Efficient solution methods for Quasiparticle Random Phase Approximation equations

Jussi Toivanen
Department of Physics, University of Jyväskylä, Finland

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QRPA solver project

We want to solve hard QRPA problems with modest resources...

- Lowest QRPA eigenmodes without full diagonalization
- QRPA strength functions without full diagonalization
- Deformed nuclei (axial/triaxial/isospin mixing)
- As few approximations and truncations as possible (HFB and QRPA consistent, full functional, all quasiparticles)
- Large basis sets
- Continuum basis (PTG)

Starting point

- Density functional with (generalized) Skyrme particle-hole part, Coulomb terms and pairing functional

$$E[\rho] = T[\rho] + U_{\text{Skyrme}}[\rho] + U_{\text{Coulomb}}[\rho] + U_{\text{Cou.ex}}[\rho] + U_{\text{Pair.}}[\bar{\rho}]$$

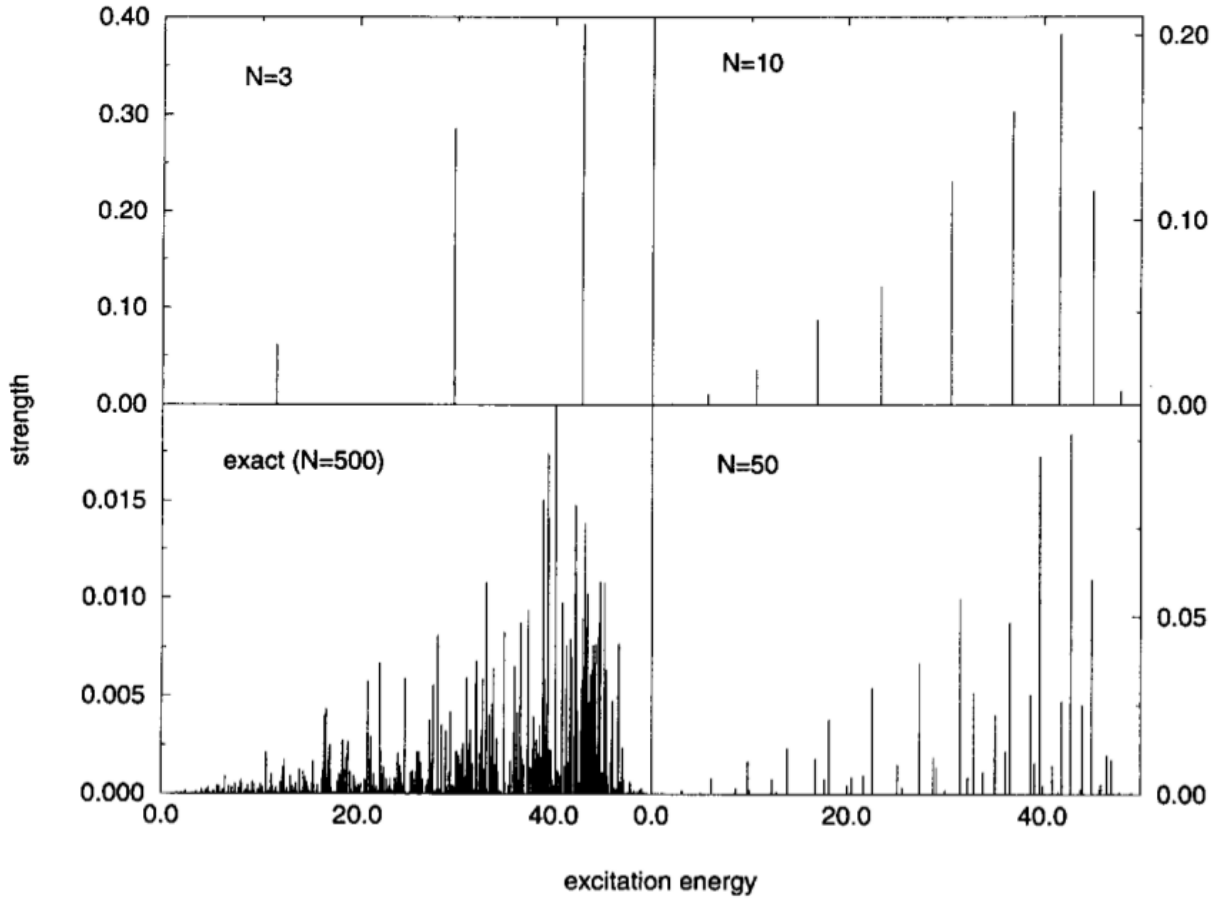
- Typical number of oscillator shells in HFB and QRPA is $15 - 25$. Maximum $70 - 80$...
- Coulomb exchange usually in Slater approximation.
- Pairing can be mixed delta pairing or finite range pairing.

$$V(|r_1 - r_2|, |r_1' - r_2'|) = Ge^{-|r_1 - r_2|^2/a^2} e^{-|r_1' - r_2'|^2/a^2}$$

- We can also just import TBMEs and/or mix with Skyrme

QRPA with Lanczos?

One can do Lanczos iteration starting from a special pivot vector:



(Johnson and Bertsch, CPC 120, 155-161 (1999))

Basic iterative Arnoldi procedure

Instead of Lanczos, we use Arnoldi method

- More stable than Lanczos for non-hermitean problems.
- Only matrix-vector products are needed.

$$\begin{pmatrix} X^{k+1} \\ Y^{k+1} \end{pmatrix} = \begin{pmatrix} W^{k} \\ W'^{k} \end{pmatrix} - \sum_{i=1}^{k} \begin{pmatrix} X^{i} \\ Y^{i} \end{pmatrix} a_{ik} + \sum_{i=1}^{k} \begin{pmatrix} Y^{i*} \\ X^{i*} \end{pmatrix} b_{ik} \,,$$

$$\begin{pmatrix} Y^{k+1*} \\ X^{k+1*} \end{pmatrix} = -\begin{pmatrix} W'^{k*} \\ W^{k*} \end{pmatrix} + \sum_{i=1}^{k} \begin{pmatrix} X^{i} \\ Y^{i} \end{pmatrix} b^{*}_{ik} - \sum_{i=1}^{k} \begin{pmatrix} Y^{i*} \\ X^{i*} \end{pmatrix} a^{*}_{ik} \,. \tag{1}$$

Krylov space (small) QRPA matrix:

$$\rightarrow \begin{pmatrix} a & b \\ -b^{*} & -a^{*} \end{pmatrix} \begin{pmatrix} x_n \\ y_n \end{pmatrix} = \hbar\omega_n \begin{pmatrix} x_n \\ y_n \end{pmatrix}$$

QRPA matrix-vector products

The QRPA matrix - vector products are calculated using *linearized RPA mean fields*, without construction of the actual matrix

$$\begin{pmatrix} W^n \\ W'^n \end{pmatrix} = \begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X^n \\ Y^n \end{pmatrix}$$

Definitions:

- U, V: Bogoliubov-Valatin transformation from HFB
- $\tilde{\rho}$, $\tilde{\kappa}$, $\tilde{\kappa}'$: Density matrix and pairing tensors of QRPA
- E: Diagonal matrix of HFB quasiparticle energies
- RPA norm: $\langle \boldsymbol{Q}_\omega | \boldsymbol{Q}_{\omega'} \rangle = \sum_{k<k'} X^{\omega *}_{kk'} X^{\omega'}_{kk'} - Y^{\omega *}_{kk'} Y^{\omega'}_{kk'}$

From TDHFB to QRPA

From linearized TDHFB equations:

- TDHFB linearized

$$\hbar\omega\tilde{\mathcal{R}} = \left[\mathcal{H}(\mathcal{R}_{g.s.}), \tilde{\mathcal{R}}\right] + \left[\mathcal{H}^1(\tilde{\mathcal{R}}), \tilde{\mathcal{R}}_{g.s.}\right]$$

