

从手征核力到原子核第一性原理计算 _{许甫荣}

- 1. 手征有效场论核力(三体力)
- 2. 第一性原理计算:含共振和连续谱
 - > 把手征核力、重整化、ab initio多体方法推广到复能量空间
 - ➢ 弱束缚, 4n体系

低能核理论的二个最基本问题:

- 1) Nuclear force (核力)
- 2) Many-body correlations (多体量子关联)

什么叫核结构第一性原理计算 (ab initio, first principles)?

1)从 realistic nuclear forces出发

2) "严格"处理量子多体关联 ("严格"—数值计算收敛)

I. Realistic nuclear forces



	Chadwick (1932): Neutron		
1930's	Heisenberg (1932): First Phenomenology (Isospin)		
	Yukawa (1935): Meson Hypothesis		
1940's	Discovery of the pion in cosmic ray (1947) and in the Berkeley Cyclotron Lab (1948). Nobelprize awarded to Yukawa (1949).		
	Taketani, Nakamura, Sasaki (1951): 3 ranges.		
1950's	Taketani, Nakamura, Sasaki (1951): 3 ranges. One-Pion-Exchange (OPE): o.k.		
1950's	Taketani, Nakamura, Sasaki (1951): 3 ranges. One-Pion-Exchange (OPE): o.k. Multi-pion exchanges: Problems!		
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1950's <i>"Pion</i> <i>Theories "</i>	Taketani, Nakamura, Sasaki (1951): 3 ranges. One-Pion-Exchange (OPE): o.k. Multi-pion exchanges: Problems! Taketani, Machida, Onuma (1952); Brueckner, Watson (1953).		





1990s: 高精度核力 high-precision modern nuclear forces

$$\chi^{2} = \sum_{i=1}^{i=N} \frac{\left(z_{i}^{theory} - z_{i}^{\exp}\right)^{2}}{\left(\Delta z_{i}^{\exp}\right)^{2}}$$

(about 6000 NN Data below 350 MeV)

 χ^2 /datum \rightarrow 1

1993 Nijmegen: high-precision phase shift analysis

1994-2001: High-precision NN potentials: Nijmegen I, II, AV18, CD-Bonn, N³LO ...



1970s-1980s QCD: Quark cluster model

从QCD做核结构计算?

4000	Effective Field Theory (EFT):
1990 -	Weinberg (1990); Ordonez, Ray, van Kolck (1994/96)
today	成功的pion theory,拥有QCD一样的对称性
touay	特别是 chiral symmetry and broken spontaneously

QCD=quarks + gluons (symmetries: spin, isospin, parity, chiral symmetry broken spontaneously)

Chiral EFT=nucleon + pion (symmetries: spin, isospin, parity, chiral symmetry broken spontaneously)

50s: multi-pion exchange 失败, Why? 因为当时还不知道如何表达手征对称 性及其破缺! 写出的场论拉氏量不合 适!



Weinberg (1990's)

At low energy, the effective degrees of freedom are nucleon and pion, rather than quark and gluon!

- QCD at low energy is strong. Perturbation is inapplicable !
- Quarks and gluons are confined into colorless hadrons.
- •Nuclear forces are residual color forces (similar to van der Waals forces)

$$\frac{\text{Chiral EFT}}{\text{Chiral EFT}}: \quad \mathcal{L}_{\text{eff}} = \mathcal{L}_{\pi\pi} + \mathcal{L}_{\pi N} + \mathcal{L}_{NN} + \cdots$$

