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跃迁求和规则作为近似方法的判据

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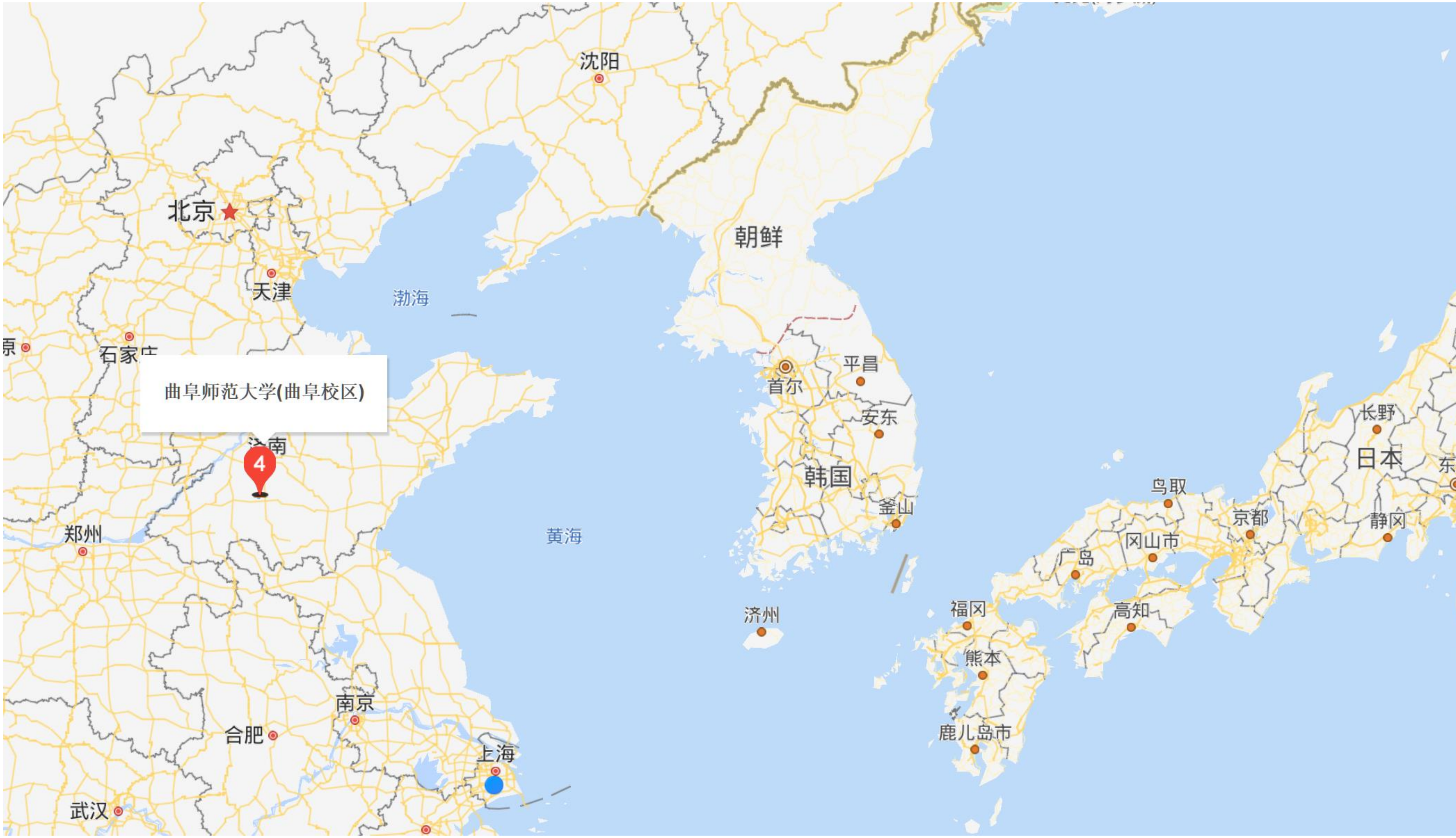

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Transition sum rules as a test stone

1. Derivation of transition sum rules
2. Code Implementation
3. Application: test of Brink-Axel hypothesis, calculation of TRK sum rules.
4. (New) Shell model v.s. HF&PHF v.s. NPA: sum rules from ground states.

Collaborators:

Calvin W. Johnson, San Diego State University

Ken Luu, San Diego State University

单体跃迁算符

$$\hat{O}_{KM} = \sum_{ab} F_{ab}[K]^{-1}[c_a^\dagger \otimes \tilde{c}_b]_{KM}$$

$$\begin{aligned} B(J_i \to J_f) &= \frac{1}{2J_i+1} \sum_{M_f M_i M} |\langle J_f M_f | O_{KM} | J_i M_i \rangle|^2 \\ &= \frac{1}{2J_i+1} \sum_{M_f} \sum_{M_i M} (J_i M_i K M | J_f M_f)^2 |\langle J_f || O_K || J_i \rangle|^2 \\ &= \frac{2J_f+1}{2J_i+1} |\langle J_f || O_K || J_i \rangle|^2 \end{aligned}$$

求和规则

$$S(E_i, E_x) \equiv \sum_f \delta\left(E_x - E_f + E_i\right) B(F; i \rightarrow f)$$

$$S_k(E_i) = \int (E_x)^k \, S(E_i, E_x) \, dE_x.$$

Non-energy weighted sum rule $S_0(E_i) = \int S(E_i, E_x) dE_x$

e.g. **Ikeda sum rule** of *Gamow-Teller transitions*

$$S_0(GT_-) - S_0(GT_+) = 3(N - Z)g_A^2$$

Energy-weighted sum rule $S_1(E_i) = \int E_x S(E_i, E_x) dE_x$

e.g. **Thomas-Reiche-Kuhn** sum rule of *electric dipole transitions*

In atomic physics: $S_1 = \frac{3e^2\hbar^2}{2m_e} N_e$ (for a multi-electron atom)