- Matrix elements between occupied and unoccupied states give QRPA equations

$$\begin{aligned} \hbar\omega\tilde{Z} &= E\tilde{Z} + \tilde{Z}E + \tilde{W} \\ -\hbar\omega\tilde{Z}'^{\dagger} &= E\tilde{Z}'^{\dagger} + \tilde{Z}'^{\dagger}E + \tilde{W}'^{\dagger} \end{aligned}$$

QRPA matrix-vector products in more detail

From linearized TDHFB equations:

- Transformation from quasiparticle amplitudes to density matrices

$$\begin{aligned}\tilde{\rho} &= UX^nV^T + V^*Y^{n\dagger}U^\dagger \\ \tilde{\kappa} &= UX^nU^T + V^*Y^{n\dagger}V^\dagger, \quad \tilde{\kappa}' = VX^nV^T + U^*Y^{n\dagger}U^\dagger\end{aligned}$$

- Calculation of normal and pairing fields

$$\tilde{h}_{kk'} = \sum_{ll'} \bar{v}_{kl'k'l}\tilde{\rho}_{ll'} + \ldots \quad \tilde{\Delta}_{kk'} = \frac{1}{2}\sum_{ll'} \bar{v}_{kk'll'}\tilde{\kappa}_{ll'} + \ldots$$

- Transforming back to quasiparticle amplitudes

$$\begin{aligned}X^{n+1} &= U^\dagger\tilde{h}V^* - V^\dagger\tilde{h}^TU^* + U^\dagger\tilde{\Delta}U^* + V^\dagger\tilde{\Delta}'^\dagger V^* + EX^n + X^nE \\ Y^{n+1} &= -U^T\tilde{h}^TV + V^T\tilde{h}U + U^T\tilde{\Delta}'^\dagger U + V^T\tilde{\Delta}V + EY^n + Y^nE\end{aligned}$$

Done with modified mean-field code (HOSPHE)

Starting the Arnoldi iteration: Pivot vector

The initial vector, *pivot*, is important with strength functions.

- QRPA satisfies odd energy weighed sum rules (EWSR) and violates even ones
- Iterative Arnoldi satisfies all odd EWSR up to k^{th} after k iterations, if we set

$$\begin{aligned} X^1_{kk'} &= (U\mathcal{O}V^T - V\mathcal{O}^T U^T)_{kk'}, \\ Y^1_{kk'} &= 0. \end{aligned}$$

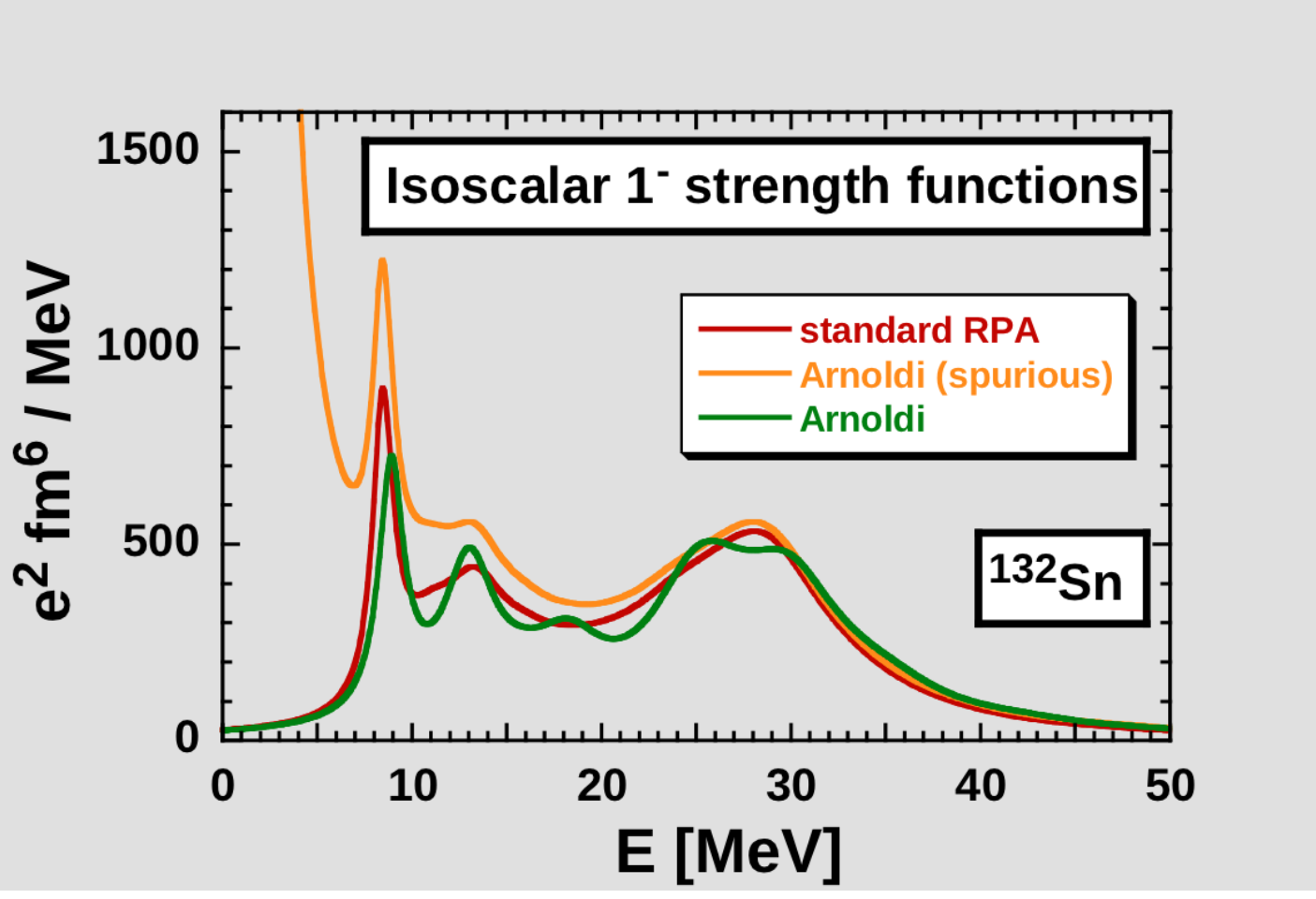
  $\mathcal{O}$ is the matrix of EM transition operator elements.

- pnQRPA satisfies the Ikeda sum rule
- Iterative Arnoldi satisfies the Ikeda sum rule also, if we set

$$\begin{aligned} X^{1,\text{pn}}_{kk'} &= (U_p\mathcal{O}_{GT-}V_n^T - V_p\mathcal{O}^T_{GT-}U_n^T)_{kk'}, \\ Y^{1,\text{pn}}_{kk'} &= 0. \end{aligned}$$

  And similarly for the beta+ channel.

Spurious mode mixing



Spurious QRPA modes

Each broken symmetry of the ground state wave function produces a pair of large amplitude RPA modes (spurious & boost).

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} \boldsymbol{S} \\ \boldsymbol{S}^* \end{pmatrix} = 0$$

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} \boldsymbol{B} \\ \boldsymbol{B}^* \end{pmatrix} = \delta\lambda \begin{pmatrix} \boldsymbol{S} \\ \boldsymbol{S}^* \end{pmatrix}$$

Both modes have RPA norm zero, $\langle \boldsymbol{S}|\boldsymbol{S}\rangle = \langle \boldsymbol{B}|\boldsymbol{B}\rangle = 0$, but their overlap $\langle \boldsymbol{S}|\boldsymbol{B}\rangle$ is non-zero.

$$Q_S^\dagger = \sum_{k<k'} S_{kk'}\beta_k^\dagger\beta_{k'}^\dagger + S_{kk'}^*\beta_{k'}\beta_k \qquad Q_B^\dagger = \sum_{k<k'} B_{kk'}\beta_k^\dagger\beta_{k'}^\dagger + B_{kk'}^*\beta_{k'}\beta_k$$

Spurious RPA mode generation

- Tanslational invariance: both are known beforehand ($Q_S = \boldsymbol{P}$, $Q_B = \boldsymbol{R}$)
- Particle number non-conservation and rotational invariance violation: Use a different method to find the boost mode ($Q_S = \boldsymbol{J}$, $Q_S = \hat{N}$).

$$\begin{aligned} B_{kk'} &= (V_{12}^* U_{12}^T)_{kk'} \,, \\ U_{12} &= U_0^\dagger U_1 + V_0^\dagger V_1 \,, \\ V_{12} &= U_0^T V_1 - V_0^T U_1 \,. \end{aligned}$$

  The boost mode amplitudes are generated using Thouless theorem.