- π π Lagrangian: $\mathcal{L}_{\pi\pi}^{(2)} = \frac{f_{\pi}^2}{4} \operatorname{Tr} \left[\partial_{\mu} U \partial^{\mu} U^+ + m_{\pi}^2 \left(U + U^+ \right) \right];$ $m_{\pi} \operatorname{and} f_{\pi} \operatorname{are fixed} (f_{\pi} = 92.4 \text{ MeV}).$ No free parameters.
- π -N Lagrangians: $L_{\pi N}^{(1)} = \bar{N} \left[i\partial_0 \frac{1}{4f_{\pi}^2} \tau \cdot (\pi \times \partial_0 \pi) \frac{g_A}{2f_{\pi}} \tau \cdot (\vec{\sigma} \cdot \vec{\nabla}) \pi \right] N$ $g_A = 1.29$, no free parameters. $L_{\pi N}^{(2)}$: 4 parameters. $L_{\pi N}^{(3)}$: 4 parameters. $L_{\pi N}^{(3)}$: 4 parameters. $L_{\pi N}^{(3)}$: 4 parameters.
- N-N Lagrangian ("Contacts" N3LO): 24 essentially free parameters.



NLO or NNLO, only 9 parameters

$$\begin{split} V_{\rm LO}^{\rm cont} &= C_S + C_T \left(\vec{\sigma}_1 \cdot \vec{\sigma}_2 \right) \\ V_{\rm LO}^{\rm OPE} &= -\frac{g_A^2}{4F_\pi^2} \, \tau_1 \cdot \tau_2 \frac{\left(\vec{\sigma}_1 \cdot \vec{q} \right) \left(\vec{\sigma}_2 \cdot \vec{q} \right)}{q^2 + M_\pi^2} & \vec{q} = \text{t-channel mom. transfer} \\ V_{\rm NLO}^{\rm cont} &= C_1 q^2 + C_2 k^2 + \left(C_3 q^2 + C_4 k^2 \right) \left(\vec{\sigma}_1 \cdot \vec{\sigma}_2 \right) + i C_5 \frac{1}{2} \left(\vec{\sigma}_1 + \vec{\sigma}_2 \right) \cdot \left(\vec{q} \times \vec{k} \right) \\ &+ C_6 \left(\vec{\sigma}_1 \cdot \vec{q} \right) \left(\vec{\sigma}_2 \cdot \vec{q} \right) + C_7 \left(\vec{\sigma}_1 \cdot \vec{k} \right) \left(\vec{\sigma}_2 \cdot \vec{k} \right) & \vec{k} = \text{u-channel mom. transfer} \\ V_{\rm NLO}^{\rm TPE} &= -\frac{\tau_1 \cdot \tau_2}{384 \pi^2 F_\pi^4} L(q) \left[4 M_\pi^2 \left(5 g_A^4 - 4 g_A^2 - 1 \right) + q^2 \left(23 g_A^4 - 10 g_A^2 - 1 \right) \\ &+ \frac{48 g_A^4 M_\pi^4}{4 M_\pi^2 + q^2} \right] - \frac{3 g_A^4}{64 \pi^2 F_\pi^4} L(q) \left[\left(\vec{q} \cdot \vec{\sigma}_1 \right) \left(\vec{q} \cdot \vec{\sigma}_2 \right) - q^2 \left(\vec{\sigma}_1 \cdot \vec{\sigma}_2 \right) \right] \end{split}$$

2003 N³LO : Entem and Machleidt,, PRC 68, 041001(R) (2003);

R. Machleidt, D.R. Entem, Physics Reports 503, 1 (2011)

Table 4

Number of parameters needed for fitting the *np* data in phase shift analysis and by a high-precision *NN* potential *versus* the total number of *NN* contact terms of EFT based potentials to different orders.

