RPA strength functions in nuclei with iterative Arnoldi diagonalization

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Outline

1. Nuclear energy density functional.
2. Basics of the fast RPA and QRPA + Arnoldi method
3. Tricks of the trade.
4. Results for the multipole vibrations in spherical nuclei
5. Scaling properties
6. Plans and perspectives.

Nuclear Energy Density Functional

We consider the EDF in the form,

$$\mathcal{E} = \int d^3r \mathcal{H}(r),$$

where the energy density $\mathcal{H}(r)$ can be represented as a sum of the kinetic energy and of the potential-energy isoscalar ($t = 0$) and isovector ($t = 1$) terms,

$$\mathcal{H}(r) = \frac{\hbar^2}{2m}\tau_0 + \mathcal{H}_0(r) + \mathcal{H}_1(r),$$

which for the time-reversal and spherical symmetries imposed read:

$$\mathcal{H}_t(r) = C_t^\rho \rho_t^2 + C_t^\tau \rho_t \tau_t + C_t^{\Delta\rho} \rho_t \Delta\rho_t + \tfrac{1}{2} C_t^J J_t^2 + C_t^{\nabla J} \rho_t \nabla \cdot J_t.$$

Following the parametrization used for the Skyrme forces, we assume the dependence of the coupling parameters C_t^ρ on the isoscalar density ρ_0 as:

$$C_t^\rho = C_{t0}^\rho + C_{t\mathrm{D}}^\rho \rho_0^\alpha.$$

The standard EDF depends linearly on 12 coupling constants,

$$C_{t0}^\rho,\ C_{t\mathrm{D}}^\rho,\ C_t^\tau,\ C_t^{\Delta\rho},\ C_t^{\mathrm{J}},\ \text{and}\ C_t^{\nabla\mathrm{J}},$$

for $t = 0$ and 1.

Iterative methods to solve RPA have been proposed and used often in the past:

- P. G. Reinhard, Ann. Phys. 1, 632 (1992) – P, Q method, related to iterative diagonalization
- C. W. Johnson, G. F. Bertsch and W. D. Hazelton, Computer Physics Communications **120**, 155-161 (1999), physics/9802014v1 – Non-hermitian Lanczos, satisfies some energy weighed sum rules
- T. Nakatsukasa et al., PRC 76, 024318 (2007). – Efficient way to calculate RPA matrix-vector products (finite amplitude method)
- S. Tretiak et al., J. Chem. Phys. 130, 054111 (2009). – RPA + Lanczos for large molecules, photoabsorption spectra
- Iterative RPA solvers already in popular electronic structure packages (e.g. GAMESS UK)

In nuclear physics iterative RPA solvers not readily available

Fast RPA and QRPA + Arnoldi method

Within RPA, let ρ denote the one-body projective density matrix, $\rho^2 = \rho$, and $h(\rho) = \partial E/\partial\rho$ denote the mean-field Hamiltonian calculated for ρ. The TDHF equation for $\rho(t)$ then reads:

$$i\hbar\frac{d}{dt}\rho = [h(\rho), \rho].$$

The RPA method approximates the TDHF solution by a single-mode vibrational state $\rho(t)$ in the vibrating mean field $h(t) = h(\rho(t))$:

$$\rho(t) = \rho_0 + \tilde{\rho}e^{-i\omega t} + \tilde{\rho}^+e^{i\omega t}, \qquad h(t) = h_0 + \tilde{h}e^{-i\omega t} + \tilde{h}^+e^{i\omega t}$$

where ρ_0 is the self-consistent solution, $[h_0, \rho_0] = 0$ for $h_0 = h(\rho_0)$, $\tilde{\rho}$ is the RPA amplitude, and $\tilde{h} = h(\tilde{\rho})$. This allows for transforming the TDHF into the RPA equation in the form

$$\hbar\omega\tilde{\rho} = \mathrm{H}_0\tilde{\rho} = [h_0, \tilde{\rho}] + [\tilde{h}, \rho_0],$$

by which the right-hand side becomes a linear operator H_0 depending on ρ_0 and acting on $\tilde{\rho}$.

