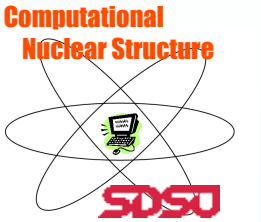
Multidisciplinary Workshop on RPA
UPMC Paris, 26-29 Jan 2010



How *APPROXIMATE* is THE RANDOM PHASE *APPROXIMATION*?

Comparing RPA against full configuration-interaction calculations

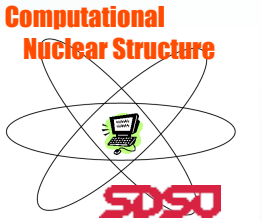
Calvin W. Johnson San Diego State University

Ionel Stetcu Louisiana State University & University of Washington

I. Stetcu and C. W. Johnson, Phys. Rev. C **66** 034301 (2002)
I. Stetcu and C. W. Johnson, Phys. Rev. C. **67**, 043315 (2003)
I. Stetcu and C. W. Johnson, Phys Rev. C **69**, 024311 (2004)
C. W. Johnson and I. Stetcu, Phys. Rev. C 80, 024320 (2009)

This work was supported by grants from the Department of Energy

Systematic Investigation of RPA
or
Outline of my talk!



Review of RPA

Overview of previous "benchmarking" of RPA

Configuration-interaction (CI) calculations and our code SHERPA

Two tests:

(1) Correlation energies

(2) Transitions in RPA and pnRPA

"Collapse" of RPA

Conclusions ... and future work

Review of RPA

RPA models excited states as
small oscillations about the mean-field.

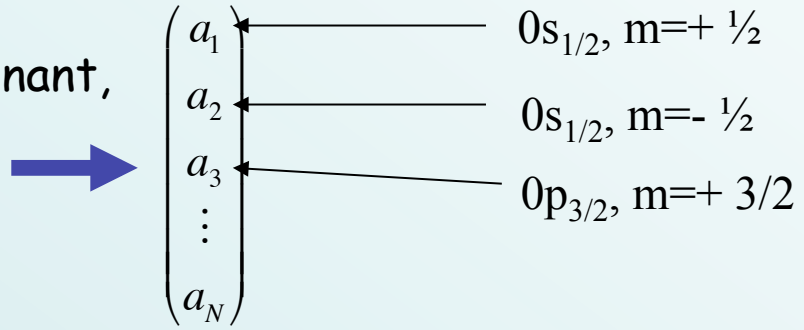
One can put RPA in the same framework
as configuration-interaction (CI) calculations

using an occupation-space (shell-model) basis

The nuclear landscape

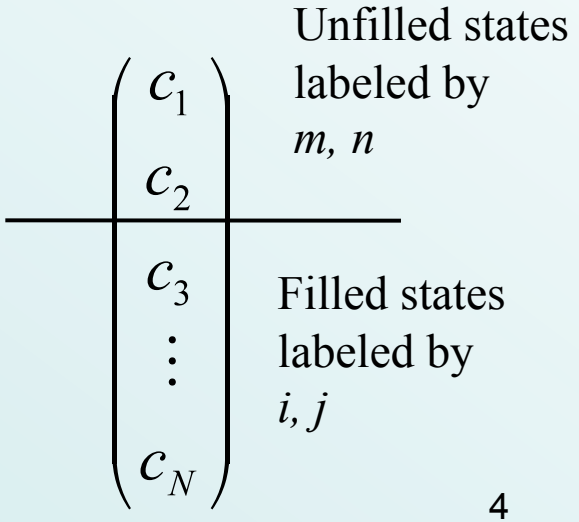
Hartree-Fock based upon variational principle:
minimize $\langle \Psi | \hat{H} | \Psi \rangle$

Here Ψ is a Slater determinant,
a product of single-particle wfns
each of which can be written
as a vector :



A Slater determinant is a product wavefunction,
by filling single-particle states

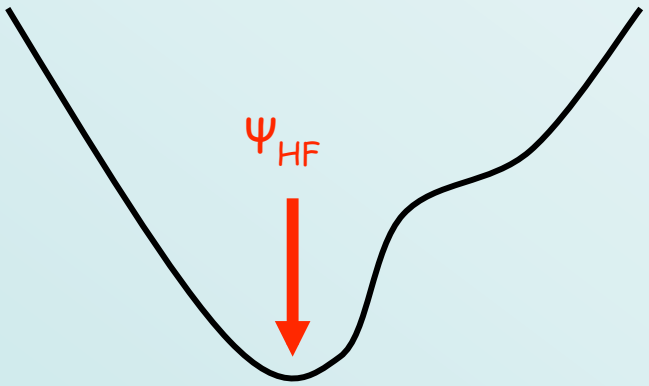
$$|\Psi\rangle = \hat{c}_1^+ \hat{c}_2^+ \hat{c}_3^+ \ldots \hat{c}_n^+ |0\rangle$$



The nuclear landscape

There are many ways to derive the random phase approximation (RPA):
eqns of motion, time-dependent Hartree-Fock, linear response...

I prefer quantization of the energy surface:



$$V(x) \approx V(x_0) + \tfrac{1}{2} V''(x_0)(x - x_0)^2$$

We often approximate a potential by a harmonic oscillator

In occupation space, the second derivatives are given by the **A** and **B** matrices:

$$A_{mi,nj} \cong \left\langle mi^{-1} \middle| H \middle| nj^{-1} \right\rangle$$

$$\left| mi^{-1} \right\rangle = \hat{c}_m^+ \hat{c}_i \left| HF \right\rangle$$

$$B_{mi,nj} \cong \left\langle mi^{-1} nj^{-1} \middle| H \middle| HF \right\rangle$$

The nuclear landscape

For details, see the excellent monograph *The Nuclear Many-Body Problem* **by P. Ring and P. Schuck**

brought into diagonal form using a Bogoliubov (quasiboson) transformation

$$E(0) - \tfrac{1}{2} Tr\mathbf{A} + \sum_{\lambda} \hbar\Omega_{\lambda} \left(\hat{\beta}^{+}_{\lambda} \hat{\beta}_{\lambda} + \tfrac{1}{2} \right)$$

$$\hat{\beta}_{\lambda} = \sum_{mi} X_{mi,\lambda} \hat{b}_{mi} - Y_{mi,\lambda} \hat{b}^{+}_{mi}$$

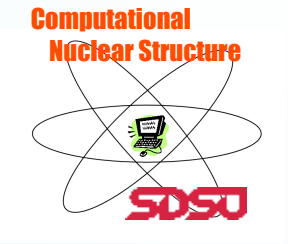
and

$$\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ -\mathbf{B}^{*} & -\mathbf{A}^{*} \end{pmatrix} \begin{pmatrix} \vec{X}_{\lambda} \\ \vec{Y}_{\lambda} \end{pmatrix} = \hbar\Omega_{\lambda} \begin{pmatrix} \vec{X}_{\lambda} \\ \vec{Y}_{\lambda} \end{pmatrix}$$

The RPA matrix equation

There is a correction to the Hartree-Fock energy due to "zero-point motion" or, correlations among the nucleons:

$$E_{RPA} = E(0) - \tfrac{1}{2} Tr\mathbf{A} + \sum_{\lambda} \hbar\Omega_{\lambda} \left(\tfrac{1}{2} \right)$$



Historical validation of RPA

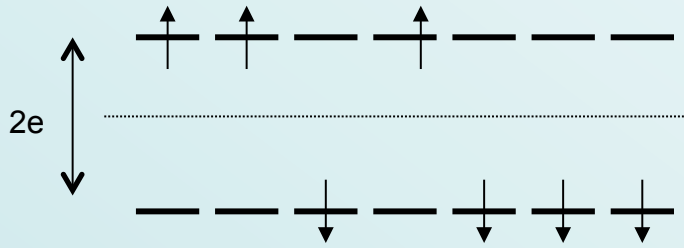
Benchmarking RPA

Despite its widespread use, RPA has generally been only tested against toy models (in nuclear physics)

A typical exampe are Lipkin-type models:

Parikh & Rowe, Phys Rev **175** (1968) 1293
Hagino & Bertsch, PRC C **61** (2000) 024307

acts like parity conservation



The 2-body interaction promotes or demotes 2 particles at a time

N particles, each either up or down... simple quasispin Hamiltonian

Your basic Lipkin model has only 2 independent parameters: N, the number of particles and ratio of 2-body to single-particle spitting, V/ε

Benchmarking RPA

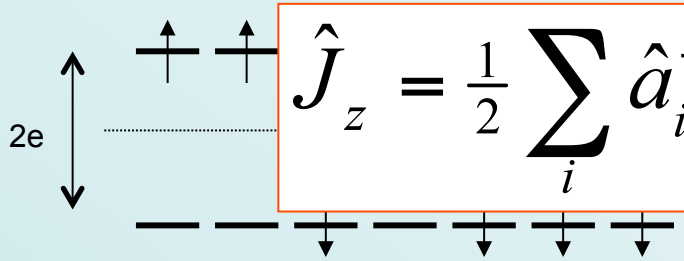
Despite its widespread use, RPA has generally been only tested against toy models

A typical exampe are Lipkin-type models:

$$\hat{H}_{LMG} = \varepsilon \hat{J}_z - V\left(\hat{J}_+^2 + \hat{J}_-^2\right)$$

175 (1968) 1293
61 (2000) 024307

acts like parity conservation



$$\hat{J}_z = \frac{1}{2}\sum_i \hat{a}_{i\uparrow}^+ \hat{a}_{i\uparrow} - \hat{a}_{i\downarrow}^+ \hat{a}_{i\downarrow}$$

