Configuration mixing: the Generator Coordinate Method

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Configuration mixing

We have learned that to restore symmetries one should take linear combinations of HFB states

- Generated by the application of the symmetry operator
- with weights dictated by the underlying group structure.

The same idea can be applied to take into account long range correlations

$$|\Psi_\sigma\rangle = \int dQ f_\sigma(Q)|\Phi(Q)\rangle$$

be choosing an appropriate set of "generating coordinates" Q. The weights can be determined, for instance, recurring to the variational principle on the energy

$$E_\sigma = \frac{\int\int dQdQ' f^*_\sigma(Q) f_\sigma(Q')\langle\Phi(Q)|H|\Phi(Q')\rangle}{\int\int dQdQ' f^*_\sigma(Q) f_\sigma(Q')\langle\Phi(Q)|\Phi(Q')\rangle}$$

Please note that the set $|\Phi(Q)\rangle$ is not necessarily orthogonal with respect to the Q variable

The weights are determined by imposing

$$\frac{\delta E}{\delta f^*} = 0$$

Hill-Wheeler equation

$$\int dQ' h(Q, Q') f_\sigma(Q') = E_\sigma \int dQ' n(Q, Q') f(Q')$$

with $n(Q, Q') = \langle \Phi(Q) | \Phi(Q') \rangle$ and

$$h(Q, Q') = \langle \Phi(Q) | H | \Phi(Q') \rangle$$

How to choose Q ?

Good question but no answer ....

- The choice of Q depends on the physics you want to describe.
- Typically Q is a multipole moment of the mass distribution $Q_{2\mu}$ $Q_{3\mu}$, etc
- but it can be ΔN^2 (or any other order parameter associated to a broken symmetry).
- Ideally as many as possible should be chosen, but the computational cost increases with the square of the number of "generating coordinate" and calculations with more than two are exceptional. The extreme case would be to take all the parameters of the Thouless parametrization (more later)

Solution of the HW equation

Discretize $Q \implies q_i, i = 1, \ldots, N$ to render HW into an algebraic equation

$$\sum_j h_{i,j} f_j^\sigma = E_\sigma \sum_j n_{i,j} f_j^\sigma$$

Diagonalize the norm overlap $n_{i,j}$ (hermitian, positive)

$$n_{i,j} = \sum_k D_{i,k} n_k D_{j,k}^*$$

Get rid of eigenvalues smaller than some threshold $\epsilon \approx 10^{-4}$
Define $g_k = \sum_j f_j D_{j,k}^* n_k^{1/2}$ and $|k\rangle = \sum_j |\Phi_j\rangle D_{jk} n_k^{-1/2}$

$$\tilde{h}_{k,k'} = \sum_{ij} D_{ik} h(i,j) D_{jk'} n_k^{-1/2} n_{k'}^{-1/2}$$

HW becomes

$$\sum_{k'} \tilde{h}_{k,k'} g_{k'}^\sigma = E_\sigma g_k^\sigma$$

The GCM wave function in the "natural" basis $|k\rangle$

$$|\Psi_\sigma\rangle = \sum_k g_k |k\rangle$$

$|k\rangle$ orthogonal and therefore $|g_k|^2$ has the meaning of a probability (unlike f which is an amplitude for non-orthogonal basis)
Mean values $\langle\Psi|O|\Psi\rangle = \sum_k g_k^* O_{kk'} g_{k'}$
Restoring symmetries on $|\Psi\rangle$ is easy as the projector P **only** adds another set of integrals