The RPA equation can be written explicitly in terms of the particle-hole and hole-particle matrix elements as:

$$\begin{aligned}\hbar\omega\tilde{\rho}_{\omega,mi} &= (\epsilon_m - \epsilon_i)\,\tilde{\rho}_{\omega,mi} + \tilde{h}_{\omega,mi}\,,\\ \hbar\omega\tilde{\rho}_{\omega,im} &= (\epsilon_i - \epsilon_m)\,\tilde{\rho}_{\omega,im} - \tilde{h}_{\omega,im}\,,\end{aligned}$$

We solve this problem by using an iterative method that during each iteration only needs to know the product of the RPA matrix and a density vector, that is, the right-hand sides of the preceding equations:

$$\begin{aligned}W^k_{mi} &= (\epsilon_m - \epsilon_i)\,X^k_{mi} + \tilde{h}_{mi}(\mathcal{X}^k,\mathcal{Y}^k) = \left(A\mathcal{X}^k + B\mathcal{Y}^k\right)_{mi}\,,\\ W'^k_{mi} &= (\epsilon_i - \epsilon_m)\,Y^k_{mi} - \tilde{h}_{im}(\mathcal{X}^k,\mathcal{Y}^k) = \left(-B'^*\mathcal{X}^k - A'^*\mathcal{Y}^k\right)_{mi}\,,\end{aligned}$$

where index k labels iterations and the mean fields $\tilde{h}(\mathcal{X}^k,\mathcal{Y}^k)$ depend linearly on the density vectors $\mathcal{X}^k$ and $\mathcal{Y}^k$. :

$$\begin{pmatrix}\mathcal{W}^k_+\\ \mathcal{W}'^k_+\end{pmatrix} = \begin{pmatrix}A & B\\ -B'^* & -A'^*\end{pmatrix}\begin{pmatrix}\mathcal{X}^k\\ \mathcal{Y}^k\end{pmatrix}, \quad \begin{pmatrix}\mathcal{W}^k_-\\ \mathcal{W}'^k_-\end{pmatrix} = \begin{pmatrix}A & B\\ -B'^* & -A'^*\end{pmatrix}\begin{pmatrix}\mathcal{Y}^{k*}\\ \mathcal{X}^{k*}\end{pmatrix}$$

In exact arithmetic $A = A'$ and $B = B'$ and therefore either of these equations could be used in the iteration procedure with equivalent results. Nevertheless, below we use them both to stabilize the iteration process.

Fast and converging algorithm is obtained by using the following tricks:

1. Calculate the mean fields $\tilde{\rho}_{\omega,mi} \Longrightarrow \tilde{h}_{\omega,mi}$ in three steps that are exactly analogous to the HF method for ρ_0, namely:
   - $\psi_m(\vec{r}\sigma') = \sum_i \tilde{\rho}_{\omega,mi}\phi_i(\vec{r}\sigma), \quad \tilde{\rho}(\vec{r}\sigma'\sigma) = \sum_m \phi_m(\vec{r}\sigma')\psi^*_m(\vec{r}\sigma)$
   - $\tilde{h}(\vec{r}\sigma'\sigma) = \delta E/\delta\tilde{\rho}^*(\vec{r}\sigma'\sigma)$
   - $\tilde{h}_{\omega,mi} = \int \mathrm{d}^3\vec{r} \sum_{\sigma'\sigma} \phi^*_m(\vec{r}\sigma')\tilde{h}(\vec{r}\sigma'\sigma)\phi_i(\vec{r}\sigma)$
2. Reduce the numerical errors in the matrix-vector products by symmetrization to get the final stabilized RPA matrix-vector product,
$$\begin{pmatrix} \mathcal{W}^k \\ \mathcal{W}'^k \end{pmatrix} = \frac{1}{2}\begin{pmatrix} \mathcal{W}^k_+ - \mathcal{W}'^{\,k*}_- \\ \mathcal{W}'^{\,k}_+ - \mathcal{W}^{k*}_- \end{pmatrix}$$
3. Use the non-hermitian Arnoldi method instead of the non-hermitian Lanczos method, that is, orthogonalize each new basis vector against all previous basis vectors and their opposite norm partners:
$$\begin{pmatrix} \tilde{\mathcal{X}}^{k+1} \\ \tilde{\mathcal{Y}}^{k+1} \end{pmatrix} = \begin{pmatrix} \mathcal{W}^k \\ \mathcal{W}'^k \end{pmatrix} - \sum_{p=1}^{k} \begin{pmatrix} \mathcal{X}^p \\ \mathcal{Y}^p \end{pmatrix} a_{pk} + \sum_{p=1}^{k} \begin{pmatrix} \mathcal{Y}^{p*} \\ \mathcal{X}^{p*} \end{pmatrix} b_{pk}$$
   where a_{pk} and b_{pk} are the overlap matrices.