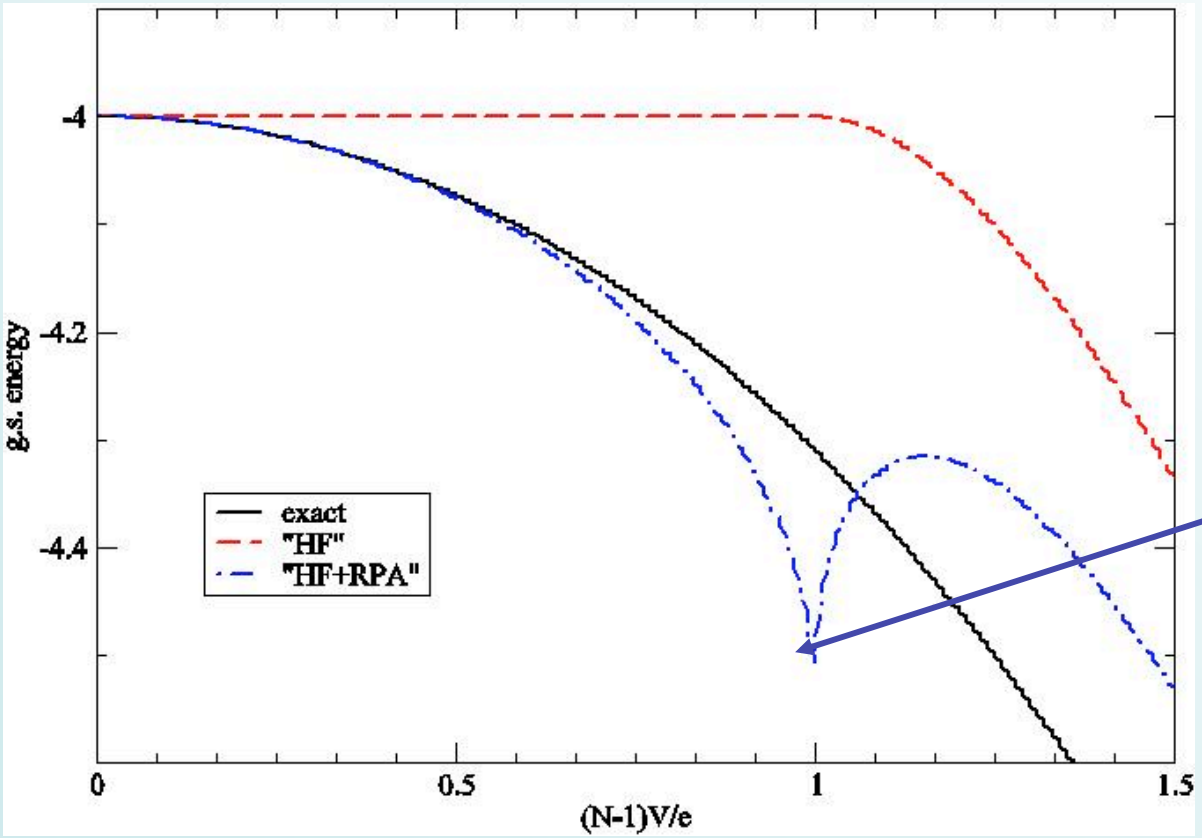
raction promotes or
cles at a time

N particles, each up or down... simple quasispin Hamiltonian

$$\hat{J}_+ = \sum_i \hat{a}_{i\uparrow}^+ \hat{a}_{i\downarrow}$$

Your basic Lipkin model has
independent parameters:
number of particles and
f 2-body to single-particle
g, V/ε

Benchmarking RPA



I'll return to this point later...

Benchmarking RPA

Other tests of RPA...

two-level pairing — Hagino & Bertsch, Nucl. Phys. **A679** (2000) 163

schematic interaction in small SM space — Ullah & Rowe, Phys. Rev. **188** (1969) 1640.

+ handful of others...

The Shell-Model Basis and configuration-interaction calculations

and a flexible RPA code in the shell model

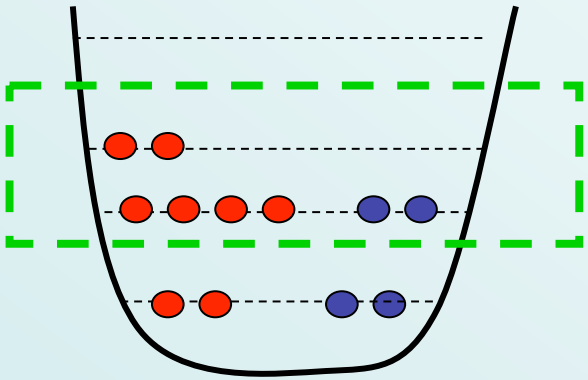
Diagonalization of a Hamiltonian in a shell-model basis
(a.k.a. configuration-interaction or CI)
yields **"exact"** (for that space) and **nontrivial** numerical results

Let's compare RPA against these numerical CI results

How a CI code works

Nuclear CI codes, such as OXBASH, ANTOINE,
or REDSTICK/BIGSTICK, (also called 'shell-model codes'
in the nuclear structure community) writes the Schrodinger eqn as a
matrix eigenvalue equations

One defines a single-particle basis ...



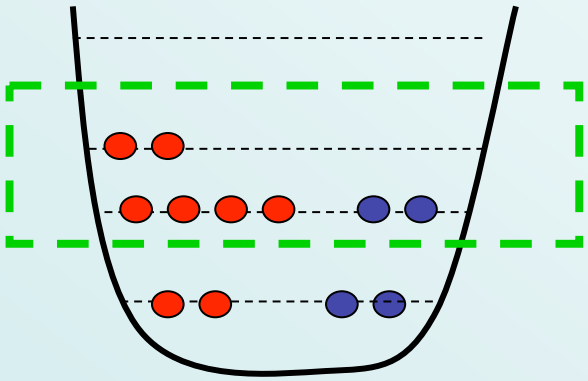
...selects a valence space...

....puts in valence nucleons...

...possibly assuming an inert core.

How a CI code works

The basis is the set of Slater determinants
of all (sort of) possible configurations
in the valence space



The interaction Hamiltonian
is specified as
single-particle energies
plus
two-body matrix elements
(the "residual interaction")

These are read in to the
program as a list of numbers

How a CI code works

We solve $\mathbf{H}\left|\Psi\right\rangle = E\left|\Psi\right\rangle$

in a large but finite-dimension space (eigenvalue problem)

$\left|\Psi\right\rangle = \sum c_\alpha \left|\alpha\right\rangle$ ← basis states are *Slater determinants*

$\left|\alpha\right\rangle = \prod \hat{a}_i^+ \left|0\right\rangle$ ← single particle states taken from the valence space

i = $(0s_{1/2,1/2})_\pi$, etc.

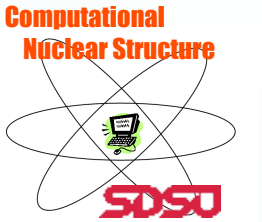
How a CI code works

$$\hat{H} = \sum_i \varepsilon_i \hat{a}_i^+ \hat{a}_i + \tfrac{1}{4} \sum_{ij\,kl} V_{ij\,kl} \hat{a}_i^+ \hat{a}_j^+ \hat{a}_l \hat{a}_j$$

$$V_{ij\,kl} = \int dx dx' \phi_i^*(x) \phi_j^*(x') V(x,x') \left[\phi_k(x) \phi_l(x') - \phi_l(x) \phi_k(x') \right]$$

The V_{ijkl} enter the code as *pre-computed numbers*, so there is *no* limitation on the form of the interaction.

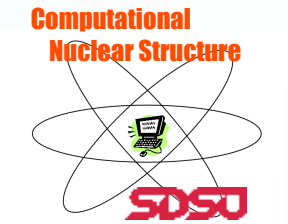
How a CI code works



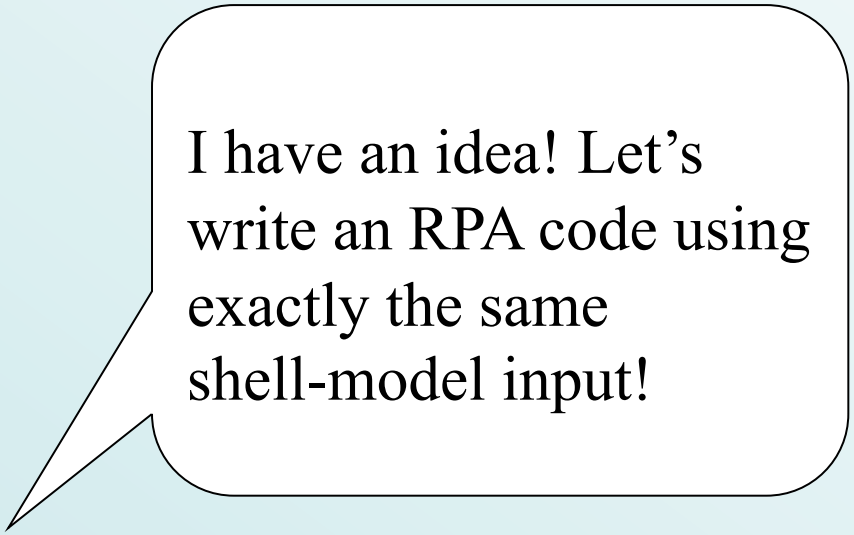
The hard part is actually computing *efficiently*
the many-body matrix elements
from the two-body matrix elements

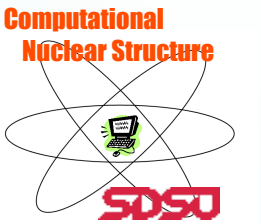
That is, $\langle \alpha | \hat{H} | \beta \rangle$ from the V_{ijkl}

The final result is the low-lying energy spectrum
and the corresponding wavefunctions
(the coefficients in the Slater determinant basis)



Diagonalization of a Hamiltonian in a shell-model basis
yields **"exact"** (for that space) and **nontrivial** numerical results





SHEll-model RPA code (Stetcu PhD LSU 2003)

Shell-model input compatible with REDSTICK:

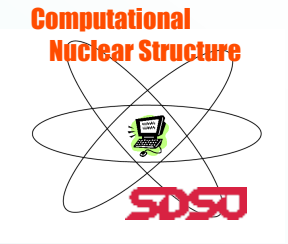
list of single-particle orbits ($0s_{1/2}$, $0p_{3/2}$ etc.)
list of two-body matrix elements $\langle ab; JT|H|cd;JT\rangle$
fair to compare output with REDSTICK results

Fully self-consistent Hartree-Fock:

no restrictions on Slater determinant → arbitrary deformations within model space
(except, wfns purely real)

Standard RPA:

