.*, see Ref. [20]). The symplectic Sp$(3,\mathbb{R})$ symmetry applied in a microscopic framework is directly related to the particle position and momentum coordinates, and naturally describes rotations and vibrations of an equilibrium deformation[21–22]. The existence of this symmetry and its slight symmetry breaking emerges

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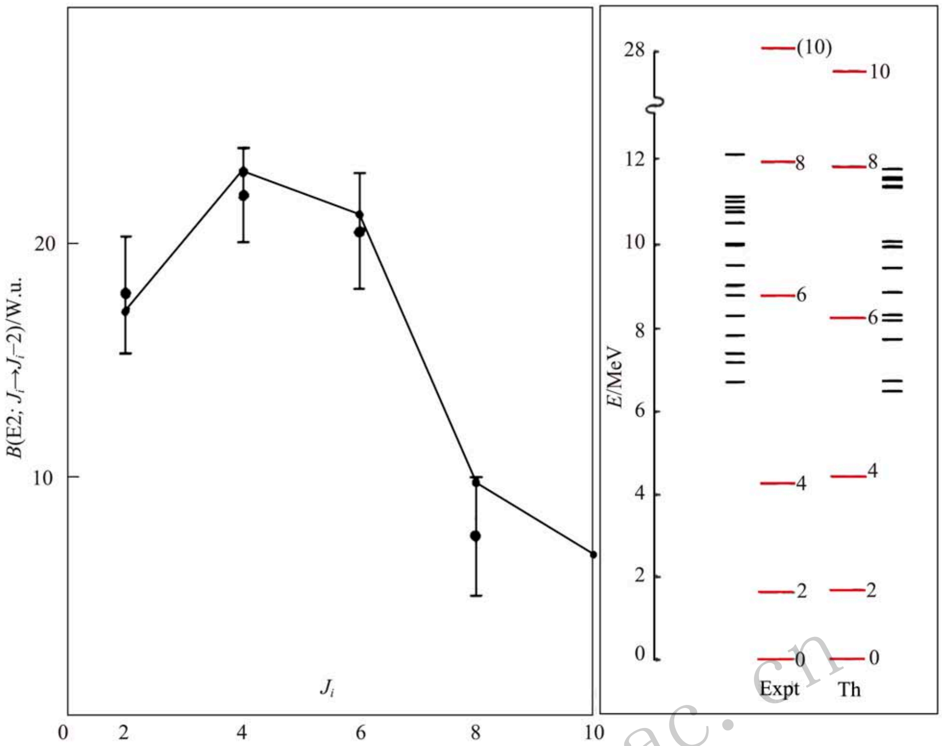

Fig. 1 (color online) Microscopic symplectic model with a set of effective single-particle energies, a $Q \cdot Q$-type interaction+pairing for ^{20}Ne. Left: Calculated $B(\mathrm{E2}\downarrow)$ transition strengths *without effective charges* fall within the uncertainties of the corresponding experimental measurements. Right: Calculated energy spectrum for ^{20}Ne as compared to the experiment. Figure adapted from Ref. [12].

naturally from first principles, as has been revealed in recent *ab initio* symmetry-adapted no-core shell model (SA-NCSM) studies[22–23]. The SA-NCSM is a microscopic theory, which by exploiting exact and approximate symmetries exposes simple symmetry patterns that underpin nuclear structure.

Informed by the emergence of the symplectic symmetry from *ab initio* studies, the fully microscopic no-core symplectic shell model (NCSpM)[24] uses the symplectic symmetry and a schematic interaction, and can approach model spaces beyond the reach of *ab initio* theories. Using this tool, we can probe the physics of the Hoyle state in ^{12}C, including the associated rotational band, plus the nature of other positive- and negative-parity states in ^{12}C and its giant resonance modes. This can be extended to the properties of other highly deformed intermediate-mass nuclei. The NCSpM is able to describe bound states within a model space that is a small fraction of the complete space, through reorganizing the complete model space into irreducible representations (irreps) of $\mathrm{Sp}(3,\mathbb{R})$ (that is, into physically relevant “vertical cones”).

2 Approximate symmetries in nuclei

Emergent symmetries from first principles – The *ab initio* SA-NCSM[23] is a no-core shell model with a symmetry-adapted (SA) basis that is either $SU(3)$-coupled or $\mathrm{Sp}(3,\mathbb{R})$-coupled. In its $SU(3)$ realization, the many-particle basis states are organized with respect to the deformation-related $SU(3)_{(\lambda\,\mu)} \overset{\kappa}{\supset} SO(3)_L$ subgroup chain[22, 25]. In a given complete $N_{\max}$ space, results obtained in the SA-NCSM are exactly equivalent to the NCSM results using the same interaction. The symmetry-guided organization scheme used in the SA-NCSM allows for the consideration of only the most physically-relevant subspace of a complete $N_{\max}$ model space.