4. For the positive norm of the residual vector $\tilde{N}^{k+1} = \langle \tilde{X}^{k+1}, \tilde{Y}^{k+1} | \tilde{X}^{k+1}, \tilde{Y}^{k+1} \rangle > 0$, define the new normalized positive-norm basis vector as

$$X_{mi}^{k+1} = \frac{1}{\sqrt{\tilde{N}^{k+1}}} \tilde{X}_{mi}^{k+1}, \quad Y_{mi}^{k+1} = \frac{1}{\sqrt{\tilde{N}^{k+1}}} \tilde{Y}_{mi}^{k+1}.$$

If $\tilde{N}^{k+1} < 0$, the new normalized positive norm basis vector is defined as

$$X_{mi}^{k+1} = \frac{1}{\sqrt{-\tilde{N}^{k+1}}} \tilde{Y}_{mi}^{k+1*}, \quad Y_{mi}^{k+1} = \frac{1}{\sqrt{-\tilde{N}^{k+1}}} \tilde{X}_{mi}^{k+1*}.$$

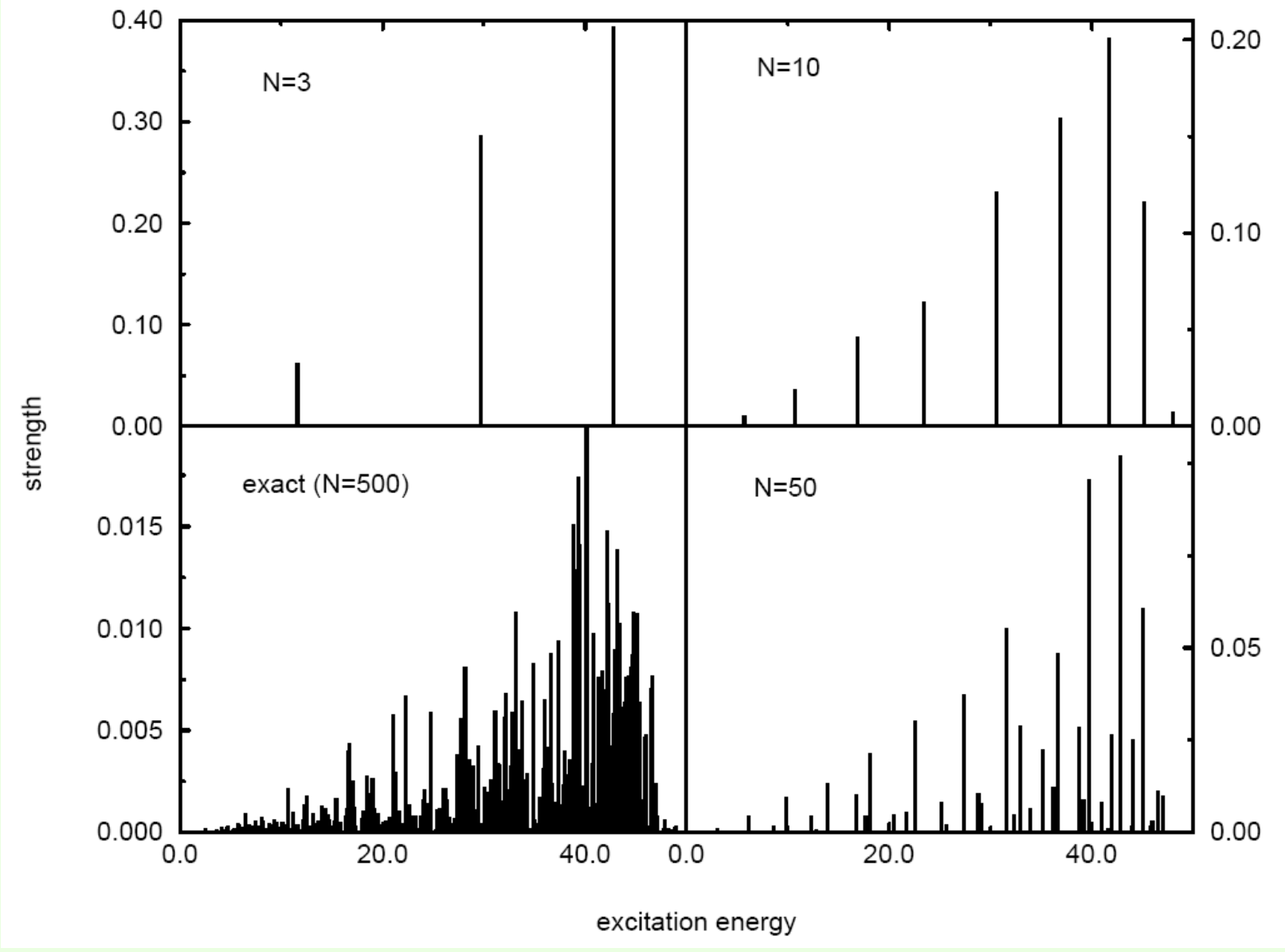
5. During the Arnoldi iteration orthogonalize the basis with respect to the position and momentum vectors:

$$\begin{pmatrix} \mathcal{X}_k \\ \mathcal{Y}_k \end{pmatrix}_{phys.} = \begin{pmatrix} \mathcal{X}_k \\ \mathcal{Y}_k \end{pmatrix} - \lambda \begin{pmatrix} \mathcal{P} \\ \mathcal{P}^* \end{pmatrix} - \mu \begin{pmatrix} \mathcal{R} \\ \mathcal{R}^* \end{pmatrix}$$

where the overlaps λ and μ are defined as

$$\lambda = \frac{\langle R, R^* | X^k, Y^k \rangle}{\langle R, R^* | P, P^* \rangle}, \quad \mu = -\frac{\langle P, P^* | X^k, Y^k \rangle}{\langle R, R^* | P, P^* \rangle}.$$

Figure taken from C. W. Johnson, G. F. Bertsch and W. D. Hazelton, Computer Physics Communications **120**, 155-161 (1999).



