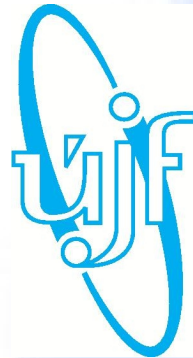


Computational challenges in nuclear energy density functional methods



Petr Veselý

Nuclear Physics Institute, Czech Academy of Sciences

www-ucjf.troja.mff.cuni.cz/~vesely/

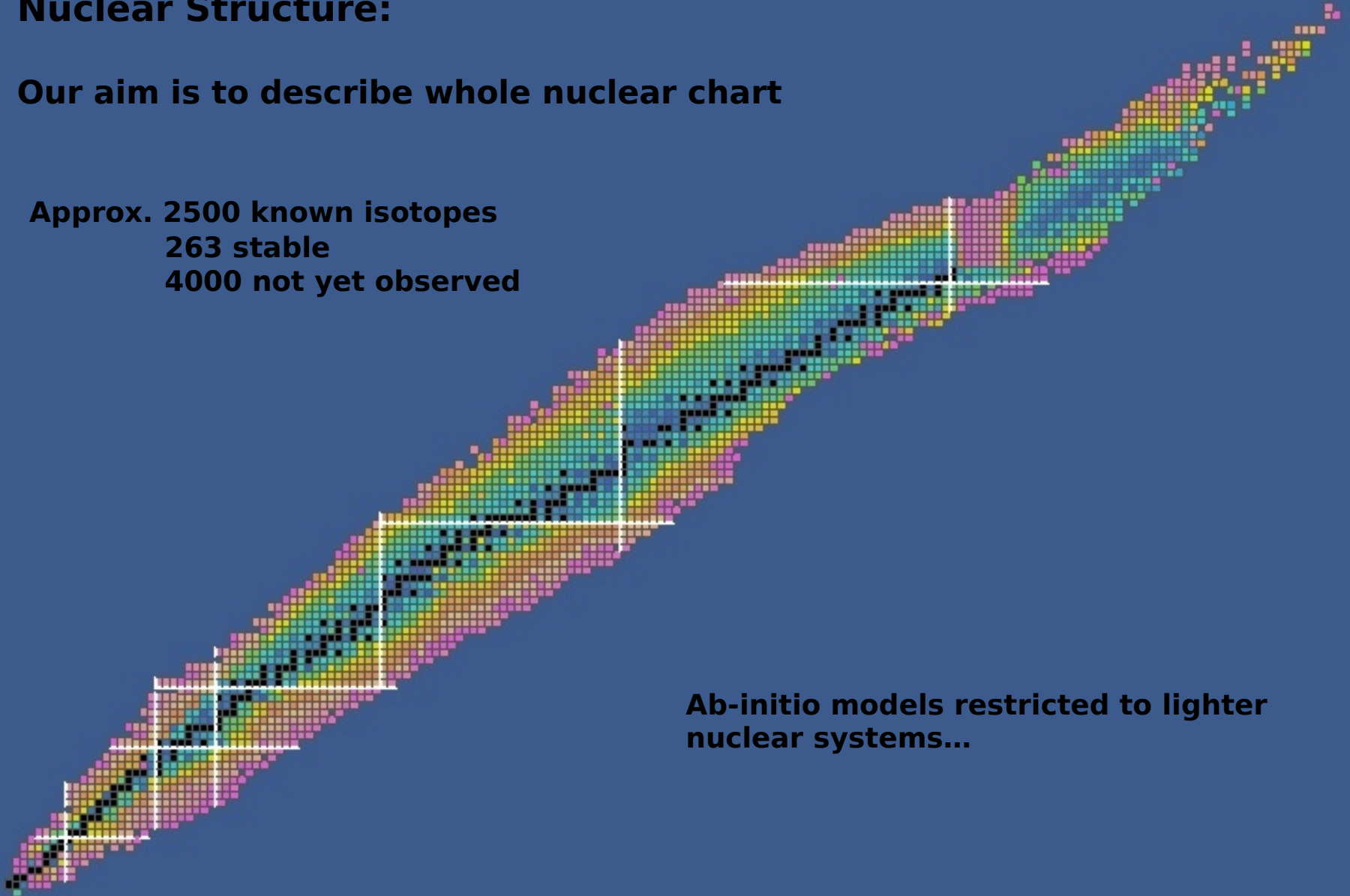
April 2017

Introduction

Nuclear Structure:

Our aim is to describe whole nuclear chart

Approx. 2500 known isotopes
263 stable
4000 not yet observed



Ab-initio models restricted to lighter nuclear systems...

Introduction

“Domain“ of ab-initio models - taken from V. Soma, lectures of 28th Indian-Summer School 2016