- U_0 and V_0 are from HFB ground state calculation, U_1 and V_1 from another HFB calculation with slightly changed cranking frequency/chemical potential, $\lambda' = \lambda + \delta\lambda$, $\omega' = \omega + \delta\omega$.

Spurious RPA mode removal

The spurious and boost mode components are removed with a Gram-Schmidt procedure

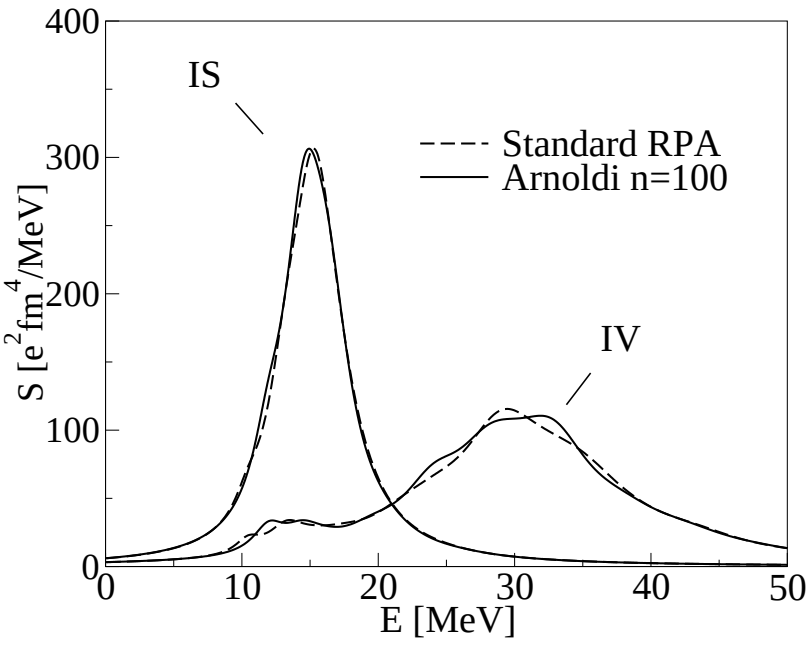
$$\begin{pmatrix} X^{k,2} \\ Y^{k,2} \end{pmatrix} = \begin{pmatrix} X^{k} \\ Y^{k} \end{pmatrix} + \sum_{i=1}^{n_s} \left(\begin{pmatrix} S^{i} \\ S^{i*} \end{pmatrix} \frac{\langle \boldsymbol{B}_i | \boldsymbol{Q}_k \rangle}{\langle \boldsymbol{S}_i | \boldsymbol{B}_i \rangle} - \begin{pmatrix} B^{i*} \\ B^{i} \end{pmatrix} \frac{\langle \boldsymbol{S}_i | \boldsymbol{Q}_k \rangle}{\langle \boldsymbol{S}_i | \boldsymbol{B}_i \rangle} \right)$$

It is not sufficient to remove just the spurious components!

Arnoldi applications: EM strength functions

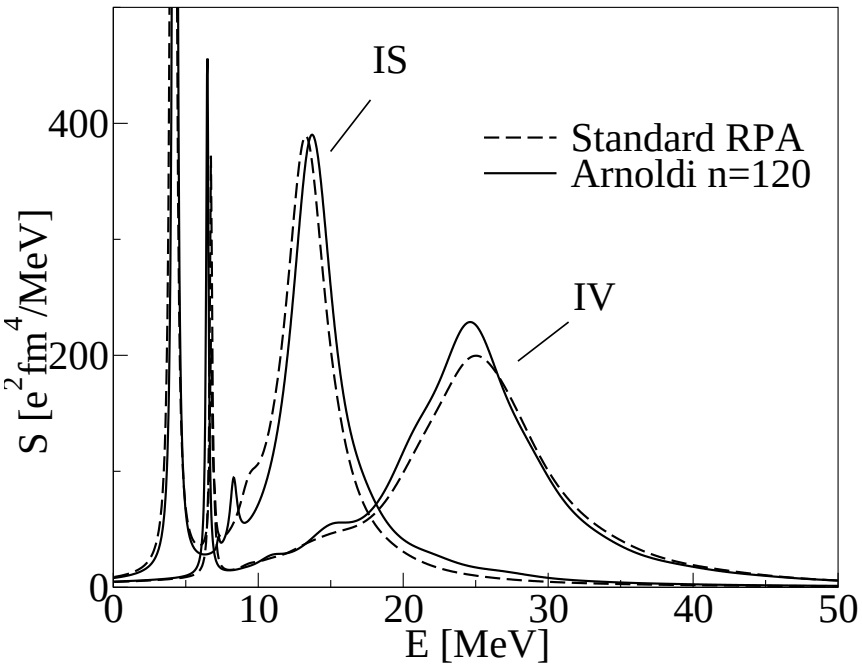
J. Toivanen et al., "Linear response strength functions with iterative Arnoldi diagonalization", Phys. Rev. C 81, 034312 (2010)

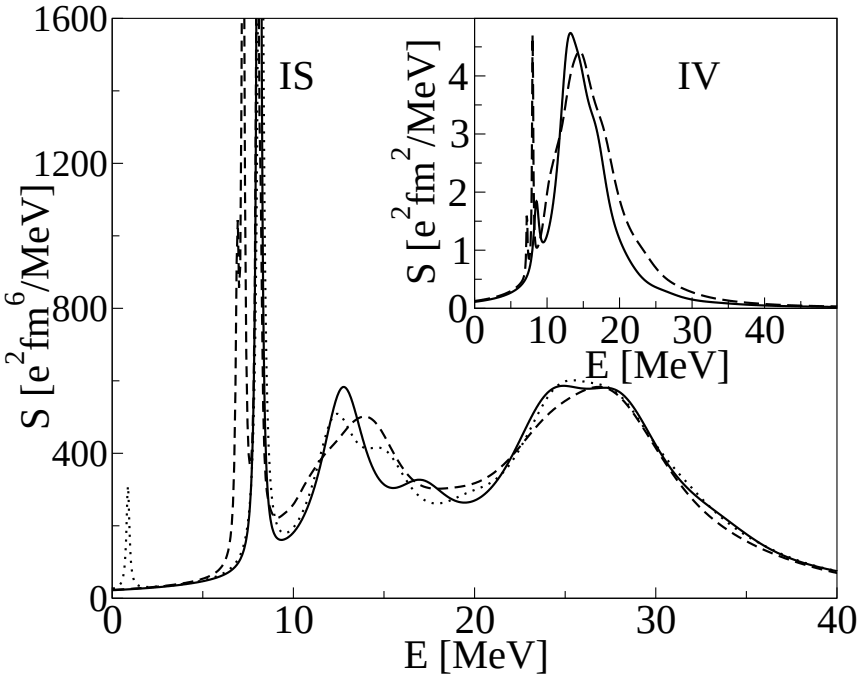
- RPA satisfies odd-order sum rules
- *pivot* vector X-amplitudes equal to EM operator
- vector Y-amplitudes zero
- Arnoldi iteration generates moments of EM strength and preserves the odd ones (S_1, S_3, S_5, ...)