In nuclear physics: $S_1 \sim \frac{NZe^2\hbar^2}{Am_N}$

0阶求和规则：总跃迁强度

We can define $\mathcal{F}_{ba} \equiv (-1)^{1+j_a+j_b} F^*_{ab}$, and

$$\mathcal{F}_{K-M} \equiv (-1)^M \hat{F}^\dagger_{KM} = [K]^{-1} \sum_{ab} \mathcal{F}_{ba} (\hat{b}^\dagger \otimes \tilde{a})_{K-M}.$$

$$\begin{aligned}
B(F) &= \frac{1}{2J_i+1} \sum_{M_i M M_f} |\langle J_f M_f | \hat{F}_{KM} | J_i M_i \rangle|^2, \\
S_0(F) &= \frac{1}{2J_i+1} \sum_{M_i M M_f J_f \ \alpha} \langle J_i M_i | \hat{F}^\dagger_{KM} | J_f M_f, \alpha \rangle \langle J_f M_f, \alpha | \hat{F}_{KM} | J_i M_i \rangle \\
&= \frac{1}{2J_i+1} \sum_{M_i} \langle J_i M_i | \sum_{M} \hat{F}^\dagger_{KM} \hat{F}_{KM} | J_i M_i \rangle \\
&= \langle J_i M_i | (-1)^K [K] (\mathcal{F}_K \otimes \hat{F}_K)_{00} | J_i M_i \rangle
\end{aligned}$$

1阶求和规则：能量权重求和规则

$$
\begin{aligned}
S_1 &= \frac{1}{2J_i+1}\sum_{M_f M_i M} |\langle J_f M_f|O_{KM}|J_i M_i\rangle|^2 (E_f - E_i) \\
&= \frac{1}{2J_i+1}\sum_{M_f M_i M} \langle J_i M_i|O^\dagger_{KM}|J_f M_f\rangle\langle J_f M_f|O_{KM}|J_i M_i\rangle (E_f - E_i) \\
&= \frac{1}{2(2J_i+1)}\sum_{M_f M_i M} (\langle J_i M_i|O^\dagger_{KM}H|J_f M_f\rangle\langle J_f M_f|O_{KM}|J_i M_i\rangle + \langle J_i M_i|O^\dagger_{KM}|J_f M_f\rangle\langle J_f M_f|HO_{KM}|J_i M_i\rangle \\
&\quad -\langle J_i M_i|HO^\dagger_{KM}|J_f M_f\rangle\langle J_f M_f|O_{KM}|J_i M_i\rangle - \langle J_i M_i|O^\dagger_{KM}|J_f M_f\rangle\langle J_f M_f|O_{KM}H|J_i M_i\rangle \\
&= \frac{1}{2}\langle J_i M_i|\sum_{M}(2O^\dagger_{KM}HO_{KM} - HO^\dagger_{KM}O_{KM} - O^\dagger_{KM}O_{KM}H)|J_i M_i\rangle .
\end{aligned}
$$

$$
\begin{aligned}
S_1 &= \frac{1}{2}\langle J_i M_i|\sum_{M}(-1)^M (2O_{K-M}HO_{KM} - HO_{K-M}O_{KM} - O_{K-M}O_{KM}H)|J_i M_i\rangle \\
&= \frac{1}{2}\langle J_i M_i|\sum_{M}(-1)^{1+M}\left[(H,O)_{KM}, O_{K-M}\right]|J_i M_i\rangle \\
&= \frac{1}{2}\langle J_i M_i|\sum_{M}(-1)^{1+M}\left[(H,O)_{KM}, O_{K-M}\right]|J_i M_i\rangle \\
&= \langle J_i M_i|\frac{(-1)^{1+K}}{2}\sqrt{2K+1}\left[(H,O),O\right]_{00}|J_i M_i\rangle
\end{aligned}
$$

sum rule = 求和算符的期望值

$$
\begin{aligned}
S_0(\hat{F}_K, i \to all) &= \frac{1}{2J_i+1} \sum_{M_i M M_f J_f} \langle J_i M_i | \hat{F}^\dagger_{KM} | J_f M_f \rangle \langle J_f M_f | \hat{F}_{KM} | J_i M_i \rangle \\
&= \frac{1}{2J_i+1} \sum_{M_i} \langle J_i M_i | \sum_M \hat{F}^\dagger_{KM} \hat{F}_{KM} | J_i M_i \rangle \\
&= \langle J_i M_i | (-1)^K [K] (\hat{F}_K \otimes \hat{F}_K)_{00} | J_i M_i \rangle
\end{aligned}
$$

That is to say, the NEWSR equals the expectation value of an operator

$$\hat{O}_{NEWSR} = (-1)^K [K] (\hat{F}_K \otimes \hat{F}_K)_{00}.$$

$$\hat{\mathbf{O}}_{\mathbf{NEWSR}} = \sum_{\mathbf{ab}} \frac{\sum_{\mathbf{c}} \mathbf{F}^*_{\mathbf{ca}} \mathbf{F}_{\mathbf{cb}}}{[\mathbf{j_a}]} \delta_{\mathbf{j_a j_b}} (\hat{\mathbf{a}}^\dagger \otimes \tilde{\mathbf{b}})_{\mathbf{00}} + \sum_{\mathbf{abcd}} \mathbf{F}^*_{\mathbf{cb}} \mathbf{F}_{\mathbf{ad}} \begin{Bmatrix} j_a & j_d & K \\ j_c & j_b & I \end{Bmatrix} [\mathbf{I}] \left[(\hat{\mathbf{a}}^\dagger \otimes \hat{\mathbf{b}}^\dagger)_{\mathbf{I}} \otimes (\tilde{\mathbf{c}} \otimes \tilde{\mathbf{d}})_{\mathbf{I}} \right]_{\mathbf{00}}$$

Commutator to evaluate EWSRs

$$
\begin{aligned}
S_1 &= \sum_f (E_f - E_i) |\langle f|T|i\rangle|^2 = \langle i|O_{\mathrm{d.c.}}|i\rangle \\
O_{\mathrm{d.c.}} &= \frac{(-1)^K}{2}\sqrt{2K+1}\,[T_K, (H, T_K)]_0 \\
&= \sum_{ab} g_{ab}\hat{a}(a^\dagger \times \tilde{b})_0 + \frac{1}{4}\sum_{abcd}\sqrt{(1+\delta_{ab})(1+\delta_{cd})} \\
&\quad \times \sum_I \hat{I} W(abcd; I)\left[A_I^\dagger(ab) \times \tilde{A}_I(cd)\right]_0 ,
\end{aligned}
$$

