FRIB-Theory Alliance workshop

Many-Body Perturbation Theory Calculations

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Outline

I. Introduction

II. Theoretical framework and calculations

a) MBPT for closed-shell nuclei

b) MBPT (*Q*-box + folded diagrams) for open-shell nuclei

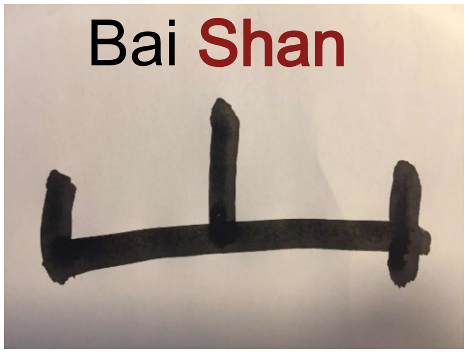
As Prof. F.R. Xu's talk

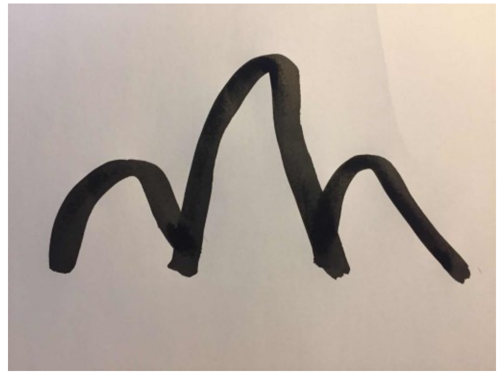
c) MBPT for nuclear reaction (RGM)

III. Summary and Outlook

Perturbation theory

takes us from a simple, exactly solvable (unperturbed) problem to a corresponding real (perturbed) problem





- **The key formulas in perturbation theory are**

$$\hat{H} = \hat{H}_0 + (\hat{H} - \hat{H}_0) = \hat{H}_0 + \hat{V} \qquad \hat{H}_0 \Phi_n = E_n^{(0)} \Phi_n$$

- **In MBPT the ambition is to include in H_0 as much "physics" as possible, so that V represents a "small" perturbation**

History of MBPT

Key tool from 1950's to 1970's

- Rayleigh-Schrödinger perturbation theory
- *G*-matrix, Brueckner-Hartree-Fock method
- Valence-space shell-model interaction (*Q*-box + folded diagram)

Great depression in 1980's

- Depending on a starting energy parameter of *G*-matrix
- Poor convergence of the intermediate-state summations (tensor part)
- Intruder states

Today MBPT is coming back ...

- RSPT with soft potential ($V_{\text{low-}k}$, SRG, UCOM, OLS)
- Bogoliubov MBPT
- Auxiliary method (importance truncation, natural orbital basis)
- Realistic Gamow shell model (Extended Kuo-Krenciglowa method)

MBPT for closed-shell nuclei

$$\hat{H} = \sum_{i=1}^{A}\left(1-\frac{1}{A}\right)\frac{\vec{p}_i^2}{2m} + \sum_{i<j}^{A}\left(\hat{V}_{NN,ij} - \frac{\vec{p}_i\cdot\vec{p}_j}{mA}\right) + \sum_{i<j<k}^{A}\hat{V}_{3N,ijk}$$

Rayleigh-Schrödinger perturbation theory

$$\hat{H} = \hat{H}_0 + (\hat{H} - \hat{H}_0) = \hat{H}_0 + \hat{V}$$

$$\hat{H}\Psi_n = E_n\Psi_n \qquad \hat{H}_0\Phi_n = E_n^{(0)}\Phi_n$$

$$\Delta E = E_0 - E_0^{(0)}$$

$$\Psi_0 = \sum_{m=0}^{\infty}\left[\hat{R}_0(E_0^{(0)})(\hat{V} - \Delta E)\right]^m\Phi_0$$

$$\Delta E = \sum_{m=0}^{\infty}\langle\Phi_0|\hat{V}\left[\hat{R}_0(E_0^{(0)})(\hat{V} - \Delta E)\right]^m|\Phi_0\rangle$$

$$\text{where } \hat{R}_0 = \sum_{i\neq 0}\frac{|\Phi_i\rangle\langle\Phi_i|}{E_0^{(0)} - E_i^{(0)}}$$

$$E_0 = E_0^{(0)} + E_0^{(1)} + E_0^{(2)} + E_0^{(3)} + \dots$$

$$E_0^{(1)} = \langle\Phi_0|\hat{V}|\Phi_0\rangle$$

$$E_0^{(2)} = \langle\Phi_0|\hat{V}\hat{R}_0\hat{V}|\Phi_0\rangle$$

$$E_0^{(3)} = \langle\Phi_0|\hat{V}\hat{R}_0(\hat{V} - \langle\Phi_0|\hat{V}|\Phi_0\rangle)\hat{R}_0\hat{V}|\Phi_0\rangle;$$

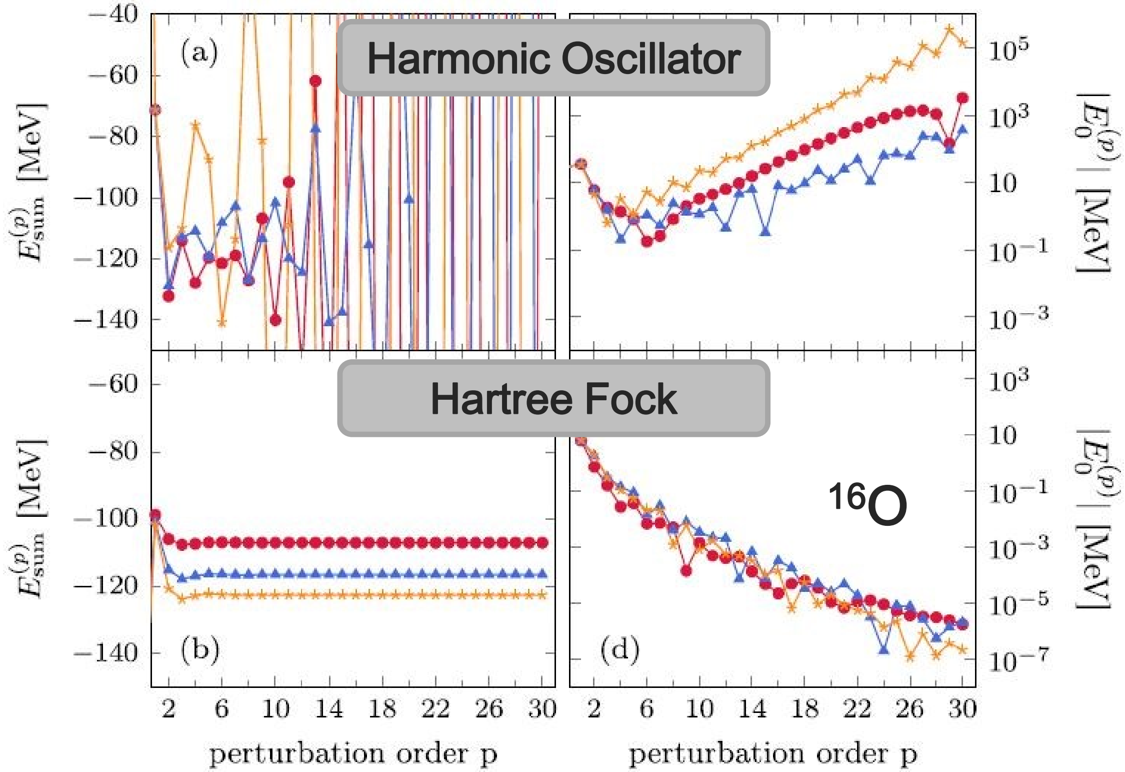
$$\Psi_0 = \Phi_0 + \Psi_0^{(1)} + \Psi_0^{(2)} + \dots$$

$$\Psi_0^{(1)} = \hat{R}_0\hat{V}|\Phi_0\rangle$$

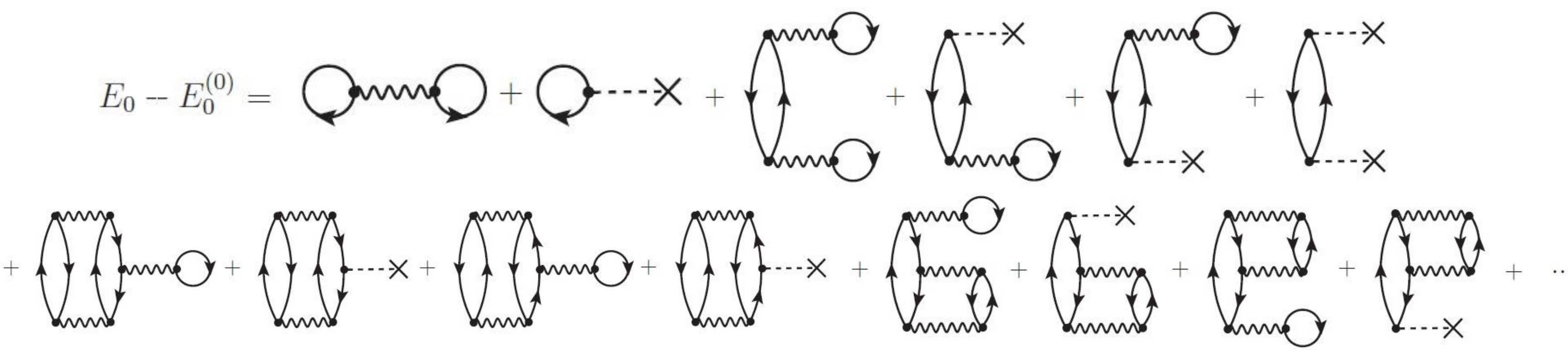
$$\Psi_0^{(2)} = \hat{R}_0(\hat{V} - E_0^{(1)})\hat{R}_0\hat{V}|\Phi_0\rangle$$

Advantages in HF basis, compared with HO basis

- **Faster convergence**
- **Some perturbation diagrams are cancelled out**
- **In HO basis, calculations could be ħω dependent, while much less in HF basis**

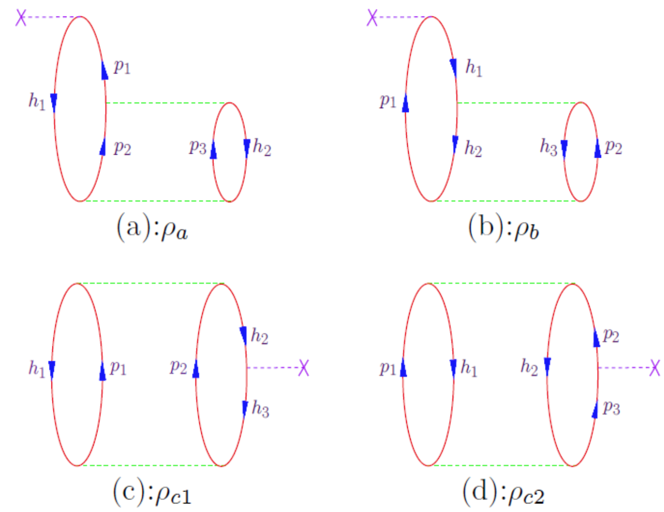


A. Tichai *et al.,* PLB 756, 283 (2016)



RSPT for closed-shell nuclei

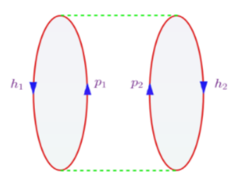
- Perform a Hartree-Fock calculation
- HF state is chosen as a reference state H_0
- In the HF basis, make RSPT corrections
  - Energy up to 3rd order
  - Wave function up to 2nd order (One-body density)