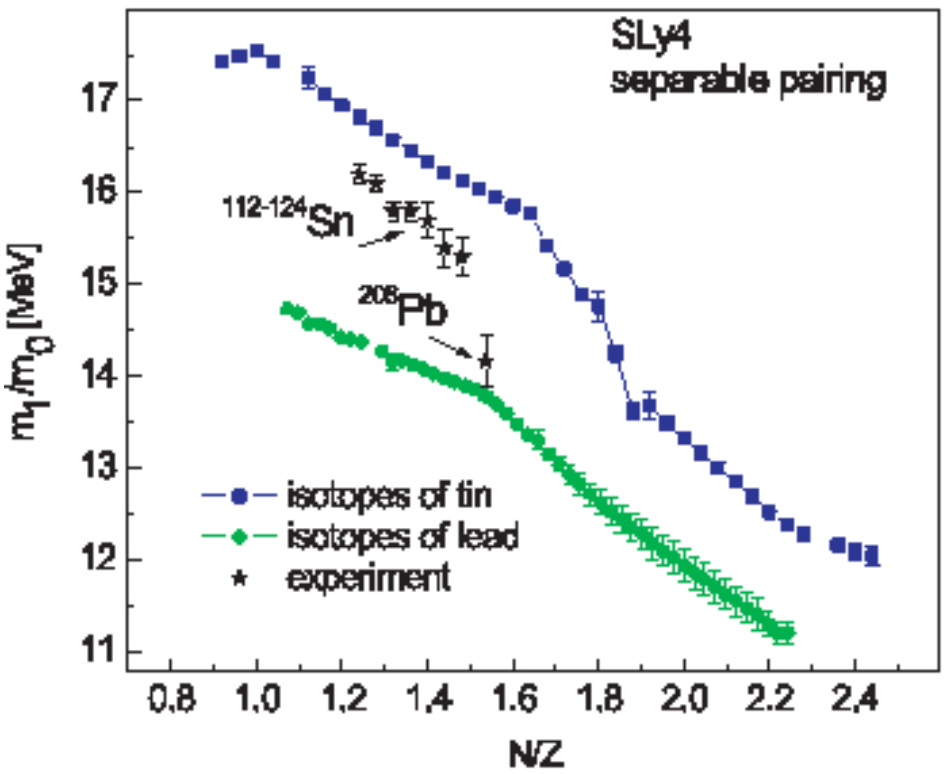
Arnoldi applications: EM strength functions

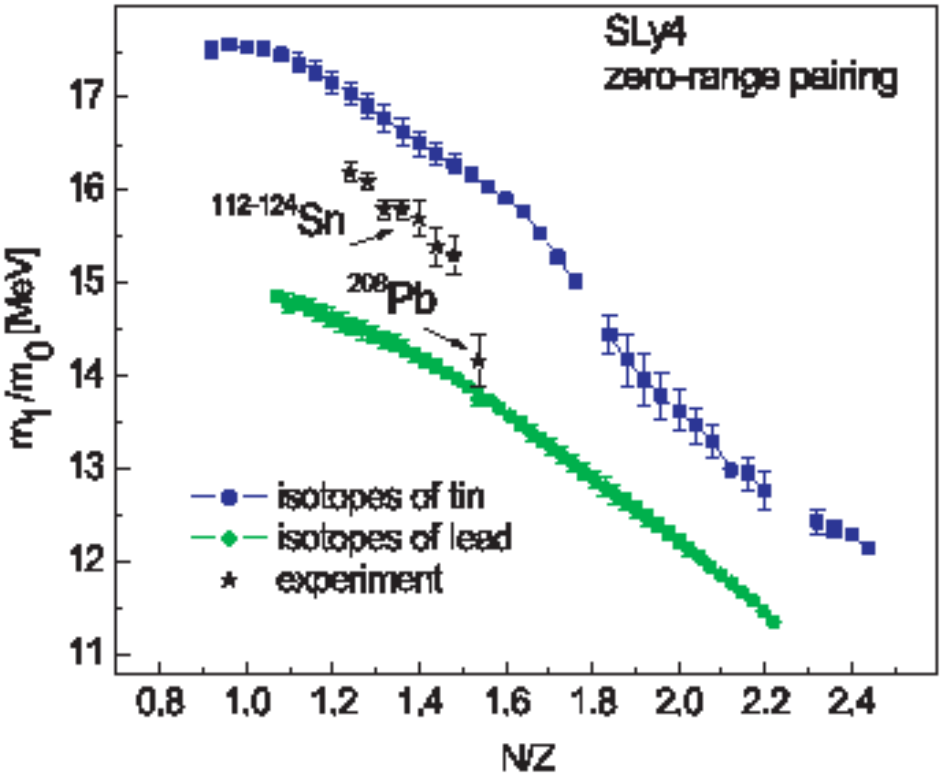
Higher multipoles (1-, 2+):





Monopole strength function and nuclear incompressibility





Finite Amplitude Method

- RPA: T. Nakatsukasa et al., Phys. Rev. C76, 024318 (2007)
- QRPA: P. Avogadro et al., Phys. Rev. C84, 014314 (2011)
- QRPA in H.O. basis: M. Stoitsov et al., Phys. Rev. C84, 041305 (2011)

$$\begin{aligned} \rho_\eta &= (V + \eta U^* X^*)^* (V + \eta U^* Y)^T \\ \kappa_\eta &= -(U + \eta V^* Y^*)^* (V + \eta U^* X)^\dagger \end{aligned}$$

$$X_{ab} = -\frac{\delta H^{20}_{ab}(\omega) - F^{20}_{ab}}{E_a + E_b - \omega + i\gamma}, \quad Y_{ab} = -\frac{\delta H^{02}_{ab}(\omega) - F^{02}_{ab}}{E_a + E_b + \omega + i\gamma}$$

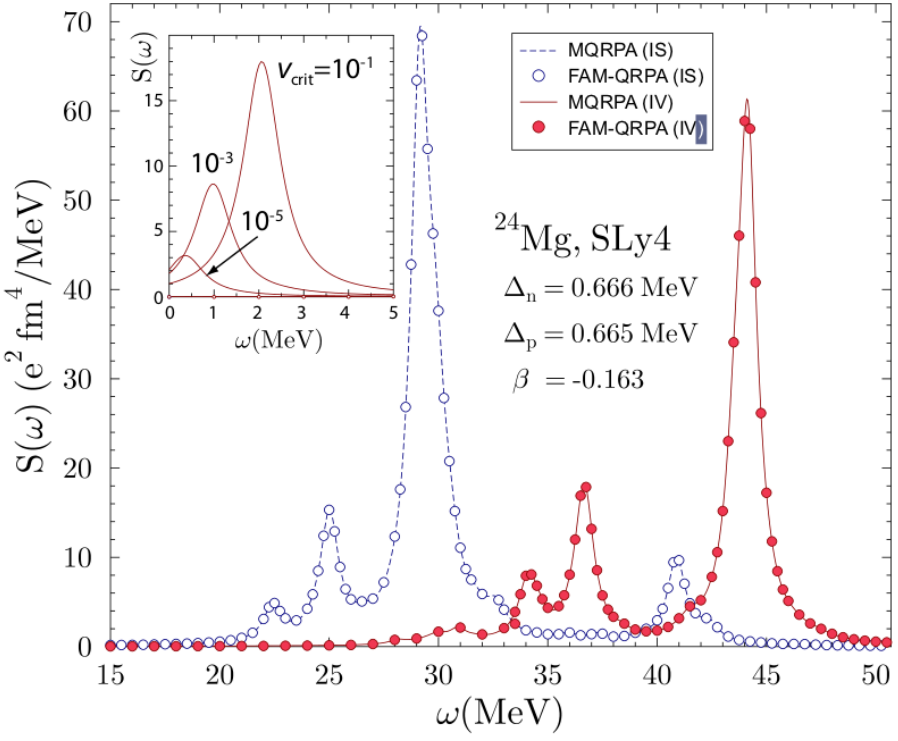
- Broyden method used to accelerate convergence

(F^{20}_{ab} external perturbing field, H^{20}_{ab} QRPA fields, γ smoothing width)

Finite Amplitude Method with H.O. basis

M. Kortelainen et al., implementation in code HFBTHO

- In FAM the energy ω can be freely chosen
- $\rightarrow$ freedom to investigate only the interesting energy range
- Must use smoothing width γ always
- $\rightarrow$ affects accuracy of QRPA amplitudes
- Work going on to implement arbitrary multipoles



Restarted Arnoldi Method

- Implicitly Restarted Arnoldi Method creates a Krylov basis set and forms an upper Hessenberg matrix H_k after k iterations.

$$MV_k = V_k H_k + f_k e_k^T \,,$$

  where M is the RPA matrix and matrix V_k contains *Arnoldi vectors* as its columns. f_k is a residual vector.