Commutator to evaluate EWSRs

$$g_{ab} = \frac{\delta_{j_a j_b}}{2(2j_a+1)} \sum_{cd} \left(-e_{ac} F_{cd} F^*_{bd} + F_{ac} e_{cd} F^*_{bd} + F^*_{ca} e_{cd} F_{db} - F^*_{ca} F_{cd} e_{db} \right), \tag{23}$$

$$W^1(abcd;J) = -\frac{1}{2}(1+\mathscr{P}_{cdJ}) \sum_{efJ'} (-1)^{J+J'} (2J'+1) \pi^{J'}_{de} \zeta_{ef} \zeta^{-1}_{cd} V_J(ab,ef) \times F_{ec} F_{fd} \begin{Bmatrix} J & K & J' \\ j_d & j_e & j_f \end{Bmatrix} \begin{Bmatrix} J & K & J' \\ j_e & j_d & j_c \end{Bmatrix}, \tag{25}$$

$$W^2(abcd;J) = -\frac{1}{2}(1+\mathscr{P}_{cdJ}) \sum_{efJ'} (2J'+1) \pi^{J'}_{cf} \zeta_{ce} \zeta^{-1}_{cd} V_J(ab,ce) \times F_{ef} F^*_{df} \begin{Bmatrix} J & K & J' \\ j_f & j_c & j_e \end{Bmatrix} \begin{Bmatrix} J & K & J' \\ j_f & j_c & j_d \end{Bmatrix}, \tag{26}$$

$$W^3(abcd;J) = (1+\mathscr{P}_{abJ})(1+\mathscr{P}_{cdJ}) \sum_{efJ'} (2J'+1) \zeta_{be} \zeta_{df} \zeta^{-1}_{ab} \zeta^{-1}_{cd} V_{J'}(be,df) \times F^*_{ea} F_{fc} \begin{Bmatrix} J & K & J' \\ j_e & j_b & j_a \end{Bmatrix} \begin{Bmatrix} J & K & J' \\ j_f & j_d & j_c \end{Bmatrix}, \tag{27}$$

$$W^4(abcd;J) = P_{ac} P_{bd} W^{1*}(abcd;J), \tag{28}$$

$$W^5(abcd;J) = P_{ac} P_{bd} W^{2*}(abcd;J), \tag{29}$$

Y. Lu, C. W. Johnson, PRC 97, 034320(2018), "Transition sum rules in the Shell Model".

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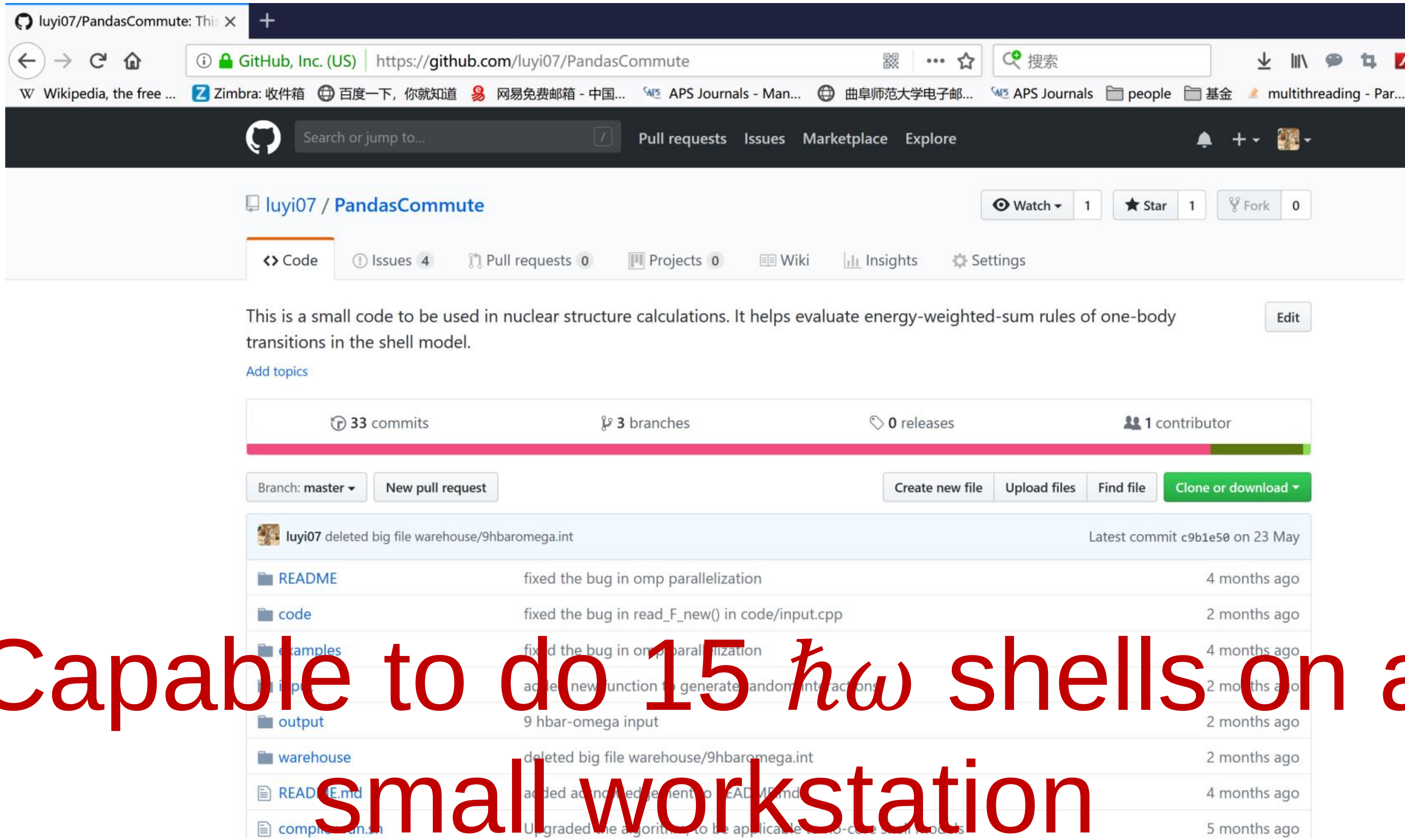
PandasCommute



