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Ab initio calculations for the nuclear shell evolution

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Content



- 1. Introduction of ab initio calculations
- 2. Shell evolution in neutron-rich nuclei
- 3. Isospin symmetry breaking



- 4. Isospin symmetry breaking for the shell evolution in proton-rich nuclei
- 5. Summary





1. Introduction of ab initio calculations

Ab initio calculations for the nuclear shell evolution



What is *ab initio* calculations?



3NF

Nuclear Force

Freedom: Pion and Nucleon

Requirement: Reproduce nucleon-nucleon scattering phase shifts **Properties**: Short-range repulsion and long-range attraction, strong repulsion **Typical Forces** / CD-Bonn, AV18, χEFT

Renormalization

Objective: To decouple high and low momentum, soften the nuclear force, and accelerate the convergence speed of many-body calculations. **Representatives:** G-Matrix, V_(low-k), SRG

Many-Body Methods

Objective: To solve the Hamiltonian of strongly interacting many-body nuclear

systems

Representatives: NCSM (A≤16), MBPT (A ~ 100), CC (A ~ 100, 208Pb), IMSRG

(A ~ 100, 208Pb), ACSE (We are developing this method)...

Many-body Method—nuclear shell model—medium-Heavy nuclear

VS-IMSRG realistic interaction vs USDB phenonological shell model interaction





S. Ragnar Stroberg, Scott K. Bogner, Heiko Hergert, Jason D. Holt Annual Review of Nuclear and Particle Science, 69 307-362 (2019)





Ab initio calculations for the nuclear shell evolution



VS-IMSRG and MBPT many-body method







Normal-ordered two-body interaction capture the main contribution of three-body forces



VS-IMSRG and MBPT many-body method





Ab initio calculations for the nuclear shell evolution

¹⁶O core



VS-IMSRG and MBPT many-body method



- **3.** Valence-space Hamiltonian can be constructed by using the unity transformation
 - $H_{eff}(s) = U(s)H_{NO}U^{\dagger}(s), (UU^{\dagger}=1)$
 - Flow equation $\frac{d}{ds}H_{eff}(s) = [\eta(s), H(s)]$
 - Generator: $\eta(s) = \frac{dU(s)}{ds}U^{\dagger}(s) = -\eta^{\dagger}(s)$
 - Unity transformation: $U(s) = e^{\Omega(s)} = e^{\int \eta(s) ds}$





Ab initio VS-IMSRG method

Ab initio Valence-Space In-Medium Similarity Renormalization Group(*Ab initio* VS-IMSRG)

➤ Mainly ides

 $H(s) = U(s)H(0)U^+(s)$



- ≻Advantage:
 - Realistic nuclear interaction (NN+3N)
 - Including CSB + CIB
 - Isospin symmetry breaking in contact and exchange terms

IMP

- No parameter introduced during the calculations
- "Exact" calculations

VS-IMSRG works for nuclei covered by shell model calculations

Ab initio calculations for the nuclear shell evolution





Ab initio

2. Shell evolution in neutron-rich nuclei

- 1 <u>J. G. Li*</u>, Phys. Lett. B 840 137892(2023)
- ② Q. Yuan, J. G. Li^{*}, H. H. Li, PLB 848 138331 (2024)
- ③ H. H. Li, J. G. Li*, M. R. Xie, W. Zuo, PRC (Letter) 109, L061304 (2024).
- ④ N. Chen, <u>J. G. Li*,</u> and H. H. Li, Phys. Rev. C 110, 034316(2024)
- (5) M. R. Xie, L. Y. Shen, <u>J. G. Li*</u>, H. H. Li, Q. Yuan and W. Zuo, CPC 48 074106(2024)
- 6 Q. Yuan, J. G. Li*, and W. Zuo, Phys. Rev. C(Letter) 109, L041301 (2024)
- (7) X. P. Wang, <u>J. G. Li*</u>, N. Chen, submitted to PRC