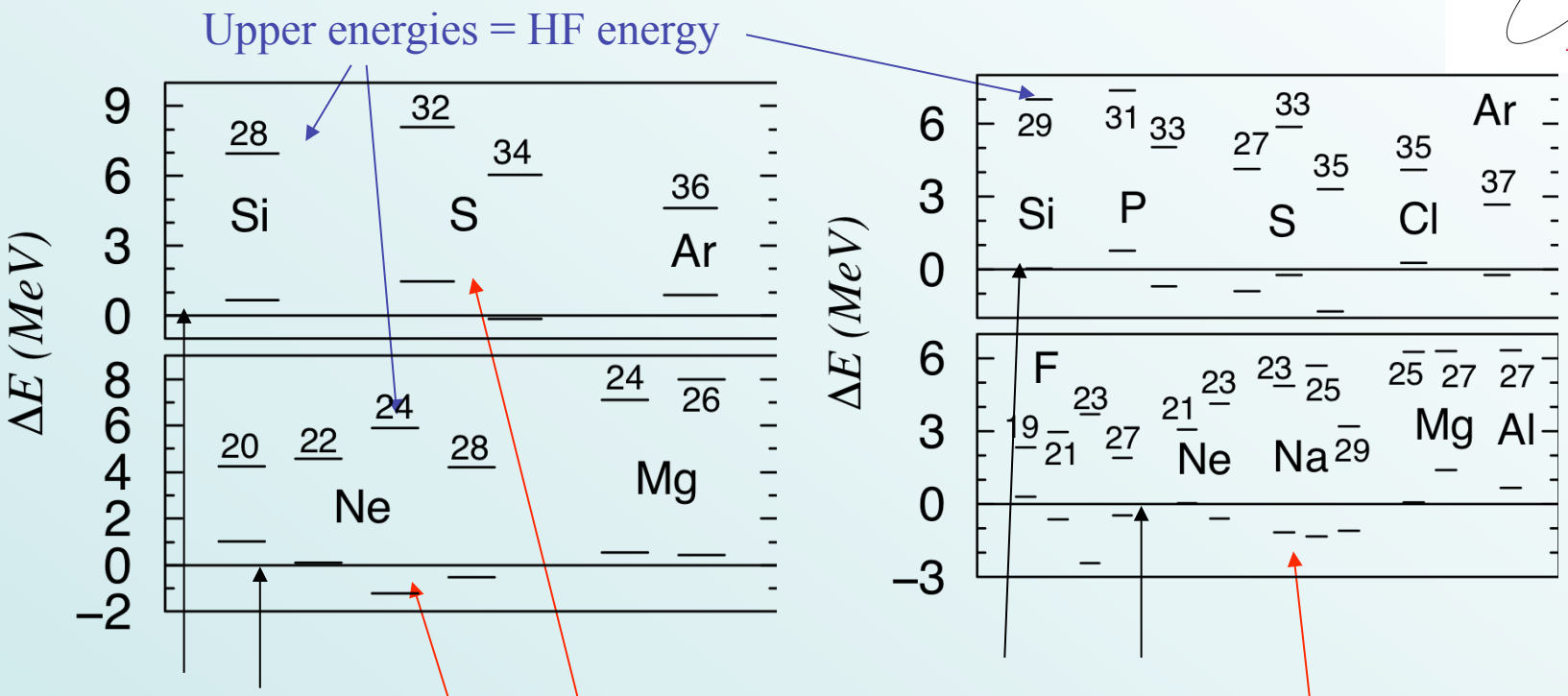
solve matrix RPA equations
see rotation of deformed HF state as zero-frequency modes;
option to do pnRPA



RPA Correlation Energies

(g.s. Binding energies beyond the mean-field)

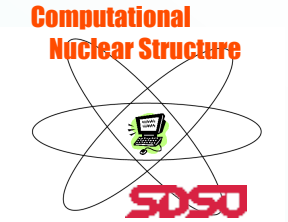
Results: Correlation energies



Poorest results for single-species calculations (oxygen, calcium isotopes)

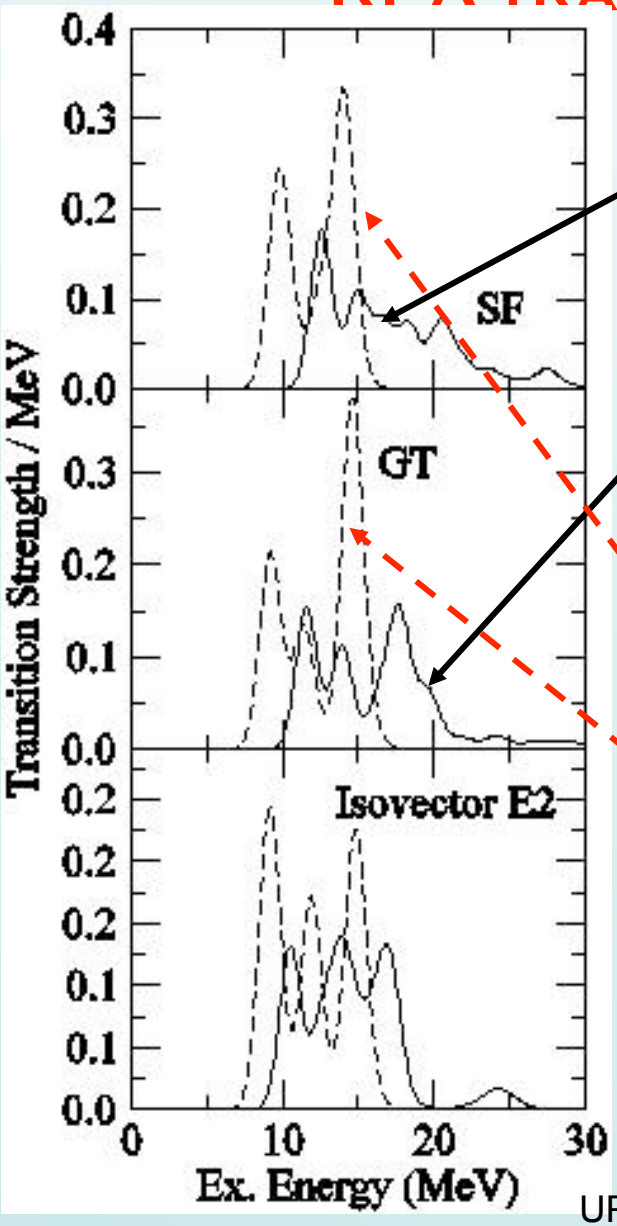
Results: Correlation energies

space	# nuclides	rms err (keV)
sd (p+n)	41	870
sd oxygen	6	1800
pf (p+n)	11	480
pf calcium	7	730



Transitions

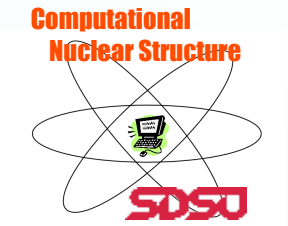
RPA transition strengths



"exact" shell model results

RPA results

Appendix: the standard energy-weighted RPA sum rule is wrong (in the presence of Goldstone modes)



We also looked at Gamow-Teller transitions in pnRPA

here there have been previous detailed comparisons with the shell model, but using spherical pnQRPA

the central question: which is more important,

pairing or deformation?

What is pnRPA?

So far we had separate proton and neutron Slater determinants

$$\left|\Psi\right\rangle = \left|\psi\right\rangle_{\pi}\left|\psi\right\rangle_{\nu}$$

The particle-hole operators conserved charge: $X^{\pi}_{\lambda,mi}\pi^{+}_{m}\pi_{i} - Y^{\pi}_{\lambda,mi}\pi^{+}_{i}\pi_{m}$

pn operators change charge $X^{pn}_{\lambda,mi}\pi^{+}_{m}\nu_{i} - Y^{pn}_{\lambda,mi}\pi^{+}_{i}\nu_{m}$

Other's Previous Work: pn-QRPA

A number of papers compared **spherical** pn-QRPA against "exact" shell –model calculations of Gamow-Teller strengths

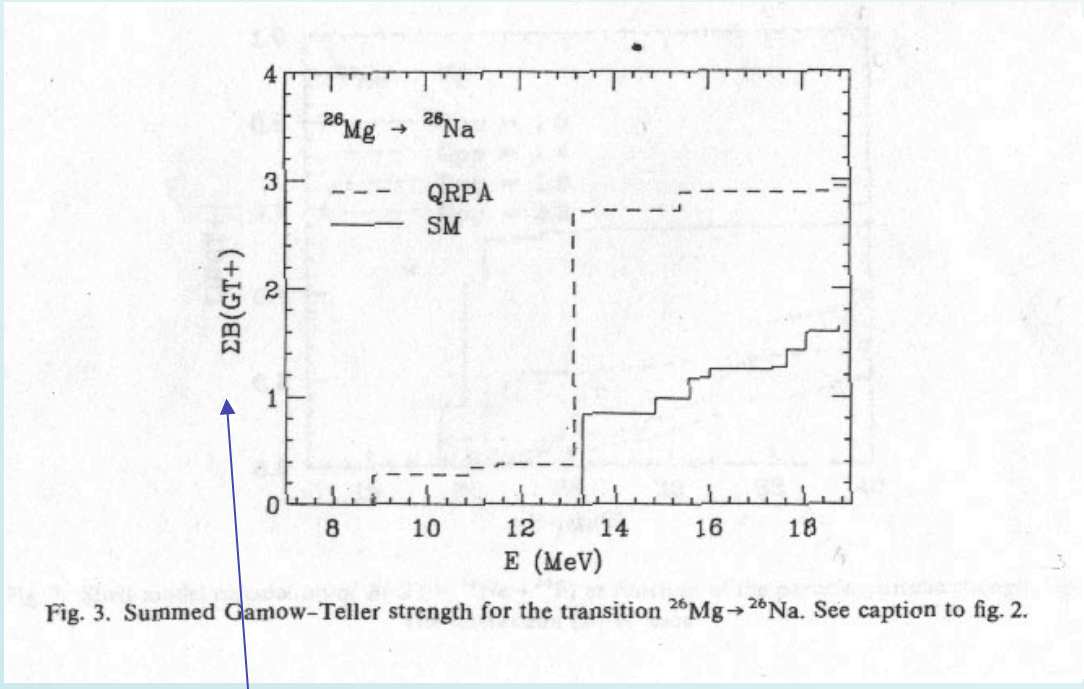


Fig. 3. Summed Gamow–Teller strength for the transition ^{26}Mg→^{26}Na. See caption to fig. 2.

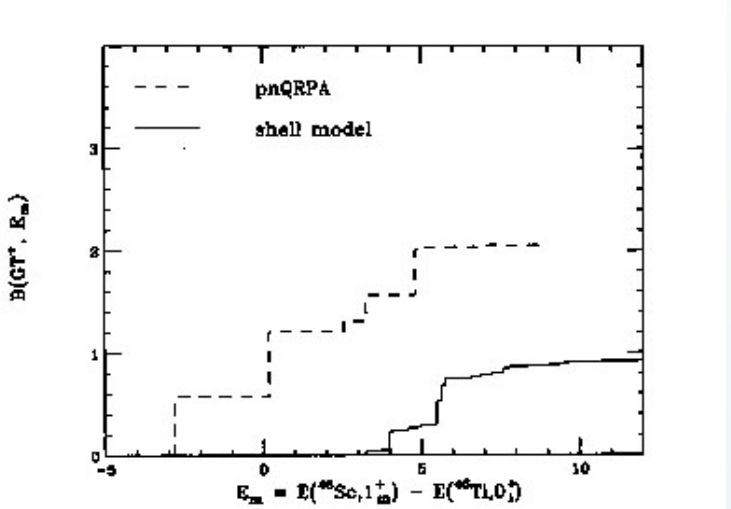


FIG. 1. Running sum of the Gamow-Teller strength $B(GT^+, E_m)$ for ^{46}Ti →^{46}Sc as a function of the ^{46}Sc 1^+ excitation energies relative to the ^{46}Ti ground state.