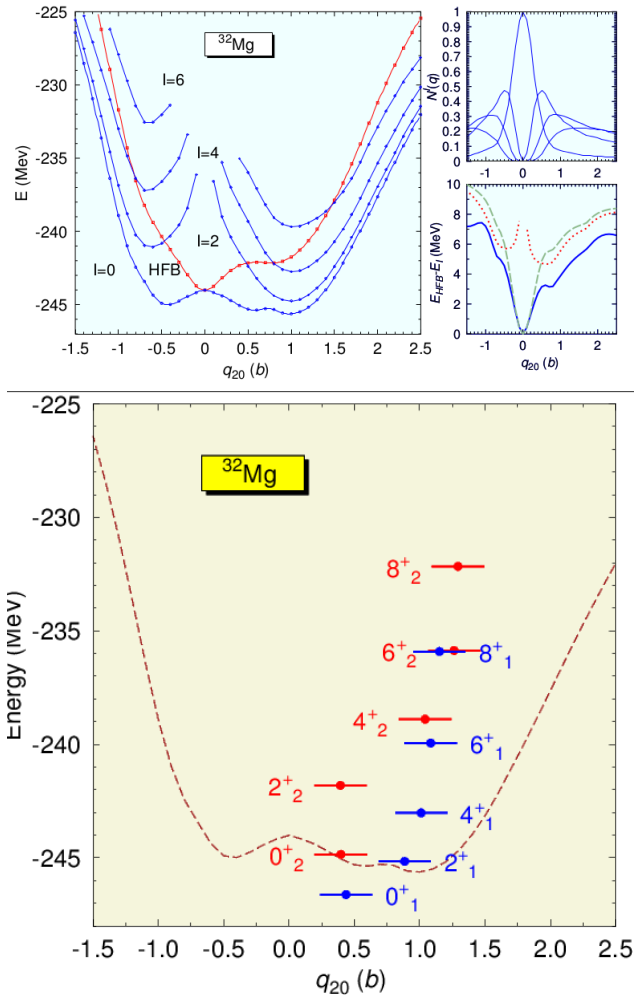
Overlaps

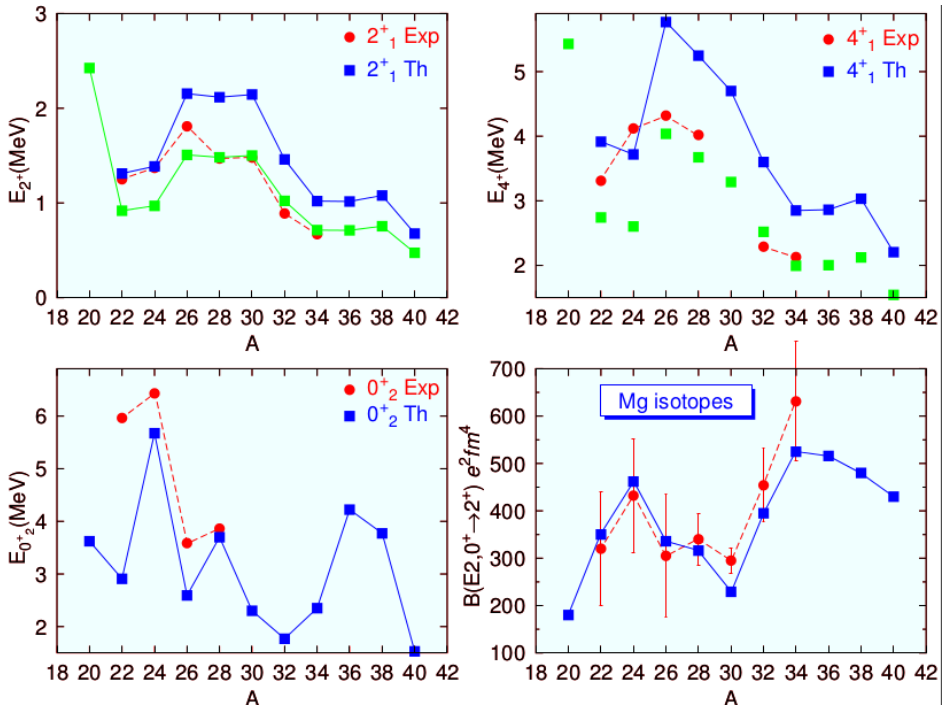
The ingredients entering the HW equation are overlaps of operators between HFB wave functions.
The pfaffian formula and the GWT of Lecture 2 will be useful, remember the kind of general overlaps we have to compute

$$\langle\varphi|\beta_i\beta_j\beta_k\beta_l c_m^+ c_n^+ c_p c_q \tilde{\beta}_r^+ \tilde{\beta}_s^+ \tilde{\beta}_t^+ \tilde{\beta}_u^+ |\tilde{\varphi}\rangle$$

leading to $11\ !! = 10\ 395$ contractions.
For density dependent forces, like Skyrme, Gogny, Relativistic mean field, etc the issue of the prescription for the density dependence to be used in the hamiltonian overlap is still problematic