Shell evolution in neutron-rich



Shell evolution is hot topic in nuclear physic

The disappearance of traditional magic number and appearance of new magic



Deep understanding of the shell evolution is important for the study of properties of heavy nuclei

Ab initio calculations for the nuclear shell evolution

1.Shape transition in ${}^{40}Mg$, ${}^{42}Si$ and ${}^{44}S$ near N = 28





Ab initio calculations for the nuclear shell evolution

2. Ab initio predictions of halo nuclei in medium-mass regio





Based on the ab initio calculations, we use the spectroscopic factor (SF) and two-nucleon amplitude (TNA) to predict the one- and two-neutron halo, respectively



H. H. Li, J. G. Li*, M. R. Xie, W. Zuo, PRC (Letter) 109, L061304 (2024).

Ab initio calculations for the nuclear shell evolution

3. Prediction of N=50 Island of inversion







Cited by

https://doi.org/10.1038/s41567-024-02680-

In-beam spectroscopy reveals competing nuclear shapes in the rare isotope ⁶²Cr

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nature physics

Article

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Motivations for Early High-Profile FRIB Experiments

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Remco G. T. Zegers ^{9,1} Vladimir Zelevinsky ^{9,1} and Xilin Zhang ⁹

Phys. Lett. B 855 (2024) 138841



Spectroscopy of N = 50 isotones with the valence-space density matrix renormalization group A. Tichai^{ab.,O}., K. Kapás^{de}, T. Miyagi^{ab.,d}, M.A. Werner^{a.,d}, Ö. Legeza^{d,b}, A. Schwenk^{ab.,O}, G. Zarand^e

⁸¹Zn@Xiaofei Yang's talk

✓ Reproduce of properties of N=40 nuclei
 ✓ Predict the existence of N=50 IoI

Ab initio calculations for the nuclear shell evolution

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N=40 and N=50 Isotones

exhibit similar properties



3. Isospin symmetry breaking in nuclear systems

- H. H. Li, Q. Yuan, J. G. Li*, M. R. Xie, S. Zhang, Y. H. Zhang, X. X. Xu, N. Michel, F. R. Xu, and W. Zuo, Phys. Rev. C 107, 014302(2023)
- ② H. H. Li, J. G. Li,* M. R. Xie, W. Zuo, Chinese Physics C 47, 12 (2023) 124101
- ③ M.Z. Sun, Y. Yu, X.P. Wang, M. Wang, J.G. Li*, Y.H. Zhang*, et al., Chin. Phys. C(2024)
- (4) Y. Yu, Y. M. Xing, Y. H. Zhang, M. Wang, X. H. Zhou, J. G. Li, H. H. Li, et al., PRL(Accepted)



Nuclear isospin symmetry breaking



- ≻Particle physics level
 - ✓ mass of u-d quark is difference✓ Coulomb forces between quarks
- >Nuclear physics level
 - ✓ Coulomb forces
 - \checkmark Nucleon-nucleon interaction
 - Charge symmetry breaking—CSB $V_{nn} V_{pp}$ (isospin vector)
 - Charge independent breaking--CIB) $2V_{np} (V_{nn} + V_{pp})$ (isospin tensor)

Isospin non-conserving force--INC

✓ Weakly-bound effects

Study the mechanism of isospin symmetry breaking: Coulomb, nuclear forces, and weakly-bound effects...



2. p-n charge difference:

 $e_p = e$, $e_n = (-4.3 \pm 7.1) \times 10^{-20} e$





Status of study of isospin symmetry breaking



> Isospin: (approximation) proton

In 1932, introduced by Heisenberg The properties of mirror nuclei should be same



> Theoretical calculations: shell model

Phenomenological ways:

Adjusting the matrix elements related to 1s1/2 to reproduce the experimental data.