- Approximate eigenvalues are calculated by making a "quasi-diagonal" decomposition of H_k. If wanted number of lowest eigenvalues have converged, the method stops.

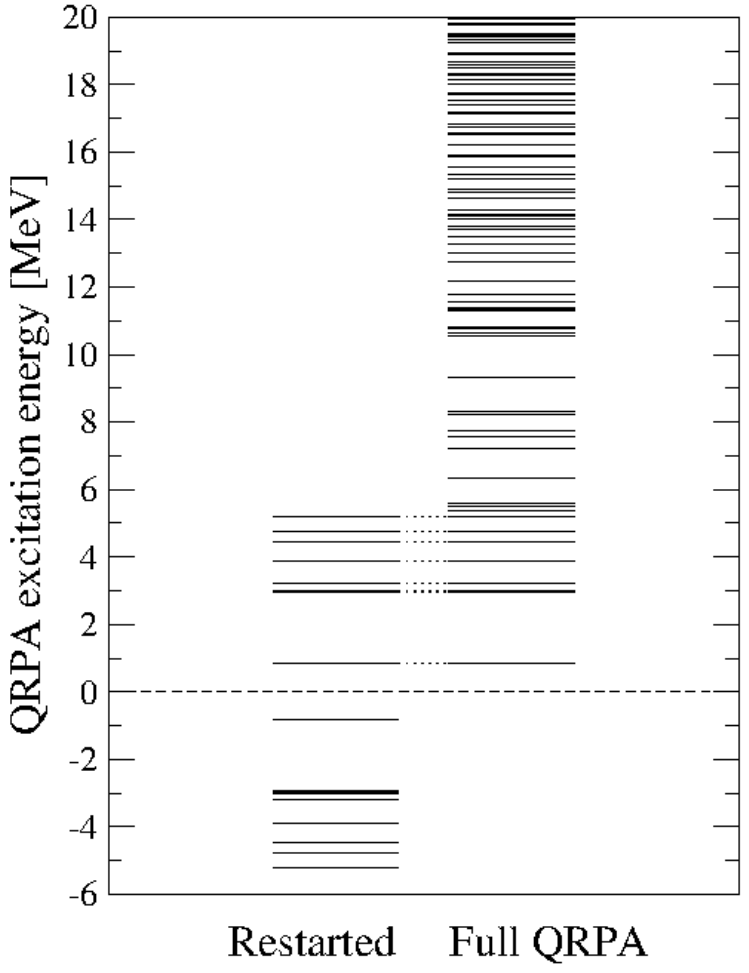
- Otherwise a new pivot is calculated using V_k and H_k decomposition and the Arnoldi iteration is restarted from the pivot.

(For more details, see e.g. Ph.D thesis of R. B. Lehoucq)

Restarted Arnoldi Method

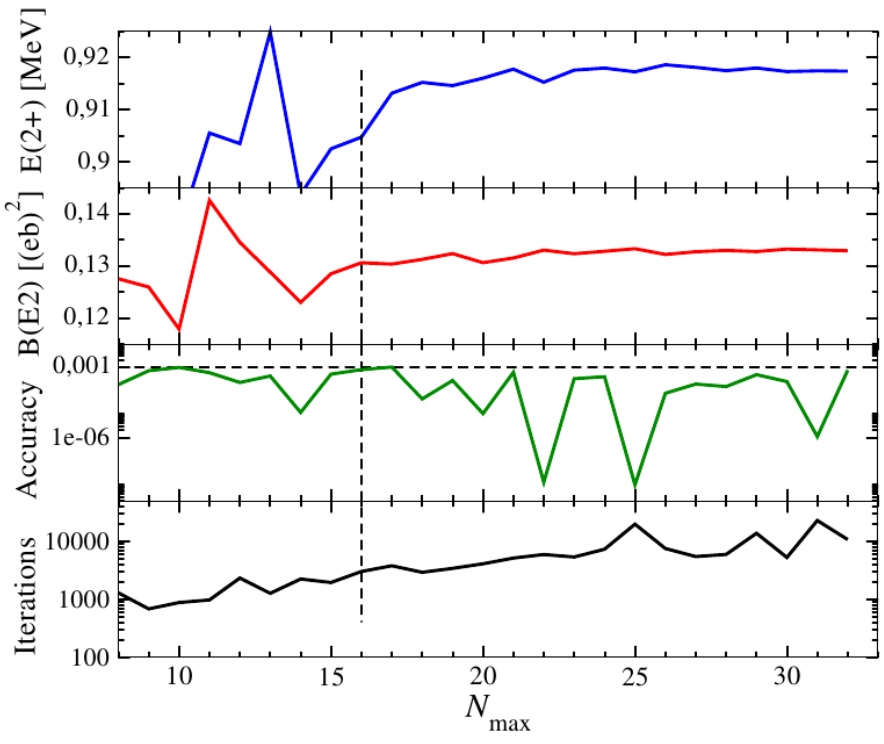
Energy spectrum example: Sixteen 2^+ states of ^{120}Sn requested, 20 harmonic oscillator shells, SkM* + separable pairing. $D = 7590$.

- Small memory footprint (100-200 Krylov vectors)
- Gives both positive and negative energy solutions (ARPACK)
- Accuracy is exact both for energies and transition amplitudes
- Very good method for deformed nuclei
- No RPA matrix...



Restarted Arnoldi Method

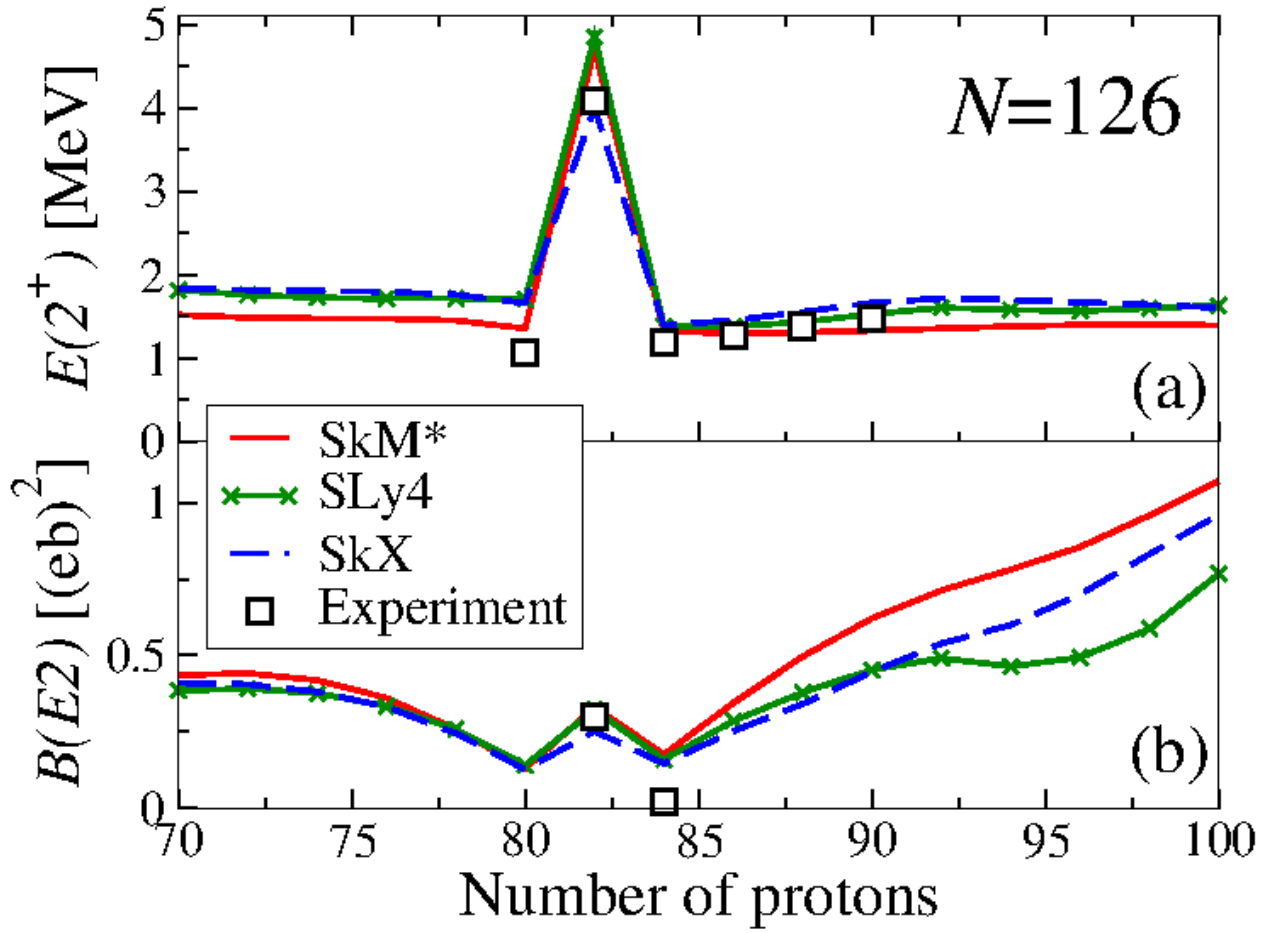
- Large basis sizes "easy"
- Convergence can be studied
- Allows less severe truncations



