Derivation of effective interactions

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CEA/Saclay

Lecture 7, 15 May 2013

Outline

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Brief Review

- Microscopic bare interactions (*NN* and *NNN*) have been derived and fit to data
- Separation into components depends on renormalization scheme
- Bare interactions reproduce *NN* scattering data up to 300-350 MeV
- Not constrained by theory or experiment for higher energies
- For purpose of these tutorials, assume accurate bare interactions
- In reduced model space, require an effective interaction
  - Must incorporate effects from outside the model space
  - Components: one-body (SPE) and two-body (TBME)
  - Explicit three-body excluded due to computational difficulties
  - Inclusion of effects at one- and two-body level?
- For historical effective interactions
  - Calculations deteriorate with increasing number of valence particles
  - Claimed that microscopic effective interactions are not practical
- Today, effective two-body component of three-body forces improves results
- Empirical correction to monopole terms provides satisfactory results
- Phenomenologically adusted effective interactions typically used for calculations
- Does not make general CI theory phenomenological!
- RG methods and MBPT provide prescriptions to construct effective interactions

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Parameterization of interaction: Two main schemes

1. Unconstrained parameterization
   - Interaction completely unknown
   - Treat all SPE and TBME as parameters
   - 66 (199) parameters in *sd* (*pf*) shell
   - Parameters become correlated through fit to data
   - Complicated fitting procedure required (singular value decomposition)
2. Constrained parameterization
   - Select fewer parameters to vary
   - For instance, only treat monopoles as free parameters
     - 6 (10) parameters in *sd* (*pf*) shell
     - Standard fitting procedures sufficient
   - Another popular procedure: fix (not fit) to experimental data
     - Fix one-body terms (SPE) to core + one nucleon
     - Fix two-body terms (TBME) to core + two nucleons

Example: ^{17}O and ^{18}O data

- For the *sd* shell, outside of the doubly magic ^{16}O core
  - Use data from ^{17}O and ^{18}O to determine effective interaction for neutrons

$$E(^{17}O; 5/2^+) - E(^{16}O; g.s.) = -4.14MeV \equiv \epsilon(0d_{5/2})(\text{SPE})$$
$$E(^{17}O; 1/2^+) - E(^{16}O; g.s.) = -3.27MeV \equiv \epsilon(1s_{1/2})(\text{SPE})$$
$$E(^{17}O; 3/2^+) - E(^{16}O; g.s.) = 0.94MeV \equiv \epsilon(0d_{3/2})(\text{SPE})$$
$$E(^{18}O; g.s.) - E(^{16}O; g.s.) = -12.19MeV$$
$$\equiv 2\epsilon(0d_{5/2}) + \langle(0d_{5/2}0d_{5/2})_{J=0}|V_{ms}|(0d_{5/2}0d_{5/2})_{J=0}\rangle$$
$$\vdots$$

  - Can obtain most important TBME in this way

$$\langle(0d_{5/2}0d_{5/2})_{J=0}|V_{ms}|(0d_{5/2}0d_{5/2})_{J=0}\rangle = -3.91MeV \text{ (TBME)}$$

  - For the remainder, G-matrix result typically used

Fitting procedure

1. Select model space of interest
2. Select free parameters to fit (constrained vs. unconstrained)
3. Select experimental data within model space for fit (typically, energy levels)
4. Initialize parameters with "microscopic" input, i.e. from RG + MBPT methods
5. Iterate by minimizing deviation with respect to data

