The Fidipro Deformed QRPA project: past, present and future

J. Toivanen
Dept. of Physics, University of Jyväskylä, Finland
-
and
The JYFL FiDiPro Team

March, 2010

The JYFL Fidipro team

FiDiPro = Finnish Distinguished Professor program

- Jacek Dobaczewski is since 2007 the Fidipro professor at JYFL
- Fidipro group of JYFL is funded by the university and by Finnish Academy of Sciences
- The group has currently 8 members, all nuclear theorists

Goal = Improve the accuracy and predictive power of nuclear energy density functionals.

The JYFL Fidipro team

Need for efficient QRPA solvers

RPA = Random Phase Approximation
DFT = Density Functional Theory
EDF = Energy Density Functional

- QRPA is needed to calculate transition amplitudes (beta, EM) across the nuclear chart.
- RPA can provide approximate nuclear correlation energies. (important for EDF fits).

Linear response theory and RPA

We describe nuclei using density functional theory.

- Hohenberg-Kohn theorem: If you know the exact exchange-correlation functional, you can describe all static nuclear properties using just the *density*
- Runge-Gross theorem: Time-dependent generalization of the Hohenberg-Kohn theorem.
- $\rightarrow$ TD-DFT methods can be used to gain information from nuclear excited states
- The small amplitude limit of time-dependent Kohn-Sham equations of Adiabatic TD-DFT has RPA form.
- $\rightarrow$ RPA limit is the simplest and most natural way to get information of excited states when we work in the density functional formalism.

The goal is to make accurate and well converged QRPA calculations across the nuclear chart, using existing and *improved* Skyrme functionals.

RPA as the small ampltide limit of TDHFB

TDHFB equation for the generalized density matrix $\mathcal{R}$:

$$i\hbar\frac{\partial\mathcal{R}}{\partial t} = [\mathcal{H}, \mathcal{R}] + \mathcal{F}(t) \tag{1}$$

gives us RPA-like equations after we set

$$\mathcal{R}(t) = \mathcal{R}_0 + \tilde{\mathcal{R}}e^{-i\omega t} + \tilde{\mathcal{R}}^\dagger e^{i\omega t} \tag{2}$$

and linearize the commutator equation in $\tilde{\mathcal{R}}$. The most used RPA variants are

- Particle-hole RPA
- pp-nnQRPA: Double-even ground state, double-even excitations
- pnQRPA: Double-even ground state, double-odd excitations

Large-scale QRPA calculations

The RPA-type eigen equation

$$\begin{pmatrix} \leftarrow 10^6 \rightarrow & \\ A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} \mathcal{X}_n \\ \mathcal{Y}_n \end{pmatrix} = \hbar\omega_n \begin{pmatrix} \mathcal{X}_n \\ \mathcal{Y}_n \end{pmatrix} \tag{3}$$