	Nijmegen partial-wave analysis [139]	CD-Bonn high-precision potential [13]	Contact potentials		
			Q ⁰ LO	Q ² NLO/NNLO	Q ⁴ N ³ LO
¹ S ₀	3	4	1	2	4
³ S ₁	3	4	1	2	4
${}^{3}S_{1} - {}^{3}D_{1}$	2	2	0	1	3
${}^{1}P_{1}$	3	3	0	1	2
³ P ₀	3	2	0	1	2
³ P ₁	2	2	0	1	2
${}^{3}P_{2}$	3	3	0	1	2
${}^{3}P_{2} - {}^{3}F_{2}$	2	1	0	0	1
${}^{1}D_{2}$	2	3	0	0	1
${}^{3}D_{1}$	2	1	0	0	1
${}^{3}D_{2}$	2	2	0	0	1
³ D ₃	1	2	0	0	1
${}^{3}D_{3}-{}^{3}G_{3}$	1	0	0	0	0
${}^{1}F_{3}$	1	1	0	0	0
${}^{3}F_{2}$	1	2	0	0	0
${}^{3}F_{3}$	1	2	0	0	0
³ F ₄	2	1	0	0	0
${}^{3}F_{4} - {}^{3}H_{4}$	0	0	0	0	0
${}^{1}G_{4}$	1	0	0	0	0
³ G ₃	0	1	0	0	0
${}^{3}G_{4}$	0	1	0	0	0
³ G ₅	0	1	0	0	0
Total	35	38	2	9	24

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PHASE SHIFTS at N4LO

 \Rightarrow Precision phase shifts with small uncertainties up to $E_{
m lab}=300\,{
m MeV}$



现实核力的最大特点:势参数由核子二体散射 数据确定(和²H),而不是核结构实验数据! NLO N2LO N3LO N4LO

ChPT Lagrangian 的合理性

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$$v_{3N}^{2\pi} = \frac{1}{(2\pi)^6} \frac{g_A^2}{8f_\pi^2} \sum_{i \neq j \neq k} \frac{(\sigma_i \cdot q_i)(\sigma_j \cdot q_j)}{(q_i^2 + M_\pi^2)(q_j^2 + M_\pi^2)} F_{ijk}^{\alpha\beta} \tau_i^{\alpha} \tau_j^{\beta}$$
$$v_{3N}^{1\pi} = -\frac{1}{(2\pi)^6} \frac{g_A c_D}{8f_\pi^4 \Lambda_\chi} \sum_{i \neq j \neq k} \frac{\sigma_j \cdot q_j}{q_j^2 + M_\pi^2} (\tau_i \cdot \tau_j) (\sigma_i \cdot q_j)$$
$$v_{3N}^{cont} = \frac{1}{(2\pi)^6} \frac{c_E}{2f_\pi^4 \Lambda_\chi} \sum_{j \neq k} \tau_j \cdot \tau_k$$

$$F_{ijk}^{\alpha\beta} = \delta^{\alpha\beta} \left[-\frac{4c_1 m_\pi^2}{f_\pi^2} + \frac{2c_3}{f_\pi^2} \boldsymbol{q}_i \cdot \boldsymbol{q}_j \right] \\ + \frac{c_4}{f_\pi^2} \varepsilon^{\alpha\beta\gamma} \tau_k^{\gamma} \boldsymbol{\sigma}_k \cdot [\boldsymbol{q}_i \times \boldsymbol{q}_j],$$

II. Renormalizations (softening) : G-matrix, V_{low-k}, OLS, SRG, UCOM...

$$\hat{H}_{int} = \sum_{i < j}^{A} \frac{(\vec{p}_i - \vec{p}_j)^2}{2mA} + \sum_{i < j}^{A} V_{NN,ij} + \sum_{i < j < k}^{A} V_{NNN,ijk}$$

- 1) 自由空间的核力软化,目的是加速数值"量子强关联多体系统"计算的收敛性
- 2) "无限"空间转化到有限空间,目的是缩小模型空间



Renormalization schemes preserving all symmetries

G-Matrix: 50年代初, Watson和Brueckner et al.