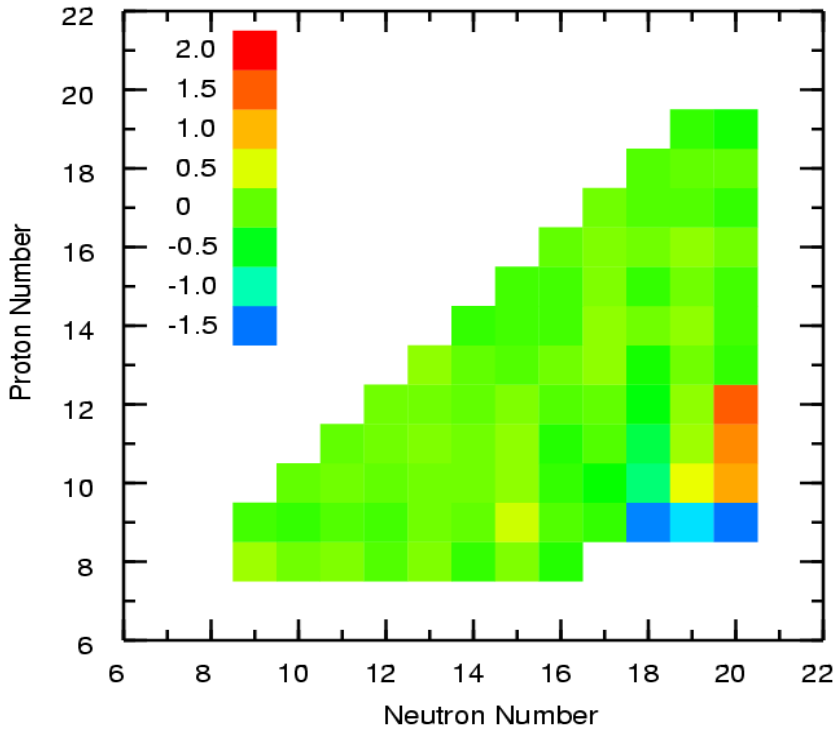
Example: USDA and USDB interactions

- Empirical universal *sd* (USD) interaction created around 1980
- As experimental capabilities extended further from stability
  - Reached nuclei beyond those included in the fit
  - Large disagreements for exotic nuclei
  - Predictive power lost in fitting procedure

Example: USDA and USDB interactions

- Empirical universal *sd* (USD) interaction created around 1980
- As experimental capabilities extended further from stability

$$BE_{exp}(Z,N) - BE_{th}(Z,N)$$



New interactions needed within *sd* shell!

Example: USDA and USDB interactions

- Brown and Richter undertook this task[a]
- 608 energy levels in *sd* shell with uncertainty $\sigma \leq 200$ keV compiled
- Procedure:

$$\begin{aligned} H(n=0) &= SPE(\text{exp}) + TBME(\text{G-matrix}) \\ &\equiv P_i(n=0) \\ i = 1-3 \qquad & P_i(n) = SPE(n) \\ i = 4-66 \qquad & P_i(n) = \frac{18}{A}^{0.3} TBME(n) \\ \{E_k(n)\} = \langle \Psi_k | H(n) | \Psi_k \rangle \quad & \overset{SVD}{\Rightarrow} \quad P_i(n+1) \end{aligned}$$

- Iteration number n increased until convergence
- Mass-dependence due to G-matrix formalism, but phenomenological

[a] B.A. Brown and W. Richter, Phys. Rev. C **74**, 034315 (2006)

Example: USDA and USDB interactions

- Brown and Richter undertook this task[a]
- 608 energy levels in *sd* shell with uncertainty $\sigma \leq 200$ keV compiled
- USDA (USDB) found from 30 (56) linear combinations of correlated parameters
- Two interactions provide a way to estimate theoretical errors
- USDA
  - More conservative
  - Smaller rms deviation from input G-matrix values
  - 170 keV rms deviation to experimental data (global rms)
- USDB
  - More accurate
  - Also determined by plateau in deviation as function of linear parameters varied
  - 126 keV global rms deviation