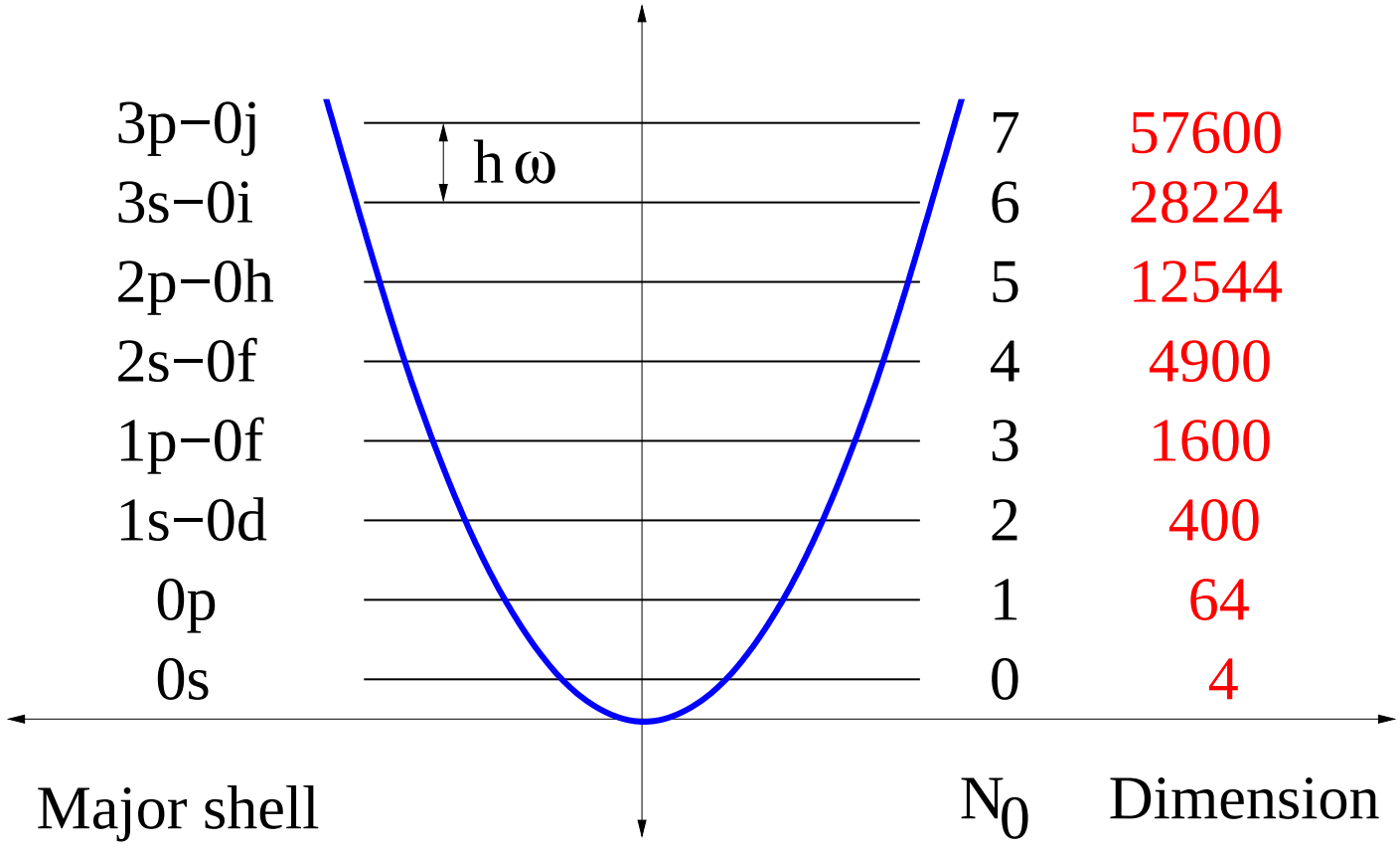
has two problems with heavy deformed nuclei:

- RPA matrix has large dimension and is dense, construction takes time
- *Full diagonalization* of large dense RPA matrix takes lots of time. Scaling of diagonalization time is $(\text{dimension})^3 = N_0^{18}$, where N_0 is the number of harmonic oscillator major shells used.

We need typically about 14 major shells of oscillator orbits to describe deformed heavy nuclei well enough.

Large-scale QRPA calculations

The dimensionality of QRPA explodes if deformation is allowed:



Large-scale QRPA calculations

Recent traditional state of the art QRPA calculations:

- J. Terasaki et al. (PRC71, 034310 (2005)): Traditional QRPA for spherical nuclei. Very large RPA dimensions, up to 40000. Calculation time was very long for each multipole (spin and parity) of each nucleus.
- C. Losa et al. (arXiv:1002.4351, submitted to PRC, thesis work): Traditional QRPA for axially deformed nuclei. Only small basis used, to have manageable QRPA dimensions.