Capable to do 15 $\hbar\omega$ shells on a small workstation

https://github.com/luyi07/PandasCommute

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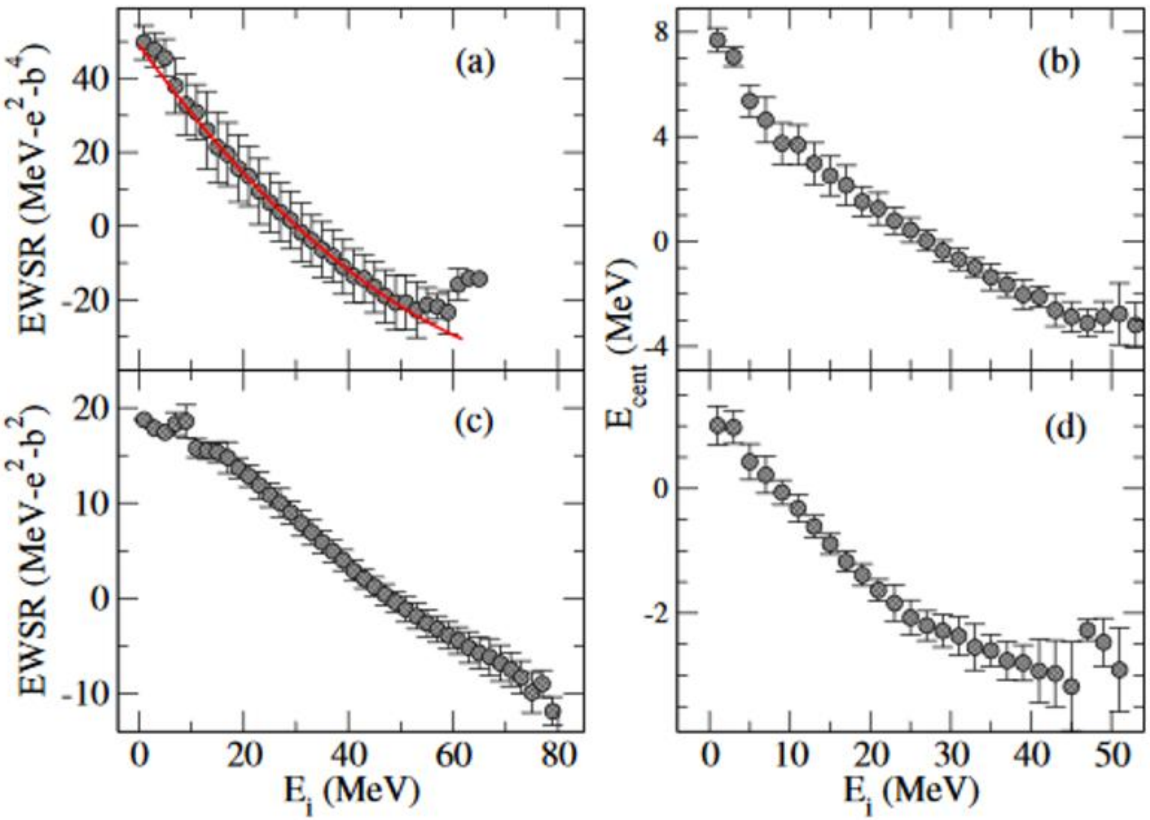
Test the Brink-Axel hypothesis

Energy-weighted sum rules (EWSR) and transition strength function centroids as a function of initial energy E_i. Results are put into 2-MeV bins with the average and root-mean-square flucutation shown; the fluctuations are not sensitive to the size of the bins. (a) EWSRs for isoscalar $E2$ for ^{34}Cl in the sd shell. The (red) solid line is the secular behavior predicted by spectral distribution theory, as described in Ref. [7]. (b) Centroids for $M1$ transitions in ^{21}Ne in the sd shell. (c) EWSR for $E1$ transitions in ^{10}B in $0p$–$1s$–$0d_{5/2}$ space. (d) Centroids for GT transitions, sum of $\beta\pm$, for ^{27}Ne in the sd shell.



Brink-Axel hypothesis: $S(E_i, E_x) \equiv \sum_f \delta\left(E_x - E_f + E_i\right) B(F; i \to f)$ is independent on E_i. If that's true, EWSR should be independent on E_i.

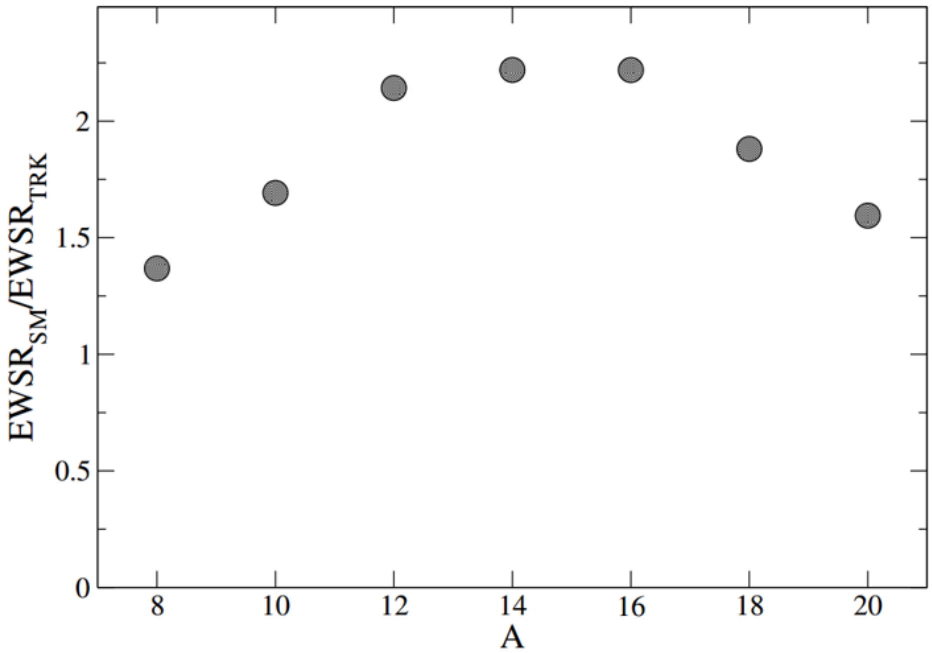
Y. Lu, C. W. Johnson, PRC 97, 034320(2018), "Transition sum rules in the Shell Model".