Results for p-shell nuclei computed in the *ab initio* SA-NCSM show the emergence, from first principles, of a simple pattern that favors large deformation and low spin (Fig. 2). For example, the $N_{\max} = 10$ SA-NCSM wave function for the 1^+ ground state of ^{6}Li computed with the bare JISP16 nucleon-nucleon (NN) interaction shows a dominance of the deformed $0\hbar\Omega$ (20) irrep and its symplectic excitations (*e.g.*, $2\hbar\Omega$ (40), $4\hbar\Omega$ (60), *etc.*). This pattern is independent of the interaction used and has been found in other p-shell nuclei, including ^{6}He, ^{8}Be, and ^{12}C. This emergent feature confirms the importance of the $SU(3)$ and $\mathrm{Sp}(3,\mathbb{R})$ symmetries in describing nuclear structure.

Clustering and collectivity in ^{12}C – The NCSpM is a fully microscopic no-core shell model based on the physically relevant symplectic $\mathrm{Sp}(3,\mathbb{R})$ group[13–14]

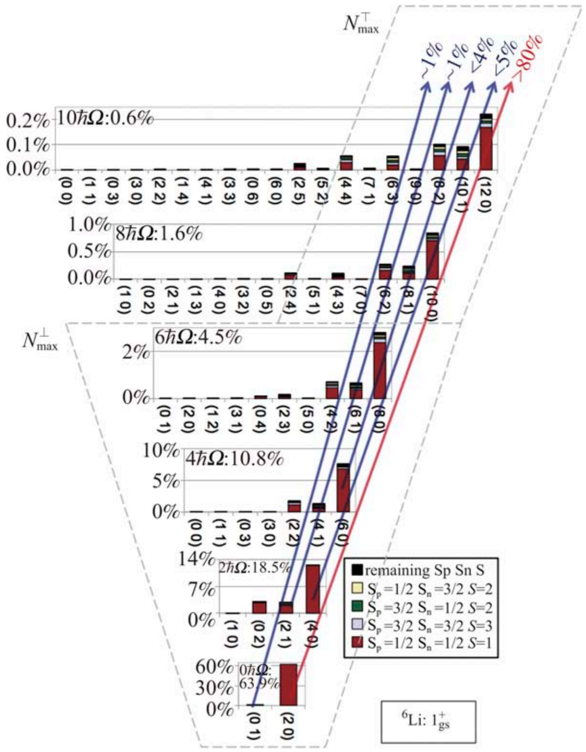

Fig. 2 (color online) Probability distributions for proton, neutron, and total intrinsic spin components ($\mathrm{S_pS_nS}$) across the deformation-related $(\lambda\,\mu)$ values for the 1^+ ground state of ^{6}Li, calculated in 12 HO shells with the JISP16 bare interaction ($\hbar\Omega=20$ MeV). The most deformed $(\lambda\,\mu)$ configurations are at the right of each subspace, where the strengths are concentrated indicating the dominance of collectivity. A symmetry-guided model-space selection takes advantage of this emergent property by including the complete space up through $N_{\max}^{\perp}$, and beyond this selecting a subset of configurations with high deformation and low spin up through $N_{\max}^{\top}$. A model space constructed in this way is labeled by $\langle N_{\max}^{\perp}\rangle N_{\max}^{\top}$. The projection onto symplectic vertical slices (with probability $\geqslant 1\%$) is schematically illustrated by arrows and clearly reveals the preponderance of a single symplectic irrep (vertical cone). Figure from Ref. [22].

and its $SU(3)$ subgroup[17–18, 26]. In the same complete $N_{\max}$ model space and using the same interaction, the NCSM and NCSpM results are identical. The NCSpM, however, organizes the space into $\mathrm{Sp}(3,\mathbb{R})$ irreps, or "vertical slices," each of which describes a single equilibrium deformation and its rotations and vibrations. Selecting only the most physically relevant vertical slices in a given $N_{\max}$ space greatly reduces the model space, and allows for the NCSpM to extend to $N_{\max}$ model spaces far beyond the current NCSM limits.