Solution: Iterative diagonalization

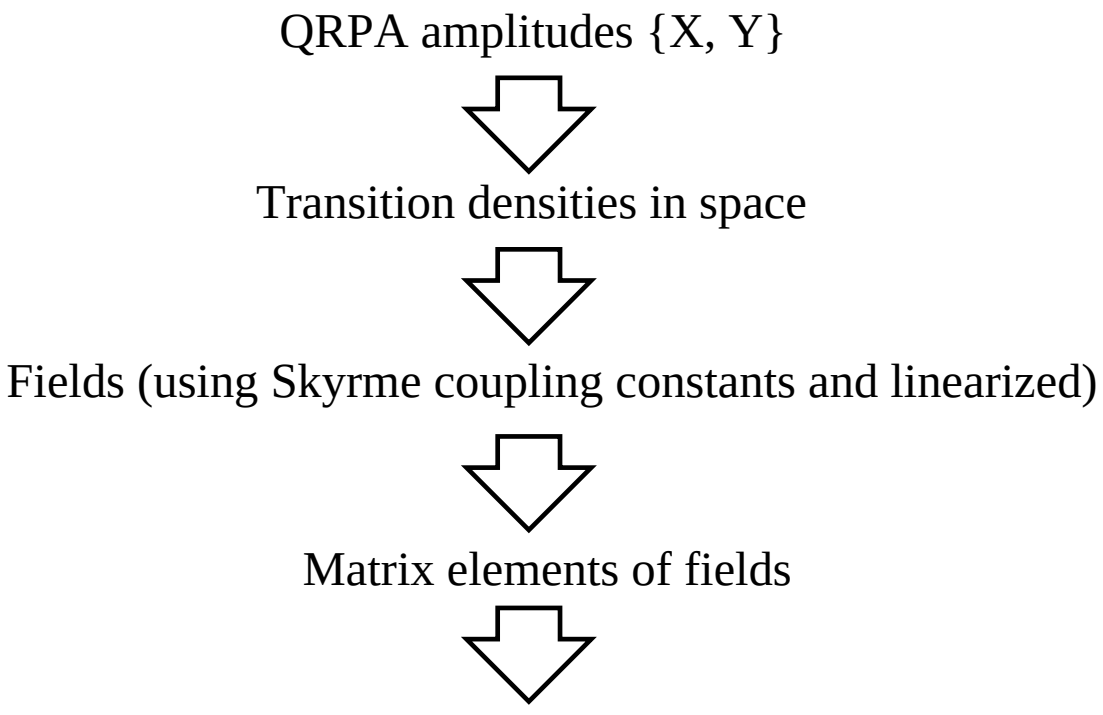
- Use non-hermitian Lanczos or Arnoldi method, do not make a full diagonalization.
- Anyway, we are not interested to know every QRPA mode exactly, only strength functions or lowest modes!

$$\begin{pmatrix} \mathcal{W}^{+} \\ \mathcal{W}'^{+} \end{pmatrix} = \begin{pmatrix} A & B \\ -B^{*} & -A^{*} \end{pmatrix} \begin{pmatrix} \mathcal{X}_n \\ \mathcal{Y}_n \end{pmatrix} \tag{4}$$

Iterative methods only need to know the result of QRPA matrix - vector products.

Modified Finite Amplitude method (FAM)

- FAM by Nakatsukasa et al. (PRC80, 044301).
- We do not have to construct the QRPA matrix at all, use time reversal non-invariant mean fields instead.



What kind of iterative diagonalization?

- Non-hermitian Arnoldi method is better than Lanczos.
- The QRPA matrix - vector products need to be stabilized.

$$\begin{pmatrix} \mathcal{W}^{+} \\ \mathcal{W}'^{+} \end{pmatrix} = \begin{pmatrix} A & B \\ -B'^{*} & -A'^{*} \end{pmatrix} \begin{pmatrix} \mathcal{X}_n \\ \mathcal{Y}_n \end{pmatrix}, \tag{5}$$

$$\begin{pmatrix} \mathcal{W}^{-} \\ \mathcal{W}'^{-} \end{pmatrix} = \begin{pmatrix} A & B \\ -B'^{*} & -A'^{*} \end{pmatrix} \begin{pmatrix} \mathcal{Y}^{*}_n \\ \mathcal{X}^{*}_n \end{pmatrix}. \tag{6}$$

$$2\begin{pmatrix} \mathcal{W} \\ \mathcal{W}' \end{pmatrix} = \begin{pmatrix} \mathcal{W}^{+} - \mathcal{W}'^{-*} \\ \mathcal{W}'^{+} - \mathcal{W}^{-*} \end{pmatrix} = \begin{pmatrix} A + A' & B + B' \\ -(B + B')^{*} & -(A + A')^{*} \end{pmatrix} \begin{pmatrix} \mathcal{X}_n \\ \mathcal{Y}_n \end{pmatrix}.$$