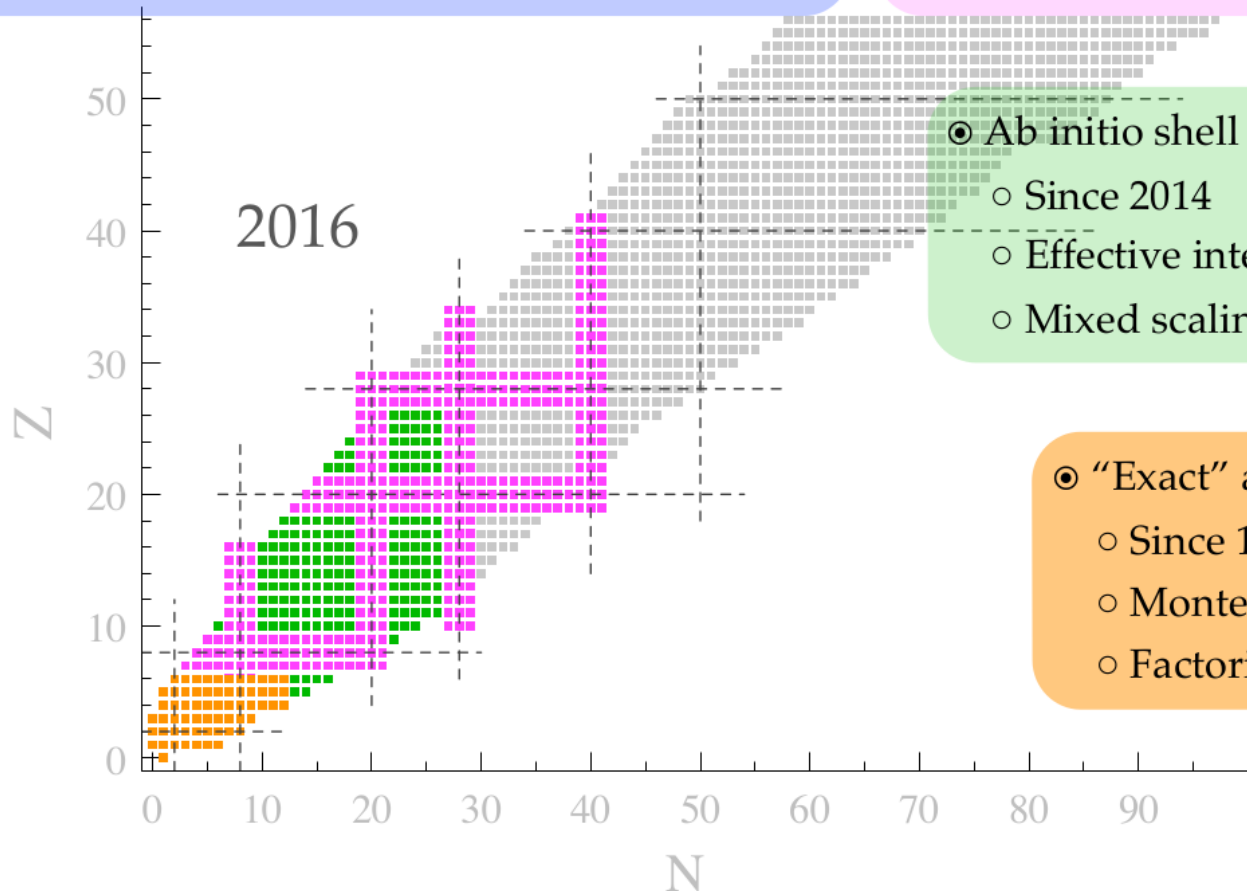
http://rafael.ujf.cas.cz/school16/presentations/Soma/GFcourse_Soma_Prague2016.pdf

Ab initio approaches for closed-shell nuclei

- Since 2000's
- SCGF, CC, IMSRG
- Polynomial scaling

Ab initio approaches for open-shell nuclei

- Since 2010's
- GGF, BCC, MR-IMSRG
- Polynomial scaling



Ab initio shell model

- Since 2014
- Effective interaction via CC/IMSRG
- Mixed scaling

“Exact“ ab initio approaches

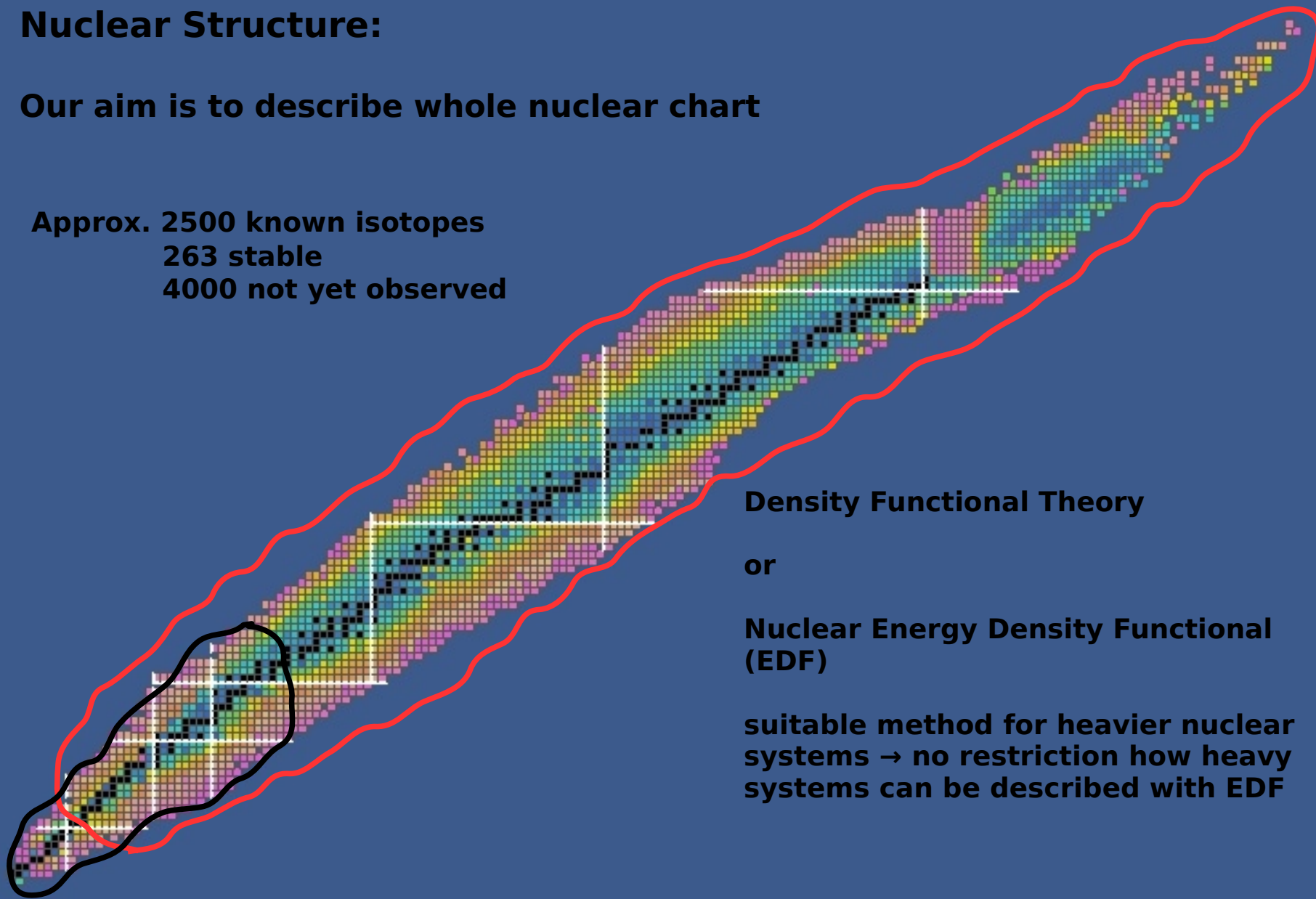
- Since 1980's
- Monte Carlo, CI, ...
- Factorial scaling

Introduction

Nuclear Structure:

Our aim is to describe whole nuclear chart

Approx. 2500 known isotopes
263 stable
4000 not yet observed



Density Functional Theory

or

Nuclear Energy Density Functional
(EDF)