Laurtizen, Nucl Phys **A489** (1988) 237.

Zhao & Brown, PRC **47** (1993) 2641

Running sum of GT strength

Other's Previous Work: pn-QRPA

Most likely explanation: pn-QRPA fails to sufficiently smear the Fermi surface → insufficient fragmentation of GT strength

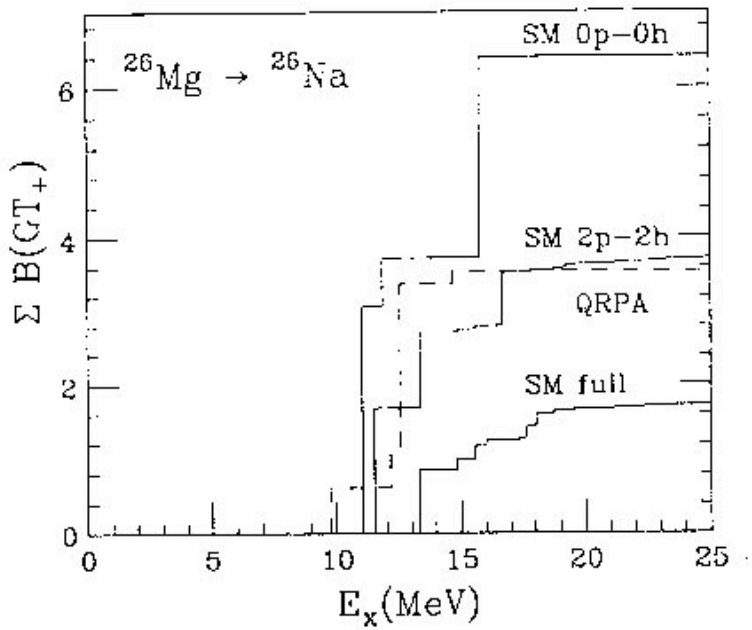


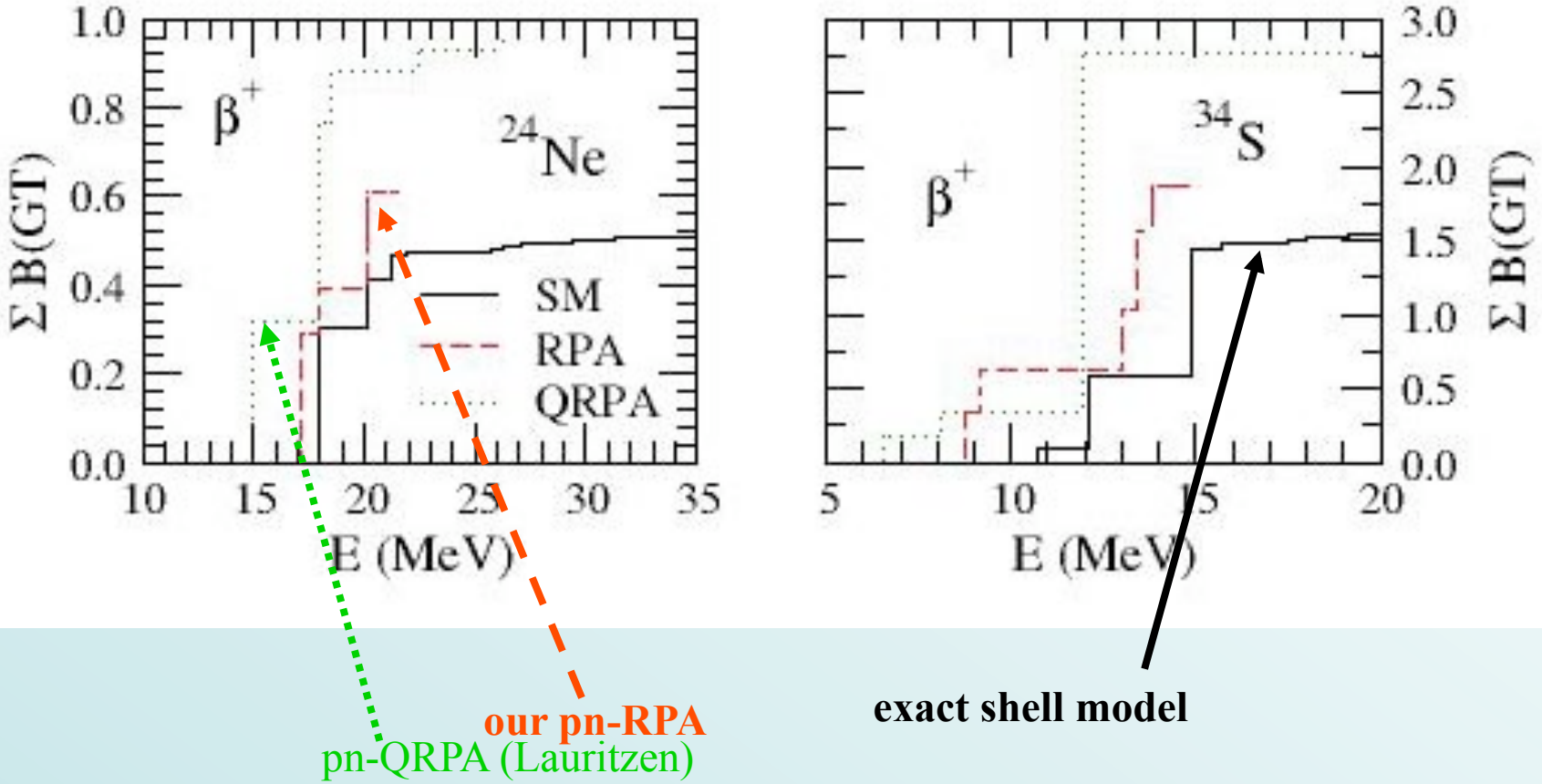
Fig. 1. Running sum of the $B(GT_+)$ values for ^{26}Mg vs. excitation energy. S_+ is the total value at $E_x = 25$ MeV. The labels correspond to the headings in table 1.

QRPA ≈ 2p-2h in spherical SM

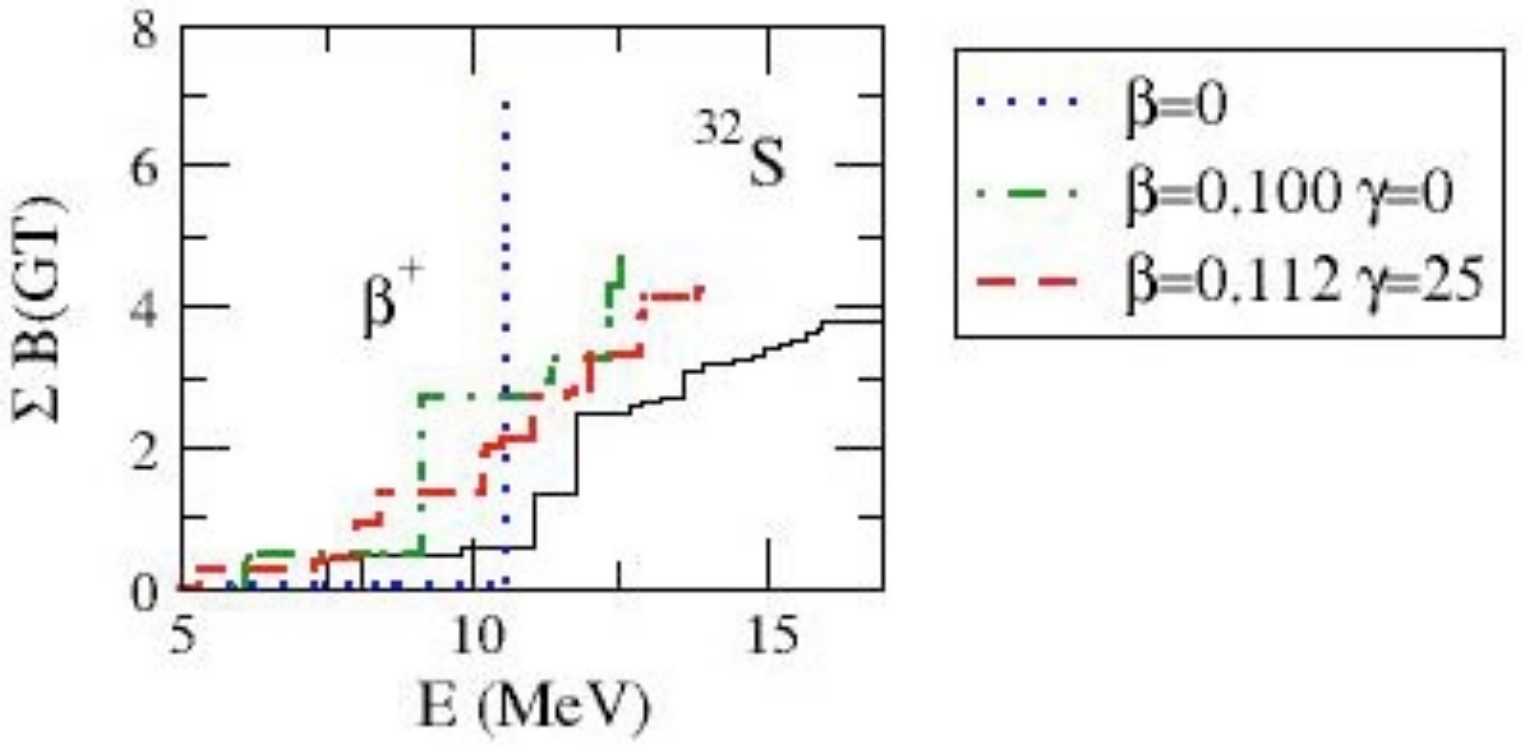
Auerbach, Bertsch, Brown & Zhao, Nucl Phys **A556** (1993) 190

Our Calculations: Deformed pn-RPA

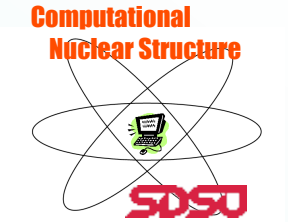
We redid this work, eschewing pairing correlations in favor of unrestricted deformations