The best iterative diagonalization

The Arnoldi procedure:

$$\begin{pmatrix} \tilde{\mathcal{X}}^{k+1} \\ \tilde{\mathcal{Y}}^{k+1} \end{pmatrix} = \begin{pmatrix} \mathcal{W}_+^k \\ \mathcal{W}'^{\,k}_+ \end{pmatrix} - \sum_{i=1}^{k} \begin{pmatrix} \mathcal{X}^i \\ \mathcal{Y}^i \end{pmatrix} a_{ik} + \sum_{i=1}^{k} \begin{pmatrix} \mathcal{Y}^{i*} \\ \mathcal{X}^{i*} \end{pmatrix} b_{ik} \,, \tag{7}$$

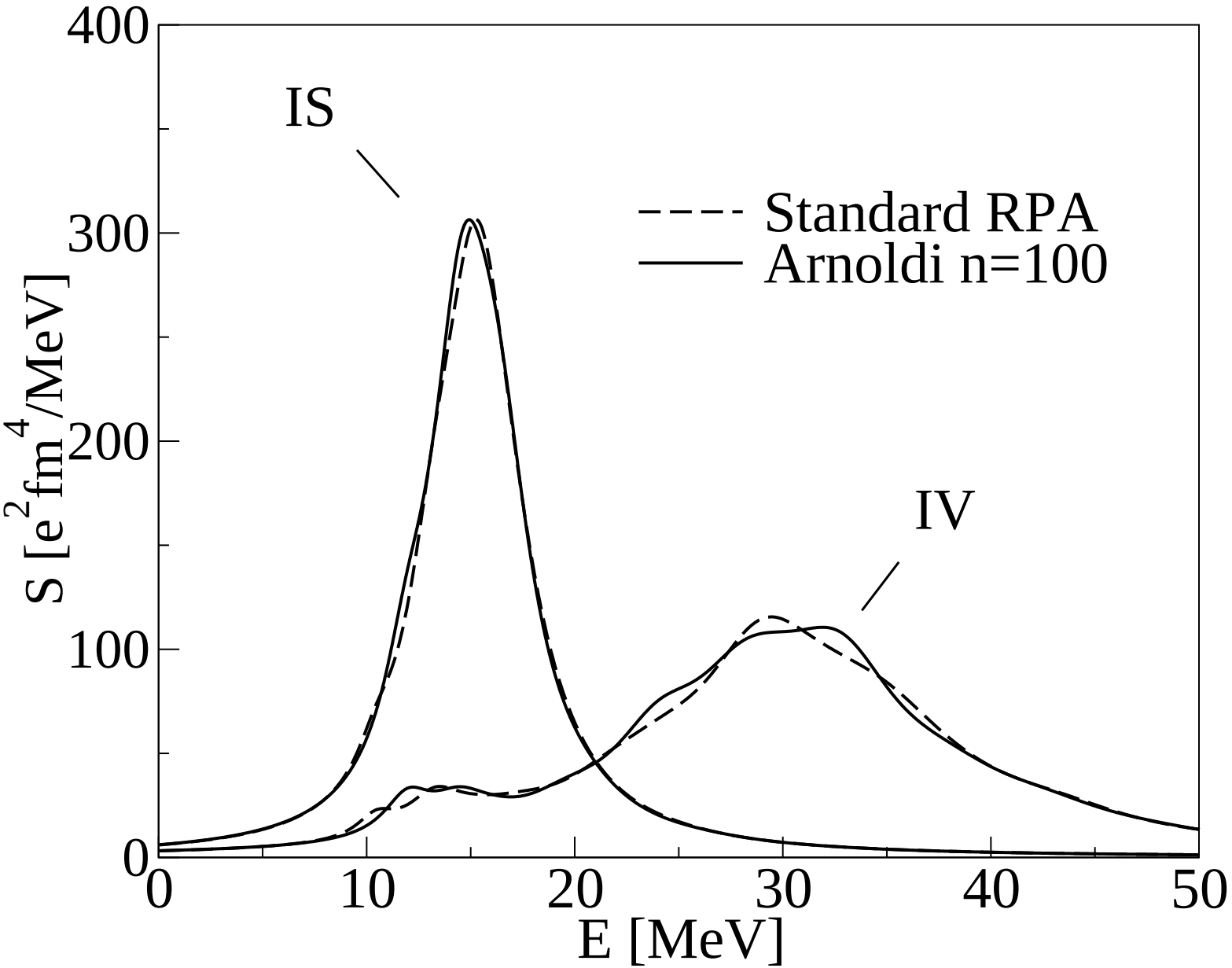
$$\begin{pmatrix} \tilde{\mathcal{Y}}^{k+1*} \\ \tilde{\mathcal{X}}^{k+1*} \end{pmatrix} = -\begin{pmatrix} \mathcal{W}_-^k \\ \mathcal{W}'^{\,k}_- \end{pmatrix} + \sum_{i=1}^{k} \begin{pmatrix} \mathcal{X}^i \\ \mathcal{Y}^i \end{pmatrix} b'^{*}_{ik} - \sum_{i=1}^{k} \begin{pmatrix} \mathcal{Y}^{i*} \\ \mathcal{X}^{i*} \end{pmatrix} a'^{*}_{ik} \,, \tag{8}$$