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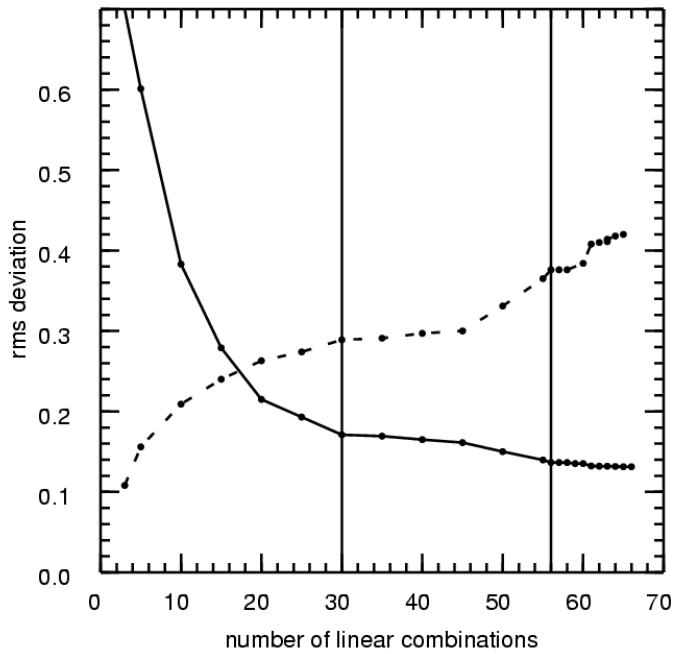

- Two interactions created based on plateau in rms deviations
- USDA more conservative (closer to G-matrix)
- USDB more accurate (smaller deviation to experimental data)

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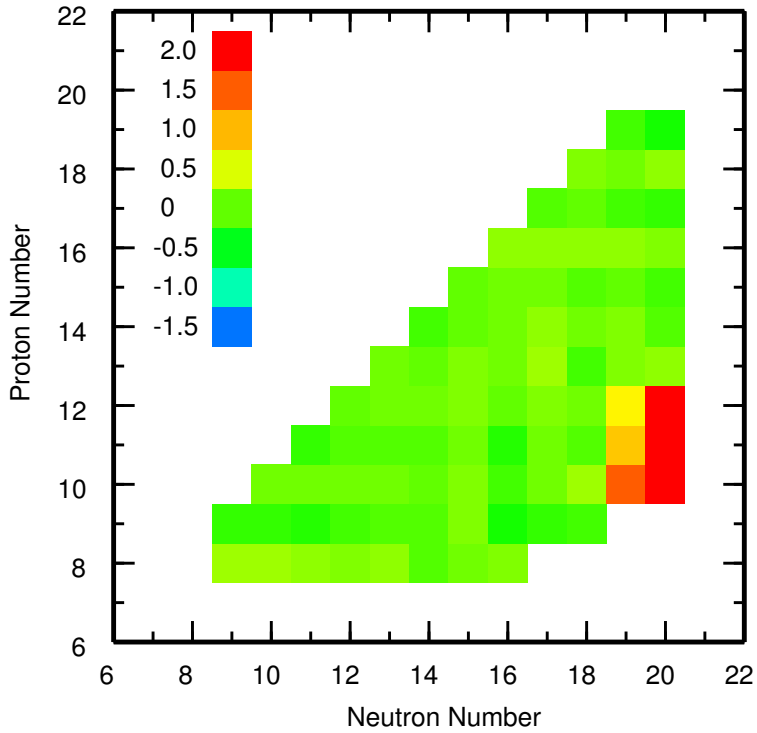

- Improvement relative to USD interaction
- Still underbound for some exotic nuclei $\rightarrow$ island of inversion region (see lecture 1)

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Outline

Motivation

- Empirical interactions are only predictive within fitting data
- Continually improve by refitting as new energy levels are observed
- Lengthy, difficult procedure to determine effective interactions
  - Requires compilation of hundreds of data
  - Iterative procedure is prohibitive for larger model spaces
  - Each model space requires this procedure
- Microscopic procedures not tuned
- Assuming sufficient data, cannot improve upon empirical parameterization
- Improvements
  1. Less time-consuming procedure to determine effective interactions
  2. No limitations on model space (number of parameters vs. data points)
  3. Theoretical error given by aspects excluded from RG+MBPT
  4. Method for explicitly determining three-body contribution

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Review

- Main topics already presented in prior two lectures (J. Holt)
  1. Select microscopic bare interactions which reproduce scattering data
  2. Soften using renormalization group methods (G-matrix, v_{lowk}, SRG, etc.)
  3. Define P and Q operators (select reduced model space and basis truncation)
  4. Employ many-body perturbation theory to determine two-body matrix elements
  5. Determine single particle energies (HF, Dyson's equation, empirically, etc.)
- NUSHELLX executable "ham" produces effective interactions
- Practical aspects of calculations must be discussed
  - Selection of basis for MBPT
  - Convergence (order of perturbation theory, $\hbar\omega$ excitations, etc.)
  - Divergences due to small energy denominators and large model spaces