Our Calculations: Deformed pn-RPA



Not only deformation, but triaxiality improves the result

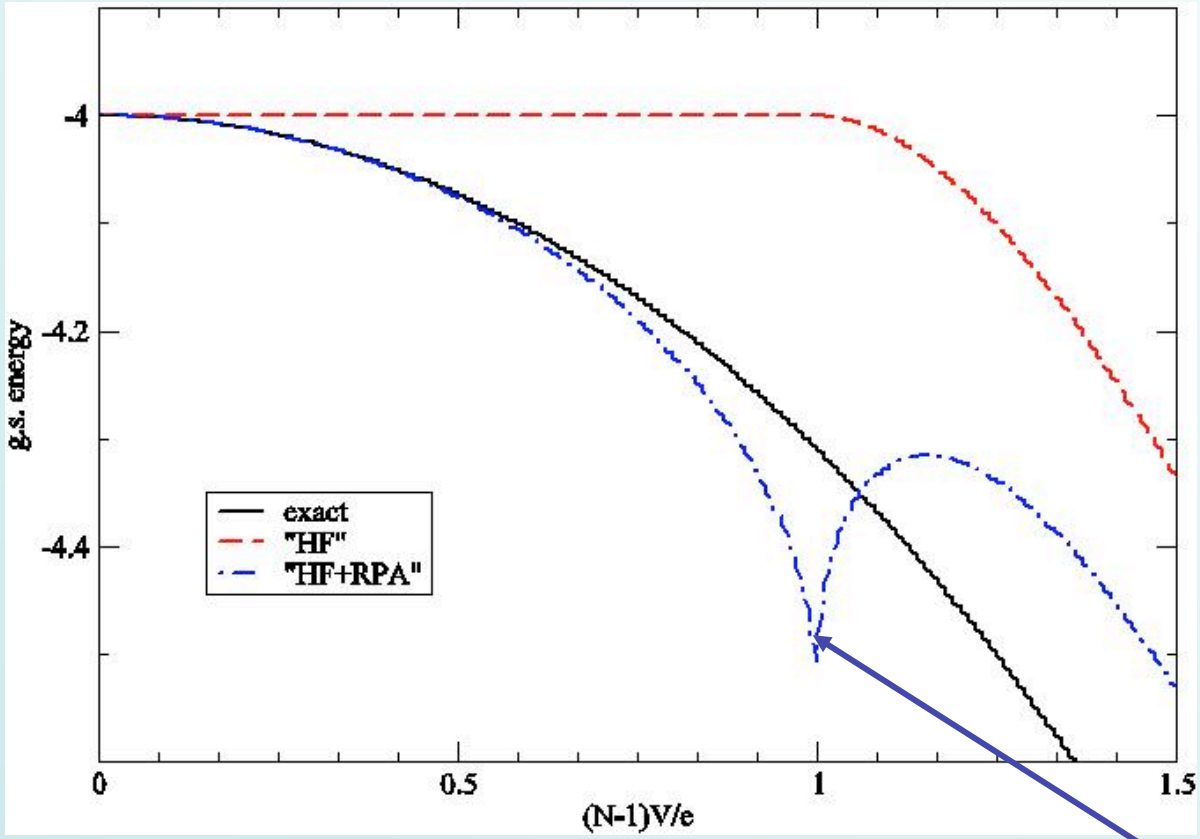


"Collapse" of RPA

at "phase transitions"

"Collapse" at "phase transitions"

Example from the **Lipkin model**....



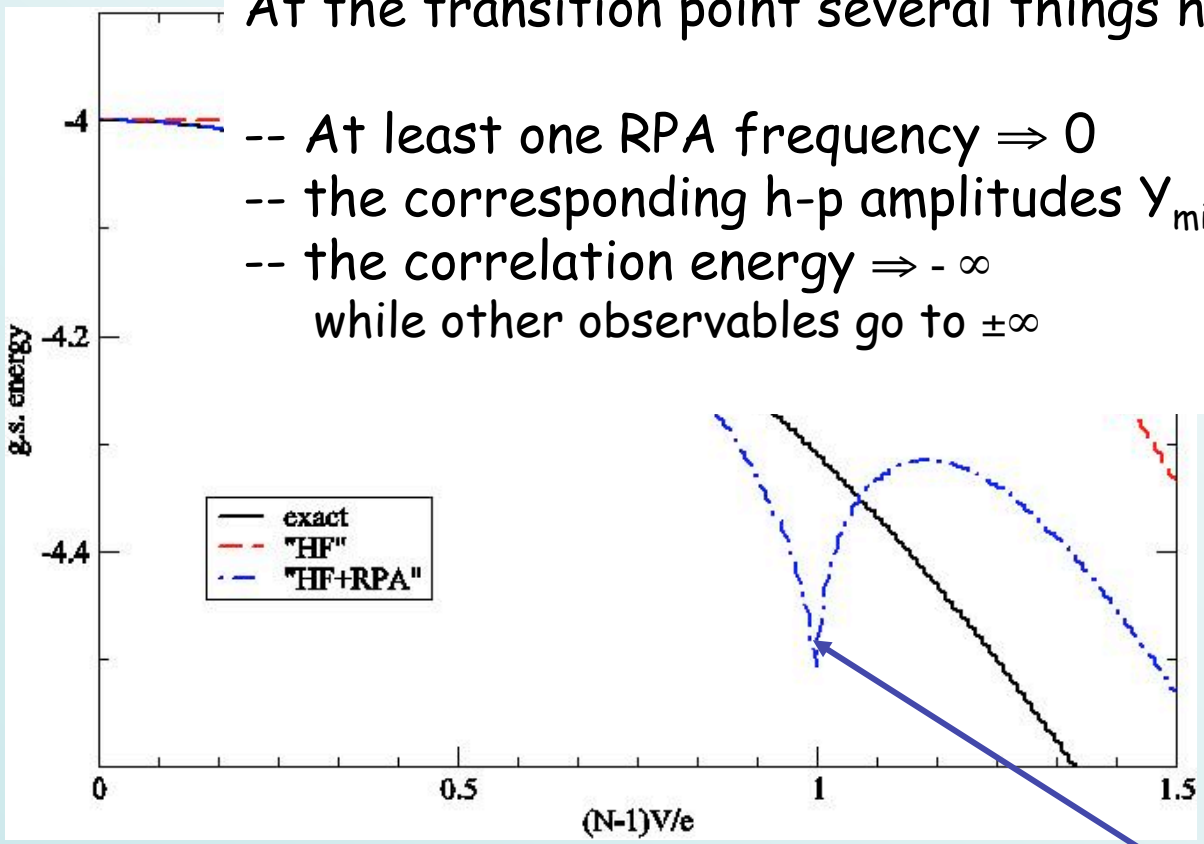
"collapse" of RPA

"Collapse" at "phase transitions"

Example f

At the transition point several things happen:

-- At least one RPA frequency $\Rightarrow$ 0
-- the corresponding h-p amplitudes $Y_{mi} \Rightarrow \infty$
-- the correlation energy $\Rightarrow -\infty$
while other observables go to $\pm\infty$

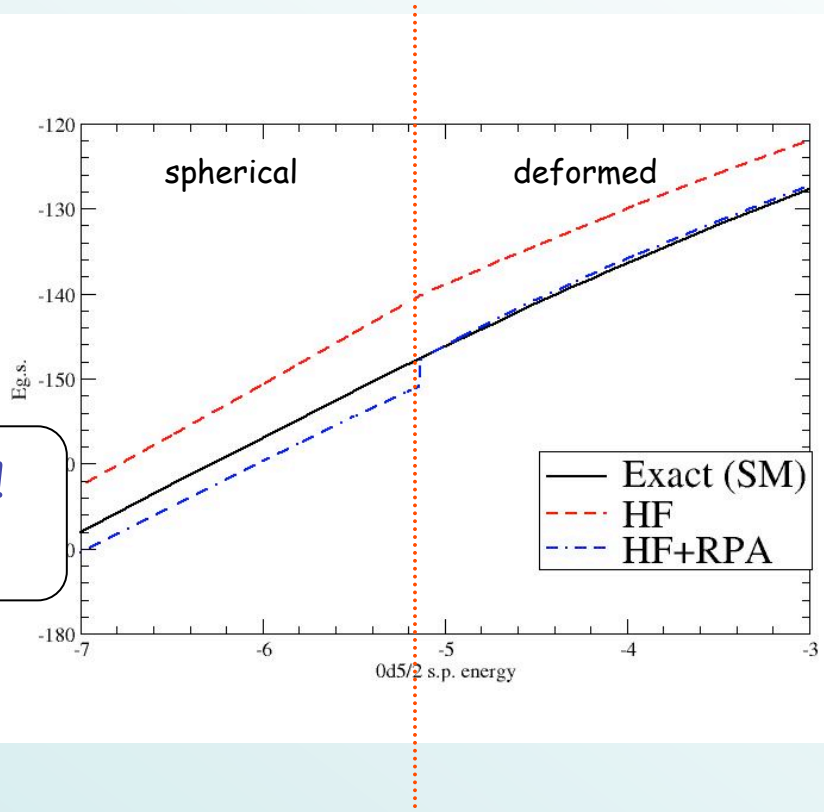


"collapse" of RPA

"Collapse" at "phase transitions"

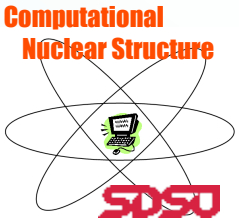
Do we see this with SHERPA?

We induced a shape transition in ^{28}Si (which normally has an oblate HF state) by lowering the $0d_{5/2}$ single-particle energy until it became spherical



No collapse of RPA!
What's going on?

"Collapse" at "phase transitions"



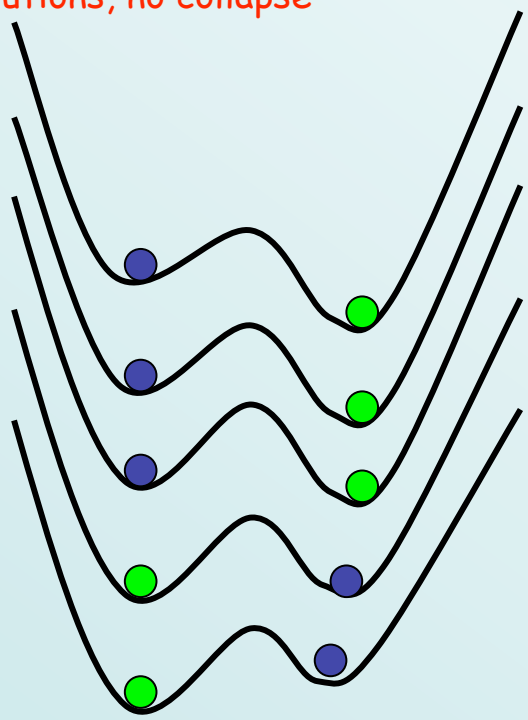
I know what's happening! I wrote about it in D.Thouless, Nucl. Phys. **22**, 78 (1961)

No collapse of RPA!
What's going on?