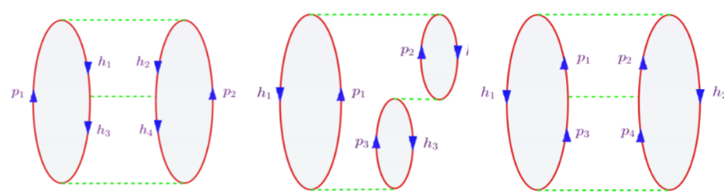
$$E=E^{(0)}+E^{(1)}+E^{(2)}+E^{(3)}+\cdots$$

$-E^{(1)}$

$E^{(2)}$

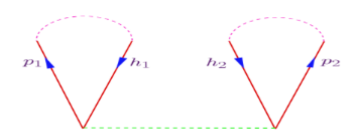


$E^{(3)}$

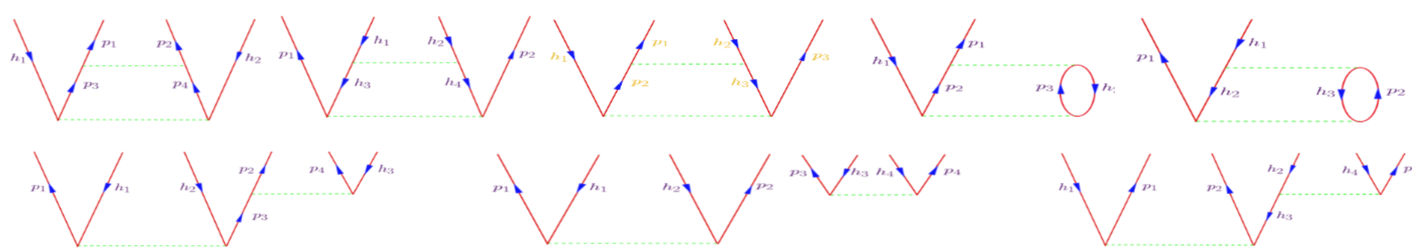


$$\Psi=\Phi_{HF}+\psi^{(1)}+\psi^{(2)}+\cdots$$

$\psi^{(1)}$



$\psi^{(2)}$



HF-RSPT calculations for ^{16}O with N^{3}LO-SRG, N_{shell}=13, ħω=35 MeV

Binding energy

	SRG flow parameter λ (fm^{-1})			
	1.5	2.0	2.5	3.0
Expt. [60]	−127.619	−127.619	−127.619	−127.619
SHF	−169.968	−133.169	−85.173	−44.102
PT2	−10.132	−29.497	−59.617	−88.326
PT3	−0.794	−1.931	−4.630	−7.339
SHF+PT2+PT3	−180.893	−164.597	−149.419	−139.767

3NF important !

B.S. Hu, F.R. Xu, *et al.*, PRC 94, 014303 (2017)

Point-proton rms radius

	SRG flow parameter λ (fm^{-1})			
	1.5	2.0	2.5	3.0
Expt.	2.581	2.581	2.581	2.581
SHF	2.098	2.096	2.201	2.345
PT2	0.011	0.011	−0.006	−0.042
$\Delta r_{c.m.}$	−0.067	−0.067	−0.070	−0.073
SHF+PT2+$\Delta r_{c.m.}$	2.042	2.040	2.125	2.230

Inclusion of 3NF

$$\hat{H} = \sum_{i=1}^{A}\left(1-\frac{1}{A}\right)\frac{\vec{p}_i^2}{2m} + \sum_{i<j}^{A}\left(\hat{V}_{NN,ij} - \frac{\vec{p}_i\cdot\vec{p}_j}{mA}\right) + \sum_{i<j<k}^{A}\hat{V}_{3N,ijk} = \sum_{i=1}^{A}\hat{H}_i^{(1)} + \sum_{i<j}^{A}\hat{H}_{ij}^{(2)} + \sum_{i<j<k}^{A}\hat{V}_{3N,ijk}$$

Normal ordering with HF reference state

$$\hat{H} = \sum_i \langle i|\hat{H}^{(1)}|i\rangle + \frac{1}{2}\sum_{ij}\langle ij|\hat{H}^{(2)}|ij\rangle + \frac{1}{6}\sum_{ijk}\langle ijk|\hat{V}_{3N}|ijk\rangle$$

$$+\sum_{pq}\left(\langle p|\hat{H}^{(1)}|q\rangle + \sum_i\langle pi|\hat{H}^{(2)}|qi\rangle + \frac{1}{2}\sum_{ij}\langle pij|\hat{V}_{3N}|qij\rangle\right) : \hat{p}^\dagger\hat{q} :$$

$\hat{H}_{\mathrm{HF}}$

$$+\frac{1}{4}\sum_{pqrs}\left(\langle pq|\hat{H}^{(2)}|rs\rangle + \sum_i\langle pqi|\hat{V}_{3N}|rsi\rangle\right) : \hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r} :$$

$$+\frac{1}{36}\sum_{pqrstu}\langle pqr|\hat{V}_{3N}|stu\rangle : \hat{p}^\dagger\hat{q}^\dagger\hat{r}^\dagger\hat{u}\hat{t}\hat{s} :$$

Discard residual 3B part: NO2B approximation

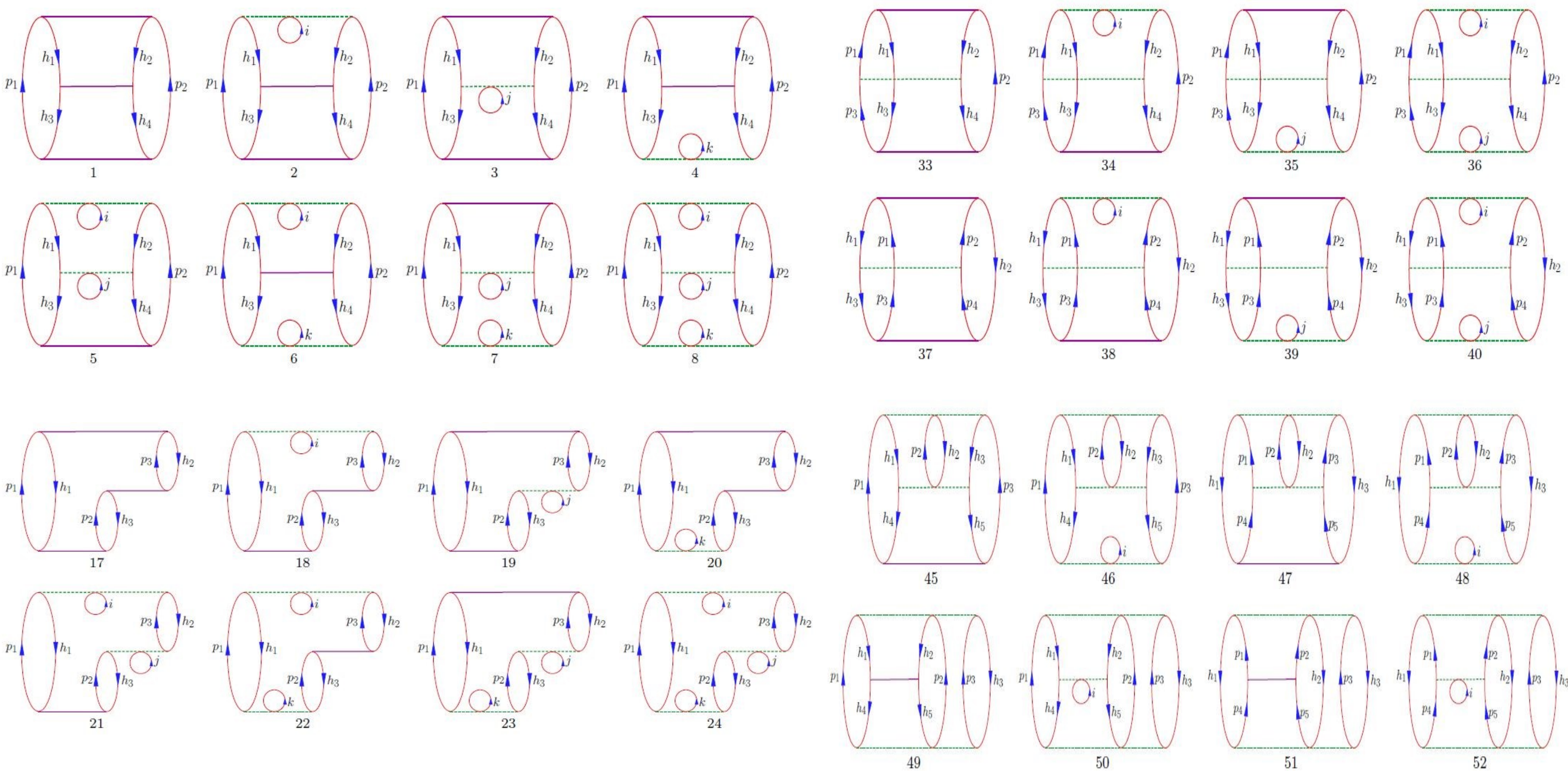
$$\hat{H} = \hat{H}_{\mathrm{HF}} + \hat{V}$$

$$\hat{V} = \frac{1}{4}\sum_{pqrs}\langle pq|\hat{W}|rs\rangle : \hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r} : + \frac{1}{36}\sum_{pqrstu}\langle pqr|\hat{V}_{3N}|stu\rangle : \hat{p}^\dagger\hat{q}^\dagger\hat{r}^\dagger\hat{u}\hat{t}\hat{s} :$$

$$\hat{W} = \left(\langle pq|\hat{H}^{(2)}|rs\rangle + \sum_i\langle pqi|\hat{V}_{3N}|rsi\rangle\right) : \hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r} :$$

ASG diagram expansion when 3NF is included

$E^{(3)}$: 56 terms (Derived for the first time)



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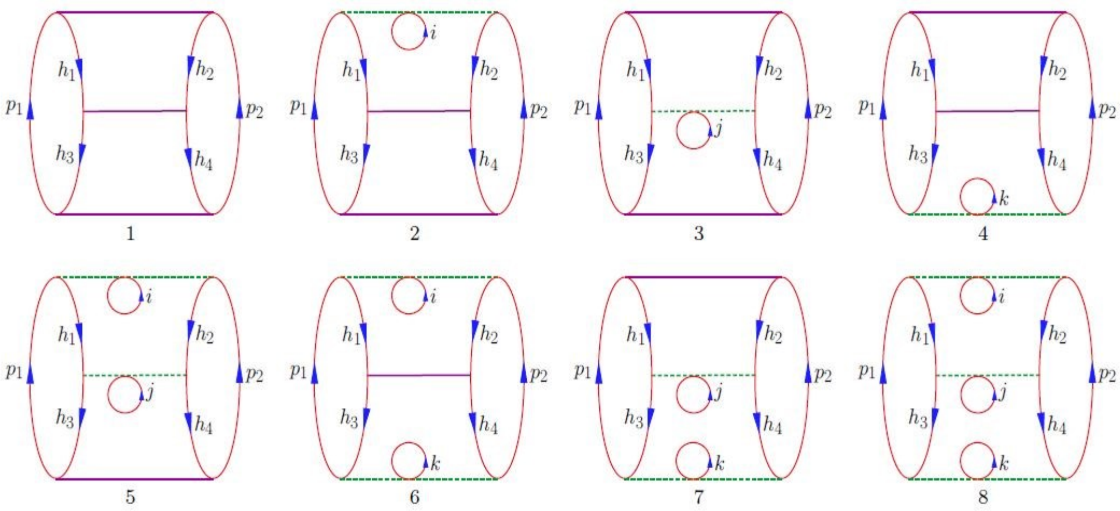
ASG diagram expansion when 3NF is included