Calculate the TRK sum rule

PandasCommute

+

BigStick



The **Thomas-Reiche-Kuhn** sum rule: $S_1 \sim \frac{NZe^2\hbar^2}{Am_N}$

Our calculation: For A=8-18 nuclei, $S_1 / \frac{NZe^2\hbar^2}{Am_N} \in (1.4, 2.3)$, which is in consistence with expr. Data, although we use a modest valence space: spd5.

Validity of Nucleon pair approximation

$$\hat{A}_r^\dagger = \sum_{ab} y(abr)(\hat{a}^\dagger \otimes \hat{b}^\dagger)_r$$

$$\hat{A}^\dagger_{J_N M_N}(\alpha_N) = |r_1 r_2 \cdots r_N; J_1 J_2 \cdots J_N; M_N\rangle = ((\hat{A}^\dagger_{r_1} \otimes \hat{A}^\dagger_{r_2})_{J_2} \cdots)_{J_N M_N}$$

Intrinsic structure of pairs are frozen (y(abr) are fixed)

	^{45}Ca			
$7/2_1^-$	0.990	0.997	0.991	0.999
$5/2_1^-$	0.975	0.986	0.990	0.999
$3/2_1^-$	0.984	0.985	0.985	0.997
$11/2_1^-$	0.977	0.987	0.987	1.000
$9/2_1^-$	0.983	0.986	0.992	0.999
$15/2_1^-$	0.979	0.996	0.995	1.000
$1/2_1^-$	0.714	0.935	0.814	0.975
$13/2_1^-$	0.058	0.937	0.711	0.977
$17/2_1^-$		0.982	0.898	0.995
$19/2_1^-$		0.931	0.528	0.998
$21/2_1^-$		0.955	0.996	1.000
$3/2_2^-$	0.566	0.847	0.670	0.925
$5/2_2^-$	0.743	0.846	0.890	0.970
$7/2_2^-$	0.434	0.842	0.697	0.884
$9/2_2^-$	0.896	0.966	0.976	0.988
$11/2_2^-$	0.643	0.957	0.873	0.981
$13/2_2^-$		0.909	0.668	0.972
$15/2_2^-$		0.570	0.098	0.987
$17/2_2^-$		0.891	0.337	0.985
$19/2_2^-$		0.870	0.540	0.970

spin$^{\text{parity}}$	SM	*SD*	FP
0^+	8 316	4	64
2^+	37 219	7	213
4^+	54 190	4	307
6^+	57 309		336
8^+	50 319		313
10^+	38 242		257

Truncations prove to be effective at low-lying states

Conjugate-gradient method: optimize pairs

$$\hat{A}_r^\dagger = \sum_{ab} y(abr)(\hat{a}^\dagger \otimes \hat{b}^\dagger)_r$$

$$\hat{A}^\dagger_{J_N M_N}(\alpha_N) = |r_1 r_2 \cdots r_N; J_1 J_2 \cdots J_N; M_N\rangle = ((\hat{A}^\dagger_{r_1} \otimes \hat{A}^\dagger_{r_2})_{J_2} \cdots)_{J_N M_N}$$

变分法：调节集体对结构系数，使得哈密顿量期望值取极小值

$$\epsilon_{NPA} = \langle NPA|\hat{H}|NPA\rangle$$

共轭梯度法是一种梯度下降算法，对结构系数一般有几十个自由参数，所以需要几十次一维优化，每次一维优化需要几十次迭代，所以一个核需要计算几百上千次，才能得到“最优参数”。适用于价核子数较少的核。

Comparison

In the same valence space, use the same effective interactions:

Shell Model

arXiv:1801.08432 [pdf, ps, other] physics.comp-ph nucl-th

BIGSTICK: A flexible configuration-interaction shell-model code

Authors: Calvin W. Johnson, W. Erich Ormand, Kenneth S. McElvain, Hongzhang Shan

NPA: PandaWarrior

ELSEVIER

Physics Reports
Volume 545, Issue 1, 1 December 2014, Pages 1-45

Nucleon-pair approximation to the nuclear shell model

Y.M. Zhao [a], A. Arima [a, b]

Hartree-Fock、Projected Hartree-Fock in the occupation space

``The random phase approximation vs. exact shell-model correlation energies," I. Stetcu and **C. W. Johnson**, Phys. Rev. C **66** 034301 (2002).

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"Scalar ground-state observables in the random phase approximations," **C. W. Johnson** and I. Stetcu, Phys. Rev. C **66**, 064304 (2002).

"Tests of the random phase approximation for transitions strengths," I. Stetcu and **C. W. Johnson**, Phys. Rev. C. **67**, 043315 (2003).

"Gamow-Teller transitions and deformation in the proton-neutron random phase approximation," I. Stetcu and **C. W. Johnson**, Phys. Rev. C. **69**, 024311 (2004).

"Collapse of the random phase approximation: examples and counter-examples from the shell model," **C. W. Johnson** and I. Stetcu, Phys. Rev C **80**, 024320 (2009).

"Projection of angular momentum by linear algebra," **C. W. Johnson** and K. D. O'Mara, Phys. Rev C **96**, 064304 (2017)