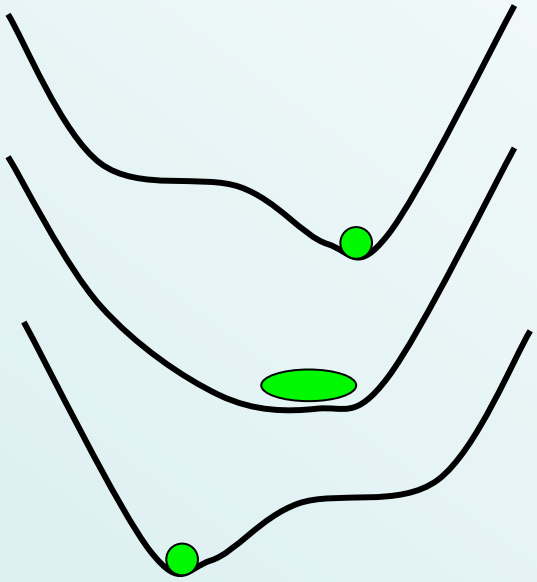
"Collapse" at "phase transitions"

There are *first-order* and *second-order* transitions!

First order: coexistence of stable solutions, no collapse

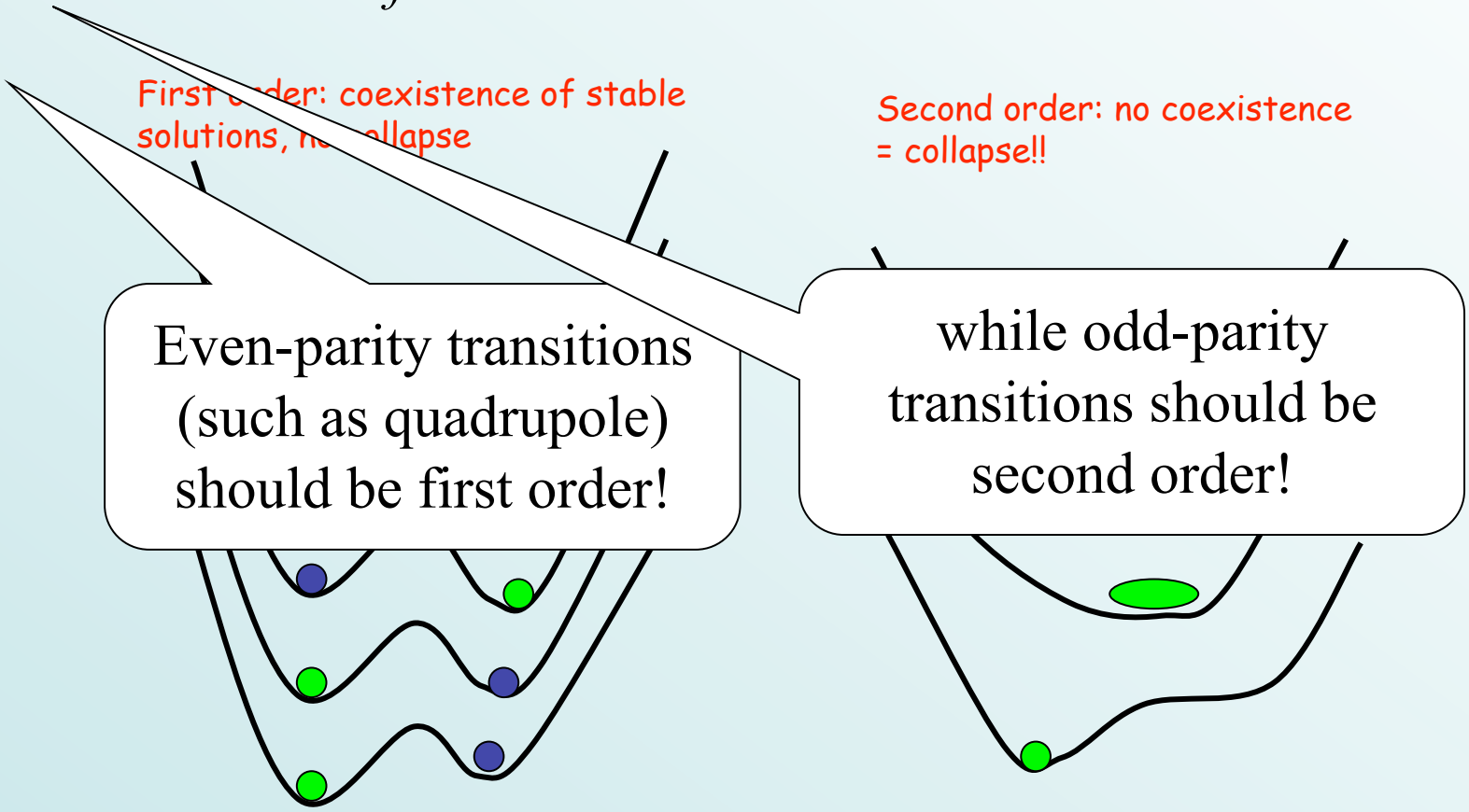


Second order: no coexistence collapse!!



"Collapse" at "phase transitions"

There are *first-order* and *second-order* transitions!

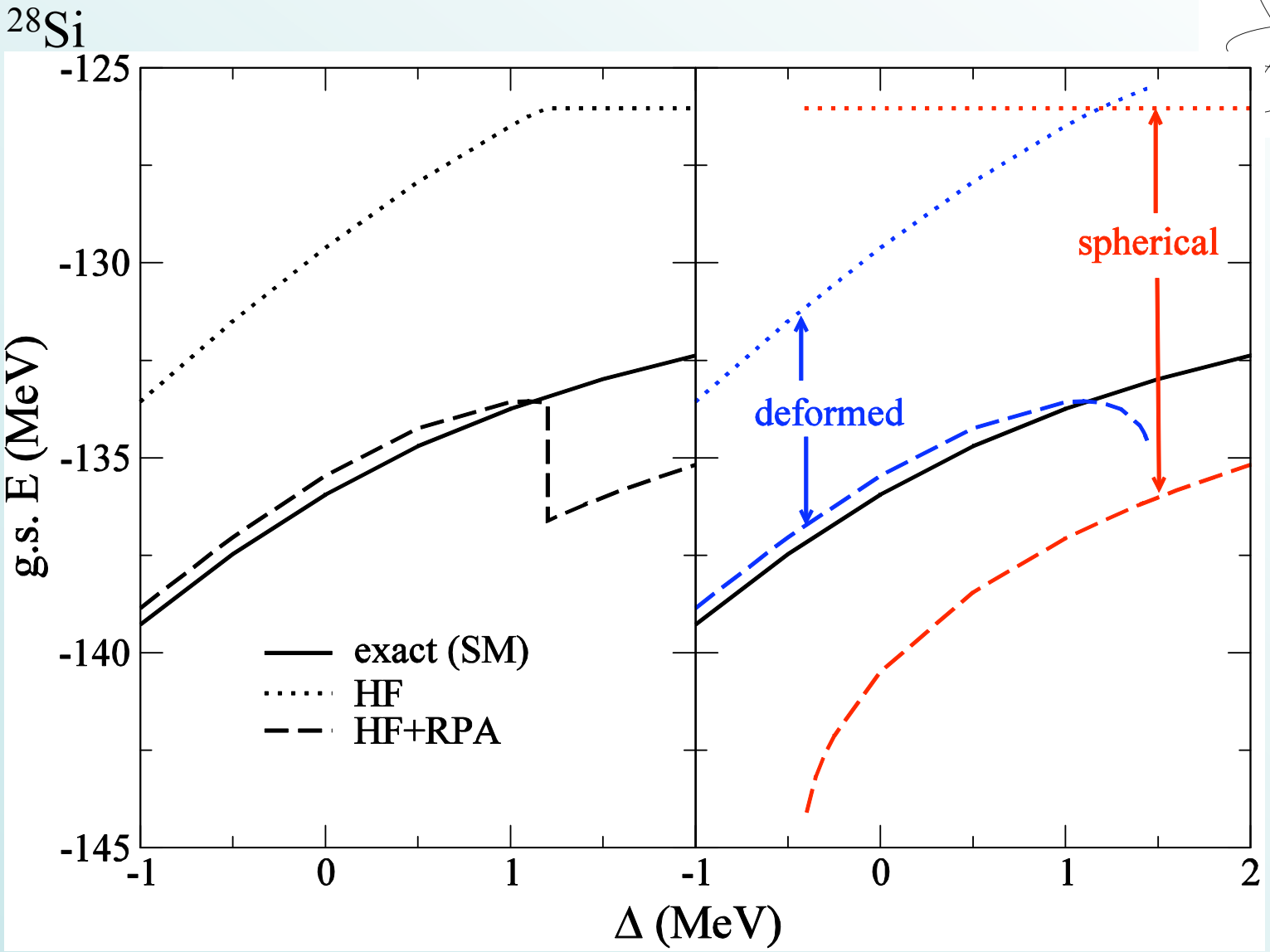


"Collapse" at "phase transitions"

Quadrupole shape transitions are first order

Lipkin model is 2nd order and is more analogous to mixing of parity across major shells