Spurious modes in RPA

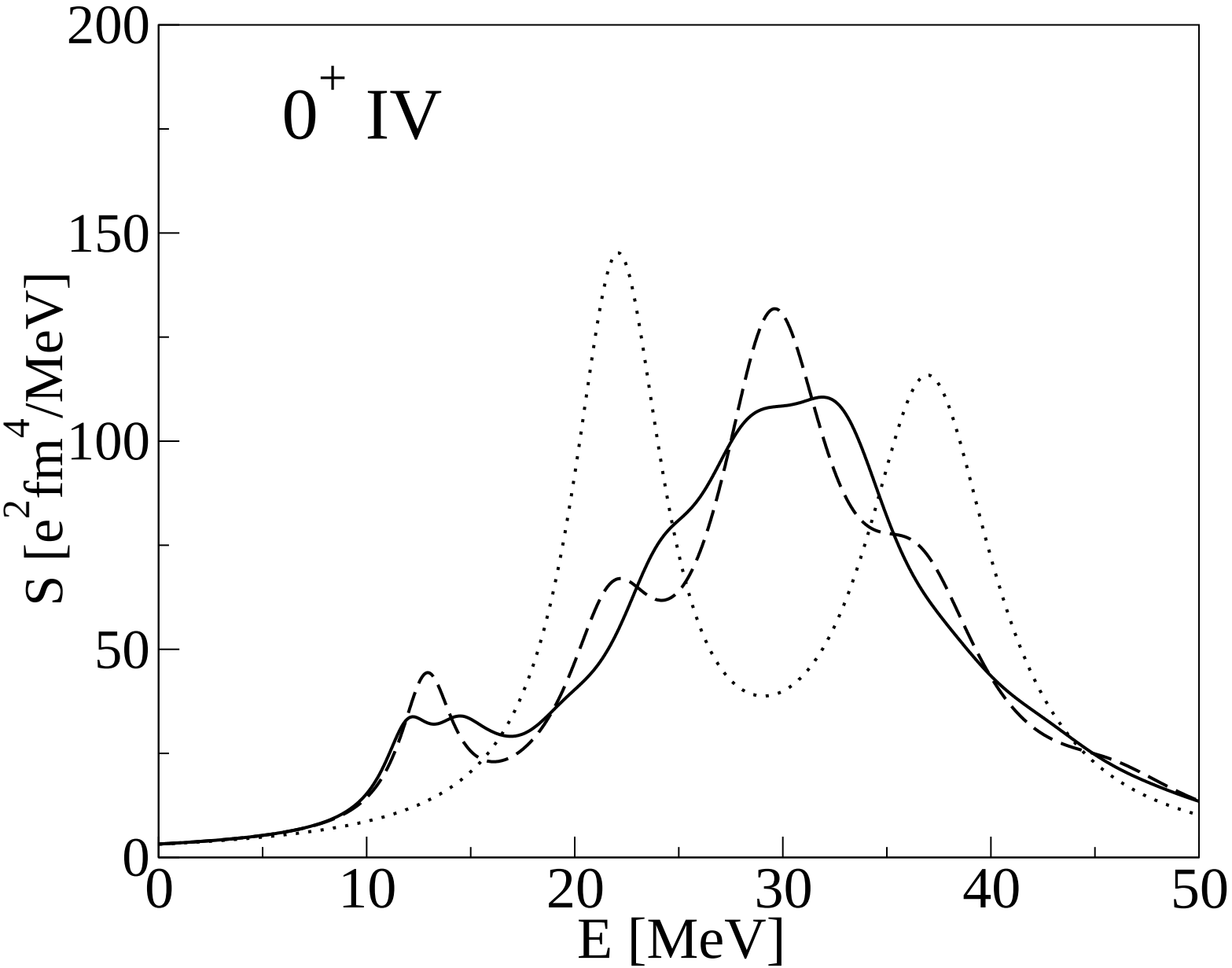
- For each broken symmetry of the mean field RPA decouples a spurious mode from the physical modes.
- In iterative diagonalization the RPA modes are constructed orthogonal to the spurious modes.