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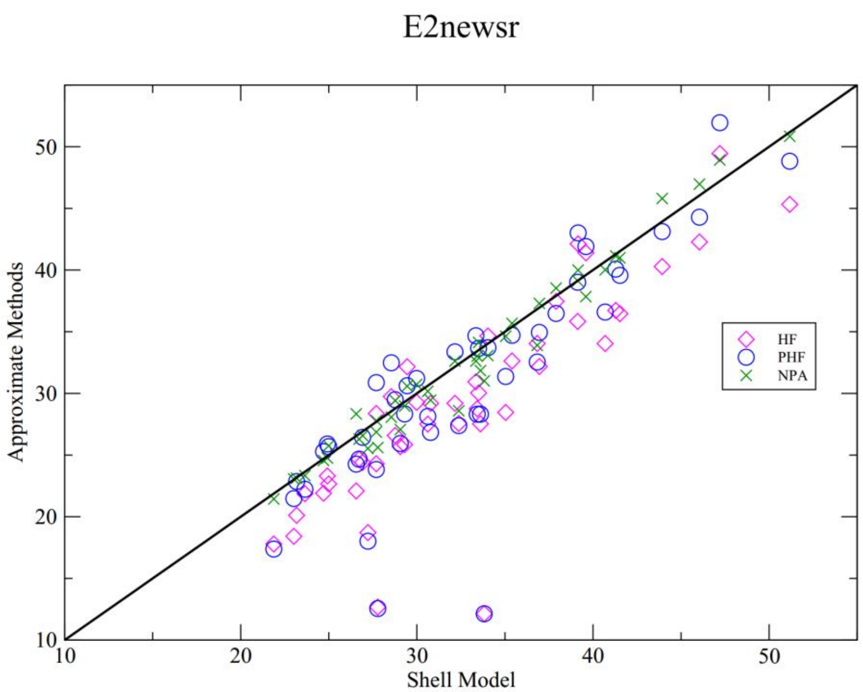
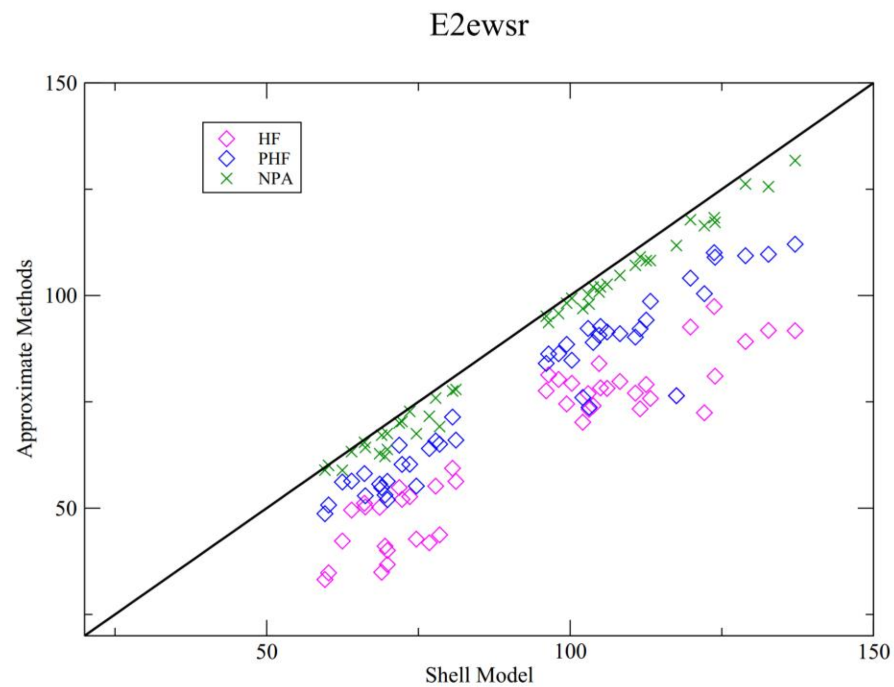
E2: non-energy-weighted sum rules & energy-weighted sum rules

Preliminary results



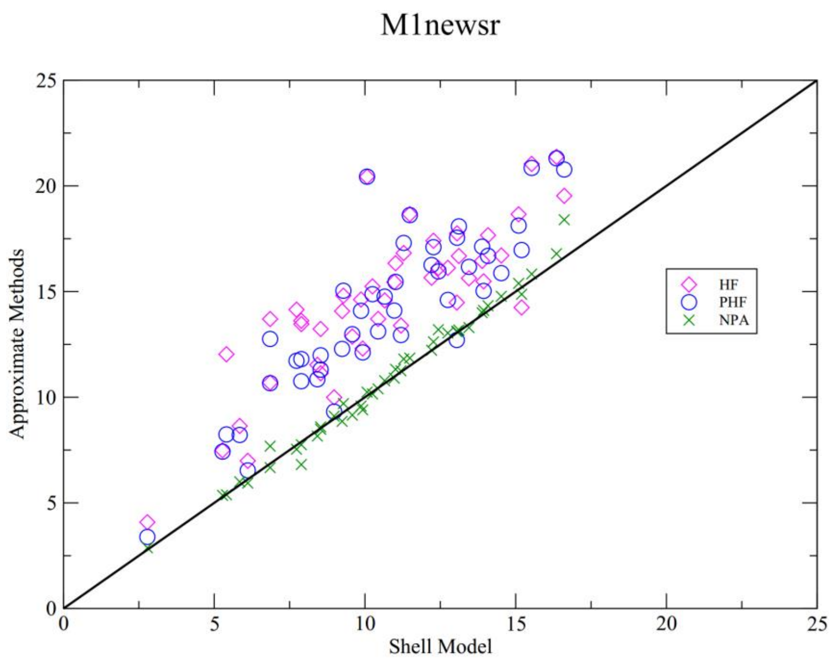


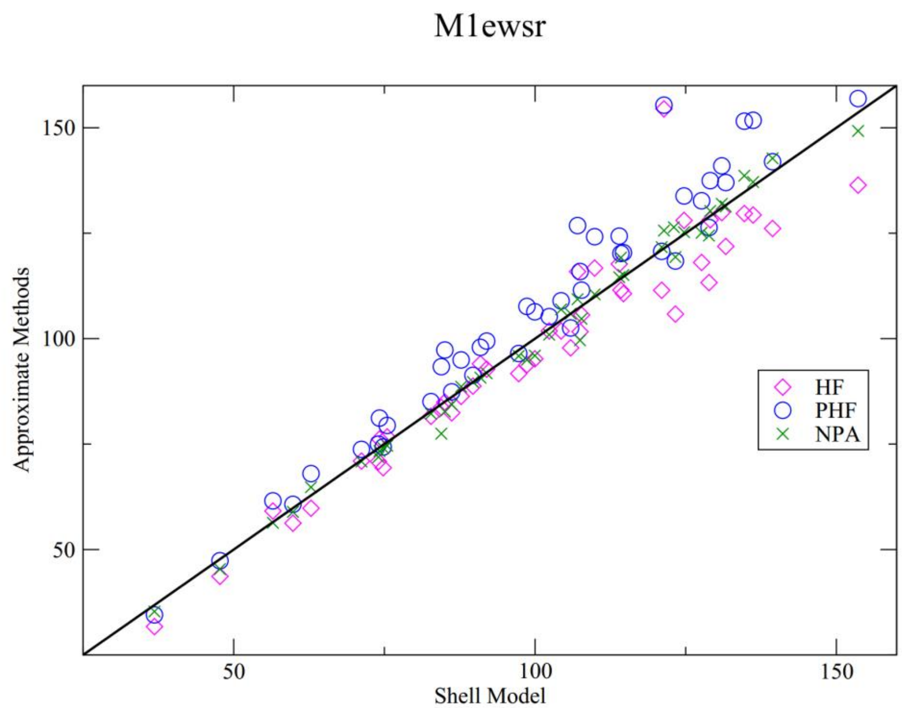
sd壳所有Z<=N的原子核基态

usdb，HF v.s. PHF v.s. NPA(SDG)