Linear response strength functions with iterative Arnoldi diagonalization

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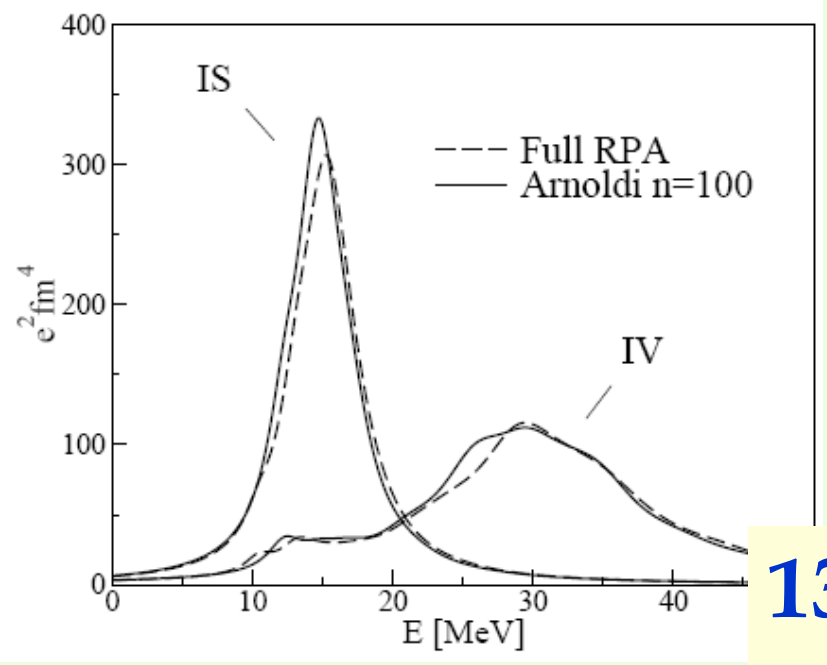
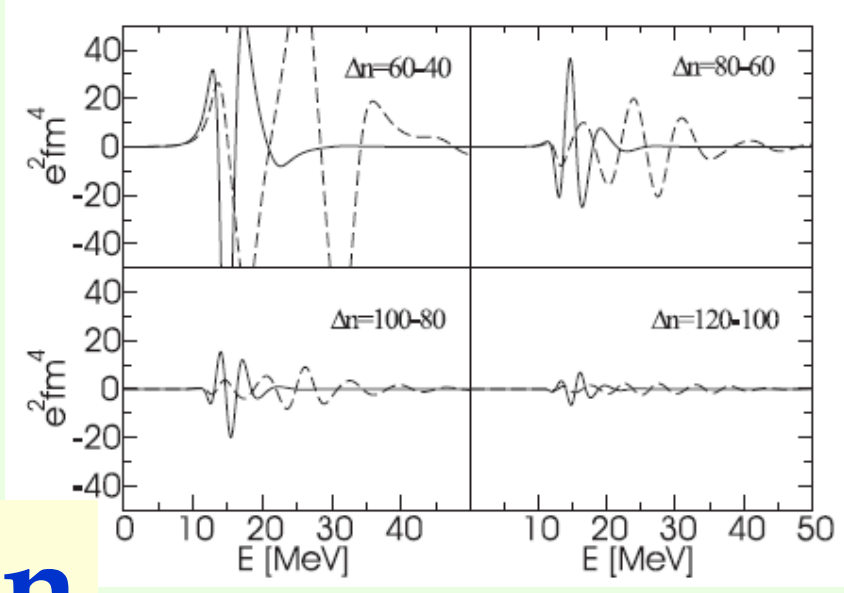
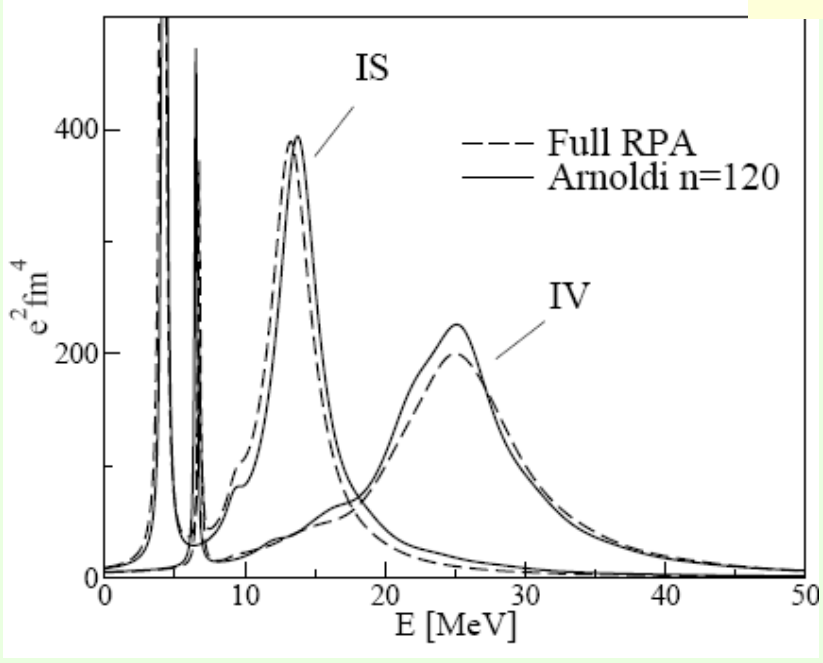