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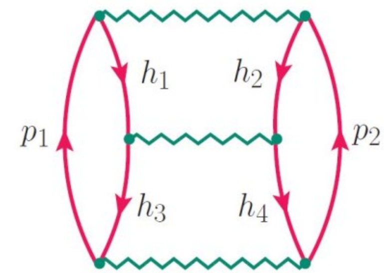
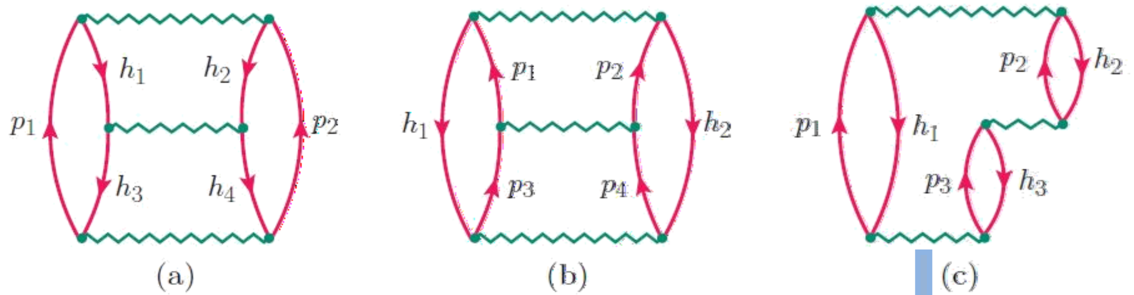
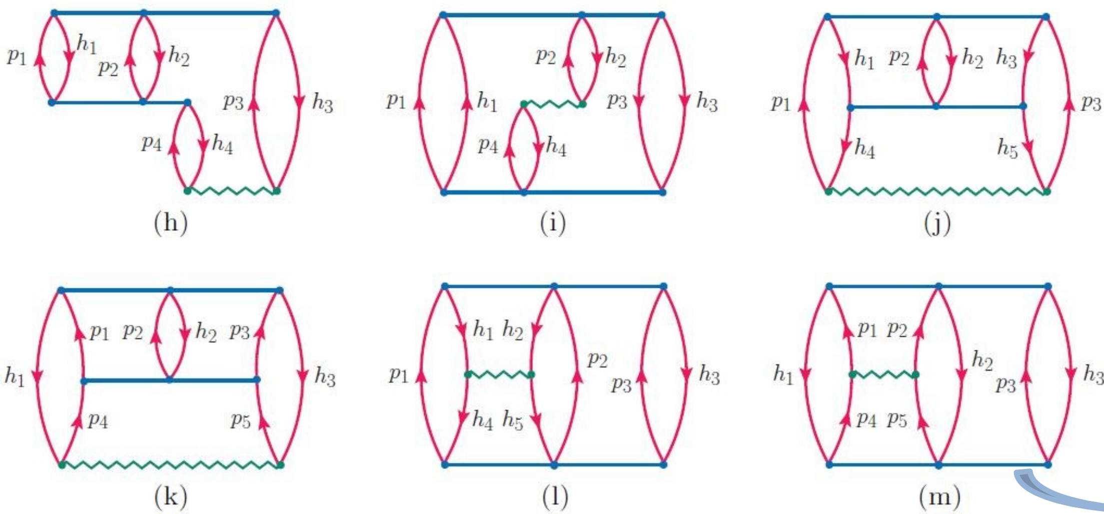


NO2B

$$\left(\langle pq|\hat{H}^{(2)}|rs\rangle + \sum_i \langle pqi|\hat{V}_{3N}|rsi\rangle\right)$$

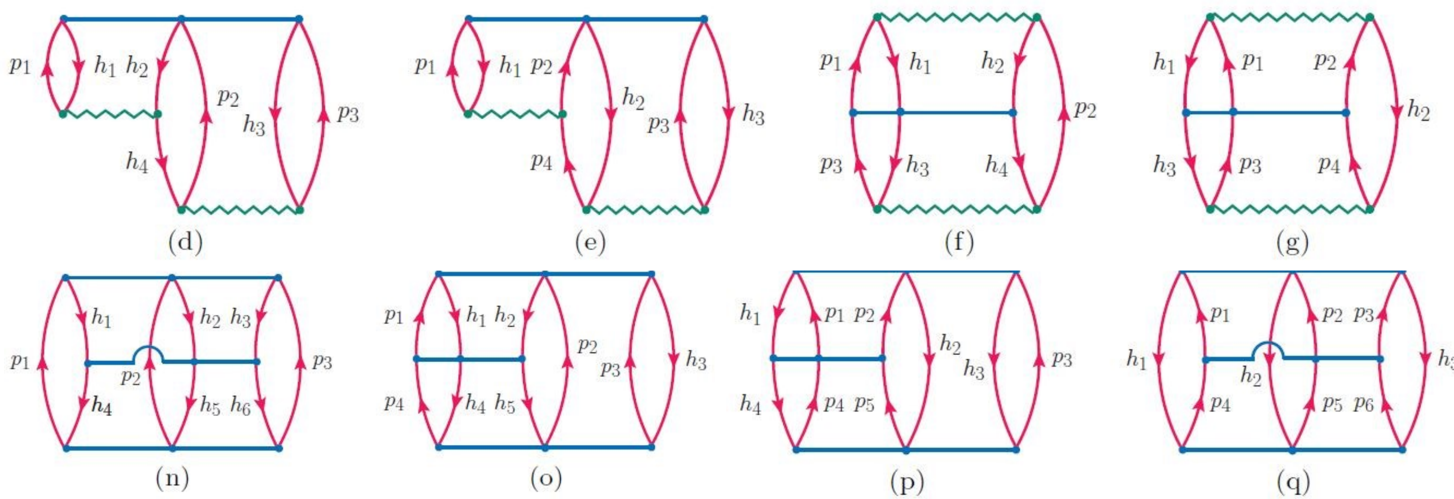
NO2B approximation:

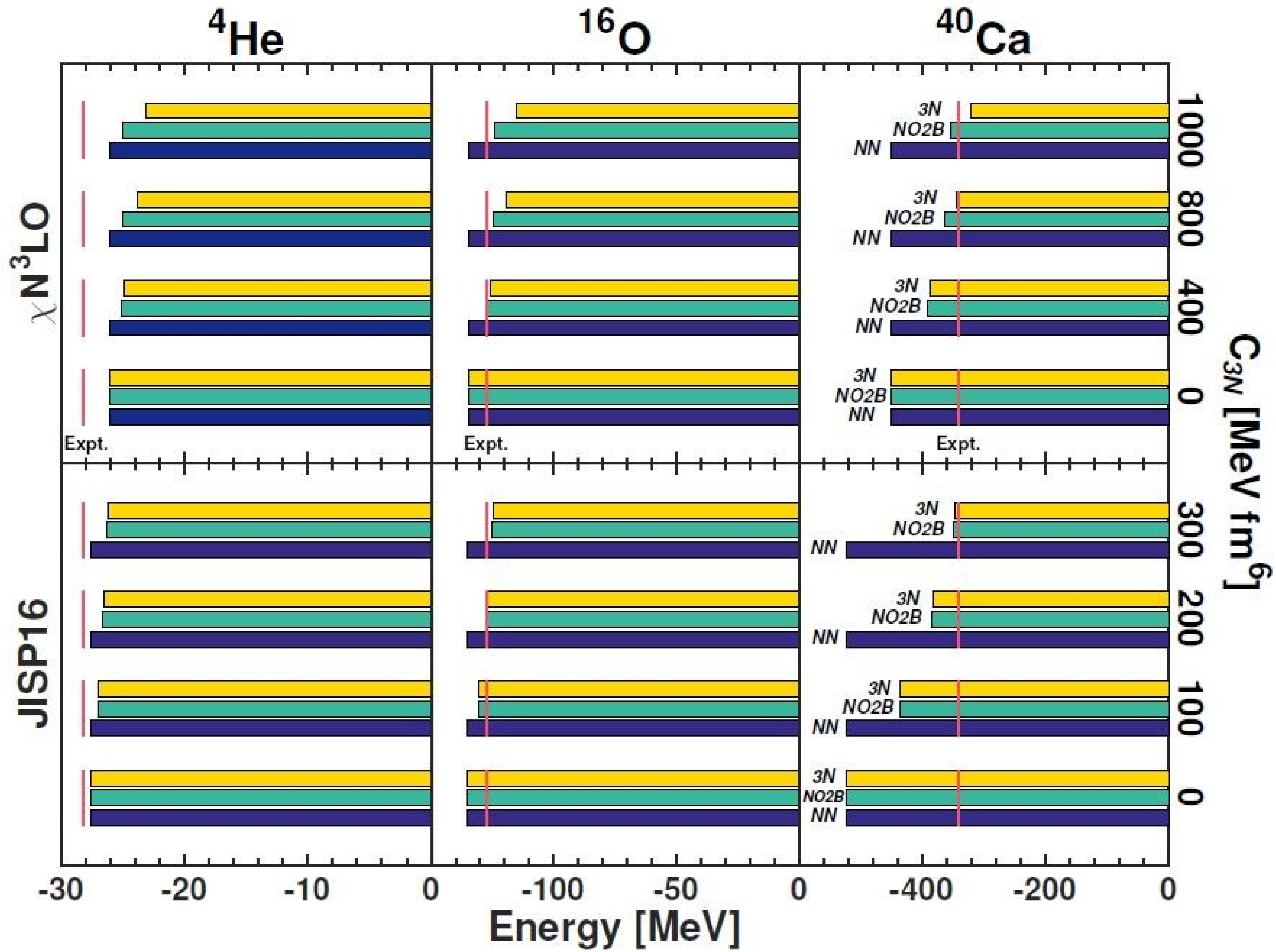




$$\left(\langle pq|\hat{H}^{(2)}|rs\rangle + \sum_i \langle pqi|\hat{V}_{3N}|rsi\rangle \right)$$

$$\langle pqr|\hat{V}_{3N}|stu\rangle$$





***NN*-only N^{3}LO-SRG**

Bare JISP16

+ $\hat{V}_{3N}^{\mathrm{ct}} = C_{3N}\delta^{(3)}(\vec{x}_1 - \vec{x}_2)\,\delta^{(3)}(\vec{x}_1 - \vec{x}_3)$

N_{shell}=7, ħω=30 MeV

HF-RSPT calculations with NO2B N^2LO_{sat}, N_{shell}=13, ħω=22 MeV

Binding energy

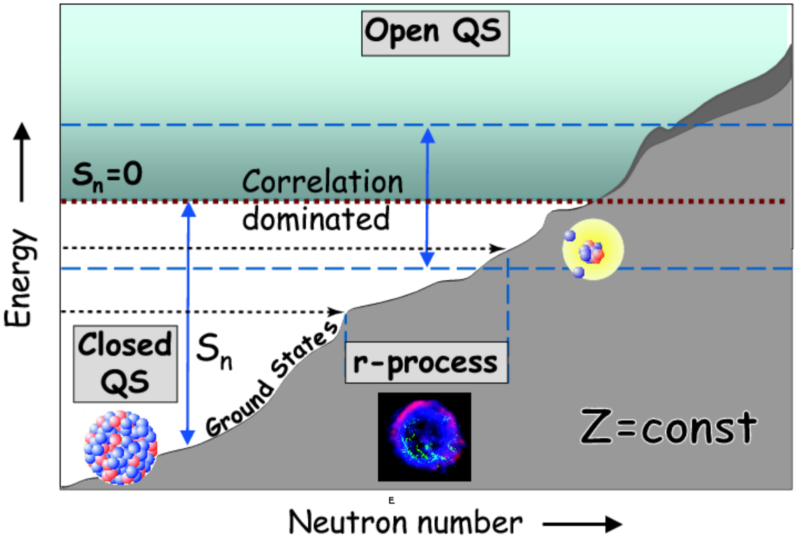
	NN		$NN+3N$		
Nucleus	IM-SRG	HF-RSPT3	IM-SRG	HF-RSPT3	Expt.
^{4}He	−27.36	−26.90	−29.09	−28.15	−28.30
^{14}C	−133.38	−132.40	−104.16	−105.06	−105.29
^{22}C	−179.72	−185.82	−114.79	−113.95	−119.18
^{16}O	−171.95	−171.08	−124.13	−125.16	−127.62
^{22}O	−242.37	−246.03	−160.02	−156.77	−162.03
^{24}O	−265.58	−269.40	−166.26	−163.12	−168.97
^{40}Ca	−610.89	−608.28	−311.47	−320.66	−342.05
^{48}Ca	−783.40	−784.52	−376.75	−370.02	−416.00