Bare force $\langle \varphi | G | \varphi \rangle = \langle \varphi | V_{NN} | \varphi' \rangle$



$$G = V_{NN} + V_{NN} \frac{Q}{\omega - QH_0Q} G$$

Illustration on how the high momentum nodes are integrated out in the Vlowk (a) and in the SRG (b) RG methods







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III. 如何"严格"求解强关联量子多体体系? Ab initio many-body methods

$$H_{\text{int}} = \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i < j} V(|\vec{r_i} - \vec{r_j}|) - \frac{P^2}{2Am} \qquad \vec{P} = \sum_{i=1}^{A} \vec{p_i}$$

$$\hat{H}_{int} = \sum_{i < j}^{A} \frac{(\vec{p}_i - \vec{p}_j)^2}{2mA} + \sum_{i < j}^{A} V_{NN,ij} + \sum_{i < j < k}^{A} V_{NNN,ijk}$$

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = H\Psi(x,t)$$

Nuclear shell model

(概念1932年由D. Ivanenko and E. Gapon提出, 1949年主要由下面三人独立发展, Nobel prize 1963)



(configuration-mixing; configuration-interaction) shell model

1950年代开始, Igal Talmi et al.

Many-body nucleus

原子核性质实验可观测吗?(定量)



我们组:

1) Nuclear forces



NN 进行中

2) 核力重整化

V_{low-k}, Similarity Renormalization Group (SRG)

- 3) Many-Body methods
 - a) Configuration-interaction Gamow shell model

b) In-medium Similarity Renormalization Group (IM-SRG) (Gamow and conventional)

Resonance and continuum





$$\psi(\mathbf{r},t)=e^{-iEt/\hbar}\varphi_E(\mathbf{r})$$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]\varphi_E(\mathbf{r}) = \mathbf{E}\varphi_E(\mathbf{r})$$

Berggren basis: T. Berggren, Nucl. Phys. A109 (1968) 265 Berggren 60年代"发展了"量子力学

用定态方法求解含时问题

 $\psi(\mathbf{r},t)=e^{-iEt/\hbar}\varphi_E(\mathbf{r})$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + \mathbf{V}(\mathbf{r})\right]\varphi_E(\mathbf{r}) = \mathbf{E}\varphi_E(\mathbf{r})$$



T. Berggren, PhD in 1966 (Lund)

But E can be complex, and $\int \varphi_E(\mathbf{r}) \varphi_E(\mathbf{r}) = 1$ (Berggren方法的一个关键)

本征值:
$$E = E_n - i \frac{\Gamma_n}{2}$$

 $\psi(\mathbf{r}, t) = e^{-iEt/\hbar} \varphi_E(\mathbf{r}) = e^{-iE_n t/\hbar} \varphi_E(\mathbf{r}) e^{-\Gamma_n t/2\hbar}$
核态有衰变寿命, decay width: $T_{1/2} = \hbar \ln 2/\Gamma$

复空间求解量子力学问题要比实空间困难得多!

Complex-momentum space: bound, resonance and continuum



ab initio Gamow Shell Model

我们发展了基于现实核力的 ab initio Gamow Shell Model



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S-, Q-box folded diagrams in complex-k Berggren basis



P + Q = 1



60年代以前,现实核力研究主要局限于核力本身的研究或用于一些少体问题研究,很难用于真正的核物理计算(计算核结构问题定量很差)

G.E. Brown 60's: 从现实核力出发计算核结构问题,

Q-box folded diagrams, V_{low-k}

核芯极化的重要性!

使得用现实核力计算原子核成为可能!





⁶He halo







⁶He correlated density distribution

 $\rho(r,\theta) = \langle \Psi | \delta(r_1 - r) \delta(r_2 - r) \delta(\theta_{12} - \theta) | \Psi \rangle$

Physics World公布2022年十大年度突破性成果



01 迎来超冷化学的新时代

02 观测到理论预言的四中子状态

两院院士评选"2022年中国/世界十大科技进展新闻"揭晓

中国科学报 2023-01-12 11:01 发表于北京

2022年世界十大科技进展新闻





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(Tetraneutron)

(大概60年前,猜想)