To study enhance deformation and clustering (Fig. 3), we use a many-body Hamiltonian comprised of two main components: a single-particle piece, consisting of the HO potential and a spin-orbit term, and a collective piece that enters through the quadrupole-quadrupole interaction:

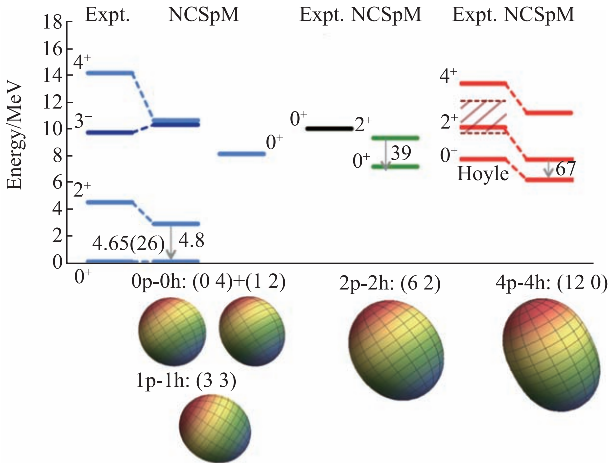

Fig. 3 (color online) Energy spectrum for ^{12}C calculated using the NCSpM with the schematic interaction (1) and the JISP16 NN interaction as the $V_{\rm NN}^{\rm SB}$ symmetry-breaking term, and using 5 $\mathrm{Sp}(3,\mathbb{R})$ irreps (the average deformation of each is also depicted) extended to $N_{\max}=20$ ($\hbar\Omega=18$ MeV), and compared to experiment[27]. The $B(E2)$ transition strengths are in W.u.

$$H_\gamma=\sum_{i=1}^{A}\left(\frac{\boldsymbol{p}_i^2}{2m}+\frac{m\Omega^2\boldsymbol{r}_i^2}{2}\right)+\frac{\chi}{2}\frac{(\mathrm{e}^{-\gamma Q\cdot Q}-1)}{\gamma}+V_{\rm NN}^{\rm SB}. \quad (1)$$

The HO Hamiltonian H_0, and the important quadrupole-quadrupole interaction, $\frac{1}{2}Q\cdot Q=\frac{1}{2}\sum_i q_i\cdot(\sum_j q_j)$ – which introduces the interaction of each particle with the total quadrupole moment of the system – preserve the symplectic $\mathrm{Sp}(3,\mathbb{R})$ symmetry.* The symmetry-breaking $V_{\rm NN}^{\rm SB}$ term can be either a realistic interaction, such as the chiral N^{3}LO interaction, or, *e.g.*, the spin-orbit term, $\sum_{i=1}^{A}\kappa l_i\cdot s_i$. The value of χ is fixed using self-consistent arguments[29] by the estimate used in an $\mathrm{Sp}(3,\mathbb{R})$-based study of ^{16}O cluster-like states[30], and the strength of the HO potential is fixed using an empirical estimate, $\hbar\Omega\approx 41/A^{1/3}$ MeV. The only adjustable parameter in the model is γ, which controls the presence of many-body interactions. Specifically, H_γ introduces many-body interactions in a hierarchical way, controlled by $\gamma<1$, such that higher-order terms in the exponential of $Q\cdot Q$ become negligible[24]. For example, we find that for ^{12}C, all terms in the expansion beyond $(Q\cdot Q)^2$ contribute negligibly to describing the ground state and its rotational band; for the Hoyle-state band, however, it is necessary to include terms up through $(Q\cdot Q)^4$.

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*The average contribution $\langle Q\cdot Q\rangle$ of $Q\cdot Q$ within a subspace of HO excitations is removed as detailed in Ref. [28] to eliminate the considerable renormalization of the zero-point energy due to the large monopole contribution of the $Q\cdot Q$ interaction.

Results for ^{12}C are shown in Figs. 3 and 4. The energy spectrum for ^{12}C, computed in the NCSpM with $N_{\max} = 20$, agree remarkably well with experiment (Fig. 3). Results are shown for $N_{\max} = 20$, ($\hbar\Omega = 18$ MeV), down-selected to include only 5 symplectic irreps. We find that the lowest 0^+, 2^+, and 4^+ states of the two 0p-0h irreps [0p-0h (4 0) and 0p-0h (1 2)] reproduce the ground state rotational band (the first 0^+, 2^+, and 4^+ of ^{12}C), the lowest 0^+ state of the 4p-4h (12 0) irrep coincides with the experimental Hoyle state, the lowest 0^+ state of the 2p-2h (6 2) irrep with the third 0^+ in ^{12}C, and the low-lying 3^- state is reproduced using the 1p-1h (3 3) irrep. In addition to the energy spectrum, the NCSpM reproduces observables such as B(E2) transition strengths (Fig. 3), matter rms radii, and electric quadrupole moments, and has been used to investigate the nature of the giant monopole and quadrupole resonances in selected light- and intermediate-mass nuclei[31]. This model has also been applied to studies of other nuclei, including ^{8}Be, as well as various *sd*-shell nuclei without the need to adjust the γ strength parameter[32–33]. This is an indication that the NCSpM captures important components of the underlying nuclear physics.