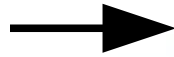
suitable method for heavier nuclear
systems → no restriction how heavy
systems can be described with EDF

Energy Density Functional

Mean Field - generated by the HF method from NN interactions



nucleons as non-interacting particles in potential well



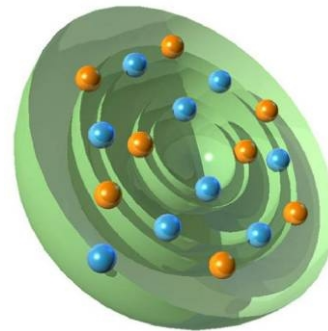
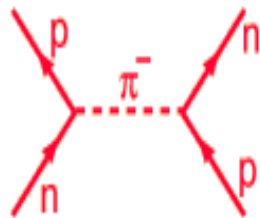
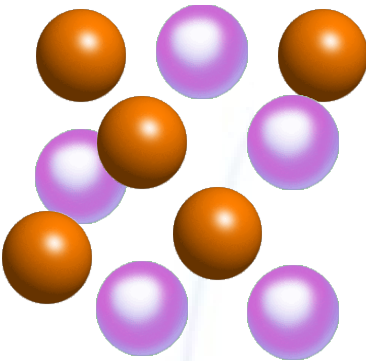
mutual interaction of nucleons creates "mean field" → nucleons move in this field

Hartree-Fock method - mean-field is generated "by itself" = self-consistence

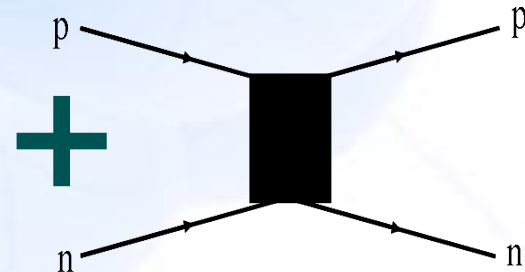
$$\sum_{ij} t_{ij} a_i^\dagger a_j$$

$$+ \frac{1}{4} \sum_{ijkl} V_{ijkl} a_i^\dagger a_j^\dagger a_l a_k = \sum_{ij} \left\{ t_{ij} + \sum_{kl} V_{kilj} \langle |a_k^\dagger a_l| \rangle \right\} a_i^\dagger a_j$$

$$+ \frac{1}{4} \sum_{ijkl} V_{ijkl} : a_i^\dagger a_j^\dagger a_l a_k :$$



mean field



residual interaction

Energy Density Functional

**Density Functional - possible to construct
Mean Field without knowledge of NN interactions**

We define energy density functional as general scalar product of densities

$$\rho(\vec{r}) = \sum_i \phi_i^*(\vec{r}) \phi_i(\vec{r})$$

$$\vec{s}(\vec{r}) = \sum_i \phi_i^*(\vec{r}) \vec{\sigma} \phi_i(\vec{r})$$

$$\tau(\vec{r}) = \sum_i \nabla \phi_i^*(\vec{r}) \cdot \nabla \phi_i(\vec{r})$$

$$\vec{j}(\vec{r}) = \sum_i (\phi_i^*(\vec{r}) \nabla \phi_i(\vec{r}) - (\nabla \phi_i^*(\vec{r})) \phi_i(\vec{r}))$$

$$\vec{T}(\vec{r}) = \sum_i \nabla \phi_i^*(\vec{r}) \cdot \vec{\sigma} \nabla \phi_i(\vec{r})$$

$$J_k(\vec{r}) = \sum_i \varepsilon_{klm} ((\nabla_l \phi_i^*(\vec{r})) \sigma_m \phi_i(\vec{r}) - \phi_i^*(\vec{r}) \sigma_m (\nabla_l \phi_i(\vec{r})))$$

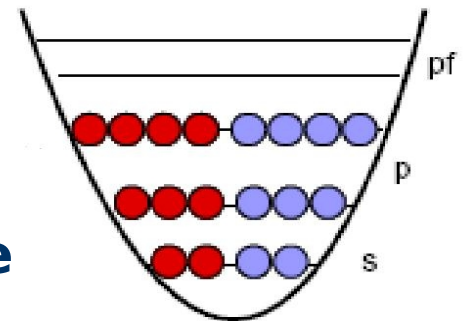
**dependence on circa 10
free parameters of the
model**

$$\begin{aligned} \mathcal{H}_{Skyrme} = & \frac{\hbar^2}{2m} \tau + \\ & + \frac{1}{2} t_0 \left[\left(1 + \frac{1}{2} x_0\right) \rho^2 - \left(x_0 + \frac{1}{2}\right) \sum_{q=n,p} \rho_q^2 \right] - \frac{1}{2} t_0 \left[\frac{1}{2} x_0 \vec{s}^2 - \frac{1}{2} \sum_{q=n,p} \vec{s}_q^2 \right] \\ & - \frac{1}{16} t_1 \left(1 + \frac{1}{2} x_1\right) \left[3\rho \Delta \rho - 4(\rho \tau - \vec{j}^2) \right] - \frac{1}{16} t_1 \left(1 + 2x_1\right) \sum_{q=n,p} \left[-\frac{3}{2} \rho_q \Delta \rho_q + 2(\rho_q \tau_q - \vec{j}_q^2) \right] \\ & + \frac{1}{16} t_1 x_1 \left[-\frac{3}{2} \vec{s} \Delta \vec{s} + (\vec{s} \cdot \vec{T} - \vec{J}^2) \right] - \frac{1}{16} t_1 \sum_{q=n,p} \left[-\frac{3}{2} \vec{s}_q \Delta \vec{s}_q + (\vec{s}_q \cdot \vec{T}_q - \vec{J}_q^2) \right] \\ & + \frac{1}{16} t_2 \left(1 + \frac{1}{2} x_2\right) \left[\rho \Delta \rho + 4(\rho \tau - \vec{j}^2) \right] + \frac{1}{16} t_2 \left(1 + 2x_2\right) \sum_{q=n,p} \left[\frac{1}{2} \rho_q \Delta \rho_q + 2(\rho_q \tau_q - \vec{j}_q^2) \right] \\ & + \frac{1}{16} t_2 x_2 \left[\frac{1}{2} \vec{s} \Delta \vec{s} + (\vec{s} \cdot \vec{T} - \vec{J}^2) \right] + \frac{1}{16} t_2 \sum_{q=n,p} \left[\frac{1}{2} \vec{s}_q \Delta \vec{s}_q + (\vec{s}_q \cdot \vec{T}_q - \vec{J}_q^2) \right] \\ & + \frac{1}{8} t_3 \left[\left(1 + \frac{1}{2} x_3\right) \rho^2 - \left(x_3 + \frac{1}{2}\right) \sum_{q=n,p} \rho_q^2 \right] \rho^\alpha - \frac{1}{8} t_3 \left[\frac{1}{2} x_3 \vec{s}^2 - \frac{1}{2} \sum_{q=n,p} \vec{s}_q^2 \right] \rho^\alpha \\ & - \frac{1}{2} t_4 \sum_{q_1 q_2} (1 + \delta_{q_1 q_2}) \left[(\vec{\nabla} \times \vec{j}_{q_1}) \cdot \vec{s}_{q_2} + \rho_{q_2} \vec{\nabla} \cdot \vec{J}_{q_1} \right] \end{aligned}$$