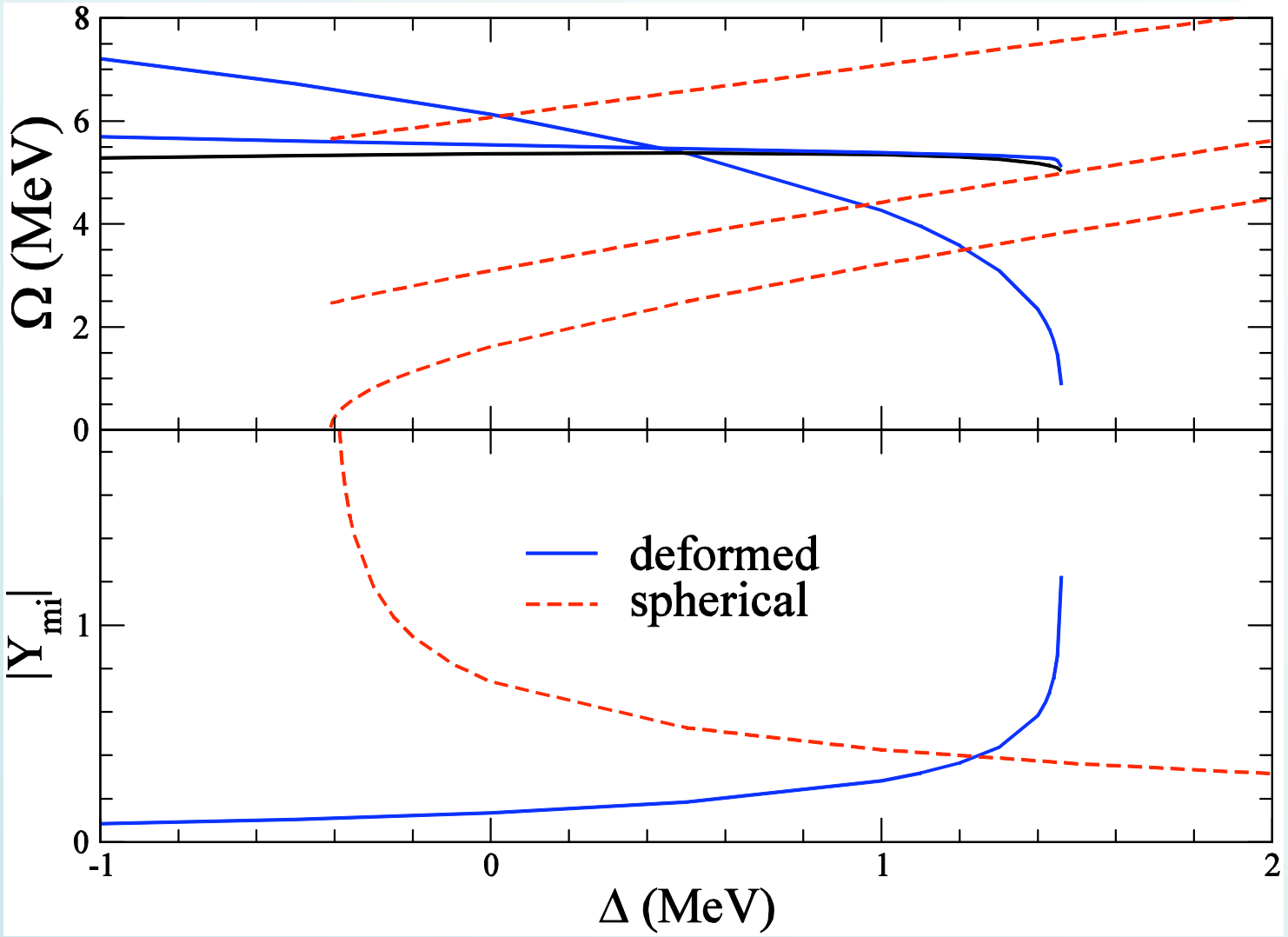
Example: 0p1/2-0d5/2 model space displays true "collapse"


^{28}Si
-125
-130
-135
-140
-145
g.s. E (MeV)
-1
0
1
-1
0
1
2
Δ (MeV)
exact (SM)
HF
HF+RPA
deformed
spherical

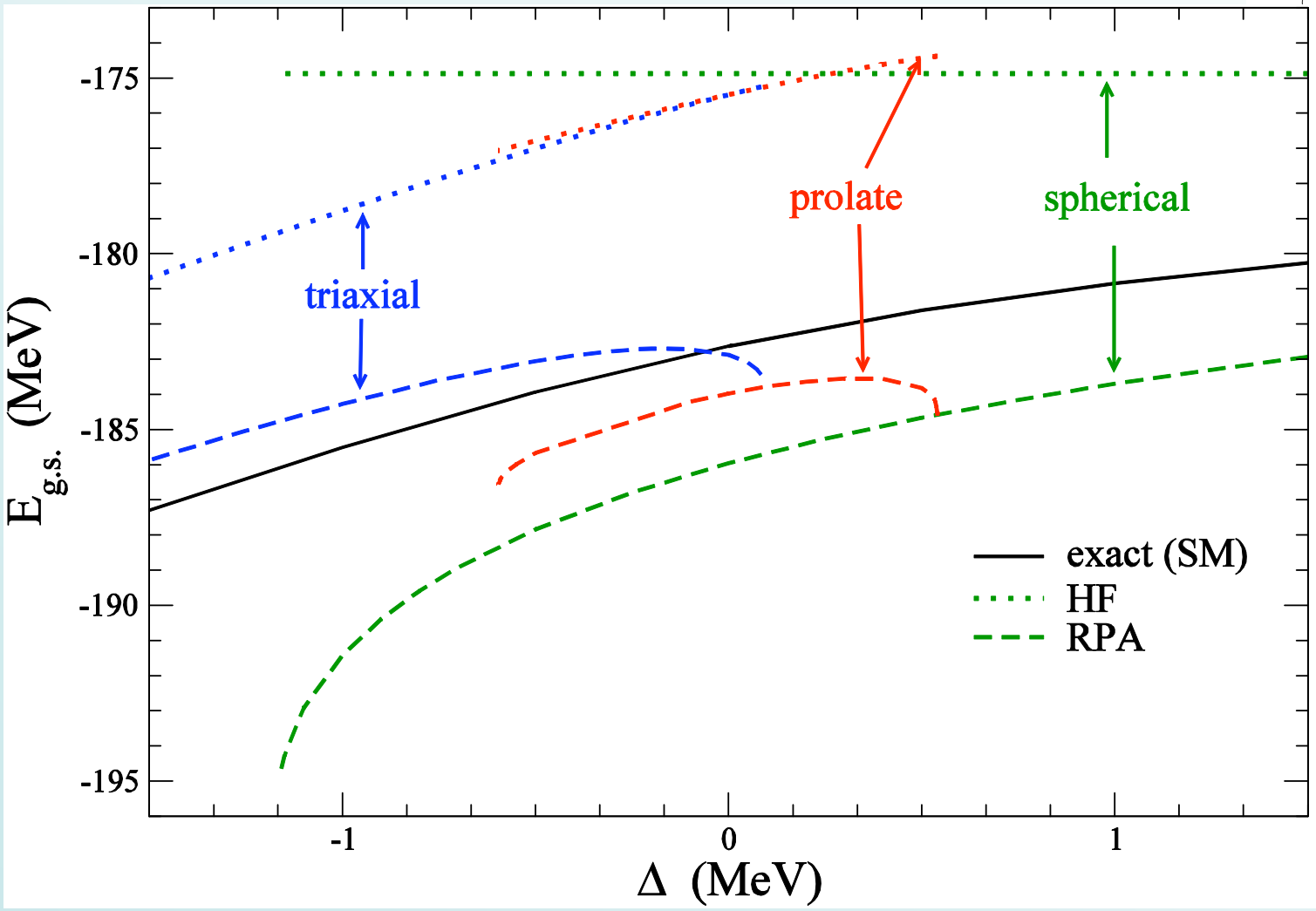
Computational Nuclear Structure

SDSU

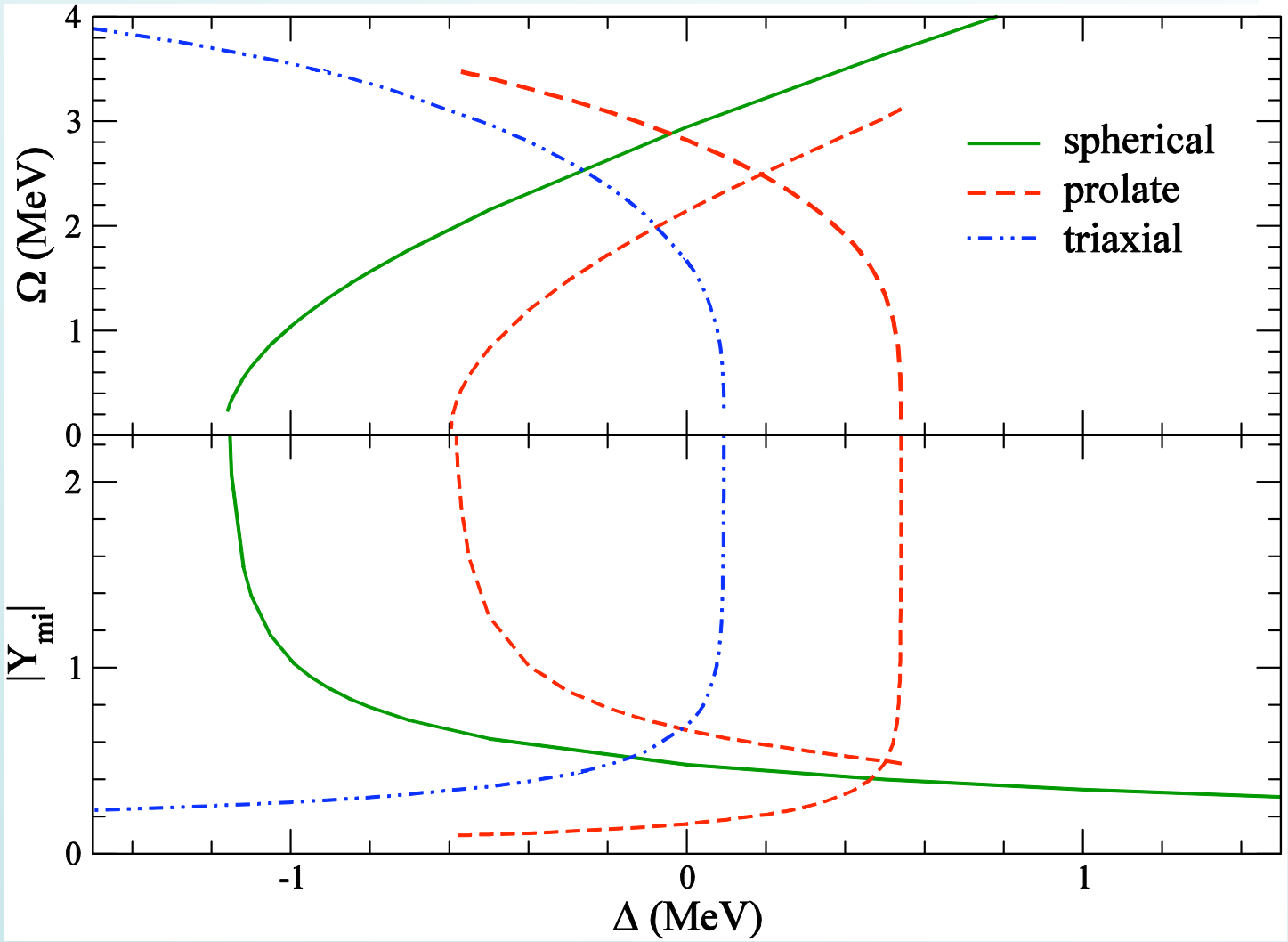
^{28}Si



^{32}S


-175
-180
-185
-190
-195
$E_{g.s.}$ (MeV)
-1
0
1
Δ (MeV)
triaxial
prolate
spherical
exact (SM)
HF
RPA