Physicists Observe Elusive Four-Neutron System: Tetraneutron

Jun 23, 2022 by Enrico de Lazaro

Published in

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Radio Isotope Beams (SAMURAI) in Japan have experimentally observed a



M. Duer et al., Nature 606, 678 (2022)



Science News

NEWS PHYSICS

« Previous

Physicists may have finally spotted elusive clusters of four neutrons If confirmed, 'tetraneutrons' could help scientists better understand nuclear forces



Four neutrons may form a short-lived agglomeration called a tetraneutron (illustrated SONJA BATTENBERG/TUM

By Emily Conover JUNE 22, 2022 AT 11:00 AM

PHYSICAL REVIEW C 100, 054313 (2019)

Ab initio no-core Gamow shell-model calculations of multineutron systems

J. G. Li,¹ N. Michel^(D),^{2,3} B. S. Hu^(D),¹ W. Zuo,^{2,3} and F. R. Xu^(D),^{*}

¹School of Physics, and State Key Laboratory of Nuclear Physics and Technology, Peking University, Beijing 100871, China ²Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou 730000, China ³School of Nuclear Science and Technology, University of Chinese Academy of Sciences, Beijing 100049, China







PHYSICAL REVIEW LETTERS 123, 212501 (2019)

Editors' Suggestion Featured in Physics



Location of the Neutron Dripline at Fluorine and Neon

D. S. Ahn,¹ N. Fukuda,¹ H. Geissel,⁵ N. Inabe,¹ N. Iwasa,⁴ T. Kubo,^{1,*,†} K. Kusaka,¹ D. J. Morrissey,⁶ D. Murai,³ T. Nakamura,² M. Ohtake,¹ H. Otsu,¹ H. Sato,¹ B. M. Sherrill,⁶ Y. Shimizu,¹ H. Suzuki,¹ H. Takeda,¹ O. B. Tarasov,⁶ H. Ueno,¹ Y. Yanagisawa,¹ and K. Yoshida¹ ¹RIKEN Nishina Center for Accelerator-Based Science, RIKEN, 2-1 Hirosawa, Wako, Saitama 351-0198, Japan

美国物理学会选出的"2019年物理学发生的十大事件"





中子滴线停滞在元素周期表的前8个元素的中子滴线(粉线)已经20年。2019年,日本科学家将中子滴线延伸至氟(F)和氖(Ne)(绿线)

物理学家希望下一个元素的滴线不要再等上20年。下一代稀有同位素装置计划在两年内投入使用, 可能会将滴线延伸至镁元素,即元素周期表中的第12号元素。 核素版图 Nuclear Landscape



 $\mathbf{N} \rightarrow$

核天体物理: Element production



Chiral EFT 3NF (NNLO) Gamow 3NF



Chiral EFT 3NF

- 1. E. Epelbaum et al., PRC 66, 064001 (2002);
- 2. P. Navratil et al., PRL 99, 042501(2007)

Phenomenological 3NFs:

- Urbana (1995)
- Tucson-Melbourne (1975-1999)

- Illinois (2001-2010)

- CD-Bonn + Δ (Deltuva, Sauer, 2003)

GSM with ¹⁶O core: N³LO(NN) + N²LO(NNN)

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5

3

2

1

0

0.015

0.008

NN NN+3N Expt.

²⁴O

 0.03^{+12}_{-3}

0.05⁺²¹

$S_{2n}(\text{MeV})$	NN	NN+3N	Expt.
^{24}O	9.110	7.038	6.925
$^{25}\mathrm{O}$	6.254	3.568	3.453
²⁶ O	3.362	-0.150	-0.018

Ma, Xu, Coraggio, Hu, Li, Fukui, Angelis,

N.Itaco, Gargano, PLB 802, 135257 (2020)

0.037

0.016

0.058

NN NN+3N Expt.

²⁵O

(0.001)

0.088

 $(1/2^+)$

0.008

0.030

0.004

0.027

0.004

0.021 0.015

NN NN+3N Expt.