**Kohn-Sham eq.
equiv.**

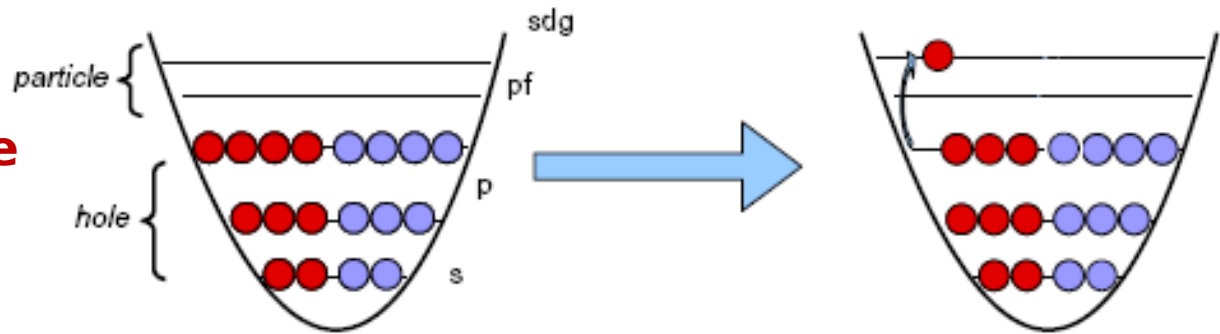
Hartree-Fock eq.

**mean field (single
particle levels)**



Random Phase Approximation

**Nuclear excitations
within 1 particle-hole
excitations**



$$|\nu\rangle = Q_\nu^\dagger |\tilde{0}\rangle = \sum_{ph} (X_{ph}^\nu a_p^\dagger a_h - Y_{ph}^\nu a_h^\dagger a_p) |\tilde{0}\rangle$$

RPA phonons

$$\langle \tilde{0} | [\delta Q_{\nu'}, [\hat{H}, Q_\nu^\dagger]] | \tilde{0} \rangle = (E_\nu - E_{\tilde{0}}) \langle \tilde{0} | [\delta Q_{\nu'}, Q_\nu^\dagger] | \tilde{0} \rangle$$

Equation of motion

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix} = \hbar \Omega_\nu \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix}$$

RPA equation

$$A_{minj} = \langle \text{HF} | [a_i^\dagger a_m [H, a_n^\dagger a_j]] | \text{HF} \rangle = (\epsilon_m - \epsilon_i) \delta_{mn} \delta_{ij} + \bar{v}_{mjin}$$

$$B_{minj} = -\langle \text{HF} | [a_i^\dagger a_m [H, a_j^\dagger a_n]] | \text{HF} \rangle = -\bar{v}_{minj}$$

**RPA matrix -
dimension (2D x 2D)**

Photoabsorption Spectrum

Photoabsorption total cross section:

$$\sigma(E\lambda\mu) = 8\pi^3 \frac{\lambda + 1}{\lambda[(2\lambda + 1)!!!]^2} \sum_{\nu} \left(\frac{\omega_{\nu}}{\hbar c}\right)^{2\lambda-1} |\langle \nu | \hat{M}(\lambda\mu) | gs \rangle|^2$$

The definition of **strength function**:

$$S(E\lambda\mu) = \sum_{\nu} B(g.s. \rightarrow \nu, \hbar\omega_{\nu}) \delta(E - \hbar\omega_{\nu})$$

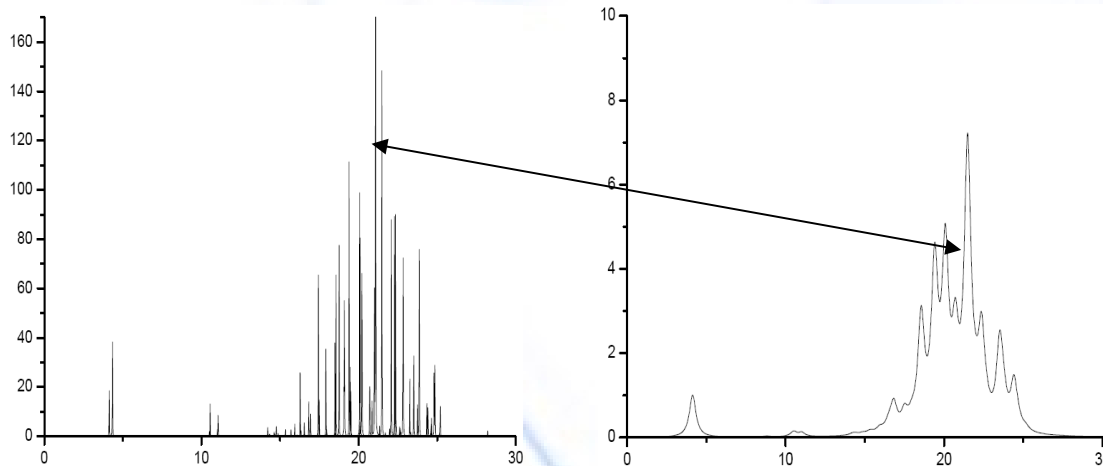
$$L = 2\lambda - 1$$

$$S_L(E\lambda\mu) = \sum_{\nu} \omega_{\nu}^L |\langle \nu | \hat{M}(\lambda\mu) | gs \rangle|^2 \zeta(\omega - \omega_{\nu})$$