M1: non-energy-weighted sum rules & energy-weighted sum rules

Preliminary results

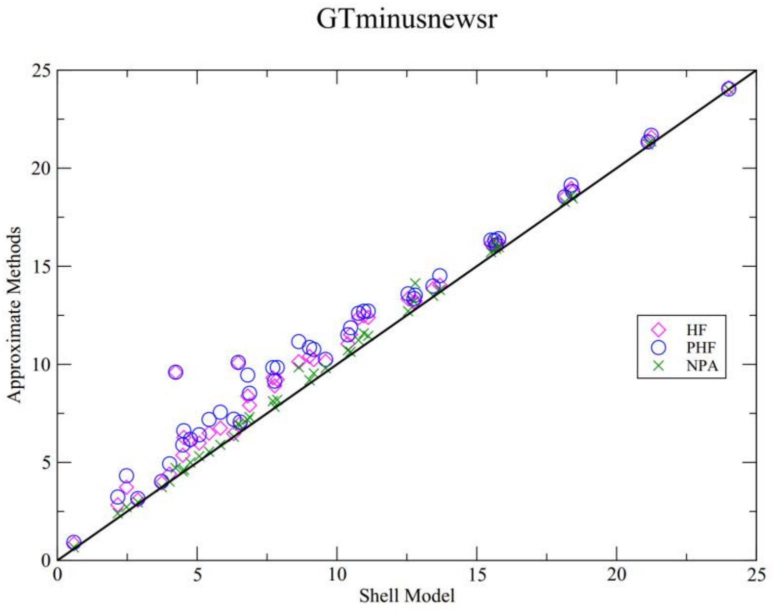


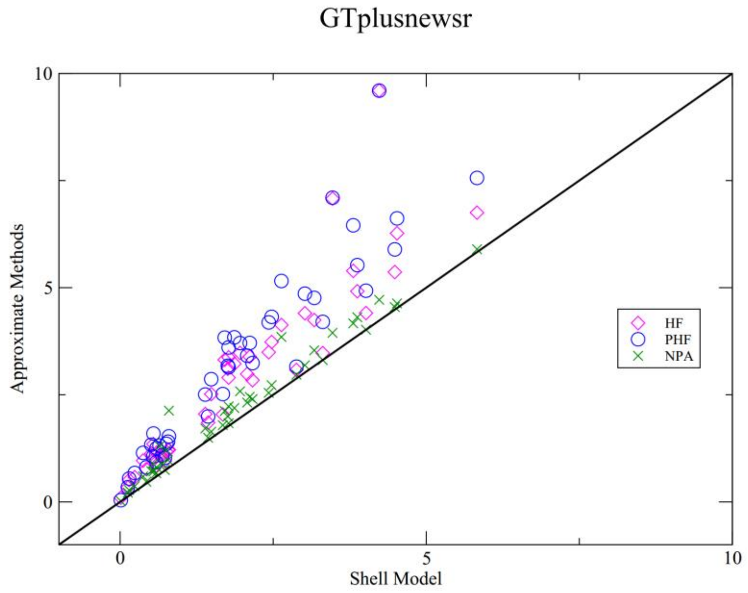


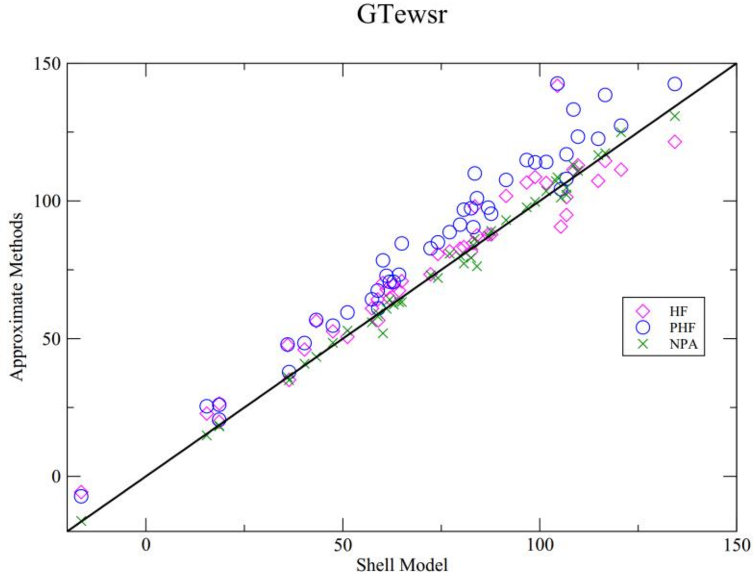
sd壳所有Z<=N的原子核基态

usdb，HF v.s. PHF v.s. NPA(SDG)