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Behavior of exotic nuclei

- Renormalization is basis-dependent (HO typical for nuclear structure applications)
- Magic numbers evolve away from stability
  - Suggests evolution of single particle shell structure
  - Not reproduced by standard HO potential in nuclear physics
- For exotic nuclei, valence orbits are often loosely bound
- Well-known problem
  - Loosely bound orbits extend farther in space
  - Huge basis required to reproduce behavior with HO wavefunctions
  - Realistic basis preferred for reasonable truncation needed computationally
- Typical realistic bases
  1. Woods-Saxon basis
  2. Skyrme Hartree-Fock (SHF) basis
  3. Gamow basis

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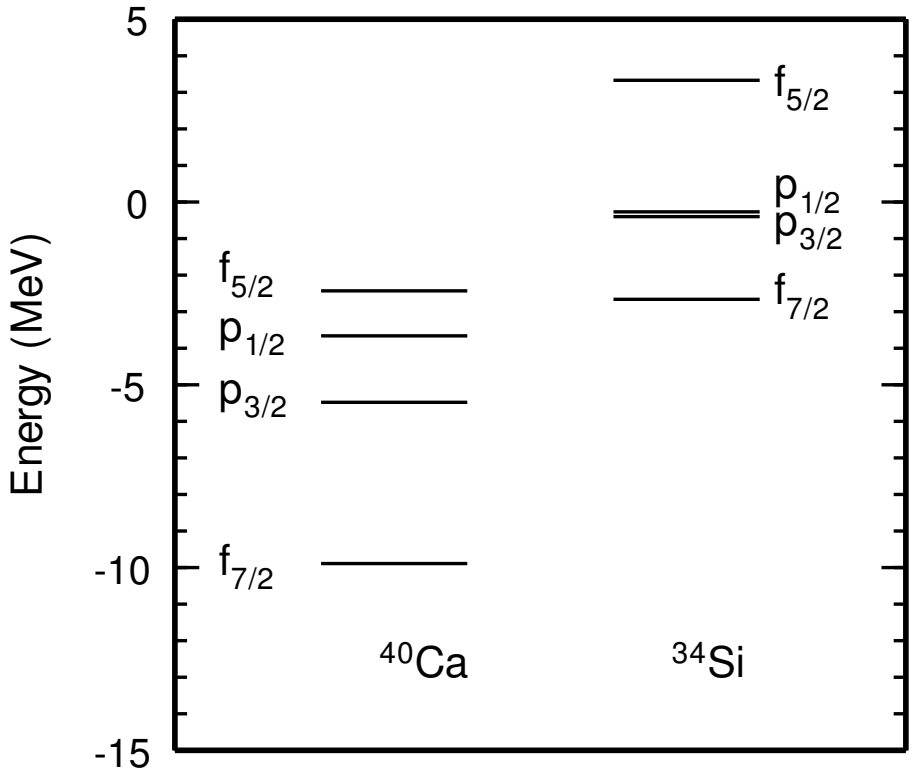
Example: *pf* neutron orbits

- Compare bases for *pf* valence space for stable ^{40}Ca and exotic ^{34}Si isotopes
- Both nuclei have $N = 20$ (same neutron occupation, same neutron valence orbits)
- HO basis energies fixed to reproduce SHF value for valence orbits (bold)

$n\ell_j$	^{34}Si HO	^{34}Si SHF	^{40}Ca HO	^{40}Ca SHF
$0s_{1/2}$	-34.59	-32.79	-39.21	-38.18
$0p_{3/2}$	-23.09	-23.10	-28.19	-29.70
$0p_{1/2}$	-23.09	-21.74	-28.19	-26.67
$0d_{5/2}$	-11.58	-13.07	-17.17	-20.20
$0d_{3/2}$	-11.58	-9.03	-17.17	-14.65
$1s_{1/2}$	-11.58	-10.04	-17.17	-15.75
$0f_{7/2}$	**-0.07**	**-2.62**	**-6.15**	**-9.89**
$0f_{5/2}$	**-0.07**	**3.33**	**-6.15**	**-2.43**
$1p_{3/2}$	**-0.07**	**-0.40**	**-6.15**	**-5.48**
$1p_{1/2}$	**-0.07**	**-0.27**	**-6.15**	**-3.66**
$0g_{9/2}$	11.44	9.22	4.87	1.15
$0g_{7/2}$	11.44	18.23	4.87	10.28