Lorentzian

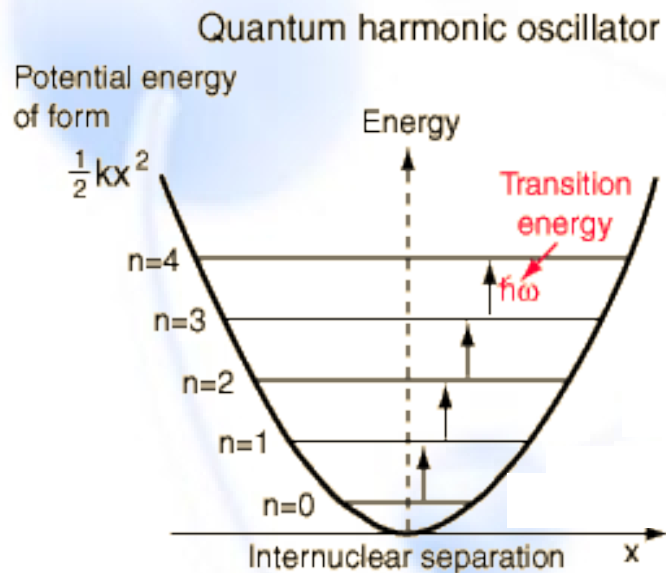
$$\zeta(\omega - \omega_j) = \frac{1}{2\pi} \frac{\Delta}{(\omega - \omega_{\nu})^2 + (\Delta/2)^2}$$

too high density of states in the region of giant resonances → Lorentzian smoothes strength function



Basis - dimensions

HO oscillator basis



single particle states

N_0	j-scheme	m-scheme
0	1	2
1	3	8
2	6	20
3	10	40
4	15	70
5	21	112
6	28	168
7	36	240
8	45	330
9	55	440
10	66	572
11	78	728
12	91	910
13	105	1120
14	120	1360
15	136	1632
16	153	1938
17	171	2280
18	190	2660
19	210	3080

j-scheme:

$$\# = (N_0+1)(N_0+2)/2$$

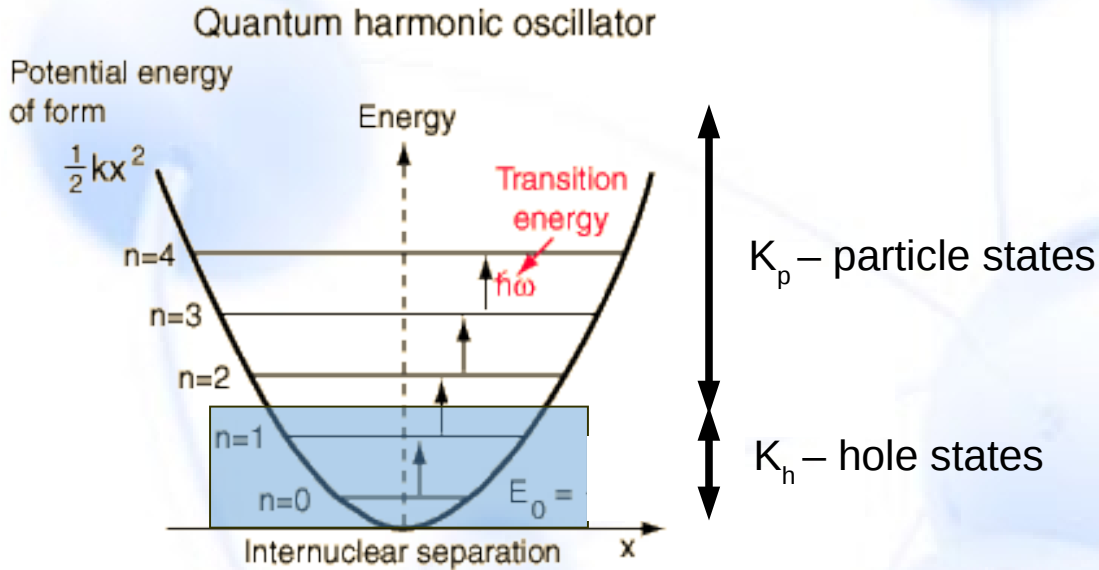
m-scheme:

$$\# = (N_0+1)(N_0+2)(N_0+3)/3$$

Spherical basis \Leftrightarrow **j-scheme**

Deformed basis \Leftrightarrow **m-scheme**

Random Phase Approximation



RPA matrix - dimension (2D x 2D)

$$|\nu\rangle = Q_\nu^\dagger |\tilde{0}\rangle = \sum_{ph} (X_{ph}^\nu a_p^\dagger a_h - Y_{ph}^\nu a_h^\dagger a_p) |\tilde{0}\rangle$$

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix} = \hbar\Omega_\nu \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix}$$

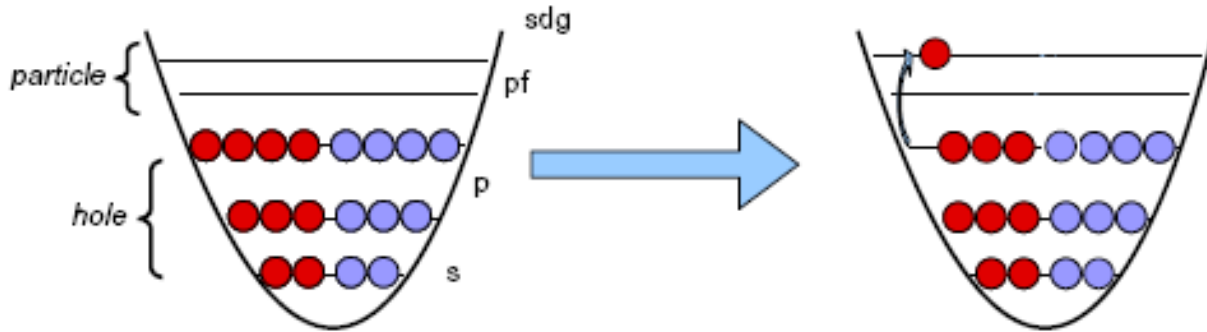
$$D = (K_p * K_h)$$

$$D \sim (N_0)^2 \quad \dots \text{ spherical}$$

$$D \sim (N_0)^3 \quad \dots \text{ deformed}$$

N_0	D - spherical	D - deformed
0	-	-
1	-	-
2	9	96
3	21	256
4	36	496
5	54	832
6	75	1280
7	99	1856
8	126	2576
9	156	3456
10	189	4512
11	225	5760
12	264	7216
13	306	8896
14	351	10816
15	399	12992
16	450	15440
17	504	18176
18	561	21216
19	621	24576