No parameter needs to be adjusted within ab initio calculations, which is suitable for the investigations of isospin symmetry breaking

Isospin symmetry breaking: Experimental results



J. Lee, X.X. Xu, et al., PRL 125,192503(2020) Y. H. Zhang et al., PRL 109, 102501(2012)

Ab initio calculations for the nuclear shell evolution

β-decay in proton-dripline nuclei-isospin symmetry breaking





Ab initio calculations for the nuclear shell evolution



1. Ab initio calculations for the mirror energy difference



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Adopting NN(bare) and NN+3N(1.8/2.0)interaction, VS-IMSRG calculations for the mirror states

PHYSICAL REVIEW C 107, 014302 (2023)

Investigation of isospin-symmetry breaking in mirror energy difference and nuclear mass with *ab initio* calculations

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MED \rightarrow isospin symmetry breaking (MED) = $E_x(n_rich) - E_x(p_rich)$



Large MED is mainly caused by the occupying of weakly-bound 1s1/2 orbital

Ab initio calculations for the nuclear shell evolution

1. Ab initio calculations for the mirror energy difference



1 Calculations of mirror states with large MED_o

Ab initio calculations well reproduce data



Ab initio VS-IMSRG can be used to predict the spectra for unknown in experiments.

Ab initio calculations for the nuclear shell evolution

(2) Predictions of low-lying states in *sd*-shell proton-dripline nuclei.



- Low-lying spectra of neutron-rich nuclei can be well produced.
- The reliability of our prediction for proton-rich nuclei.

2. Isospin symmetry—halos—mass measurement



Collaborations with IMP mass measurement group

see Prof. Yuhu Zhang's talk



M.Z. Sun, Y. Yu, X.P. Wang, M. Wang, J.G. Li^{*}, Y.H. Zhang^{*}, et al., Chin. Phys. C(2024) Y. Yu, Y. M. Xing, Y. H. Zhang, M. Wang, X. H. Zhou, J. G. Li, H. H. Li, et al., PRL(Accepted)



4. Isospin symmetry breaking for the shell evolution in proton-rich nuclei



Shell evolution—isospin symmetry breaking—shell evolutions in neutron-riching



The disappearance of traditional magic number and appearance of new magic number
 What about the shell evolutions in proton-rich nuclei? The effects of isospin symmetry breaking.

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1. ²²Si double magic nuclei---new magic number

plan to done the

experiments of

 ^{22}Si





✓ Neutron-rich double magic nuclei: ^{22}O \checkmark Isospin symmetry breaking for the magicity

Whether ²²Si is a double magic nuclei?



- The excitation energies of 22O is well reproduced with 3.2 MeV; Due to Thomas-Ehrman shift effect, the E(21+) of 22Si is 2.4 3.2 MeV
- Although the E(21+) of 22Si is small, but the ground state properties of 22Si/22O is similar.

J.G. Li,* H. H. Li, S. Zhang, Y. M. Xing,* W. Zuo,* Phys. Lett. B 846, 138197 (2023)

Ab initio calculations for the nuclear shell evolution

Summary





large MED (Thomas-Ehrman shift) is mainly caused by the occupation of 1s1/2

- 3. Isospin symmetry breaking for shell evolution in proton-rich nuclei
 - Predicted doubly magic nuclei ²²Si with small 2+ excitation energy
 - *Proton-rich nuclei near* Z=8, 20 and 28 show deformation, which belong to IOI

Thank you for your attention!

2.

三体力数范-质量-第一性原理计算





三体力效应在原子核性质中扮演着非常重要的角色

Ab initio calculations for the nuclear shell evolution

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手征有效场论



N³LO两体力+N²LO三体力

Ab initio calculations for the nuclear shell evolution

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现实核力 (NN+3N)

□ 同位旋对称性破缺:接触项和π介子交换项

Isospin breaking contributions to the NN interaction.