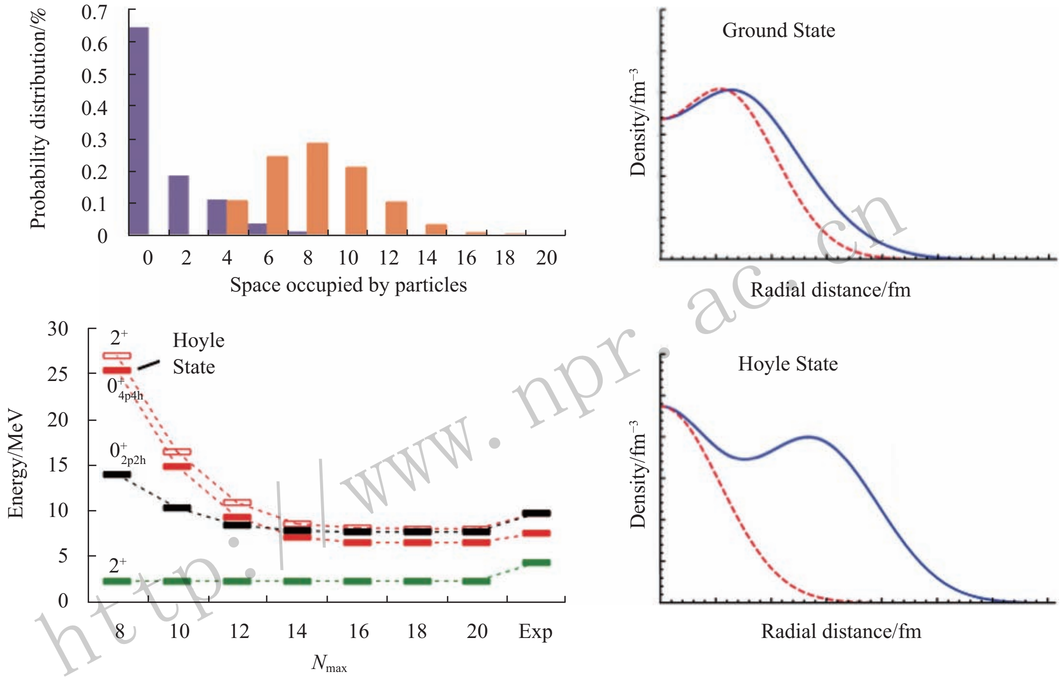
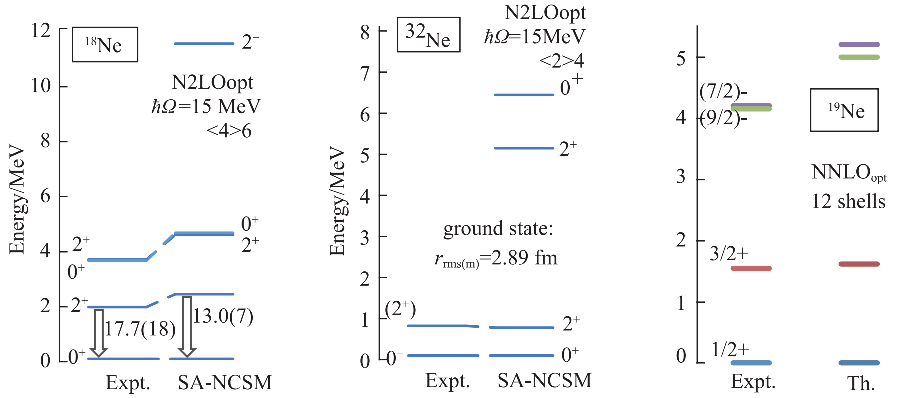


Fig. 4 (color online) left: (top) Probability distribution shown across total HO quanta excitations for the ^{12}C 0^+_{gs} (purple) and 0^+_2 (orange) states, computed with the NCSpM with $N_{\max} = 20$ and $\hbar\Omega = 18$ MeV, and (bottom) the dependence of their energies on $N_{\max}$. right: One-body densities, shown along the x-axis (red, dashed) and z-axis (blue, solid) of the intrinsic frame for (top) the ground state and (bottom) the 0^+_2 state.