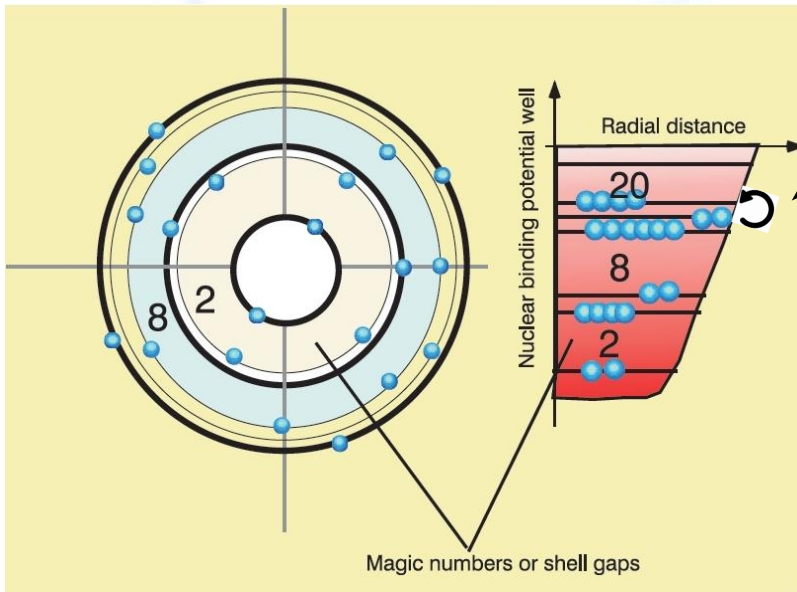
“Quasiparticles” in nuclei



particle-hole excitations

we need to distinguish
occupied and **unoccupied**
levels

nuclei with semi-closed shell



nucleons “jumping” between
energetically very close levels



“smearing” of Fermi energy

occupations of levels

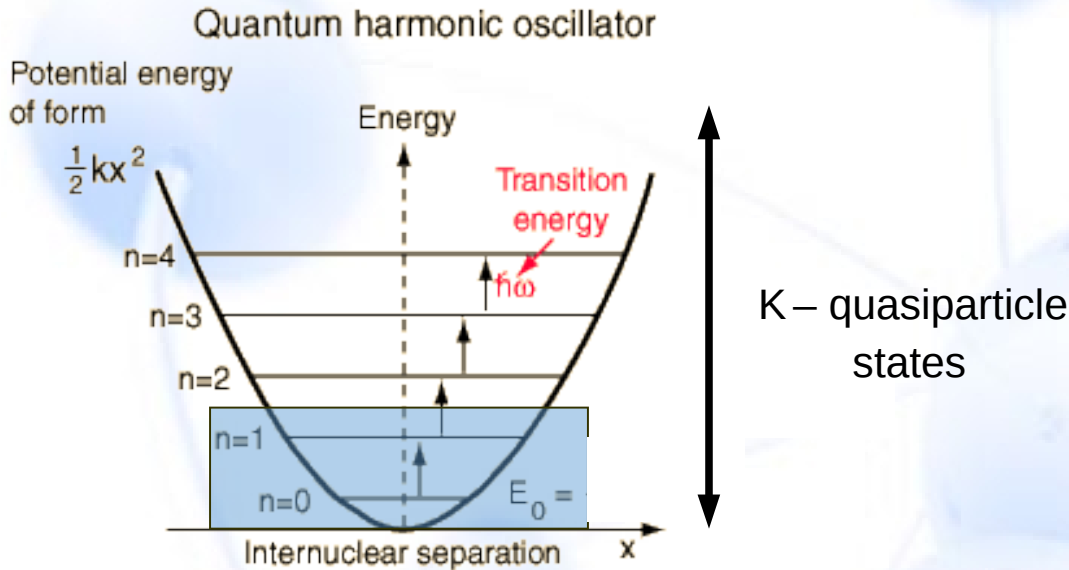
$$0 < V_i^2 < 1$$

becomes probabilistic

quasiparticle states - partially occupied orbits

Random Phase Approximation

Quasiparticle formulation



Quasiparticle formulation of RPA matrix - dimension (2D x 2D)

$$Q_\nu^+ = \frac{1}{2} \sum_{ij} (X_{ij}^{(\nu)} \alpha_i^+ \alpha_j^+ - Y_{ij}^{(\nu)} \alpha_j \alpha_i)$$

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X'' \\ Y'' \end{pmatrix} = \hbar\Omega_\nu \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} X'' \\ Y'' \end{pmatrix}$$

$$D = K*(K-1)/2$$

$$D \sim (N_0)^4 \quad \dots \text{ spherical}$$

$$D \sim (N_0)^6 \quad \dots \text{ deformed}$$

N_0	D - spherical	D - deformed
0	-	-
1	3	28
2	15	190
3	45	780
4	105	2415
5	210	6216
6	378	14028
7	630	28680
8	990	54285
9	1485	96580
10	2145	163306
11	3003	264628
12	4095	413595
13	5460	626640
14	7140	924120
15	9180	1330896
16	11628	1876953
17	14535	2598060
18	17955	3536470
19	21945	4741660

Random Phase Approximation

Quasiparticle formulation

Matrices $\sim (10^7 \times 10^7)$

→ **methods to solve** the eigenvalue problem only for a subset of states **without** generating the **full RPA** matrix

Quasiparticle formulation of RPA matrix - dimension (2D x 2D)

$$Q_\nu^+ = \frac{1}{2} \sum_{ij} (X_{ij}^{(\nu)} \alpha_i^+ \alpha_j^+ - Y_{ij}^{(\nu)} \alpha_j \alpha_i)$$

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X^r \\ Y^r \end{pmatrix} = \hbar \Omega_r \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} X^r \\ Y^r \end{pmatrix}$$

$$D = K*(K-1)/2$$

$$D \sim (N_0)^4 \quad \dots \text{ spherical}$$

$$D \sim (N_0)^6 \quad \dots \text{ deformed}$$

N_0	D - spherical	D - deformed
0	-	-
1	3	28
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Arnoldi Diagonalization Method

Arnoldi Diagonalization Method – an iterative method to calculate RPA strength functions without construction and diagonalization of the full RPA matrix

PHYSICAL REVIEW C **81**, 034312 (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. Veselý¹

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 24 March 2010)

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.