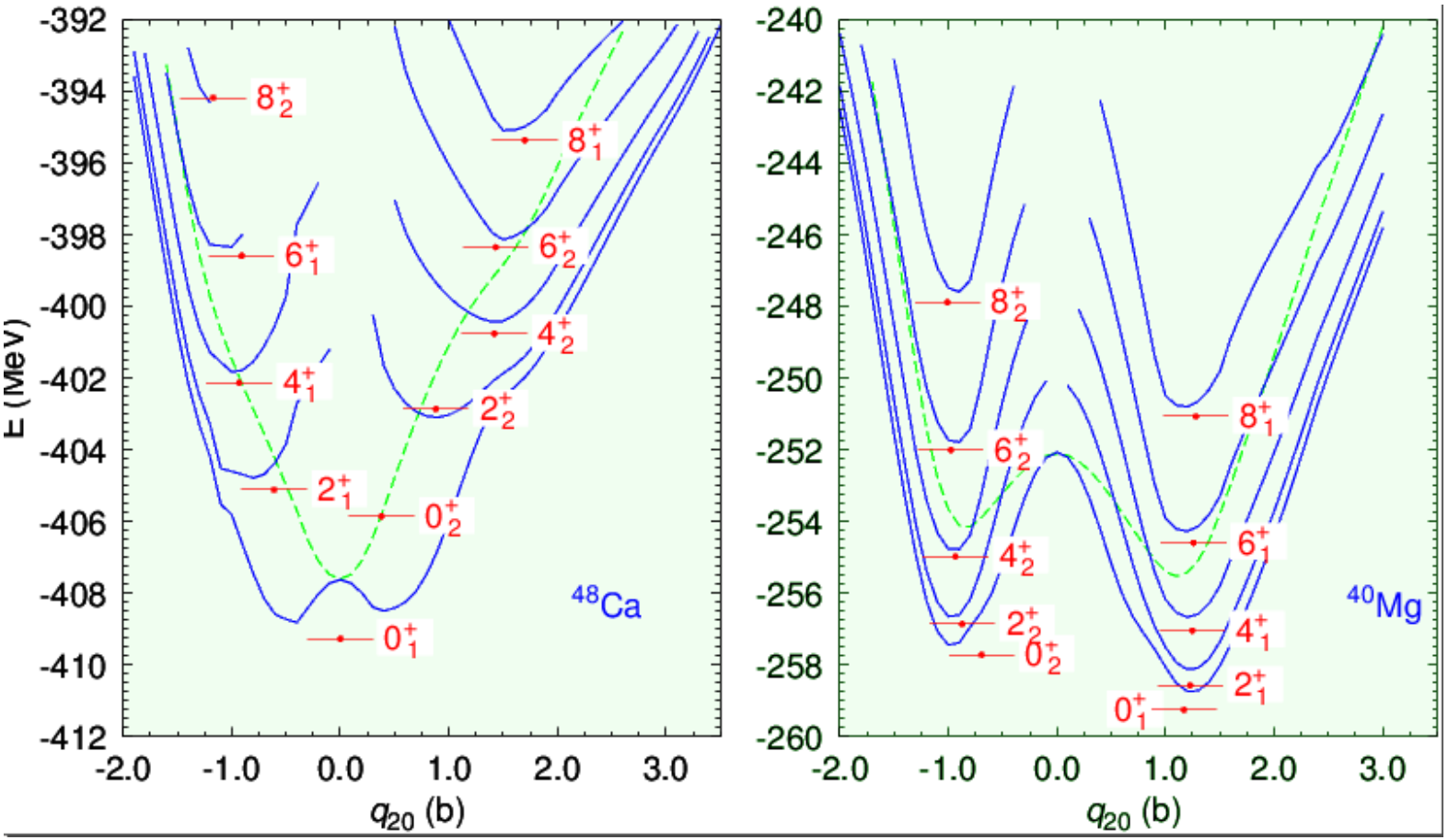
Example



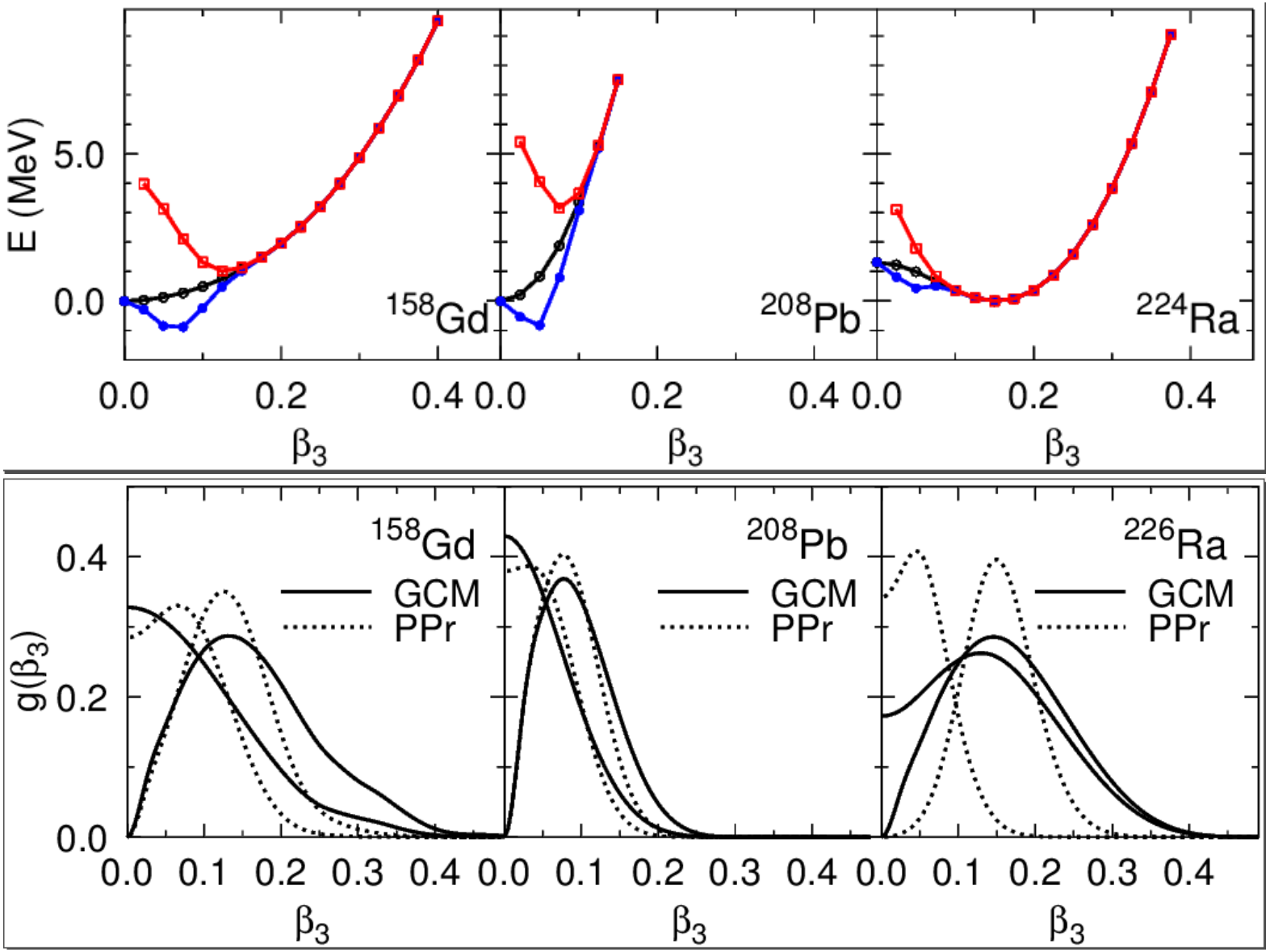


Gogny D1S calculation, Yoccoz vs Thouless moment of inertia

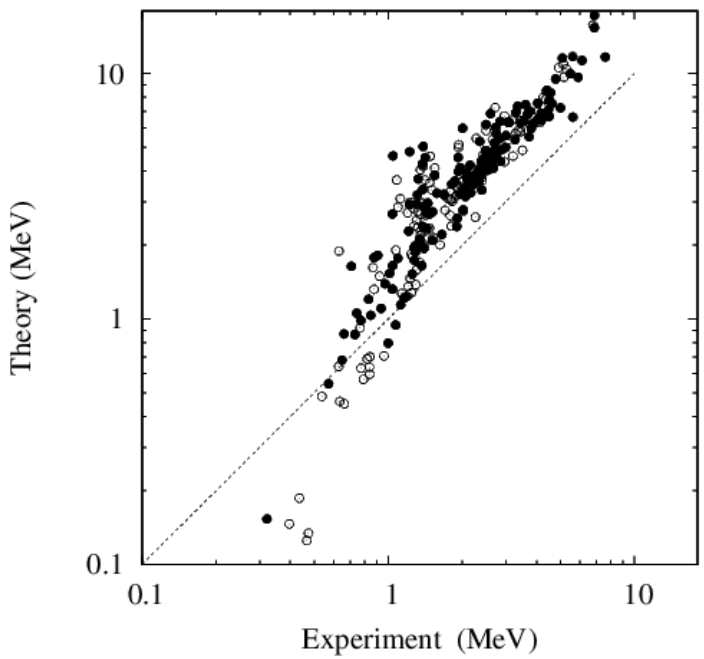
Spherical and deformed

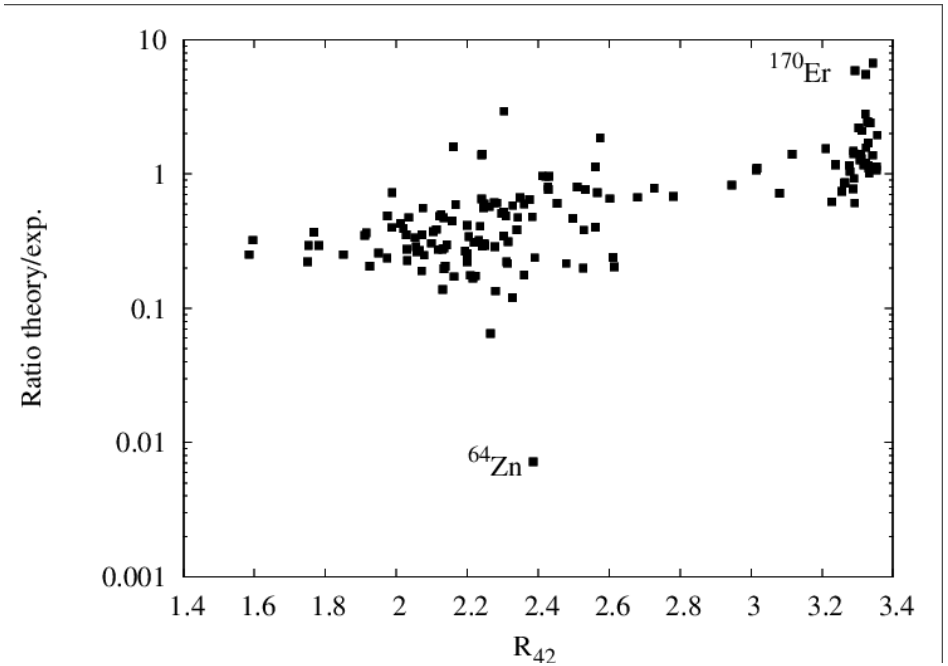


Octupole correlations

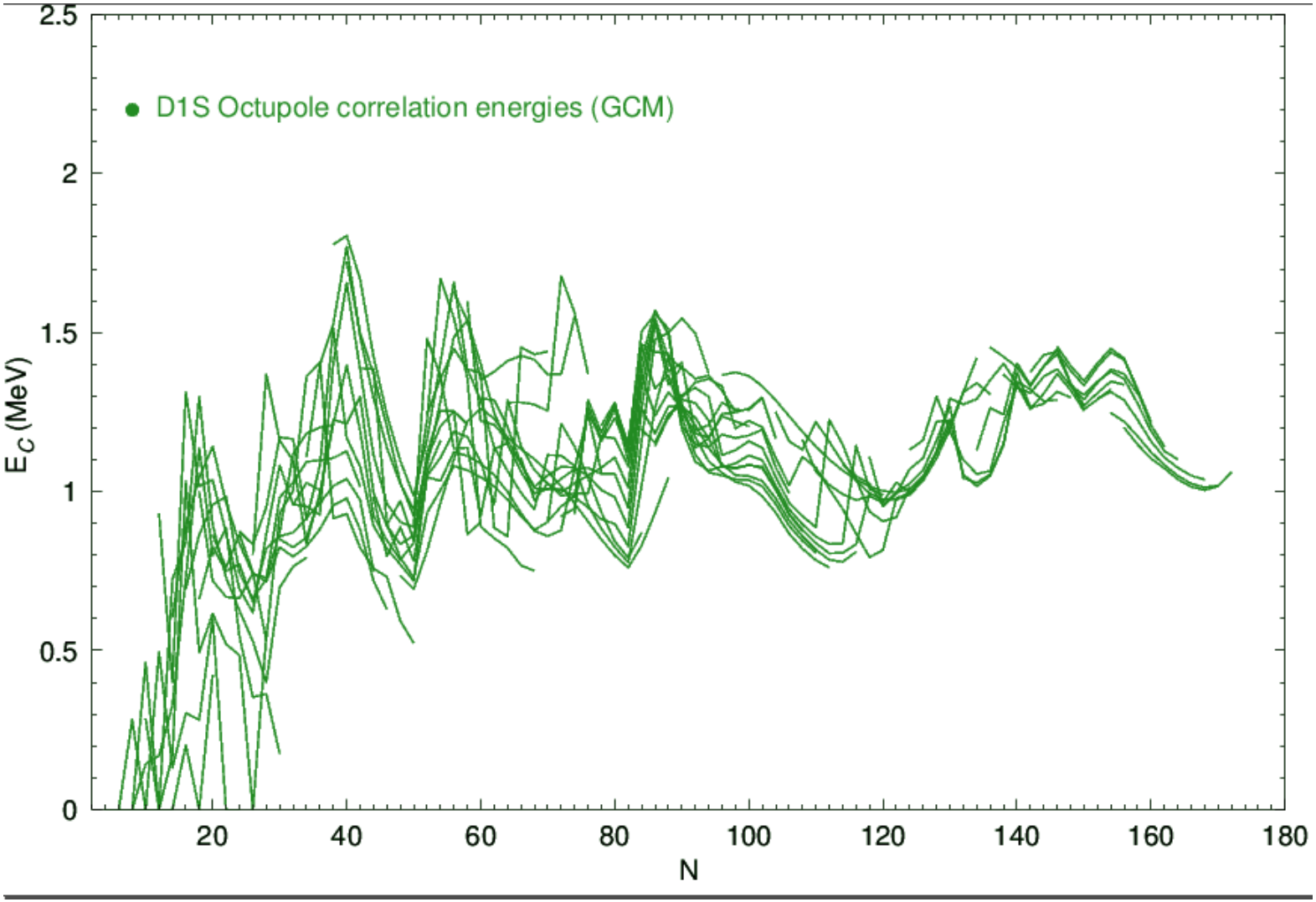


Octupole correlations





Octupole correlations



Relevant for mass tables ?

The GCM - RPA connection

The RPA is usually viewed as the small amplitude limit of TDHFB, but can also be derived from the GCM