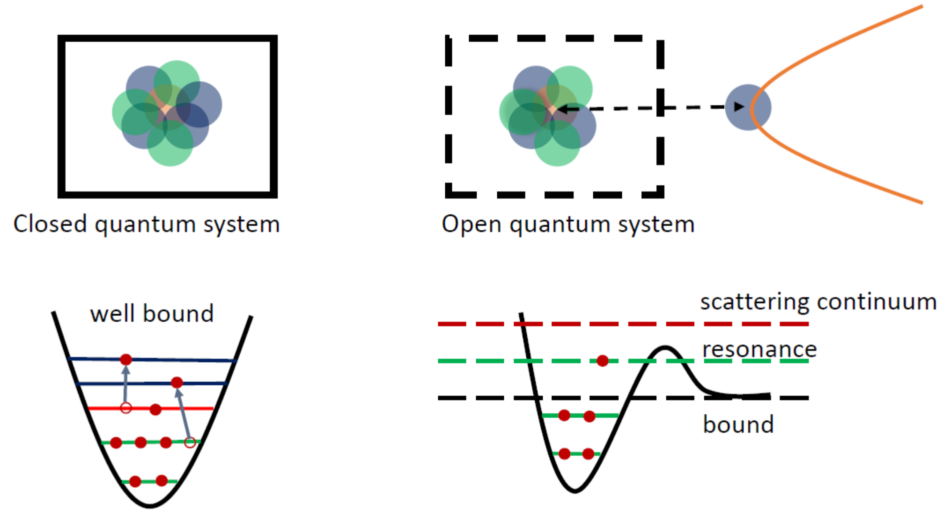
B.S. Hu, T. Li, F.R. Xu, in preparation (2018)

Charge radius

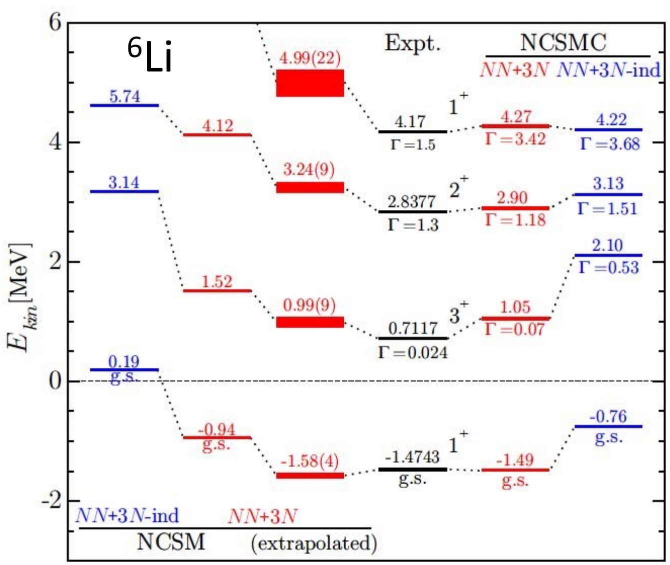
	NN		$NN+3N$		
	IM-SRG	HF-RSPT1	IM-SRG	HF-RSPT1	Expt.
^{4}He	1.64	1.66	1.69	1.75	1.6755(28)
^{14}C	2.10	2.10	2.43	2.57	2.5025(87)
^{22}C	2.05	2.02	2.53	2.63	—
^{16}O	2.20	2.20	2.67	2.78	2.6991(52)
^{22}O	2.13	2.10	2.66	2.75	—
^{24}O	2.14	2.10	2.70	2.78	—
^{40}Ca	2.61	2.58	3.40	3.49	3.4776(19)
^{48}Ca	2.55	2.51	3.38	3.46	3.4771(20)

Nucleus as an open quantum system

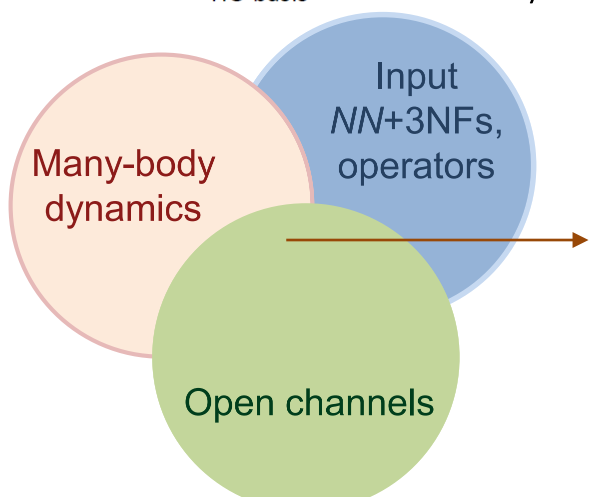




J. Phys. G: Nucl. Part. Phys. 36(2009) 013101



G. Hupin, S. Quaglioni, P. Navratil, PRL114, 212502 (2015)



- Neutron/Proton-rich isotopes
- Clustering in nuclei
- New magic numbers
- Intrinsic resonance
- New collective modes
- Halo

Bound, resonant and scattering states may be strongly coupled. Need nuclear theory including the continuum.

MBPT for open-shell nuclei

Realistic Gamow shell model Workflow

As Prof. F.R. Xu's talk

Bare forces:
Strong repulsion,
tensor force ,
slow convergence

V_{low-k},
SRG,
OLS, ...

$$\langle ab|V_{\rm osc}|cd\rangle \approx \sum_{\alpha\leqslant\beta}^{N}\sum_{\gamma\leqslant\delta}^{N}\langle ab|\alpha\beta\rangle\langle\alpha\beta|V_{\text{low-}k}|\gamma\delta\rangle\langle\gamma\delta|cd\rangle$$

pp,nn: $\langle ab|\alpha\beta\rangle = \frac{\langle a|\alpha\rangle\langle b|\beta\rangle - (-1)^{J-j_\alpha-j_\beta}\langle a|\beta\rangle\langle b|\alpha\rangle}{\sqrt{(1+\delta_{ab})(1+\delta_{\alpha\beta})}}$

pn: $\langle ab|\alpha\beta\rangle = \langle a|\alpha\rangle\langle b|\beta\rangle$

$$\hat{H} = \hat{H}_0 + (\hat{H} - \hat{H}_0) = \hat{H}_0 + \hat{H}_1$$

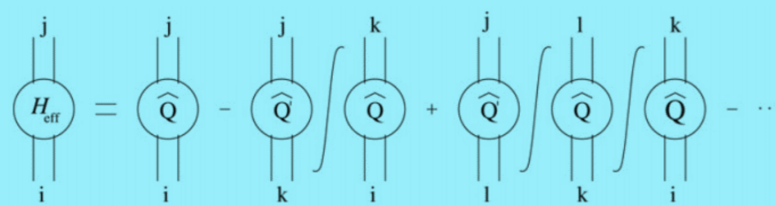
$$\hat{Q}(E) = P\hat{H}_1P + P\hat{H}_1Q\frac{1}{E - Q\hat{H}Q}Q\hat{H}_1P$$

$$\frac{1}{E - Q\hat{H}Q} = \sum_{n=0}^{\infty}\frac{1}{E - Q\hat{H}_0Q}\left(\frac{Q\hat{H}_1Q}{E - Q\hat{H}_0Q}\right)^n$$

Up to third order

HO/HF;
Gamow-Berggren
basis (a,b):
WS/GHF

Extended
Kuo-Krenciglowa
method (EKK)

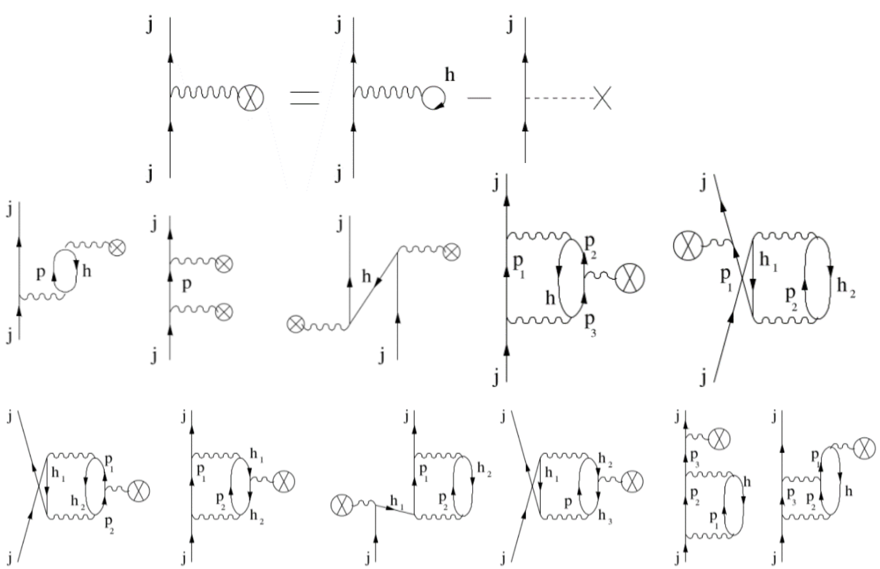


$$H_{\rm eff} - E = PH_0P - E + \hat{Q}(E) + \sum_{k=1}^{\infty}\frac{1}{k!}\frac{d^k\hat{Q}(E)}{dE^k}\{H_{\rm eff} - E\}^k$$

Valence-space effective interactions
Complex shell model code
(Jacobi-Davidson, N. Michel)

Advantages in HF basis, compared with HO basis

- **Faster convergence**
- **Some perturbation diagrams are cancelled out**
- **In HO basis, calculations could be ħω dependent, while much less in HF basis**