Example: *pf* neutron orbits

- Compare bases for *pf* valence space for stable ^{40}Ca and exotic ^{34}Si isotopes
- Both nuclei have $N = 20$
- Focus on model space orbits



Model Space Neutron Orbits in SHF Basis

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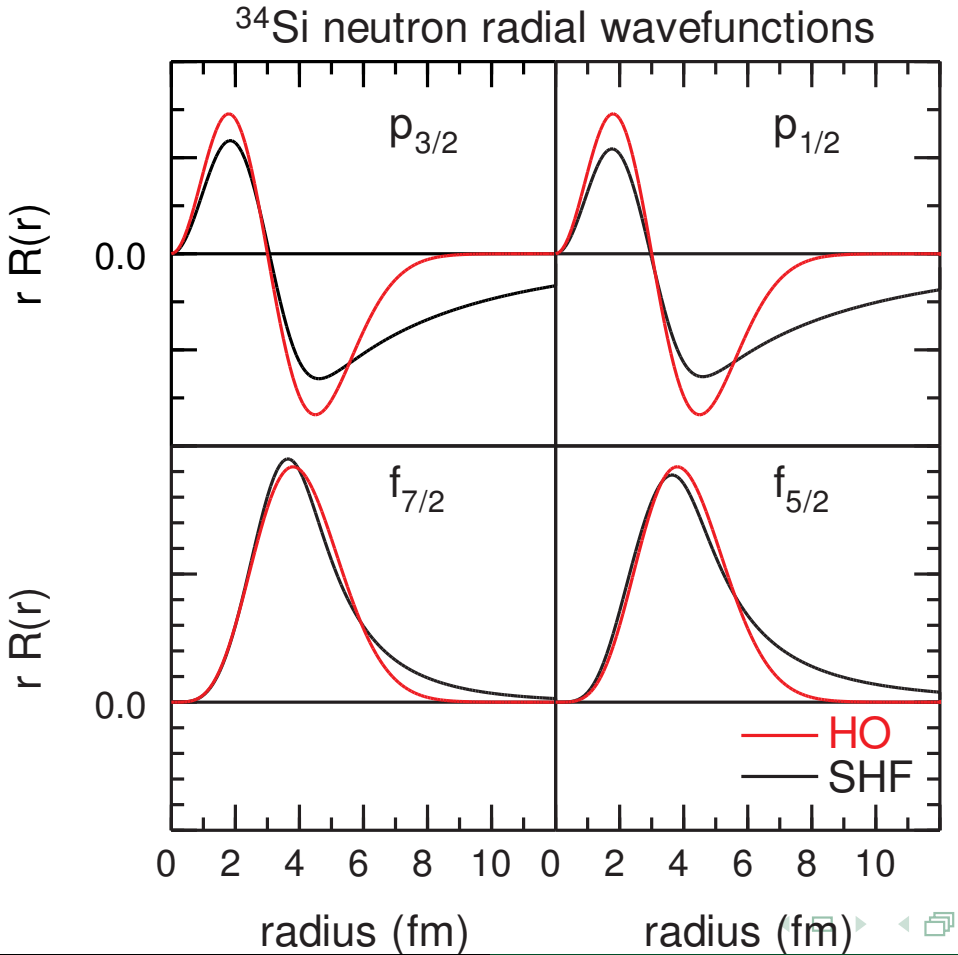
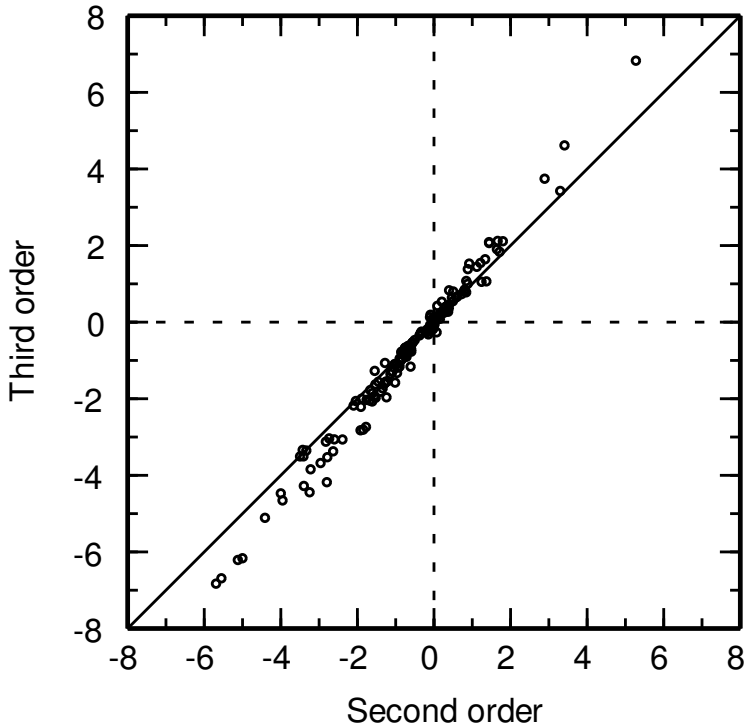