- Take as generating coordinates **all** the parameters of the Thouless formula

$$|\mathbf{Z}\rangle = \exp(\sum_{\mu\nu} Z_{\mu\nu}\alpha^+_\mu\alpha^+_\nu)|\psi_0\rangle$$

and

$$|\Psi\rangle = \int d\mathbf{Z} f(\mathbf{Z})|\mathbf{Z}\rangle$$

- Expand $\langle\mathbf{Z}'|\hat{H}|\mathbf{Z}\rangle/\langle\mathbf{Z}'|\mathbf{Z}\rangle$ up to second order
- Assume Gaussian overlaps $\langle\mathbf{Z}'|\mathbf{Z}\rangle \propto \exp(-\mathbf{Z}'^*\mathbf{Z})$
- Introduce the above in the Hill-Wheeler equation
- After some manipulations the RPA equation is obtained

(*) Jancovici&Schiff, Brink &Weiguny

Approximations: GOA and Collective hamiltonian

- The HW equation is an integral equation dealing with non-local quantities like the hamiltonian and norm overlaps.
- Typical count: $Q_2 - Q_3$ calculation with 50 quadrupole deformations and 20 octupole deformations $\Longrightarrow$ 500.000 overlaps to compute with a computational cost two times larger than a typical HFB iteration. Requires 10 times more time than the whole HFB calculation.
- In addition, when quadrupole and octupole moments in the overlap $\langle Q_2 Q_3 | H | Q_2' Q_3' \rangle$ are really different the overlap is very small
- Typically $\langle Q_2 Q_3 | Q_2' Q_3' \rangle \approx \exp(-\sum_{ij} \gamma_{ij} (Q_i - Q_j')^2)$. The norm behaves like a gaussian (Gaussian overlap approximaton GOA)
- $\langle Q_2 Q_3 | H | Q_2' Q_3' \rangle / \langle Q_2 Q_3 | Q_2' Q_3' \rangle$ is a smooth function and can be approximated by a Taylor expansion