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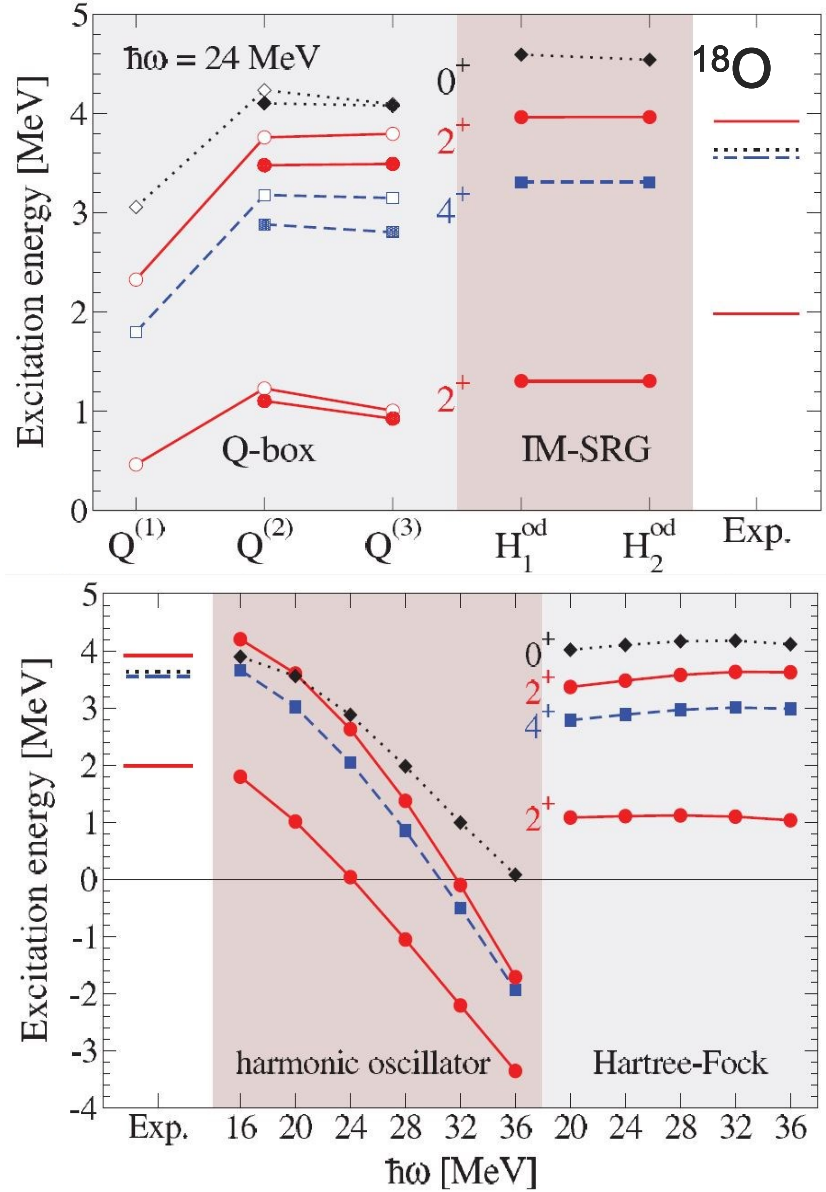
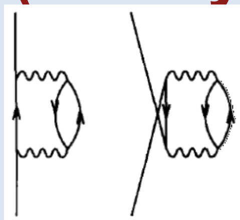


K. Tsukiyama, *et al.*, PRC 85, 061304(R) (2012)

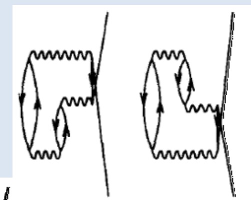
Diagrammatic expansion

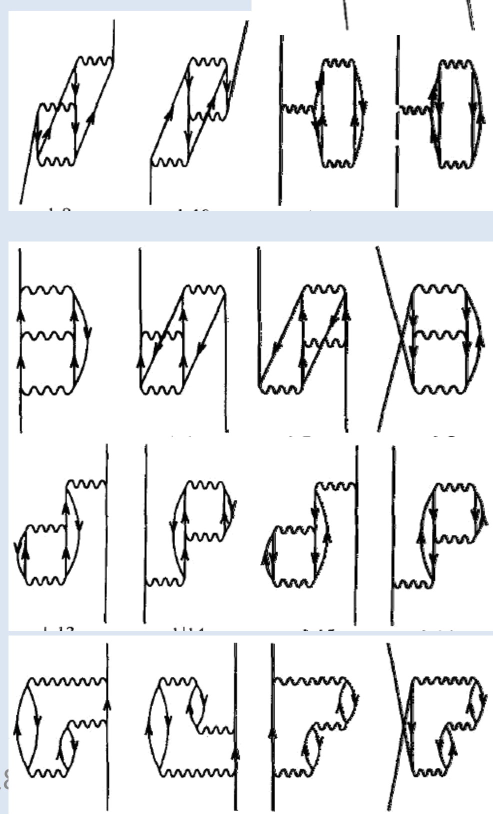
S-box (1-body)

2nd



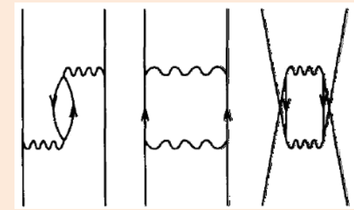
3rd



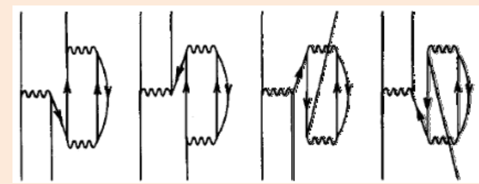


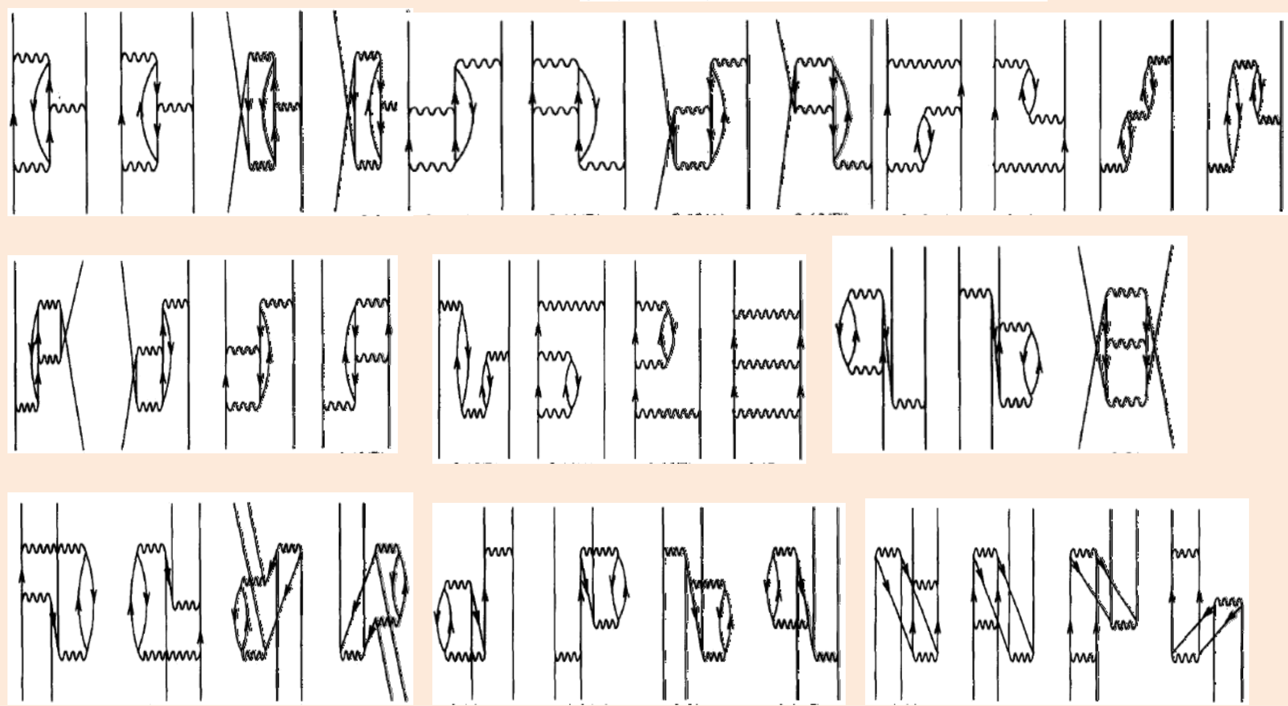
Q-box (2-body)

2nd



3rd





The pictures are taken from M. Hjorth-Jensen, *et al.*, Physics Reports 261 (1995) 125.

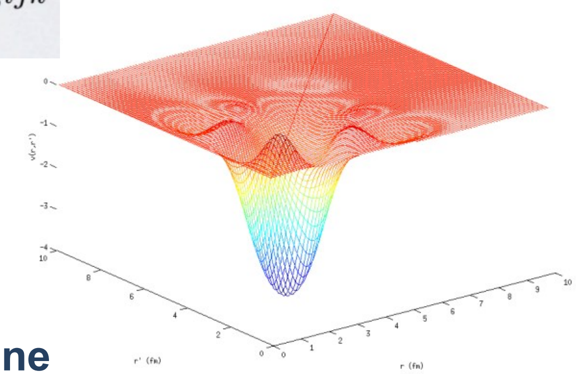
Gamow Hartree-Fock

Step ❶: Solve the Hartree-Fock equations in HO representation using H_{int},

$$H_{\text{int}} = \sum_{i=1}^{A}\left(1-\frac{1}{A}\right)\frac{\vec{p}_i^{\,2}}{2m} + \sum_{i<j}^{A}\left(V_{NN,ij} - \frac{\vec{p}_i\cdot\vec{p}_j}{mA}\right) + \sum_{i<j<k}^{A} V_{NNN,ijk}$$

Step ❷: Extract the non-local HF potential *υ(r,r')*

$$h_{ij}^{\text{HF}} = \langle i|t|j\rangle + \langle i|v|j\rangle = \langle i|t|j\rangle + \sum_{k=1}^{A}\langle ik|V|jk\rangle$$



Step ❸: Obtain the radial wave function *u(r)/r* in complex-*k* plane

$$u''(r) = \left[\frac{l(l+1)}{r^2} + v^{(\text{loc})}(r) - k^2\right]u(r) + \int_0^{+\infty} v^{(\text{non-loc})}(r,r')u(r')dr'$$

$$u(\widetilde{e},r) \sim C_0 r^{l+1}, \quad r \to 0, \qquad \widetilde{e_n} = \frac{\hbar^2 k_n^2}{2m} = e_n - i\frac{\gamma_n}{2}$$

$$u(\widetilde{e},r) \sim C^+ H_{l\eta}^+(kr) + C^- H_{l\eta}^-(kr), \quad r \to +\infty.$$

Exterior complex scaling

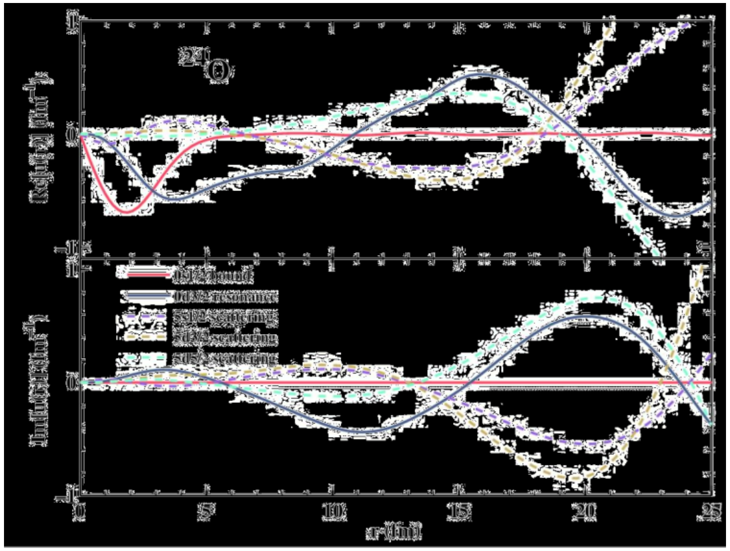
$$\int_0^{+\infty} u(\widetilde{e},r)^2 dr = \int_0^{R} u(\widetilde{e},r)^2 dr + (C^+)^2 \int_R^{+\infty} H_{l\eta}^+(kr)^2 dr$$