Convergence

- Many-body perturbation theory derived up to third order

TBME in *sd* shell including $6\hbar\omega$ excitations in SHF basis



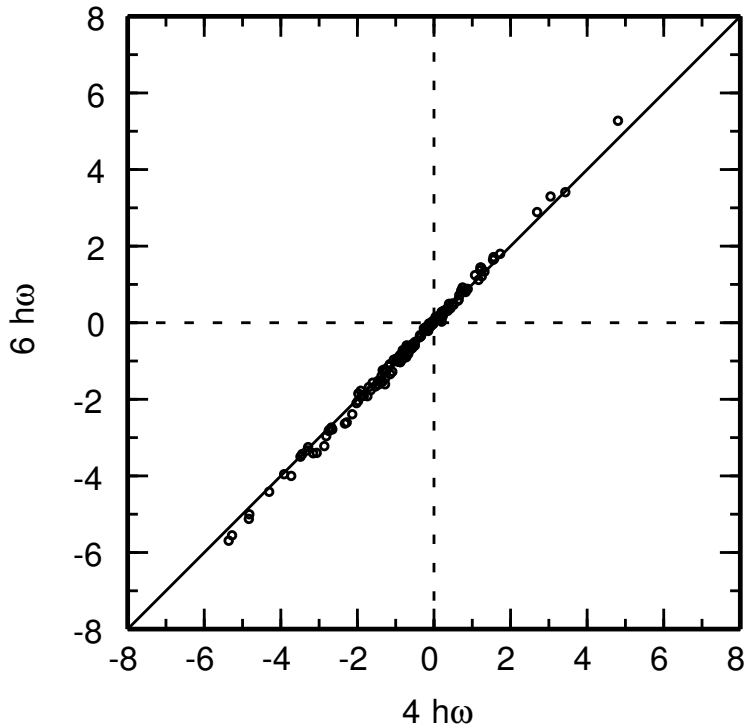
- Results with HO basis do not converge at third order[a]
- Better convergence expected with realistic basis, but not achieved at third order

[a] M. Hjorth-Jensen et al., Phys. Lett. B **248**, 243 (1990)