$$\begin{pmatrix} \tilde{\mathcal{X}}^{k+1} \\ \tilde{\mathcal{Y}}^{k+1} \end{pmatrix} = \begin{pmatrix} \tilde{\mathcal{X}}^{k+1} \\ \tilde{\mathcal{Y}}^{k+1} \end{pmatrix} - \lambda \begin{pmatrix} \tilde{\mathcal{P}} \\ \tilde{\mathcal{P}}^{*} \end{pmatrix} - \mu \begin{pmatrix} \tilde{\mathcal{R}} \\ \tilde{\mathcal{R}}^{*} \end{pmatrix}$$

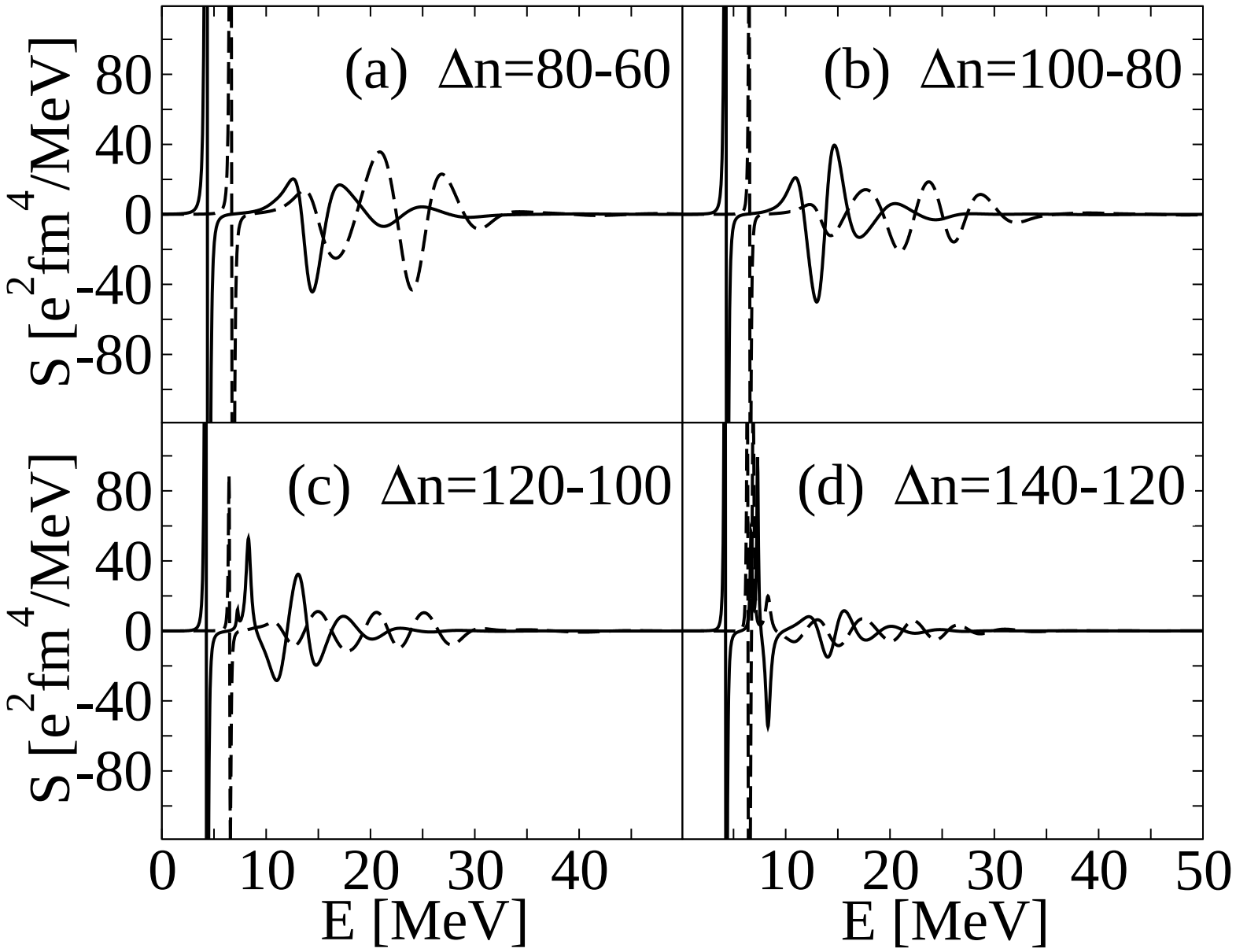
Arnoldi + stabilization, $J^\pi = 0^+$



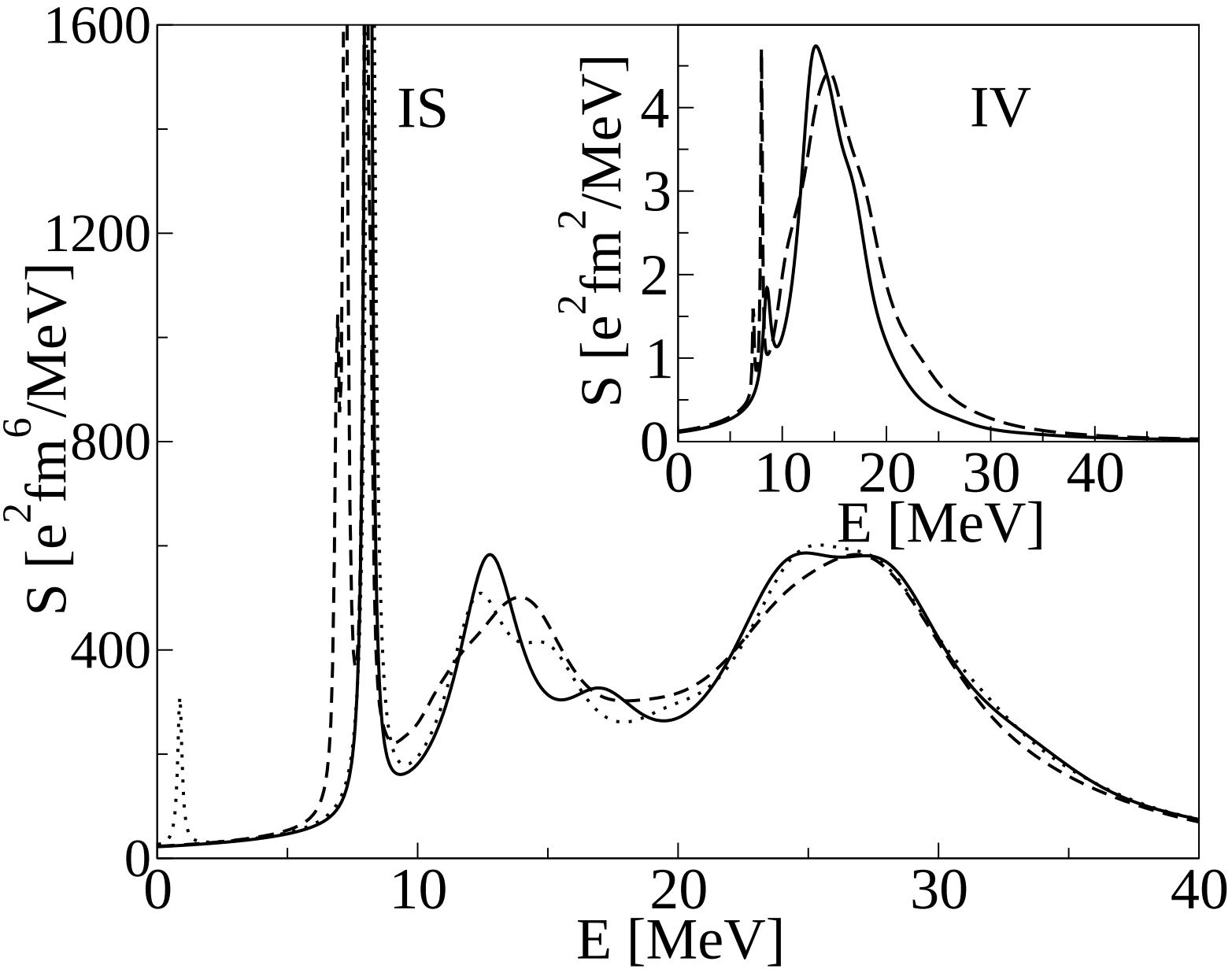
Arnoldi + stabilization, $J^\pi = 0^+$



Arnoldi + stabilization, $J^\pi = 2^+$



Arnoldi + stabilization, $J^\pi = 1^-$



The code HOSPHE

Solution of self-consistent equations for the N^{3}LO nuclear energy density functional in spherical symmetry. The program HOSPHE (v1.00)

B.G. Carlsson[a], J. Dobaczewski[a,b], J. Toivanen[a], P. Veselý[a]

[a] *Department of Physics, P.O. Box 35 (YFL), FI-40014 University of Jyväskylä, Finland*
[b] *Institute of Theoretical Physics, University of Warsaw, Hoża 69, PL-00681 Warsaw, Poland*

Abstract

We present solution of self-consistent equations for the N^{3}LO nuclear energy density functional. We derive general expressions for the mean fields expressed as differential operators depending on densities and for the densities expressed in terms of derivatives of wave functions. These expressions are then specified to the case of spherical symmetry. We also present the computer program HOSPHE (v1.00), which solves the self-consistent equations by using the expansion of single-particle wave functions on the spherical harmonic oscillator basis.