GT: non-energy-weighted sum rules & energy-weighted sum rules

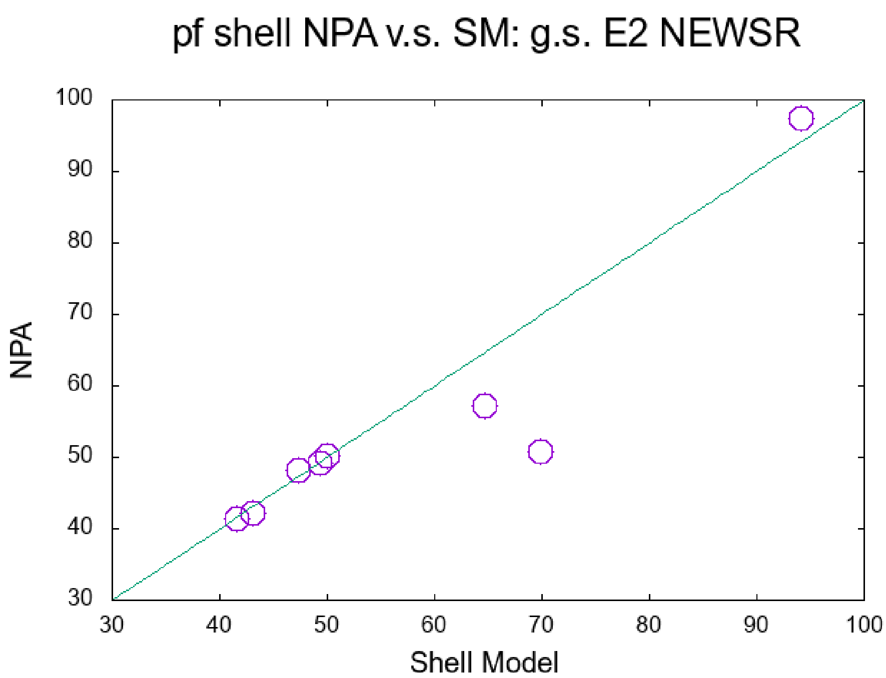


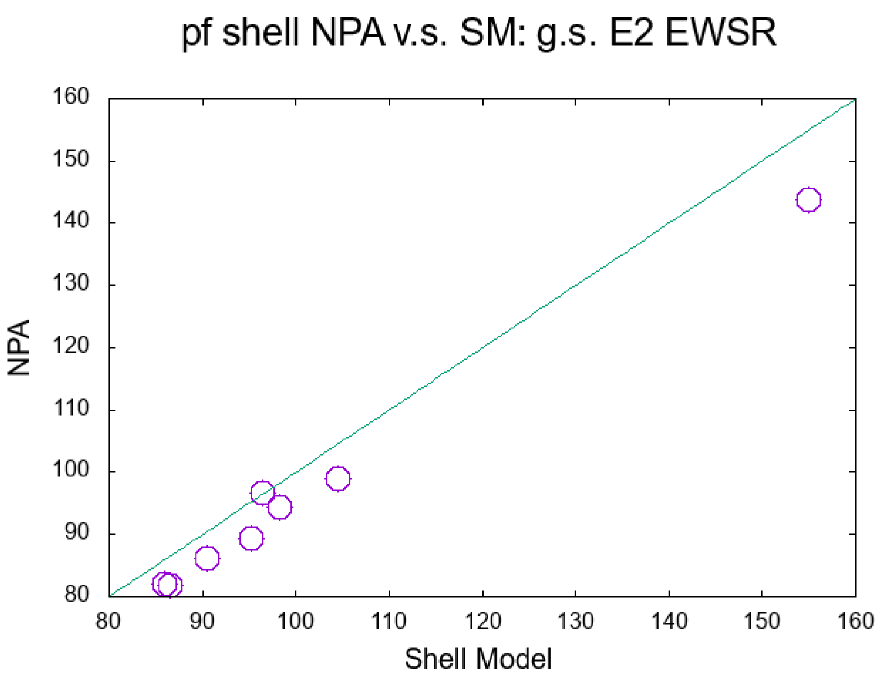




E2: non-energy-weighted sum rules & energy-weighted sum rules

Preliminary results



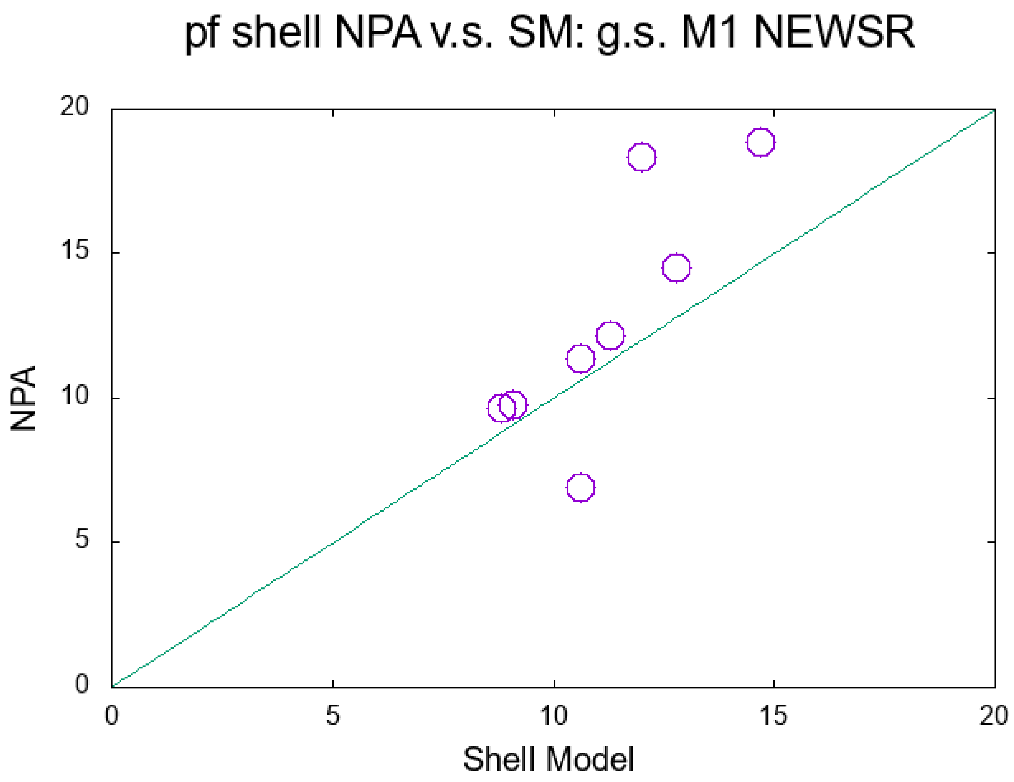


pf壳部分原子核基态

gx1a，HF v.s. PHF v.s. NPA(SDGI)

M1: non-energy-weighted sum rules

Preliminary results



pf壳部分原子核基态

gx1a，HF v.s. PHF v.s. NPA(SDGI)

Summary

1. 对于sd壳、pf壳一些开壳核，SDG/SDGI可以描述基态。

2. Transition sum rules 是Model-independent的判据，可以用来测试近似方法，配对截断与严格对角化结果非常接近。

3. 原则上，Configuration-Interaction 的方法都可以通过sum rule 检验波函数是否互相一致！

谢谢！