Convergence

- Computational limit (typical laptop/desktop): $10\hbar\omega$ in *sd* shell

TBME in *sd* shell renormalized to second order in SHF basis



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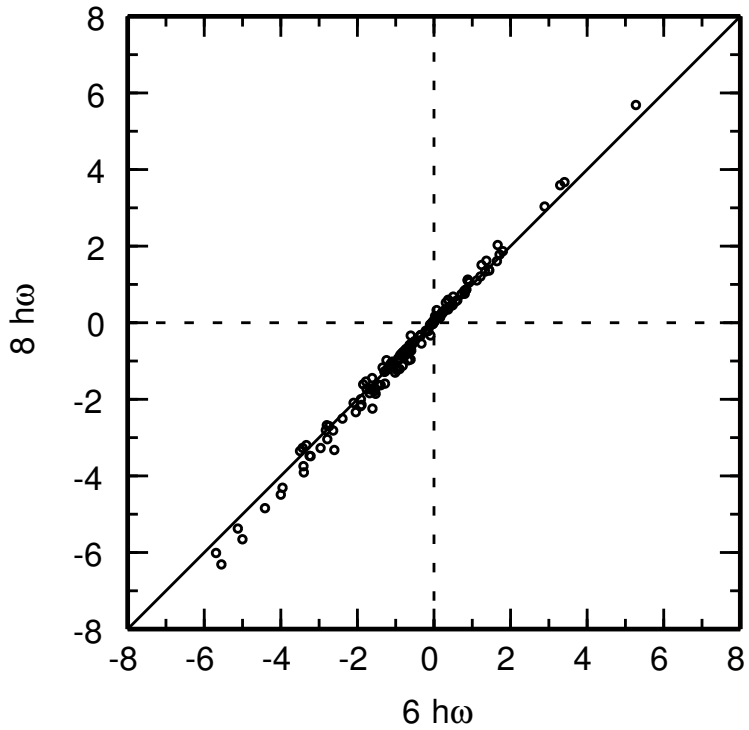

Convergence

- Lack of convergence as a function of excitations and order of perturbation theory
- More attractive interaction for higher excitations and order of perturbation theory
- Must be aware of possible dependence
  - Few percent from $4\hbar\omega$ to $6\hbar\omega$ excitations
  - $\sim 20\%$ for third order in *sd* shell example
- Evaluate error bars by various renormalization procedures?
- Less dependence for low-energy states in even-even nuclei
  - Statement not proven in these lectures
  - Effect on pairing matrix elements ($J = 0$) reduced relative to effect of basis
- Be consistent and honest in procedure
  - NUSHELLX 'ham' executable uses second order and 6 $\hbar\omega$ by default
  - Best to evaluate dependence if possible
  - At least, state explicitly parameters used
  - Realize calculations are dependent on RG+MBPT scheme

Divergences

- Small or null energy denominators result in infinite matrix elements in MBPT
- Very common (almost automatic) with any basis
- Primary way to avoid
  - Introduce constant valence energy for all model space orbits
  - Provide starting energy (typically twice the valence energy)
  - In energy denominators of two-body diagrams
    - Use starting energy $\pm\delta\epsilon$ in place of valence orbit energy
- In model spaces comprised of orbits from multiple oscillator shells
  - Intruder states enter MBPT renormalization
  - Requires calculation of Q-box to higher order to resolve divergences
  - In practice: artificially place all model space orbits in same oscillator shell
  - Current area of research in nuclear structure theory
- Divergences
  - More common with third order of MBPT
  - More common with realistic SHF basis
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Implementation

- Simplest procedure to create interactions
  1. In NUSHELLX, run executable 'ham'
  2. Select model space in proton-neutron formalism (i.e., *sdpn* in sps folder, not *sd*)
  3. Select target nucleus with closed subshell single particle structure
- Remaining parameters have default values printed out in *.inf file
  - Modify as desired
  - Copy *.inf file to ham.ini
  - Rerun ham to include updated parameters
- RG calculation performed by ham only if output file *.reint is nonexistent
- If parameters of RG procedure are modified (e.g. change in cutoff Λ)
  - Must enforce new RG calculation
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  - Copy *.inf file to ham.ini
  - Rerun ham to include updated parameters
- RG calculation performed by ham only if output file *.reint is nonexistent
- If parameters of RG procedure are modified (e.g. change in cutoff Λ)
  - Must enforce new RG calculation
  - Create new directory and copy ham.ini to the new directory
- More advanced options can be modified by hand
- See comment lines in bhf.ini and renorm.ini