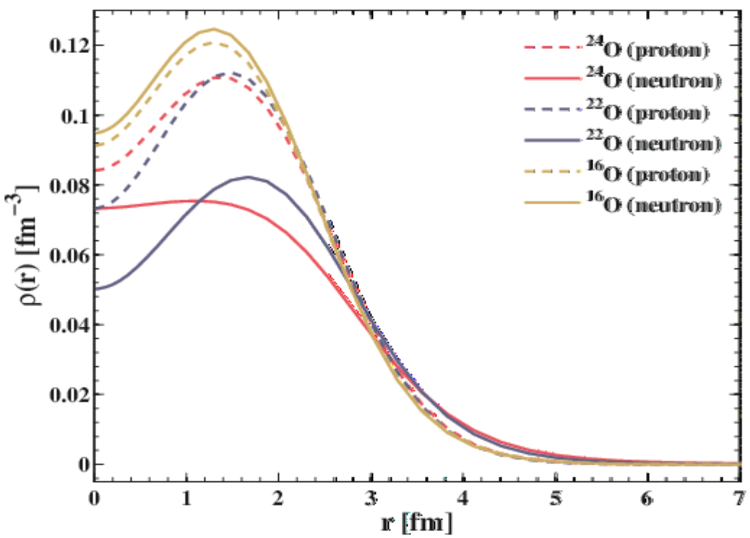
$$= \int_0^{R} u(\widetilde{e},r)^2 dr + (C^+)^2 \int_0^{+\infty} H_{l\eta}^+(kR + kxe^{i\theta})^2 e^{i\theta} dx$$

Outgoing solution at large distance

$$u_n(\widetilde{e_n},r) \sim O_l(k_n r) \sim e^{ik_n r}$$

Results of GHF





sp energies (MeV)

	^{16}O		^{22}O		^{24}O		^{28}O	
	Re(E)	Im(E)	Re(E)	Im(E)	Re(E)	Im(E)	Re(E)	Im(E)
$0s_{1/2}$	−48.858	0.000	−57.720	0.000	−59.313	0.000	−55.076	0.000
$0p_{3/2}$	−22.735	0.000	−27.729	0.000	−28.132	0.000	−28.101	0.000
$0p_{1/2}$	−13.863	0.000	−23.501	0.000	−22.669	0.000	−21.674	0.000
$0d_{5/2}$	–	–	− 3.251	0.000	−3.993	0.000	−6.687	0.000
$1s_{1/2}$	–	–	− 0.964	0.000	−2.374	0.000	−3.978	0.000
$0d_{3/2}$	–	–	3.014	−0.626	2.312	−0.368	1.088	−0.081