²⁶O

0.033

null



[3] Otsuka, Suzuki, Holt, Schwenk, Akaishi, PRL 105 (2010) 032501.[31] Hagen, Hjorth-Jensen, Jansen, Machleidt, Papenbrock, PRL108 (2012) 242501.

N³LO(NN): Entem and Machleidt, PRC **66**, 014002 (2002).

N²LO(NNN): c_D =-1, c_E =-0.34, Navrátil, Gueorguiev, Vary, Ormand, A. Nogga, PRL 99, 042501 (2007).

Summary



Ab initio nuclear structure calculations with resonance and continuum considered

- 1. Complex EFT 3NF at N²LO
- 2. Ab initio Gamow shell model with a core

calculating complex S-box and Q-box folded diagrams

Both the continuum coupling and 3NF are important in nuclei around driplines



胡柏山,马远卓,孙中浩,张爽,吴强,袁琪... 李健国, Michel, 左维 Coraggio, Fukui, ...





CIB: charge independence breaking, a violation of rotation invariance in isospin space.

T=1 NN interaction: Tz=+1 (pp), 0 (np) and -1 (nn)

The main reasons: $m_p \neq m_n$, π^0 , π^{\pm} mass splitting

CIB is more significant than CSB

CSB: charge symmetry breaking, a violation of rotation invariance by 180° Only for *pp* and *nn*

S. Zhang, Y.Z. Ma, J.G. Li, B.S. Hu, Q. Yuan, Z.H. Cheng, F.R. Xu, PLB 827, 136958 (2022)

Full space 本征值问题

 $H|\Psi_{\nu}\rangle = E_{\nu}|\Psi_{\nu}\rangle$

 $H = H_0 + H_1$

$$H_0 = \sum_{i=1}^{A} (t_i + U_i)$$
 One-body

$$H_1 = \sum_{i < j=1}^{A} V_{ij}^{NN} - \sum_{i=1}^{A} U_i \quad \text{Residual two-body}$$



P + Q = 1

$$P = \sum_{i=1}^{d} |\Phi_i\rangle \langle \Phi_i|$$

求解无限空间→有限空间多体问题

$$\begin{aligned} H_{\text{eff}}(E_{v})P|\Psi_{v}\rangle &= E_{v}P|\Psi_{v}\rangle \\ H_{\text{eff}}(E_{v}) &= P(H_{0} + H_{1})P + P(H_{0} + H_{1})Q \frac{1}{E_{v} - H_{QQ}}Q(H_{0} + H_{1})P \\ &= PH_{0}P + PH_{1}P + (\underline{PH_{0}Q} + PH_{1}Q) \frac{1}{E_{v} - H_{QQ}}(QH_{0}P + QH_{1}P) \\ &\stackrel{\frown}{\longrightarrow} H_{0}\underline{PQ} \\ &\stackrel{\frown}{\longrightarrow} 0 \quad (\because P, Q \boxminus H_{0} \overrightarrow{X} \nota) \end{aligned}$$

$$H_{0} &= \sum_{i=1}^{A} (t_{i} + U_{i}) \quad \text{unperturbed one-body} \\ H_{0} &= \sum_{i=1}^{A} (t_{i} + U_{i}) \quad \text{unperturbed one-body} \\ V_{\text{eff}}(E_{v}) &= PH_{1}P + PH_{1} \frac{Q}{E_{v} - QH_{0}Q}H_{1}P + PH_{1} \frac{Q}{E_{v} - QH_{0}Q}H_{1} \frac{Q}{E_{v} - QH_{0}Q}H_{1}P + \cdots \\ & 2^{\text{nd} \text{ order perturbation}} \qquad 3^{\text{rd} \text{ order perturbation} \\ &\stackrel{\frown}{\longrightarrow} \stackrel{\frown}{\longrightarrow} \stackrel{\frown}{\longrightarrow}$$

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