Of distinct importance is the ability of the NCSpM to achieve higher $N_{\max}$ model spaces than those that are currently within the reach of other NCSM studies (Fig. 4). While a smaller $N_{\max}$ model space is sufficient for convergence of the ground state rotational band, the wave function for the 0^+_2 state of ^{12}C has significant contributions from highly deformed configurations [*e.g.*, (12 0), (14 0), (16 0), *etc.*] and requires a much larger $N_{\max}$ model space in order for the collectivity of the state to fully develop and for the energy to reach convergence (Fig. 4, left). This large deformation is also seen in comparison of the one-body (matter) densities of the ground state and 0^+_2 state (Fig. 4, right). The ground state has an essentially donut-like shape, while the 0^+_2 state shows peaks in the probability density aligned along the z-axis, indicating overlapping clusters spatially extended along this axis.

Reaching heavier nuclei – Guided by the emergent simple patterns that points to the importance of the symplectic Sp(3,$\mathbb{R}$) group and its $SU(3)$ subgroup, SA-NCSM studies can now reach heavier nuclei *ab initio*, including odd-A nuclei and negative parity states (Fig. 5). Studies of such *sd*-shell nuclei as ^{22}Mg, ^{24}Si, and ^{24}Ne were first undertaken in a NCSpM framework[32], which yielded insights into the collective nature of these nuclei and the basis needed for that collectivity to fully develop. Subsequent SA-NCSM studies of these same nuclei with realistic chiral interactions, using model spaces reduced to include only the most important configurations, show impressive agreement with experiment.

Furthermore, an extension of the SA-NCSM that



(a) (b) (c)

Fig. 5 (color online) *Ab initio* SA-NCSM calculations using the chiral NNLO$_{\rm opt}$ NN interaction[34] in ultra-large model spaces ($\hbar\Omega = 15$ MeV). Energy spectrum of (a) ^{18}Ne in 9 HO major shells, along with the B(E2; $2^+ \rightarrow 0^+$) strength in W.u. reported for 33 shells, that has been a challenge for *ab initio* models, (b) ^{32}Ne in the proximity of the neutron drip line (in 7 HO major shells), and (c) the odd-A ^{19}Ne in 12 HO major shells. Simulations are performed on the Blue Waters system.

incorporates deformation from the onset in the many-body basis states is currently under development, with a very efficacious way to manage the combinatorial growth of the model-space size to reach even heavier nuclear species. For example, the Hoyle-state energy in ^{12}C calculated in the NCSpM using $N_{\rm max} = 20$ can be well reproduced by the deformed extension of the NCSpM using only $N_{\rm max} = 4$ model spaces[35].

3 Summary

In summary, we have demonstrated the emergence of simple patterns and associate symmetries in nuclei from first principles. We have shown that, by exploiting these symmetries, the NCSpM and SA-NCSM can provide incredible insights into the underlying nuclear physics. In particular, the NCSpM points to nuclear configurations that are most important for describing highly deformed structures, which, in turn, can guide *ab initio* no-core shell-model studies capitalizing on the use of SA bases into more computationally challenging regimes. And beyond this, an extension of the SA-NCSM with a novel twist that enables one to incorporate deformation from the onset in the many-body basis states is currently under development that can dramatically extend applicability of the theory to heavier and more exotic nuclear species.

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探索原子核结构的对称性主导无芯壳模型计算

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摘要： 揭示隐藏于复杂中的简单性相关的特殊对称性是核理论研究的“圣杯”，回顾了其探索历史和当前利用高性能计算设备及应用数学方法进行的从头计算无芯壳模型研究。作为对称性主导无芯壳模型(SA-NCSM)计算的实例，通过对轻核和中重质量区核素的能谱计算及与实验结果的比较，清晰地展示了群论在揭示这些当今最先进计算手段得到结果中所起的重要作用。作为SA-NCSM的有趣推广，从头引入形变的新方法提供了解决所有以探索原子核的集体性质为目的的从头计算方法都要面对的模型空间维数呈组合数增长的处理手段，并且该方法使本理论能用于描述重核及奇特核。

关键词： 无芯壳模型；对称性主导；从头计算

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