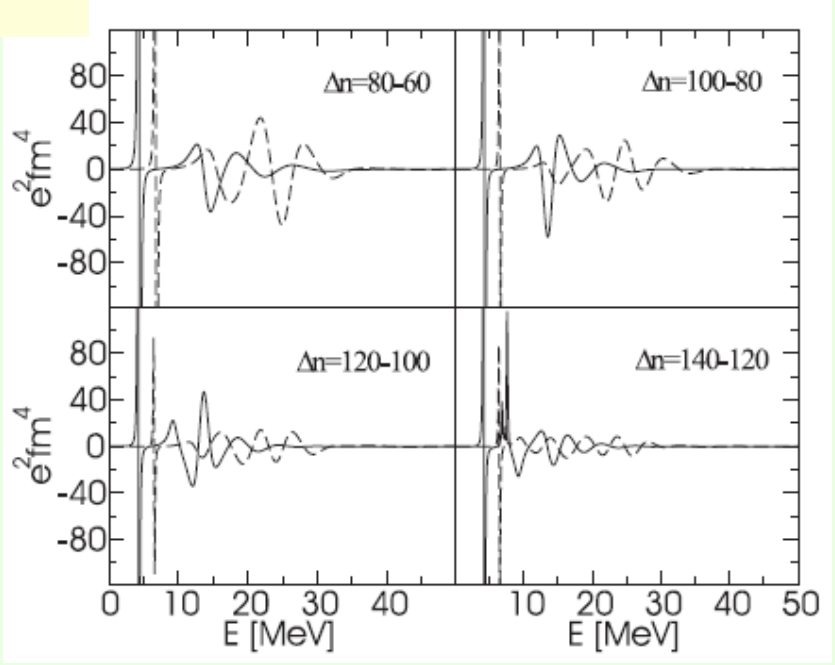
0^+



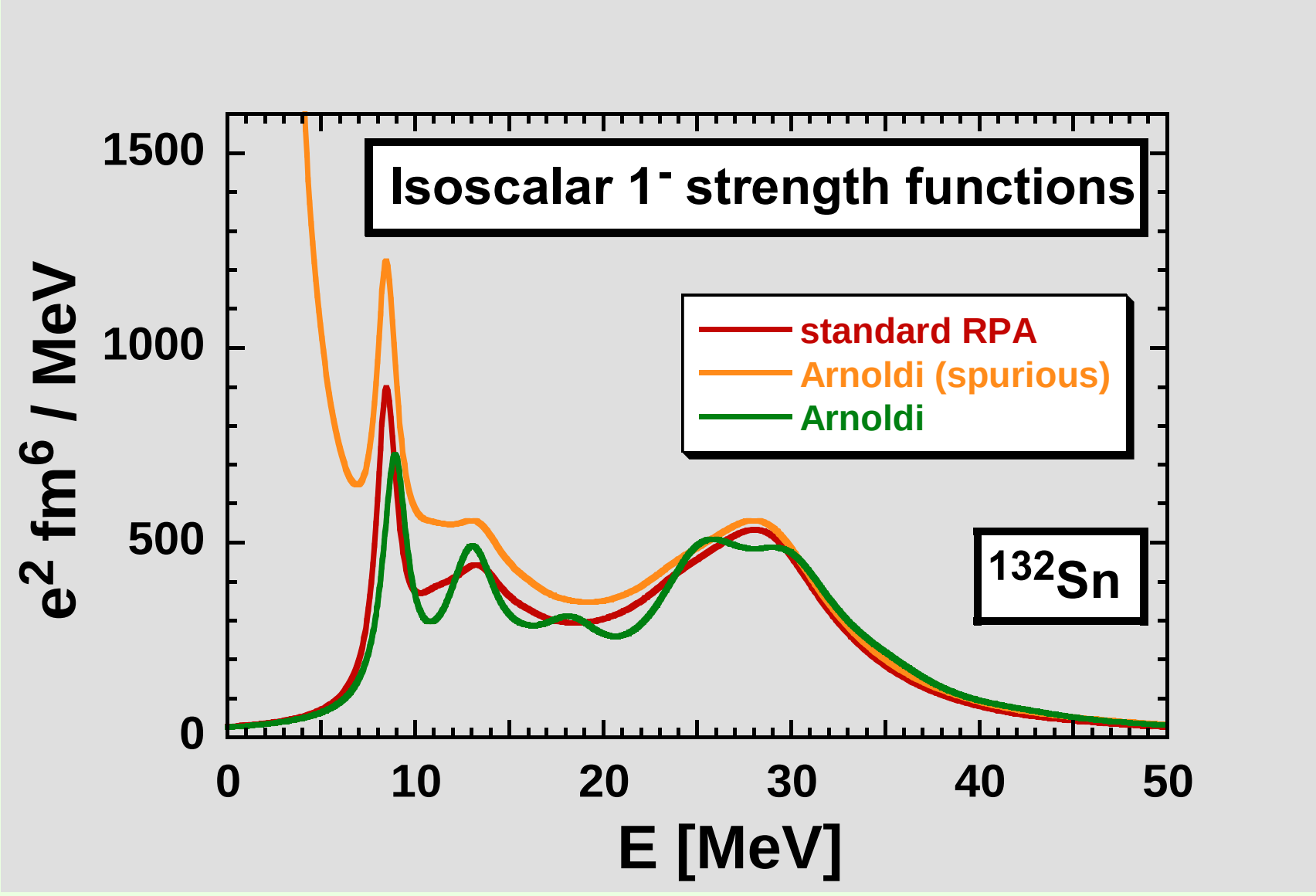
^{132}Sn



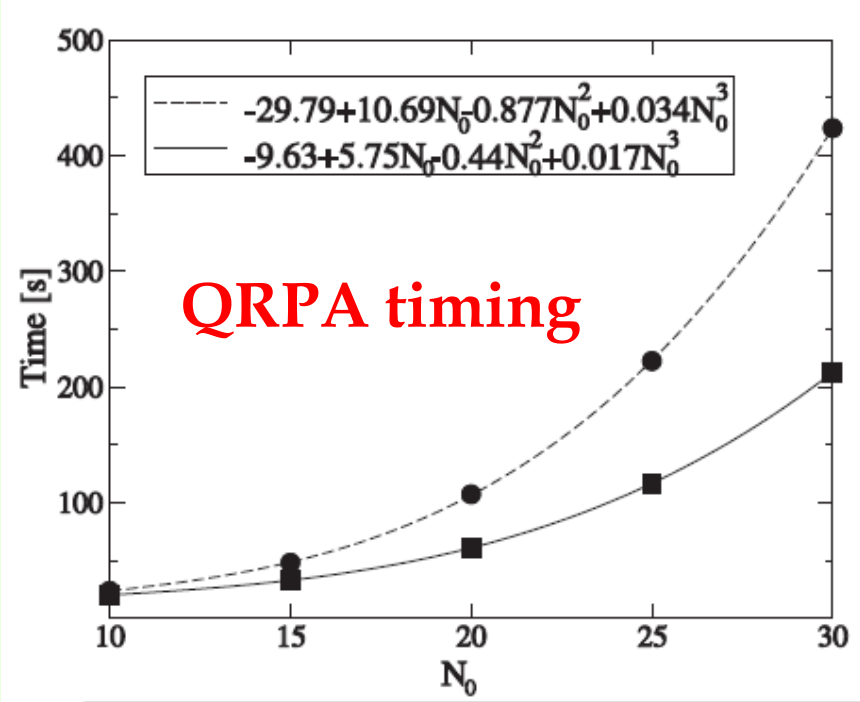
2^+



Removal of spurious modes



Scaling properties



- Spherical QRPA+Arnoldi scales linearly with the size of the single-particle space Ω.
- Deformed QRPA+Arnoldi expected to scale quadratically, that is, as Ω^2
- Standard QRPA scales quartically, that is, as Ω^4 !

Future plans:

- Full implementation and testing of the spherical QRPA + Arnoldi method in the code HOSPHE with new-generation separable pairing interactions. Systematic calculations of multipole giant-resonance modes to be used in the EDF adjustments.