DOI: [10.1103/PhysRevC.81.034312](https://doi.org/10.1103/PhysRevC.81.034312)

PACS number(s): 21.60.Jz, 71.15.Mb

Arnoldi Diagonalization Method

Arnoldi Diagonalization Method – an iterative method to calculate RPA strength functions without construction and diagonalization of the full RPA matrix

$$|\nu\rangle = Q_\nu^\dagger |\tilde{0}\rangle = \sum_{ph} (X_{ph}^\nu a_p^\dagger a_h - Y_{ph}^\nu a_h^\dagger a_p) |\tilde{0}\rangle \quad \text{RPA phonon operator}$$

We start with a **pivot vector**

$$X_{mi}^1 = \frac{e}{\sqrt{N^1}} \langle \phi_m | r^p Y_{JM} | \phi_i \rangle, \quad Y_{mi}^1 = 0,$$

→ E1 strength function
(we can choose other J^π)

We only need to know a **product** of the RPA matrix with a vector

$$\begin{pmatrix} \chi^k \\ \gamma^k \end{pmatrix}$$

$$\begin{pmatrix} \mathcal{W}_+^k \\ \mathcal{W}_+^{\nu k} \end{pmatrix} = \begin{pmatrix} A & B \\ -B'^* & -A'^* \end{pmatrix} \begin{pmatrix} \chi^k \\ \gamma^k \end{pmatrix},$$

$$\begin{pmatrix} \mathcal{W}_-^k \\ \mathcal{W}_-^{\nu k} \end{pmatrix} = \begin{pmatrix} A & B \\ -B'^* & -A'^* \end{pmatrix} \begin{pmatrix} \gamma^{k*} \\ \chi^{k*} \end{pmatrix}$$

Arnoldi Diagonalization Method

Arnoldi Diagonalization Method – an iterative method to calculate RPA strength functions without construction and diagonalization of the full RPA matrix

Iterations: if we have set of **k** vectors, we can add **(k+1)**th vector by the following

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

Moreover – we orthogonalize the **(k+1)**th state to all the **k** previous states in each iteration

where the elements \mathbf{a}_{ik} , \mathbf{b}_{ik} are defined as:

$$\mathbf{a}_{ik} = (\mathcal{X}^{i*}, \mathcal{Y}^{i*}) \begin{pmatrix} \mathcal{W}_+^{kT} \\ -\mathcal{W}_+^{kT} \end{pmatrix},$$
$$\mathbf{b}_{ik} = (\mathcal{Y}^i, \mathcal{X}^i) \begin{pmatrix} \mathcal{W}_+^{kT} \\ -\mathcal{W}_+^{kT} \end{pmatrix},$$

Arnoldi Diagonalization Method

Arnoldi Diagonalization Method – an iterative method to calculate RPA strength functions without construction and diagonalization of the full RPA matrix

In each iteration we have **d** vectors $\begin{pmatrix} x^k \\ y^k \end{pmatrix}$ which form **Krylov** subspace of full RPA space (RPA matrix with a dimension $2\mathbf{D}$).

$$\mathbf{d} \ll \mathbf{D}$$

We solve an RPA equation problem in the Krylov subspace (of dimension **d**) in each iteration...

$$\begin{pmatrix} a & b \\ -b^* & -a^* \end{pmatrix} \begin{pmatrix} x^k \\ y^k \end{pmatrix} = \hbar\omega_k \begin{pmatrix} x^k \\ y^k \end{pmatrix}$$

We obtain the eigen-energies: $\hbar\omega_k$ and calculate strength functions until the convergence is reached...

Arnoldi Diagonalization Method

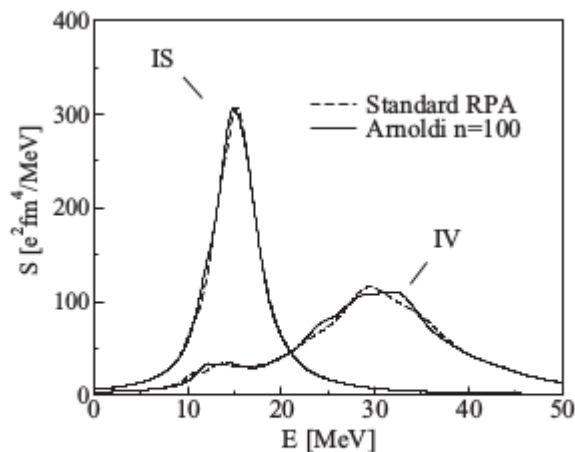


FIG. 1. The 0^+ strength functions in ^{132}Sn calculated by using 25 HO shells and 100 Arnoldi iterations for the SkM* functional (solid lines), compared with the standard RPA calculation of Ref. [17] obtained for the SkM* functional (dashed lines).

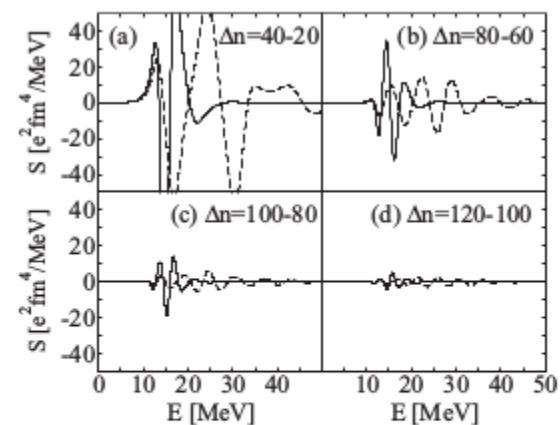


FIG. 2. Convergence of the ^{132}Sn 0^+ strength functions of Fig. 1. Solid lines are for the IS and dashed lines are for the IV strength functions. Each panel shows the difference of two strength functions, one with n iterations and the other calculated with $n - 20$ iterations.

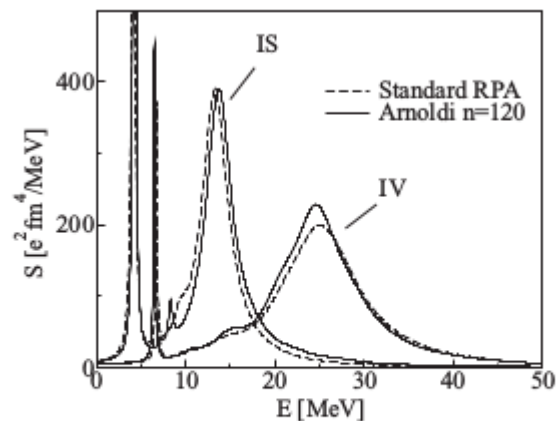


FIG. 4. Similar to Fig. 1 but for the 2^+ strength functions. All results were calculated for the SkM* functional.