Practical application: B.G. Carlsson, J. Toivanen and A. Pastore, arXiv:1203.5236v1 (published soon in PRC)

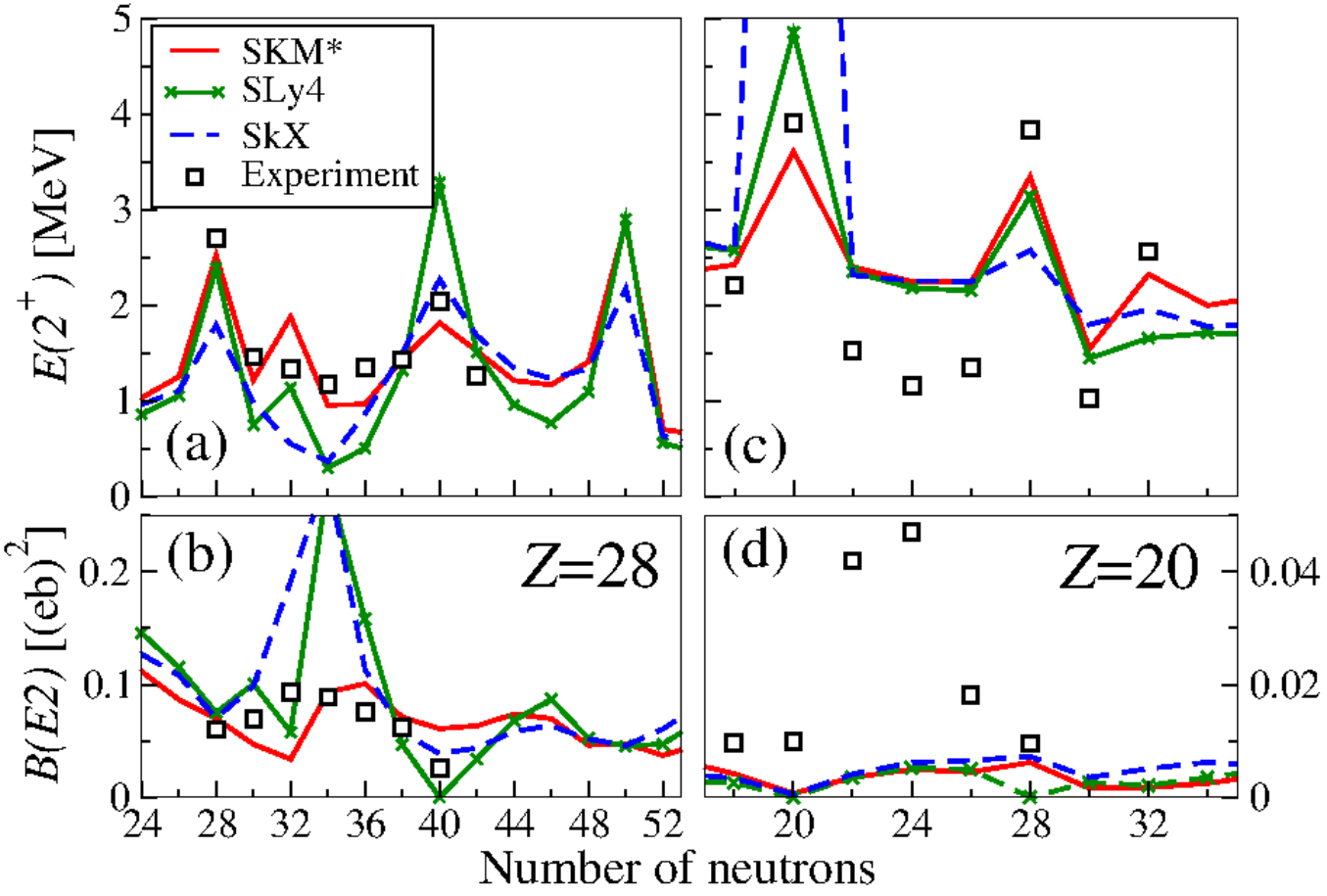
Applications: Semimagic nuclei

2^+ states of $N = 126$ isotones:



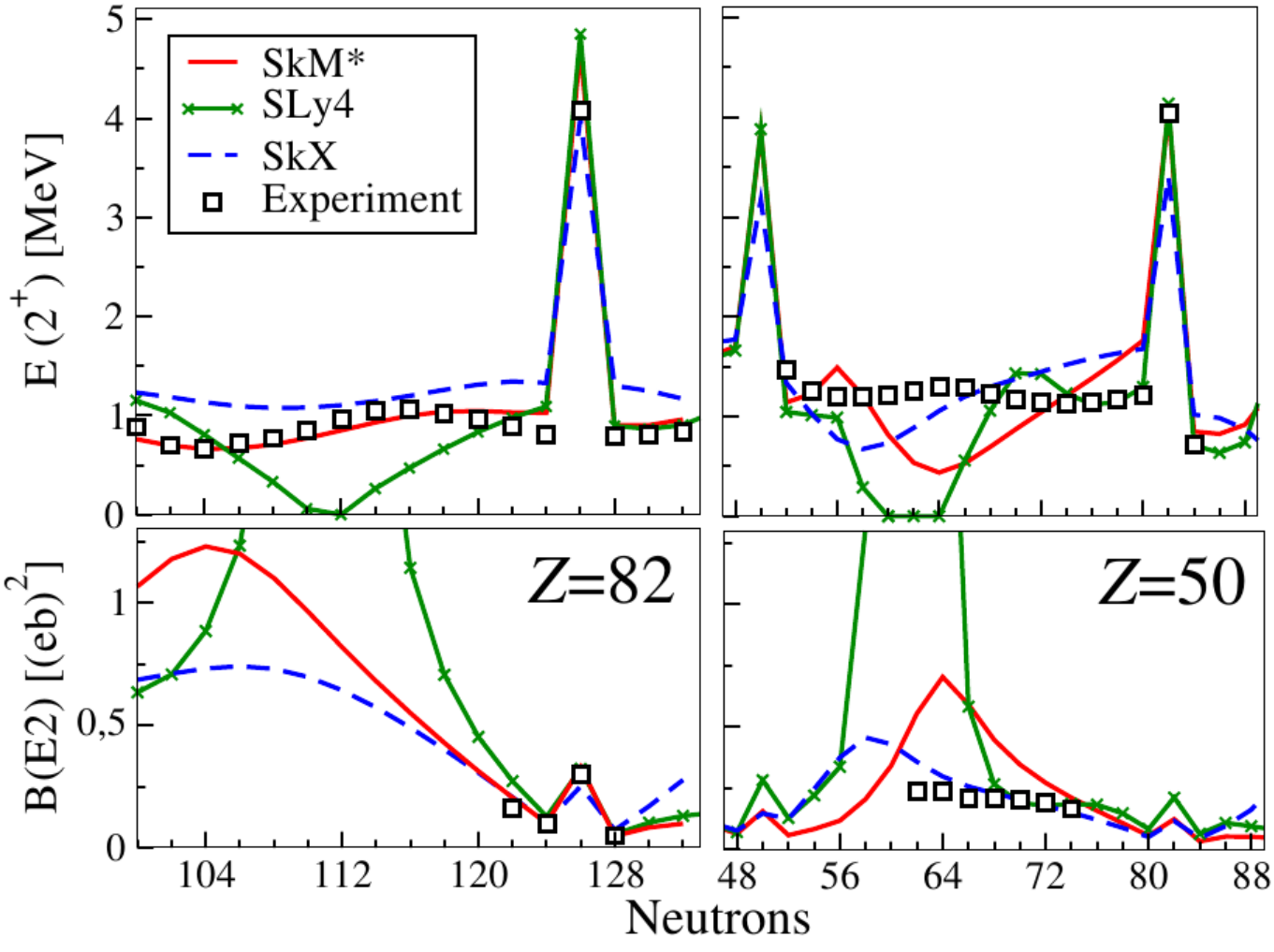
Applications: Semimagic nuclei

2^+ states of semimagic Ca and Ni isotopes:



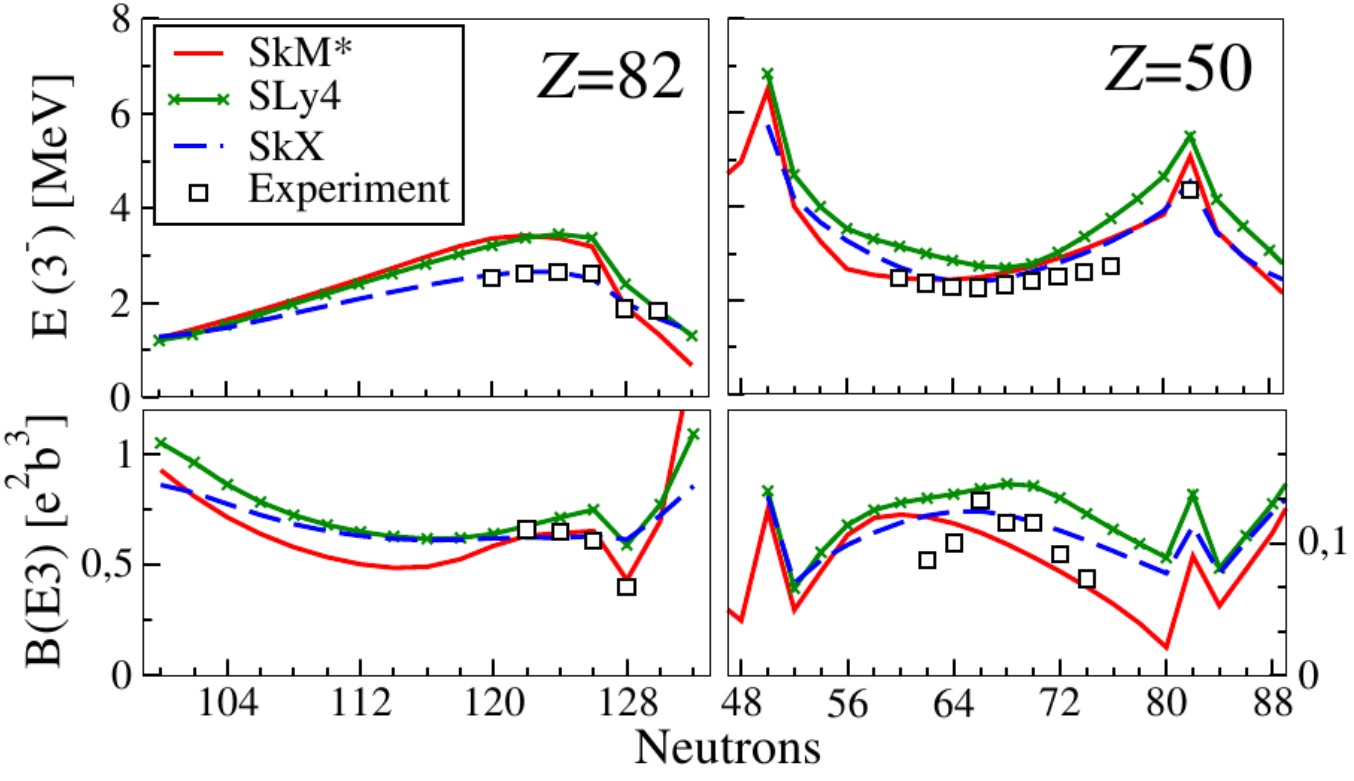
Applications: Semimagic nuclei

2^+ states of semimagic Sn and Pb isotopes:



Applications: Semimagic nuclei

3^- states of semimagic Sn and Pb isotopes:



FAM versus Arnoldi

Pros:

- Moment Arnoldi: Fastest for moments of strength function
- FAM: Free choice of energy range, finds the "real" smoothed strength function
- Restarted Arnoldi: Lowest excitations come out exactly, saves memory

Cons:

- Moment Arnoldi: Low-lying states converge slowly
- FAM: Lots of ω points have to be calculated to not miss states, must use smoothing.
- Restarted Arnoldi: Can not calculate huge number of states.

Particle-Vibration Coupling

(Dimiter Tarpanov, J.D., J.T.). PVC calculates the energy shifts when particle is added to or removed from a even-even nucleus.

$$\rho^{k}_{\alpha\beta} = \rho^{A}_{\alpha\beta} + U^{*}_{\alpha k} U_{\beta k} - V_{\alpha k} V^{*}_{\beta k}$$

PVC vertex with quasiparticle fields:

$$\langle k | H_{pv} | \omega k \rangle = \sum_{\alpha\beta} W^{k}_{\alpha\beta} X^{\omega}_{\alpha\beta} + W'^{k}_{\alpha\beta} Y^{\omega}_{\alpha\beta}$$