- Deformed QRPA + Arnoldi method implemented in the code HFODD. Systematic calculations of β-decay strengths functions and β-delayed neutron emission probabilities to be used in the EDF adjustments.

Collaborators

FIDIPRO team at the University of Jyväskylä

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Nuclear densities as composite fields

Density matrix:

$$\rho(\vec{r}\sigma,\vec{r}'\sigma') = \langle\Phi|a^+(\vec{r}'\sigma')a(\vec{r}\sigma)|\Phi\rangle$$

Scalar and vector part:

$$\rho(\vec{r},\vec{r}') = \sum\nolimits_\sigma \rho(\vec{r}\sigma,\vec{r}'\sigma)$$
$$\vec{s}(\vec{r},\vec{r}') = \sum\nolimits_{\sigma\sigma'} \rho(\vec{r}\sigma,\vec{r}'\sigma')\langle\sigma'|\vec{\sigma}|\sigma\rangle$$

Symmetries:

$$\rho^T(\vec{r},\vec{r}') = \rho^*(\vec{r},\vec{r}') = \rho(\vec{r}',\vec{r})$$
$$\vec{s}^T(\vec{r},\vec{r}') = -\vec{s}^*(\vec{r},\vec{r}') = -\vec{s}(\vec{r}',\vec{r})$$

Local densities:

Matter:	$\rho(\vec{r}) = \rho(\vec{r},\vec{r})$
Momentum:	$\vec{j}(\vec{r}) = (1/2i)[(\vec{\nabla}-\vec{\nabla}')\rho(\vec{r},\vec{r}')]_{r=r'}$
Kinetic:	$\tau(\vec{r}) = [\vec{\nabla}\cdot\vec{\nabla}'\rho(\vec{r},\vec{r}')]_{r=r'}$
Spin:	$\vec{s}(\vec{r}) = \vec{s}(\vec{r},\vec{r})$
Spin momentum:	$J_{\mu\nu}(\vec{r}) = (1/2i)[(\nabla_\mu-\nabla'_\mu)s_\nu(\vec{r},\vec{r}')]_{r=r'}$
Spin kinetic:	$\vec{T}(\vec{r}) = [\vec{\nabla}\cdot\vec{\nabla}'\vec{s}(\vec{r},\vec{r}')]_{r=r'}$
Tensor kinetic:	$\vec{F}(\vec{r}) = \frac{1}{2}[(\vec{\nabla}\otimes\vec{\nabla}'+\vec{\nabla}'\otimes\vec{\nabla})\cdot\vec{s}(\vec{r},\vec{r}')]_{r=r'}$