Order	Contributions
NLØ ($\nu = 2$)	Pion-mass splitting in 1PE,
	Static Coulomb potential.
NNLØ ($\nu = 3$)	CSB contacts without derivatives,
	Charge dependence of the pion-nucleon coupling constant in 1PE ($\sim \epsilon m_{\pi}^2 / \Lambda_{\chi}^2$).
$N^{3}LO(\nu = 4)$	CIB contacts without derivatives,
	Charge dependence of the pion-nucleon coupling constant in 1PE [$\sim e^2/(4\pi)^2$],
	Pion-mass splitting in NLO 2PE,
	Nucleon-mass splitting in NLO 2PE and LS equation,
	$\pi\gamma$ exchange,
	Relativistic corrections to the Coulomb potential ($\sim e^2 Q^2/M_N^2$),
	Further electromagnetic corrections.
$N^3LO(\nu = 4)$	CIB contacts without derivatives, Charge dependence of the pion-nucleon coupling constant in 1PE [$\sim e^2/(4\pi)^2$], Pion-mass splitting in NLO 2PE, Nucleon-mass splitting in NLO 2PE and LS equation, $\pi\gamma$ exchange, Relativistic corrections to the Coulomb potential ($\sim e^2 Q^2/M_N^2$), Further electromagnetic corrections.

Table F.2

Partial-wave LECs for two N²LO fits by the Idaho group [68] using A = 500 and 600 MeV in the regulator function f(p', p). Eq. (4.63). The \tilde{C}_i of the zero order partial-wave counterterms given in Eq. (4.39) are in units of 10^4 GeV^{-2} ; the C_i , Eq. (4.41), in 10^6 GeV^{-4} ; and the D_i , D_i , Eq.(E1), in 10^4 GeV^{-6} . The last column lists the exponent no of the regulator function, which is applied to the corresponding partial-wave counterterm.

Partial-wave LEC	$\Lambda = 500 \text{ MeV}$	$\Lambda = 600 \text{ MeV}$	n	
\widetilde{C}_{1c}^{pp}	-0.145286	-0.151165	3	
\widetilde{C}_{1c}^{nn}	-0.146285	-0.151467	3	
C ^{hp}	-0.147167	-0.151745	3	
Cir.	2.380	2.200	2	
\widehat{D}_{1c}	-2.545	-4.890	2	
D ₁₅	- 16.00	-5.84	2	
C3p.	1.487	1.548	2	
D3p.	0.245	-0.215	3	
C1p,	0.656	0.790	2	
D1p,	5.25	4.40	2	
C3p,	-0.630	-0.488	2	
D_{3p_1}	2.35	3.24	4	
\tilde{C}_{3S_1}	-0.118972496	-0.116210	3	
C35,	0.760	0.775	2	
\widehat{D}_{3}	7.00	4.8004	2	
D ₃₅	6.55	10.8654	2	
D_{3D} ,	-2.80	-2.35	2	
C _{3S1-3D1}	0.826	0.796	2	
$\widehat{D}_{3}_{5_1-3}D_1$	2.25	2.86	2	
$D_{3}S_{1}-^{3}D_{1}$	6.61	5.58	2	
D_{1}	-1.770	-1.764	4	
D_{3D_2}	-1.46	-1.27	2	
C3p2		0.54		NIDID
D_{3P_2}	2 5 6	2.55		
$D_{3P_2-3F_2}$		0.525	TIMINE	
Dan	5.66	6.26	2, 3ª	

²²Si 秋幻核结构---新幻数





- ✓ NN + 3N计算的²⁴Si/²⁴Ne 和²⁶Si/²⁶Mg的 能谱与MED与实验符合,尤其计算的 MED
- ✓ MED值较大,表明此态具有较明显的同位旋对称性破缺,同时此态的1s1/2轨道的占据较大,此²⁴Si的0₂⁺态
- ✓ 计算给出的²²Si 与²²O的E(2₁⁺) 的位置う 別为2.4 与 3.2 MeV, Thomas-Ehrman shift 致友
- ✓ 计算显示²²Si/²²O的0+与2+的组态非常接近
- ✓ 尽管²²Si的E(2₁⁺) 较低,但是与²²O相近, ²²Si依然表现幻数性质。

美国FRIB与日本RIKEN RIB均在计划测量22Si激发态

J.G. Li,* H. H. Li, S. Zhang, Y. M. Xing,* W. Zuo,* *Phys. Lett. B* 846(1):138197(2023)





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