- Then

$$\langle Q_2 Q_3 | H | Q_2' Q_3' \rangle \approx (c^0 + C^{(1)}_{Q_2} \frac{\partial}{\partial Q_2} + C^{(1)}_{Q_3} \frac{\partial}{\partial Q_3} + \cdots) \langle Q_2 Q_3 | Q_2' Q_3' \rangle$$

- Plugging the above in the HW transforms it into a differential equation

$$(-\hbar^2 \sum_{ij} M^{-1}_{ij} \frac{\partial}{\partial Q_i} \frac{\partial}{\partial Q_j} + V(Q_2, Q_3)) g_\alpha(Q_2, Q_3) = \epsilon_\alpha g_\alpha(Q_2, Q_3)$$

  where the "collective mass" tensor $M_{ij}(Q_2, Q_3)$ is a function of $C^{(0)}$, $C^{(1)}$ and $C^{(2)}$

- The "potential energy" is

$$V(Q_2, Q_3) = \langle Q_2 Q_3 | H | Q_2 Q_3 \rangle + \epsilon_0(Q_2, Q_3)$$

  where the ϵ_0 is the "zero point energy correction".

Non local kernels replaced by local quantities plus functions of derivatives

- The non-local HW is reduced to a local "collective hamiltonian equation" where the parameter (mass tensor and zero point energy correction) are evaluated locally.
- The process has to be repeated for each observable (mass moments, transition probabilities, etc) with their own "collective mass" term and "zero point" correction.
- The approximation works well whenever there are no sudden configuration changes in $|Q_2 Q_3\rangle$ like level crossings that render the hamiltonian overlap a "non-smooth" function.
- The "collective wave functions" are easy to interpret as their modulus has, at the level of approximation considered, the meaning of a probability.

Borh hamiltonian ?

- The Borh hamiltonian is a kind of collective hamiltonian for the β and γ quadrupole deformation parameters.
- It includes a collective rotational energy involving moments of inertia that change with the angular momentum of the nucleus *I*
- The "collective masses" take the form of the GCM collective hamiltonian or the form deduced from ATDHFB.
- The moments of inertia are usually the Thouless-Valatin moments of inertia computed by cranking the system with a small angular velocity ω
- Its form suggests it could be deduced from a GCM with β and γ as generating coordinates and projecting on good angular momentum.
- Such derivation in not available for the the moment
- Nicely reproduces yrast, β and γ rotational bands

Difficulties and ideas to avoid them

- The "collective hamiltonian" approximation has its own difficulties associated to a poor evaluation of the collective masses
- It is not clear how to extend to odd-A nuclei (the norm is no longer gaussian)
- It is better to stick with the HW equation but using the parabolic approximation for operator overlaps while keeping the exact values for the norm overlap to avoid level crossing problems
- Mixing these ideas with the "large deformation limit" of projection could be a reasonable and computationally feasible alternative to more sophisticated methods. (Still under development)

Multi-quasiparticle excitations

- Instead of $|\Phi(Q)\rangle$ we can choose $|\Phi\rangle$, $\alpha^+_k\alpha^+_{k'}|\Phi\rangle$, $\alpha^+_k\alpha^+_{k'}\alpha^+_{k''}\alpha^+_{k'''}|\Phi\rangle$, as generating coordinate
- or a generalization of it including some "collective" degrees of freedom $|\Phi(Q)\rangle$, $\alpha^+_k\alpha^+_{k'}|\Phi(Q)\rangle$, etc
- this idea has been successfully applied to nuclei in the Projected Shell Model of Hara and Sun but with schematic P+Q interactions.
- In this situation the pfaffian version of the GWT will be extremely useful
- Specially useful in odd-A systems where the coupling to three-quasiparticle and higher excitations are very relevant (particle-vibration coupling)