Key words: Hartree-Fock, Skyrme interaction, nuclear energy density functional, self-consistent mean-field

The code HOSPHE-RPA

PHYSICAL REVIEW C **00**, 004300 (2010)

Linear response strength functions with iterative Arnoldi diagonalization

J. Toivanen,[1] B. G. Carlsson,[1] J. Dobaczewski,[1,2] K. Mizuyama,[1] R. R. Rodríguez-Guzmán,[1] P. Toivanen,[1] and P. Veselý[1]
[1]*Department of Physics, University of Jyväskylä, FIN-40014, Finland*
[2]*Institute of Theoretical Physics, Warsaw University, PL-00681, Warsaw, Poland*
(Received 16 December 2009; published xxxxx)

We report on an implementation of a new method to calculate random phase approximation (RPA) strength functions with iterative non-Hermitian Arnoldi diagonalization method, which does not explicitly calculate and store the RPA matrix. We discuss the treatment of spurious modes, numerical stability, and how the method scales as the used model space is enlarged. We perform the particle-hole RPA benchmark calculations for double magic nucleus ^{132}Sn and compare the resulting electromagnetic strength functions against those obtained within the standard RPA.

The code HOSPHE-RPA

- HOSPHE-RPA with N3LO extended Skyrme functional (See first paper at arXiv0912.3234v1, accepted to PRC)
- Ground state and RPA calculations are consistent → no RPA collapse!
- Uses Arnoldi method to solve the RPA equations approximately.
- Orthogonalizes the physical modes against spurious RPA modes.
- Strength functions calculated using moment method.

Future of HOSPHE ... HOSPHE-QRPA

- HOSPHE-QRPA (spherical) is almost ready, uses zero-range and separable pairing (J.T., Petr Vesely, B. G. Carlsson).
- HOSPHE-pnQRPA needed for beta decay.
- Inclusion of Berggren basis to HOSPHE, continuum calculations using N3LO EDF (Nicholas Michel)
- Final stage of HOSPHE development is axial/triaxial version.

HFODD-QRPA

Persons currently involved in this project are Alessandro Pastore, Jacek Dobaczewski and J.T.

- Works for both axially and triaxially deformed nuclei
- The internal machinery of HFODD used to make QRPA matrix-vector products.

Challenges:

- Modifying an existing code can be hard
- All spurious RPA modes always present

Summary

- We know now how to make fully consistent, large-scale RPA or QRPA calculations without forming the RPA matrix and without having to construct all RPA eigenmodes (proof of principle done).
- Spherical HF/RPA code HOSPHE-RPA is ready and works, HFB/QRPA code HOSPHE-QRPA is in final stages of completion.
- The QRPA solvers will eventually be published.

Thank you!