sp resonance

Order-by-order convergence in real-energy space

Bare NNLO$_{opt}$

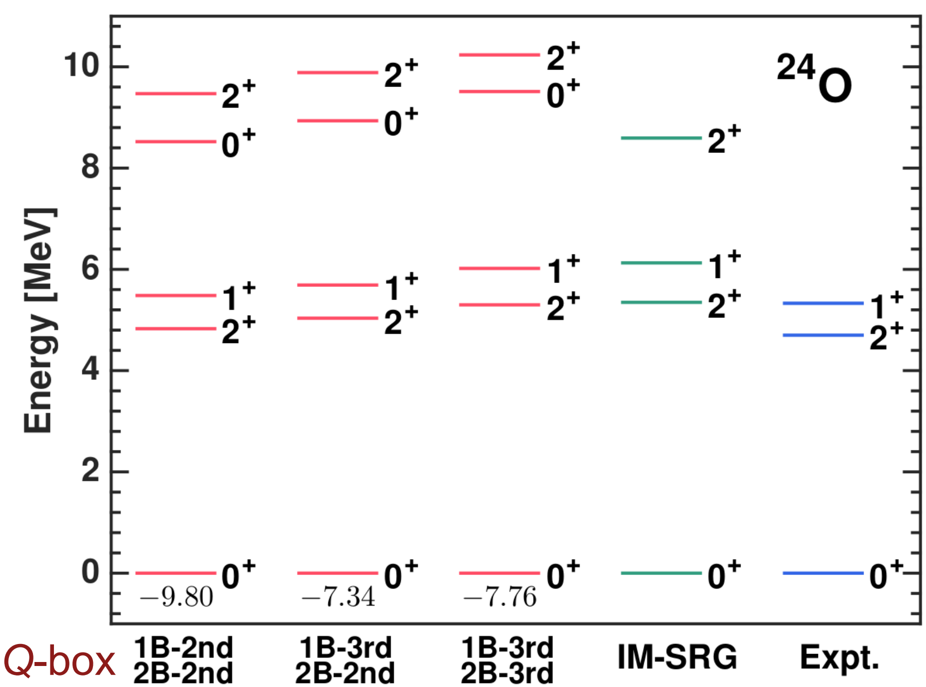
ħω=20 MeV

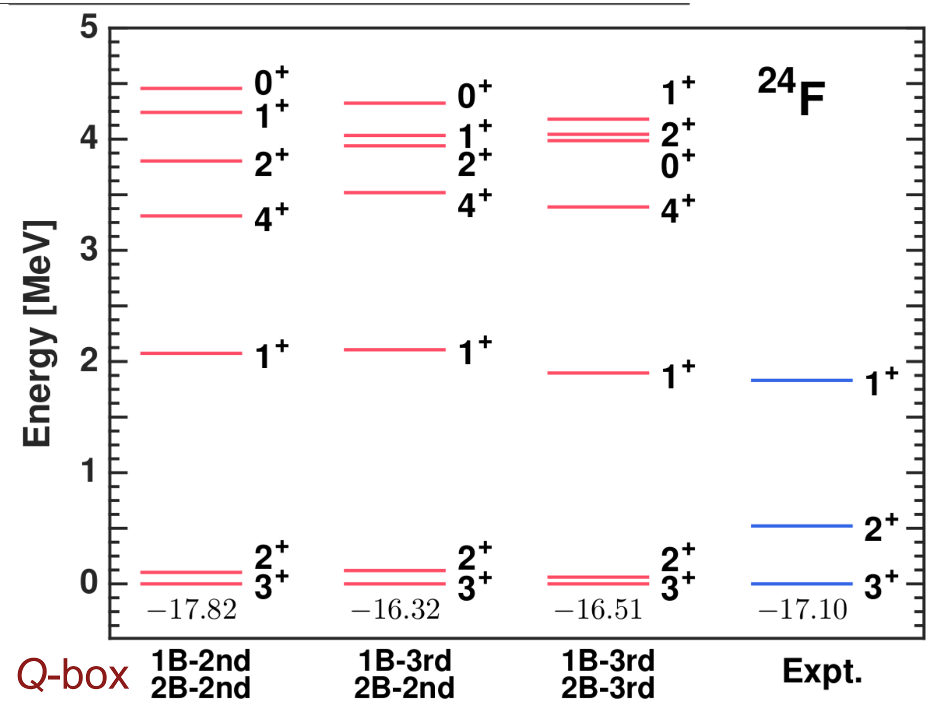
N_{shell}=12

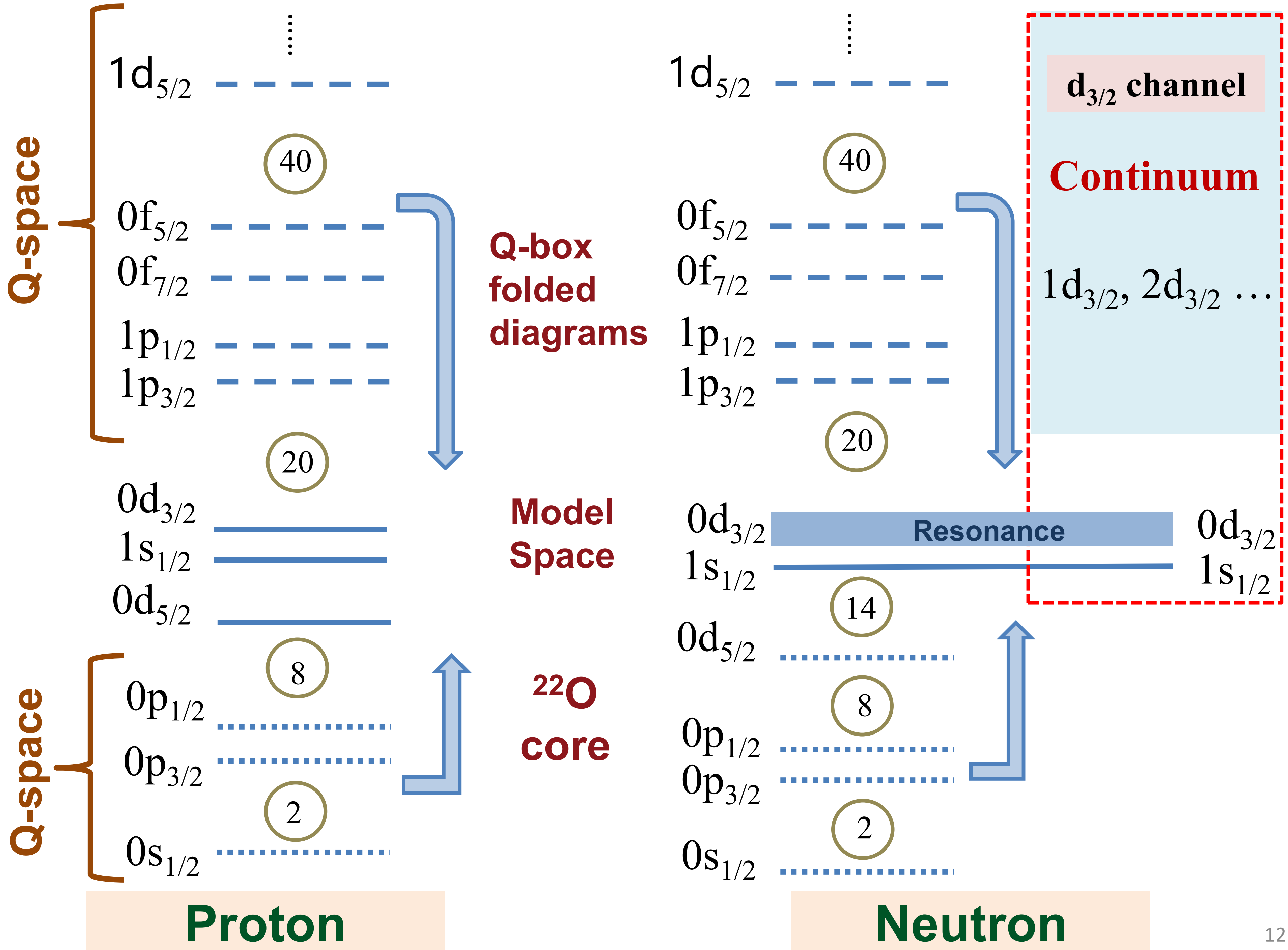
^{22}O core, *sd*-shell

SPEs

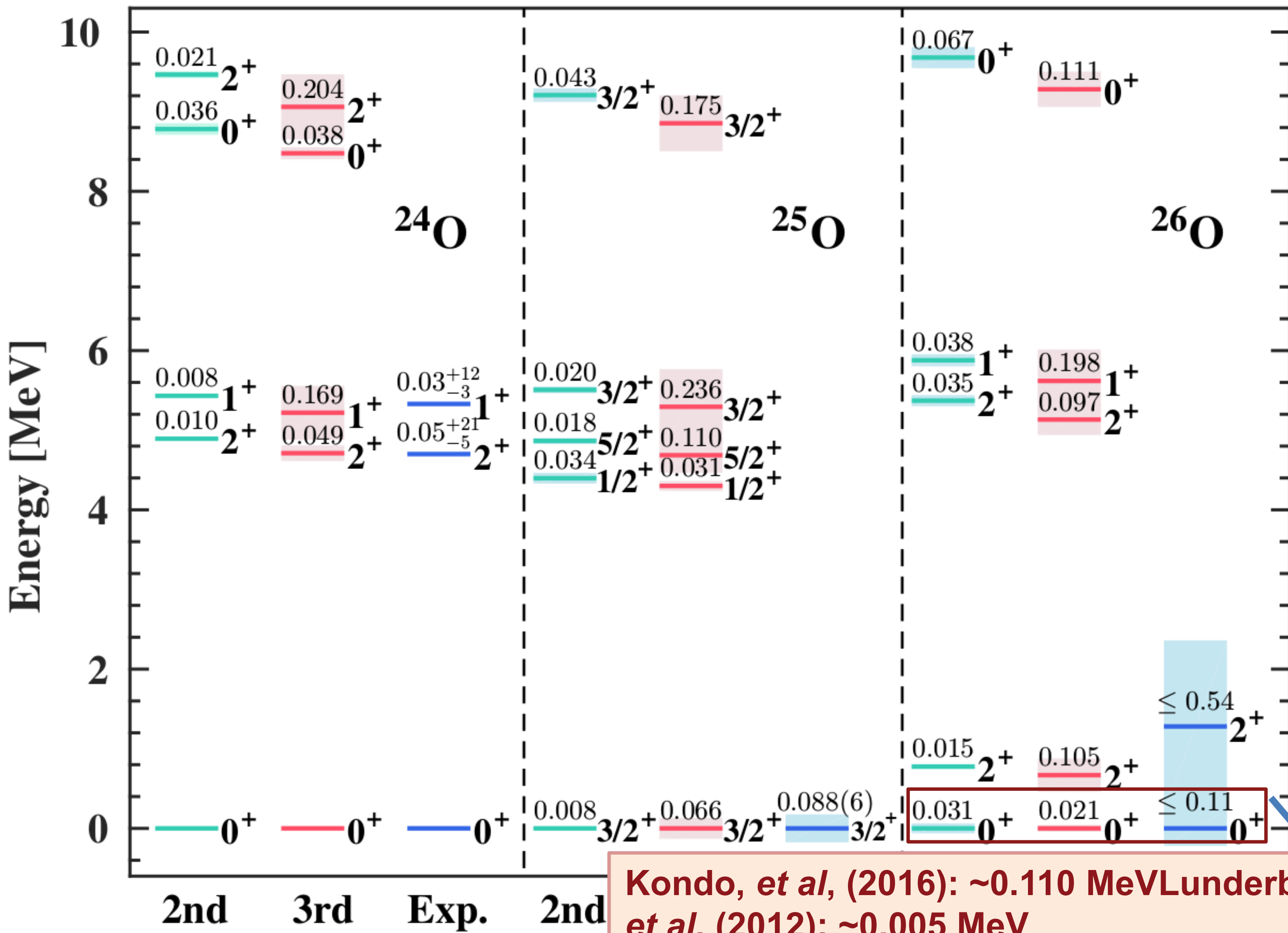
Orbit	1st	2nd	3rd	Expt.
$\pi 0d5/2$	−3.18	−12.01	−11.74	−13.26
$\pi 1s1/2$	0.70	−7.95	−7.82	−10.88
$\pi 0d3/2$	2.82	−7.15	−7.15	–
$\nu 1s1/2$	−0.07	−4.42	−3.19	−2.73
$\nu 0d3/2$	4.18	−0.12	1.31	1.26-0.2i





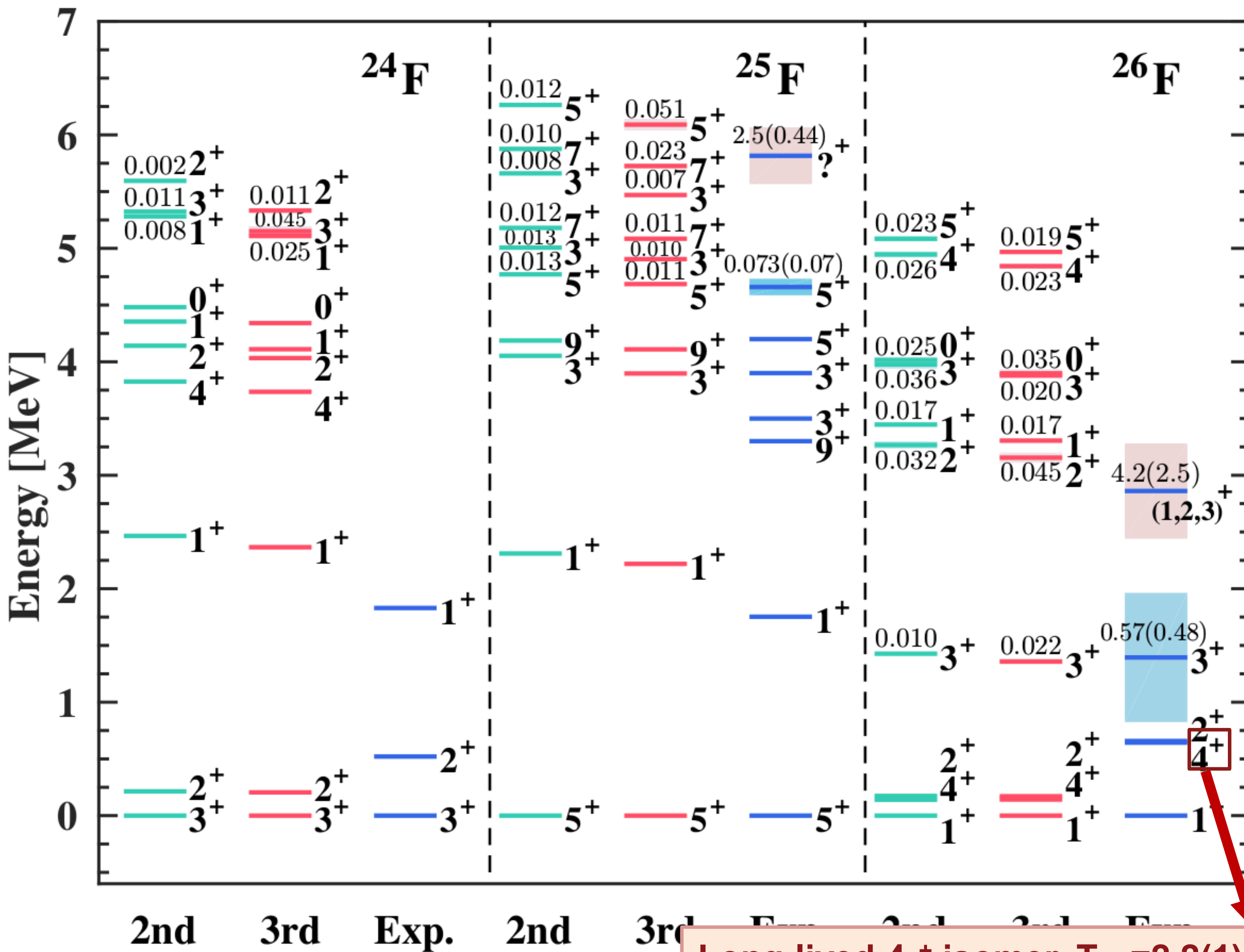

Q-space
1d5/2
40
0f5/2
0f7/2
1p1/2
1p3/2
20
0d3/2
1s1/2
0d5/2
8
0p1/2
0p3/2
2
0s1/2
Q-space
Proton
Q-box
folded
diagrams
Model
Space
22O
core
1d5/2
40
0f5/2
0f7/2
1p1/2
1p3/2
20
0d3/2
1s1/2
Resonance
14
0d5/2
8
0p1/2
0p3/2
2
0s1/2
Neutron
d3/2 channel
Continuum
1d3/2, 2d3/2 …
0d3/2
1s1/2

Oxygen isotopes from RGSM



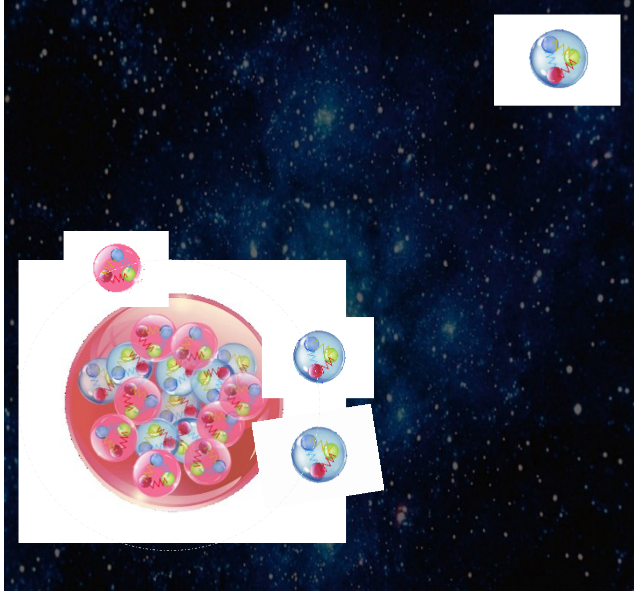
Kondo, *et al*, (2016): ~0.110 MeVLunderberg, *et al*, (2012): ~0.005 MeV
Kohley *et al*, (2013): 4.5$^{+11}_{-1.5}$(stat) $\pm$ 3 (sys) ps

Fluorine isotopes from RGSM



Long-lived 4_1^+ isomer, $T_{1/2}$=2.2(1) ms, Lepailleur, *et al.*, PRL110, 082502 (2013)

MBPT for nuclear reaction



RGSM-RGM

$$\begin{aligned}\hat{H} &= \hat{H}^{[1B]}_{\text{eff}} + \hat{H}^{[2B]}_{\text{eff}} \\ &= \hat{T} + \hat{U}_{\text{c.m.}} + \left(\hat{H}^{[1B]}_{\text{eff}} + \hat{H}^{[2B]}_{\text{eff}} - \hat{T} - \hat{U}_{\text{c.m.}}\right) \\ &= \hat{T} + \hat{U}_{\text{c.m.}} + \hat{V}\end{aligned}$$

$$|\Psi^{J_A}_{M_A}\rangle = \sum_c \int \frac{u_c(r)}{r} r^2 \, |(c,r)\rangle\rangle \, dr \qquad |(c,r)\rangle\rangle = \hat{\mathcal{A}}\left[|\Psi^{J_{\text{T}}}_{\text{T}}\rangle \otimes |\Psi^{J_{\text{P}}}_{\text{P}}\rangle\right]^{J_A}_{M_A}$$

COSM

$$\sum_c \int_0^{+\infty} \frac{u_c(r)}{r} r^2 \left(\langle\langle(c',r')|\hat{H}|(c,r)\rangle\rangle - E\langle\langle(c',r')|(c,r)\rangle\rangle\right) = 0 \qquad \vec{r} = \vec{r}_{\text{lab}} - \vec{R}_{\text{core}}$$