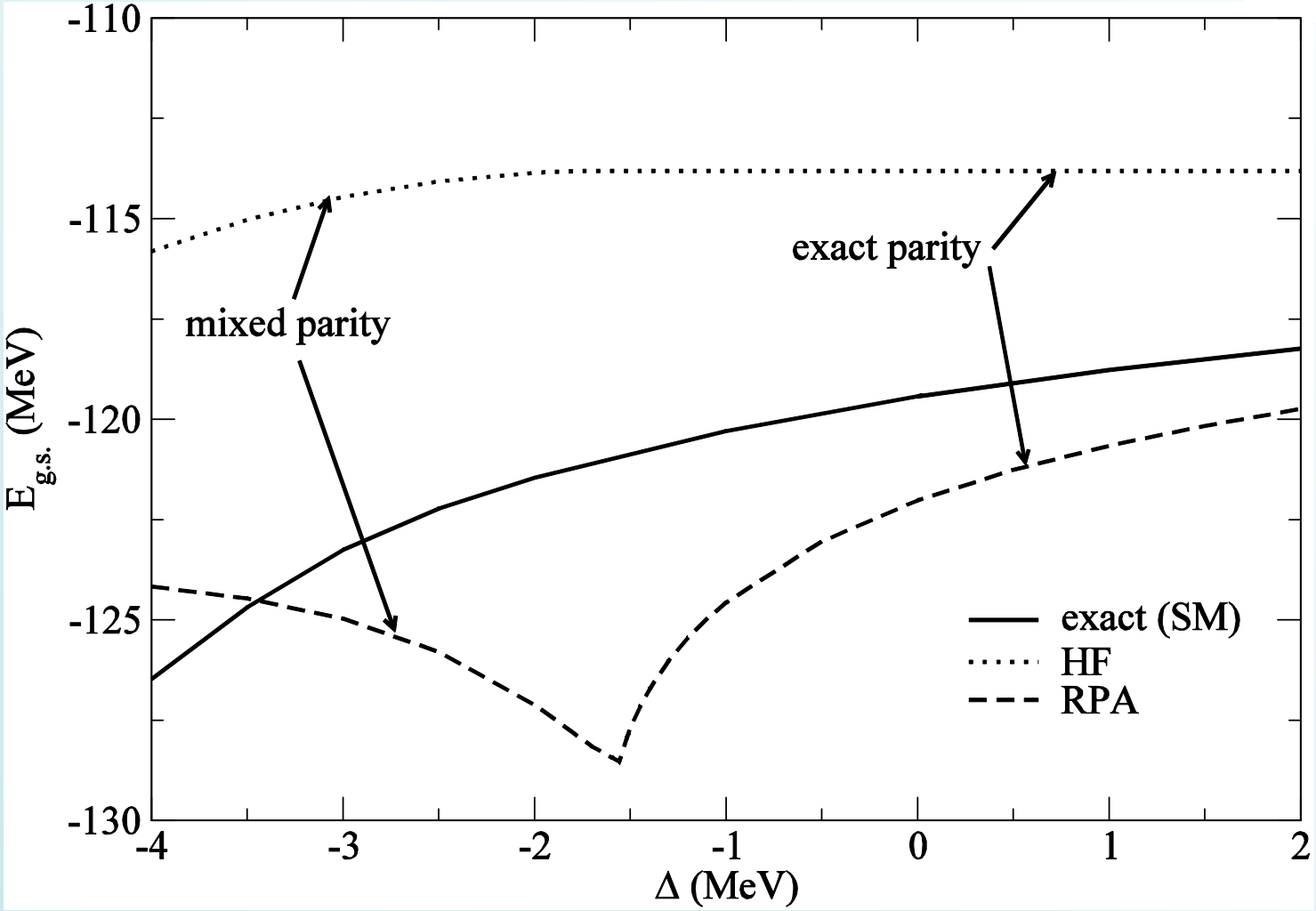
^{32}S



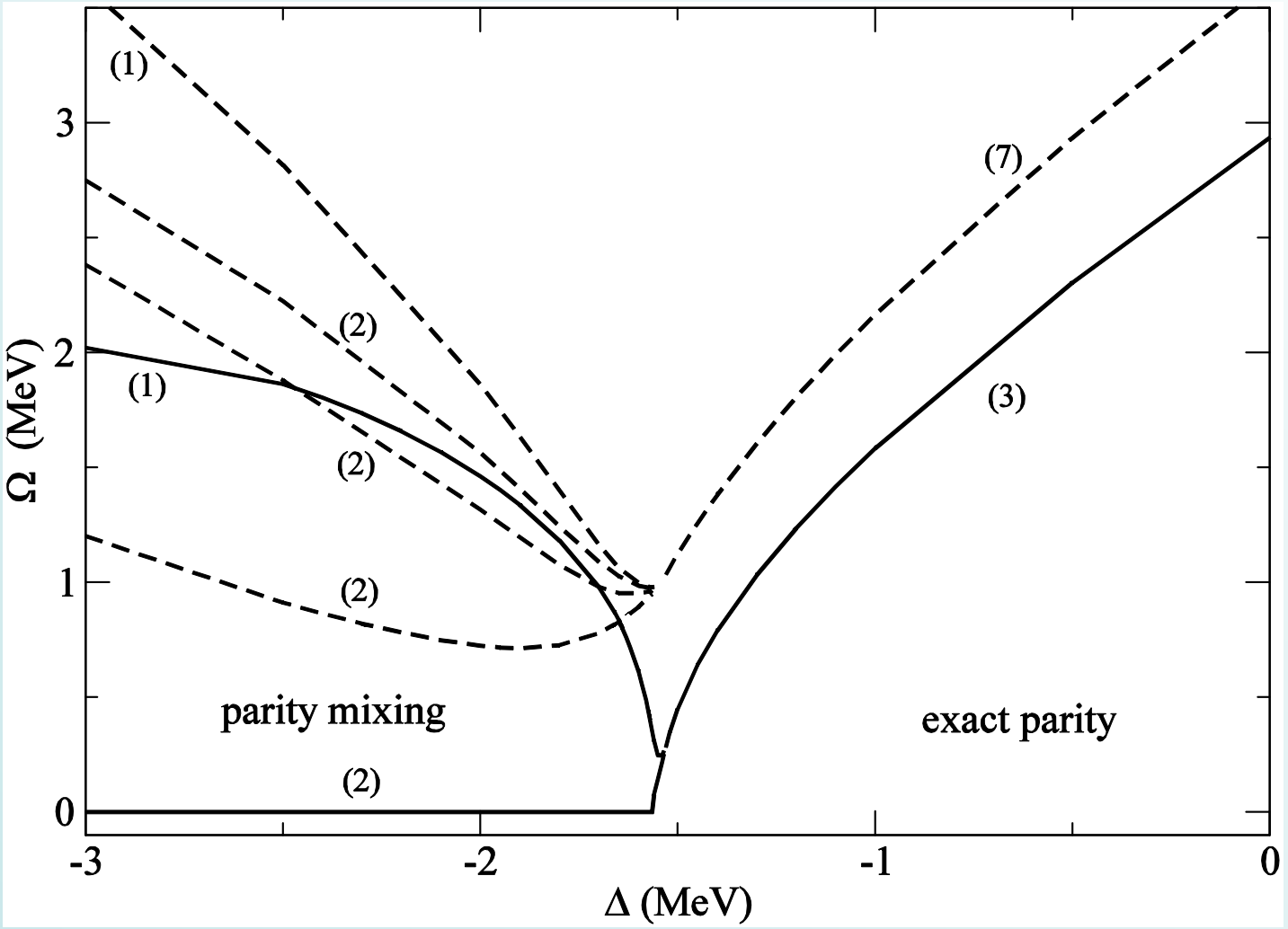
Computational Nuclear Structure

SDSU

^{16}O



^{16}O



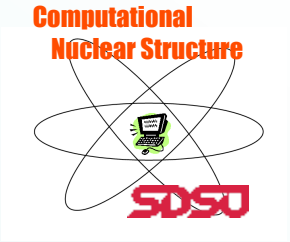
CONCLUSIONS

We have realized RPA in a non-trivial shell model framework

Tests of RPA show it to be a modest approximation to the full many-body diagonalization

We have also investigated "collapse" of RPA

We are extending this work to generator coordinate calculations, HFB+QRPA (especially for neutrinoless double-beta decay), and possibly extensions of RPA, e.g. second RPA, etc.


Computational
Nuclear Structure
SDSU

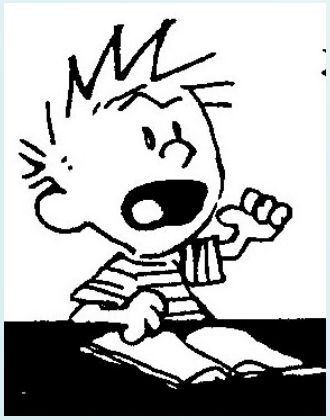
Sum Rules and Rule-Breakers

Let ***F*** be a transition operator; then the *energy-weighted sum rule* states that

$$\frac{1}{2}\left\langle HF\left|\left[\hat{F}\left[\hat{H},\hat{F}\right]\right]HF\right\rangle = \sum_{\lambda}\hbar\Omega_{\lambda}\left|\left\langle 0\left|\hat{F}\right|\lambda\right\rangle_{RPA}\right|^{2}$$

This theorem is proven in many text-books...but is wrong!

Sum Rules and Rule-Breakers



The "proof" assumes no Goldstone (zero-energy) modes

if one rederives it using those Goldstone modes one gets a correction

$$\frac{1}{2}\left\langle HF\left|\left[\hat{F}\left[\hat{H},\hat{F}\right]\right]HF\right\rangle = \sum_{\lambda}\hbar\Omega_{\lambda}\left|\left\langle 0\left|\hat{F}\right|\lambda\right\rangle_{RPA}\right|^{2}$$

$$+\sum_{\nu,\Omega=0}\frac{1}{2M_{\nu}}\left|\left[F,\hat{P}_{\nu}\right]\right|^{2}$$

Correction term (Stetcu, 2003)

Sum Rules and Rule-Breakers

The missing strength can be interpreted as transitions within a rotational band (that is, within the *intrinsic state*) while RPA models transitions within a vibrational band

if one derives it using those

This is bolstered by the fact that we see missing strength (in even-even nuclides) for E2 transitions but not for, say, spin-flip (ΔJ=1) transitions (because rotational band only allows ΔJ ≥2)

$$\frac{1}{2}\left\langle HF\left|\left[\hat{F}\left[\right.\right.\right.$$

$$+\sum_{\nu,\Omega=0}\frac{1}{2M_\nu}\left|\left[F,\hat{P}_\nu\right]\right|^2$$

Correction term (Stetcu, 2003)

Sum Rules and Rule-Breakers

The missing strength can be interpreted as transitions within a within the *intrinsic* transitions with

In addition, if we choose a spherical state (no Goldstone modes) rather than a deformed state, we regain the missing strength