Particle-Vibration Coupling

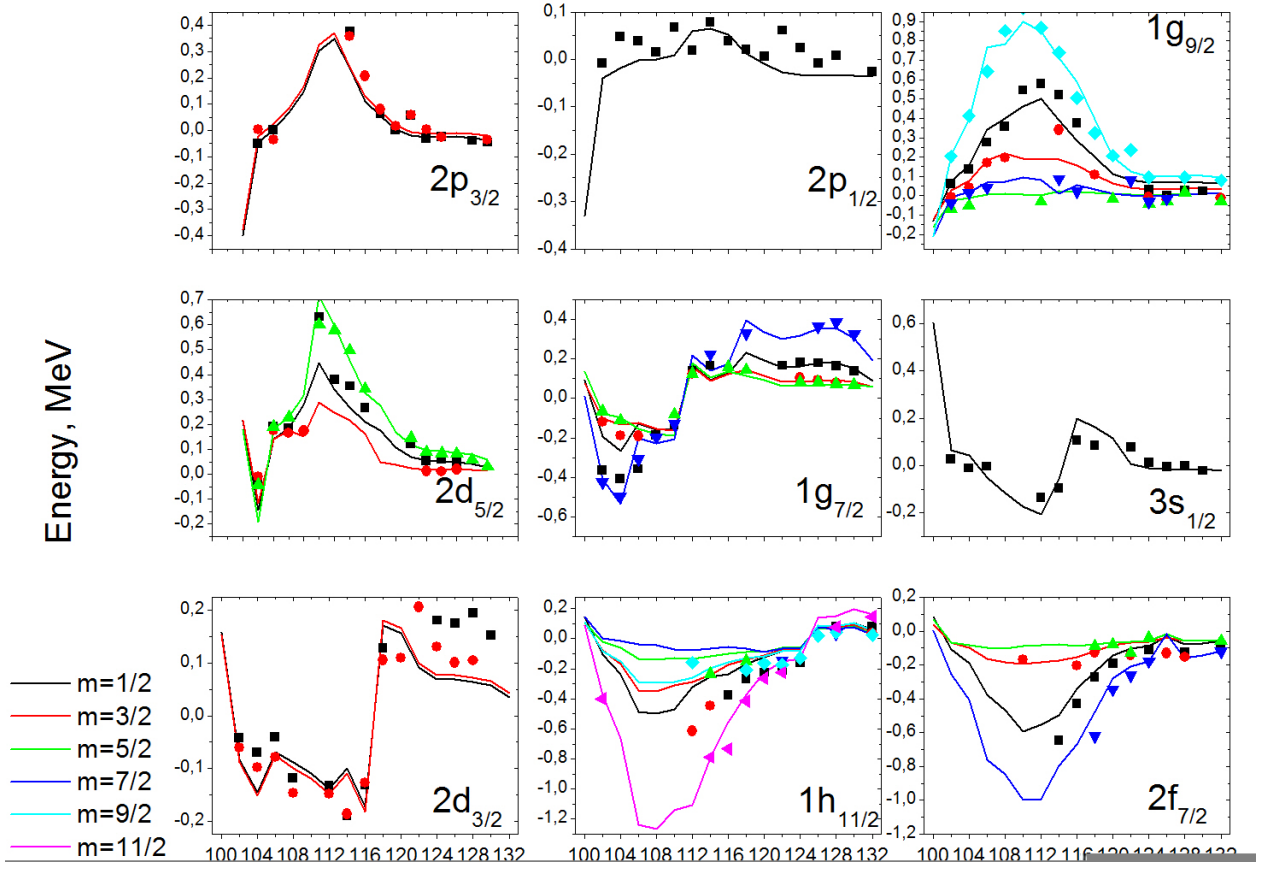
- Added (quasi)particle polarizes the nucleus. Polarization contribution is calculated with QRPA m_{-1} sum rule.

$$E_a(N+1) - E_0(N) = e_a - \sum_{\omega>0} \frac{|\langle a|H_{pv}|\omega a\rangle|^2}{\omega} + H^a_{aa} \pm \lambda$$

- Not strictly perturbation theory based. Energy shifts generally *smaller* than with second-order PT
- Comparison against blocked mean field calculations (same space and EDF) to study the accuracy.
- Useful tool with EDF fitting...

PVC

Preliminary PVC results by Dimiter Tarpanov, SLy5 + delta pairing:



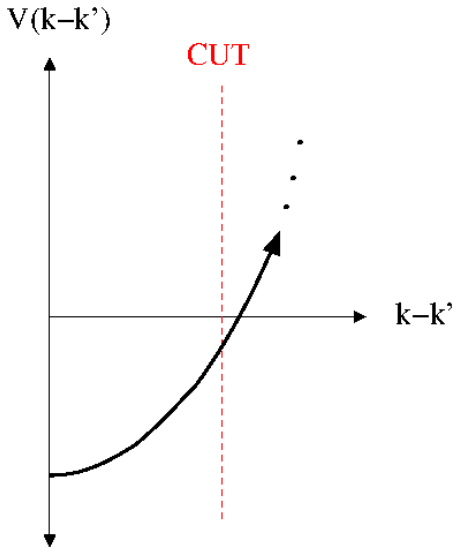
Other QRPA related projects: Correlations

Correlation energies of even-even semimagic nuclei using QRPA...

$$
\begin{aligned}
E_{corr.} &= \sum_{\omega>0} \sum_{kk'} \hbar\omega |Y^{\omega}_{kk'}|^2 \\
&= \frac{1}{4} \sum_{k<k',l<l'} \frac{|B_{kk'll'}|^2}{E_k + E_{k'} + E_l + E_{l'}} + \dots
\end{aligned}
$$

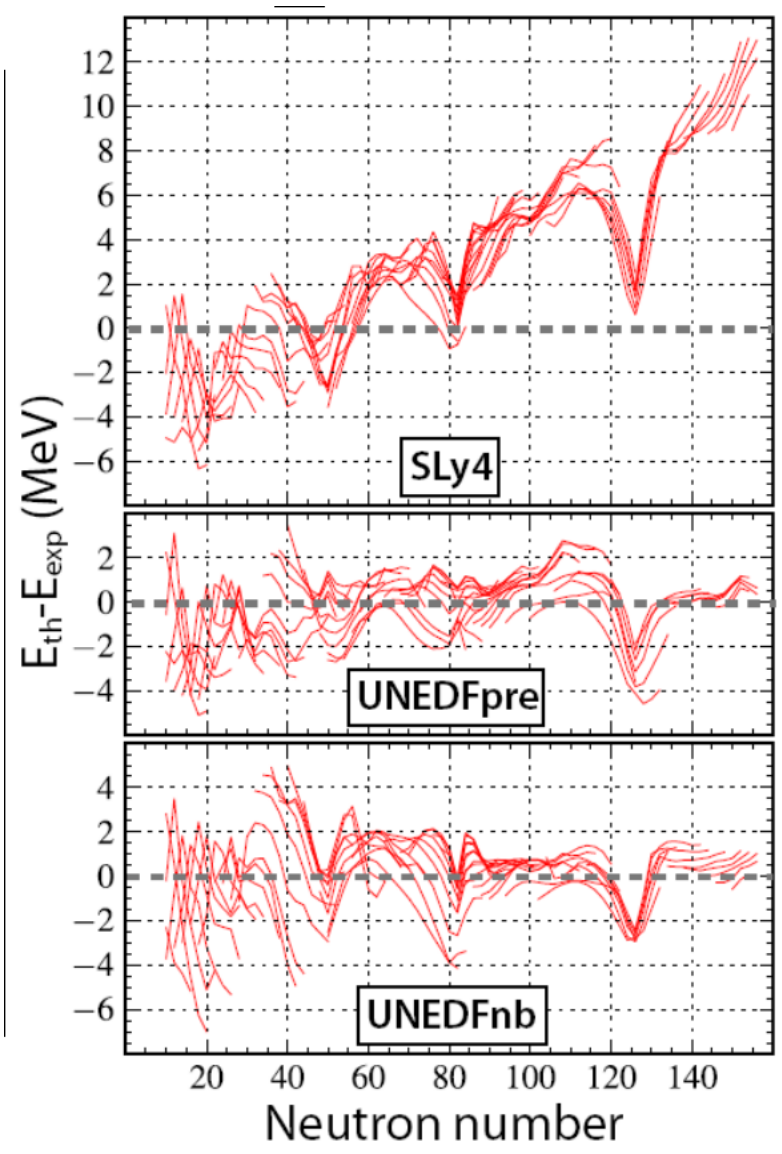
using momentum-truncated Skyrme forces.

- Skyrme ultraviolet divergence $V(k-k') \approx V_0 + \alpha(k-k')^2$
- Not a problem in very small model spaces (one major shell), but produces divergent correlation energy in large spaces.
- Skyrme forces not fitted for this...



Correlation energy

- Calculate HFB mean field and QRPA correlation energy with truncated Skyrme force and finite-range pairing force
- Fit mass formula to the total energies (HFB+QRPA)
- Study fluctuations around the average value



Summary

- We have developed some practical QRPA solution methods that fit well with the EDF prescription
- QRPA excitations without forming large matrices and without full diagonalizations (like FAM)
- Reduction of computational work
- Methods are implemented to HOSPHE, HFBTHO, HFODD