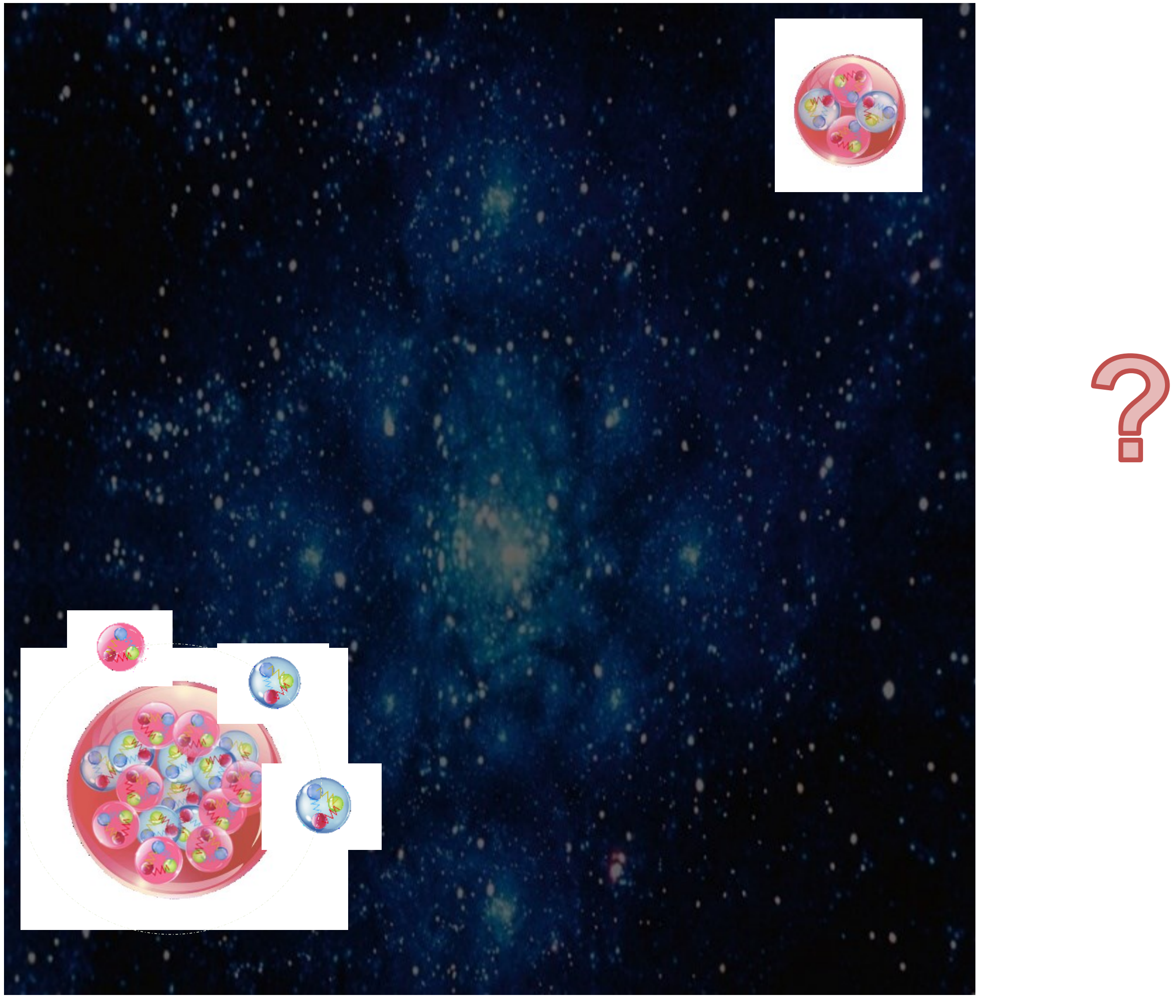
$$\begin{aligned}\langle\langle(c',r')|\hat{H}|(c,r)\rangle\rangle &= \delta_{cc'}\left[-\frac{\hbar^2}{2M_{\text{eff}}}\frac{\partial^2}{\partial r^2} + \frac{\hbar^2\ell(\ell+1)}{2M_{\text{eff}}r^2} + E_{\text{T}} + E_{\text{int}}\right]\frac{\delta(r-r')}{rr'} \\ &+ \delta_{cc'}U_{\text{c.m.}}(r,r') + \tilde{V}_{cc'}(r,r')\end{aligned}$$

$$\tilde{V}_{cc'} = \sum_{\substack{n\le n_{\max} \\ n'\le n_{\max}}} H_{cc'}(n,n')\frac{u_n(r)}{r}\frac{u_{n'}(r')}{r'} - \sum_{n\le n_{\max}} (E_{\text{T}} + E_{\text{int}} + E_{\text{c.m.}})\frac{u_n(r)}{r}\frac{u_n(r')}{r'} \qquad |r\rangle = \sum_n \frac{u_n(r)}{r}|n\rangle$$

$$H_{cc'}(n,n') = (E_{\text{c.m.}} + E_{\text{T}} + E_{\text{int}})\,\delta_{cc'}\delta_{nn'} + \sum_{\substack{\alpha,\beta \\ \gamma,\delta,\epsilon,\zeta\in T,p}} C_\alpha C_\beta \langle\gamma,\delta|\hat{V}|\epsilon,\zeta\rangle \langle\Phi_\alpha| a^+_\gamma a^+_\delta a_\epsilon a_\zeta |\Phi_\beta\rangle$$

MBPT for nuclear reaction

RGSM-RGM



Summary

- Develop HF-RSPT including the wave-function and three-body force corrections.
- Develop the third-order RGSM within HF basis
- Describe oxygen and fluorine isotopes

Outlook

- Derive the cross-shell effective interactions (*sdpf*-shell, …)
- Reconciling the microscopic valence-space effective interactions with the nuclear reaction theory (GSM-RGM)

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Thank you for your attention!

Back up

A. Gamow Hartree-Fock

The HF single-particle state $|\alpha\rangle_{\rm HF}$ can be expanded on HO basis $|p\rangle$,

$$|\alpha\rangle_{\rm HF} = \sum_p D_{p\alpha}|p\rangle. \tag{2}$$

We diagonalize the Hartree-Fock one-body Hamiltonian in HO representation,

$$\langle p|h^{\rm HF}|q\rangle = \langle p|t|q\rangle + \langle p|U|q\rangle = \langle p|t|q\rangle + \sum_{i=1}^{A}\sum_{rs}\langle pr|V|qs\rangle D^*_{ri}D_{si}. \tag{3}$$

After iterative solution of the HF equations, we can obtain the HF potential

$$\langle p|U|q\rangle = \sum_{i=1}^{A}\sum_{rs}\langle pr|V|qs\rangle D^*_{ri}D_{si}. \tag{4}$$

The the channel

$$\langle k|h^{\rm HF}|k'\rangle = (1-\frac{1}{A})\frac{\hbar^2}{2m}k^2\delta_{kk'} + \sum_{pq}\langle p|U_{\rm HF}|q\rangle\langle k|p\rangle\langle q|k'\rangle \tag{5}$$

where $\langle q|k'\rangle$ is the HO wavefunction in complex-momentum space $\langle k|$. It's noting that

$$\hat{\rho}(\vec{r}) = \sum_{k=1}^{A} \delta^3(\vec{r} - \vec{r}_k) = \sum_{k=1}^{A} \frac{\delta(r - r_k)}{r^2} \sum_{lm} Y^*_{lm}(\hat{\mathrm{r}}_k) Y_{lm}(\hat{\mathrm{r}})$$

$$\hat{\rho}(\vec{r}) = \sum_{K} \sum_{n_1 l_1 j_1} \sum_{n_2 l_2 j_2} \sum_{m_j} R_{n_1 l_1}(r) R_{n_2 l_2}(r) \frac{-Y^*_{K0}(\hat{\mathrm{r}})}{\sqrt{2K+1}} \times \left\langle l_1 \frac{1}{2} j_1 \middle| |Y_K| \middle| l_2 \frac{1}{2} j_2 \right\rangle \langle j_1 m_j j_2 - m_j | K 0 \rangle \times (-1)^{j_2 + m_j} a^\dagger_{n_1 l_1 j_1 m_j} a_{n_2 l_2 j_2 m_j}$$

$$\Psi = \Phi_0 + \Psi^{(1)} + \Psi_b^{(2)} + \Psi_c^{(2)}$$

$$\begin{aligned} \rho(\vec{r}) &= \langle \Psi | \hat{\rho}(\vec{r}) | \Psi \rangle \\ &= \langle \Phi_0 | \hat{\rho}(\vec{r}) | \Phi_0 \rangle + \langle \Phi_0 | \hat{\rho}(\vec{r}) | \Phi_0 \rangle \langle \Psi^{(1)} | \Psi^{(1)} \rangle + 2 \langle \Phi_0 | \hat{\rho}_N \middle| \Psi_b^{(2)} \rangle + 2 \langle \Phi_0 | \hat{\rho}_N \middle| \Psi_c^{(2)} \rangle + \langle \Psi^{(1)} | \hat{\rho}_N | \Psi^{(1)} \rangle \\ &= \langle \Phi_0 | \hat{\rho}(\vec{r}) | \Phi_0 \rangle + \langle \Phi_0 | \hat{\rho}(\vec{r}) | \Phi_0 \rangle \langle \Psi^{(1)} | \Psi^{(1)} \rangle + 2\rho_a + 2\rho_b + \rho_{c_1} + \rho_{c_2}, \end{aligned}$$

$$\rho_a = \frac{1}{2} \sum_{h_1, h_2} \sum_{p_1, p_2, p_3} \frac{(-1)^{j_{h_1} + j_{h_2}} \sqrt{2 j_{h_2} + 1}}{(\varepsilon_{h_1} - \varepsilon_{p_1})(\varepsilon_{h_1} + \varepsilon_{h_2} - \varepsilon_{p_2} - \varepsilon_{p_3})} \sum_J (-1)^J (2J+1) \begin{Bmatrix} j_{h_1} & j_{p_1} & 0 \\ j_{h_2} & j_{h_2} & J \end{Bmatrix}$$

$$\times \langle (h_1 h_2) J | \hat{\mathrm{H}} | (p_2 p_3) J \rangle \langle (p_2 p_3) J | \hat{\mathrm{H}} | (p_1 h_2) J \rangle \langle h_1 \| \rho \| p_1 \rangle,$$

$$\langle((n_1 l_1 j_1, n_2 l_2 j_2)J_1 T_1, n_3 l_3 j_3)J_2 T_2|\hat{\mathrm{V}}|((n_4 l_4 j_4, n_5 l_5 j_5)J_3 T_3, n_6 l_6 j_6)J_2 T_2\rangle$$

$$= C_{3N} \sum_{L_1,S_1,L_2,S_2,L_3,S_3} \begin{Bmatrix} l_1 & \frac{1}{2} & j_1 \\ l_2 & \frac{1}{2} & j_2 \\ L_1 & S_1 & J_1 \end{Bmatrix} \begin{Bmatrix} l_4 & \frac{1}{2} & j_4 \\ l_5 & \frac{1}{2} & j_5 \\ L_3 & S_3 & J_3 \end{Bmatrix} \begin{Bmatrix} L_1 & S_1 & J_1 \\ l_3 & \frac{1}{2} & j_3 \\ L_2 & S_2 & J_2 \end{Bmatrix} \begin{Bmatrix} L_3 & S_3 & J_3 \\ l_6 & \frac{1}{2} & j_6 \\ L_2 & S_2 & J_2 \end{Bmatrix}$$

$$\left\{\delta_{S_1 S_3}\delta_{T_1 T_3}\left[1-(-1)^{S_1+T_1}\right] + \hat{S}_1\hat{S}_3\hat{T}_1\hat{T}_3 \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & S_3 \\ \frac{1}{2} & S_2 & S_1 \end{Bmatrix} \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & T_3 \\ \frac{1}{2} & T_2 & T_1 \end{Bmatrix} \left[(-1)^{S_1+T_1} + (-1)^{S_3+T3} - (-1)^{S_1+T_1+S_3+T_3} - 1\right]\right\}$$

$$\frac{1}{16\pi^2}\hat{l}_1\hat{l}_2\hat{l}_3\hat{l}_4\hat{l}_5\hat{l}_6\hat{L}_2^{-2} \begin{pmatrix} l_1 & l_2 & L_1 \\ 0 & 0 & 0 \end{pmatrix}_{\mathrm{CG}} \begin{pmatrix} L_1 & l_3 & L_2 \\ 0 & 0 & 0 \end{pmatrix}_{\mathrm{CG}} \begin{pmatrix} l_4 & l_5 & L_3 \\ 0 & 0 & 0 \end{pmatrix}_{\mathrm{CG}} \begin{pmatrix} L_3 & l_6 & L_2 \\ 0 & 0 & 0 \end{pmatrix}_{\mathrm{CG}}$$

$$\int_0^\infty x^2 R_{n_1 l_1}(x) R_{n_2 l_2}(x) R_{n_3 l_3}(x) R_{n_4 l_4}(x) R_{n_5 l_5}(x) R_{n_6 l_6}(x) dx$$