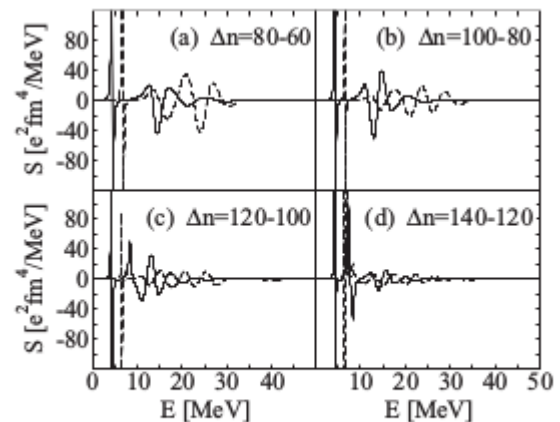


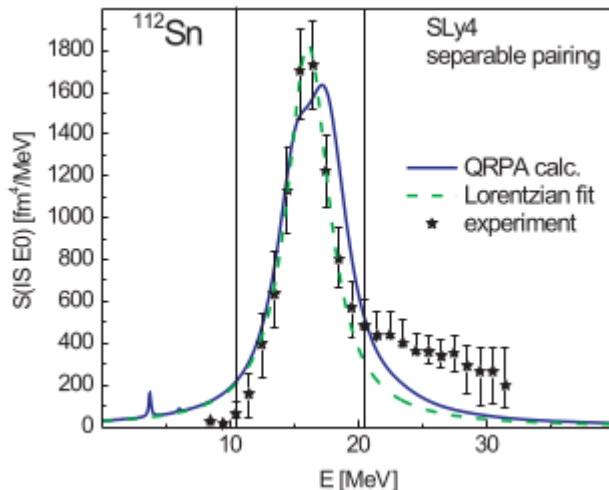
FIG. 5. Similar to Fig. 2 but for the 2^+ strength functions.

Arnoldi Diagonalization Method

Arnoldi Diagonalization Method – is meaningful only if the convergence is reached for dimension of the Krylov subspace $\mathbf{d} \ll \mathbf{D}$!

In the test calculations of the paper **PRC 81, 034312 (2010)** the convergence usually reached (within reasonable precision) for ~ 100 iterations...

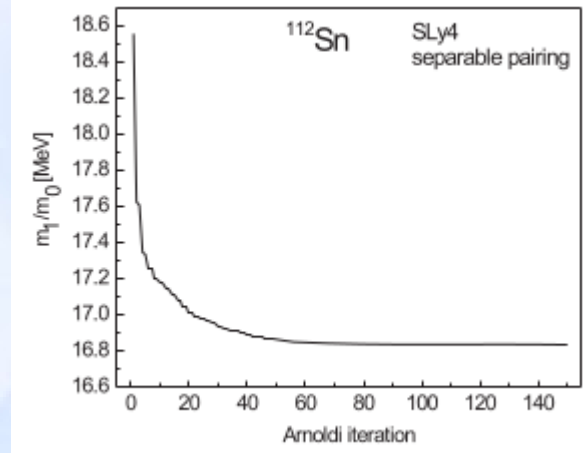
Application \rightarrow systematic study of **Giant Monopole Resonances (GMR)** in most of spherical nuclei of the chart: **Phys. Rev. C 86, 024303 (2012)**



centroid of GMR

$$E_{\text{GMR}} = \frac{m_1}{m_0}$$

m_0 , m_1 moments
of giant resonance



convergence of centroid

Arnoldi Diagonalization Method

Arnoldi Diagonalization Method – is meaningful only if the convergence is reached for dimension of the Krylov subspace $\mathbf{d} \ll \mathbf{D}$!

But important is also the **reduction** of the **time** needed for RPA calculation – useful for large systematic calculations (calculations of whole nuclear chart, fitting of parametrizations)...

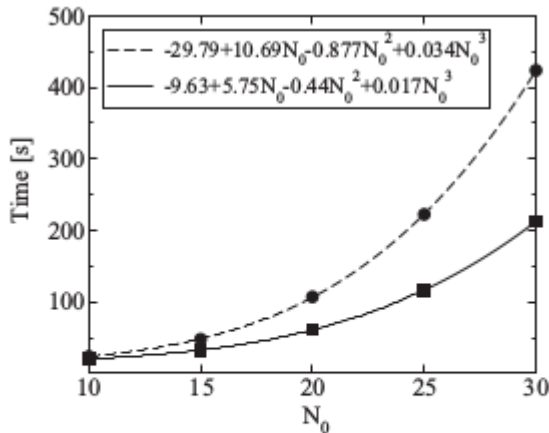


FIG. 12. Times to calculate 100 Arnoldi iterations for the spherical QRPA method applied to ^{132}Sn as functions of N_0 . Squares and circles show results for the 1^- and 2^+ modes, respectively, and lines show cubic fits.

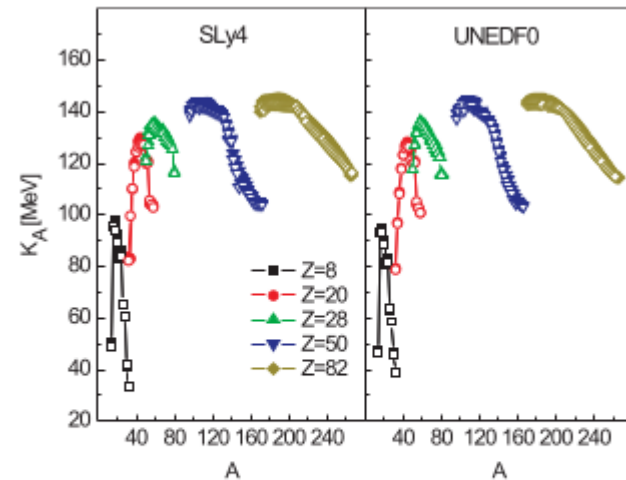


FIG. 4. (Color online) Incompressibility K_A calculated for the isotopic chains of semimagic nuclei with $Z = 8, 20, 28, 50,$ and 82 . Left and right panels show results obtained for the SLy4 and UNEDF0 functionals, respectively. Full (empty) symbols correspond to the zero-range (separable) pairing force.

RPA calculation $\sim 10^1$ sec \rightarrow allows large scale calculations...

Systematic Calculations of Nuclear Properties

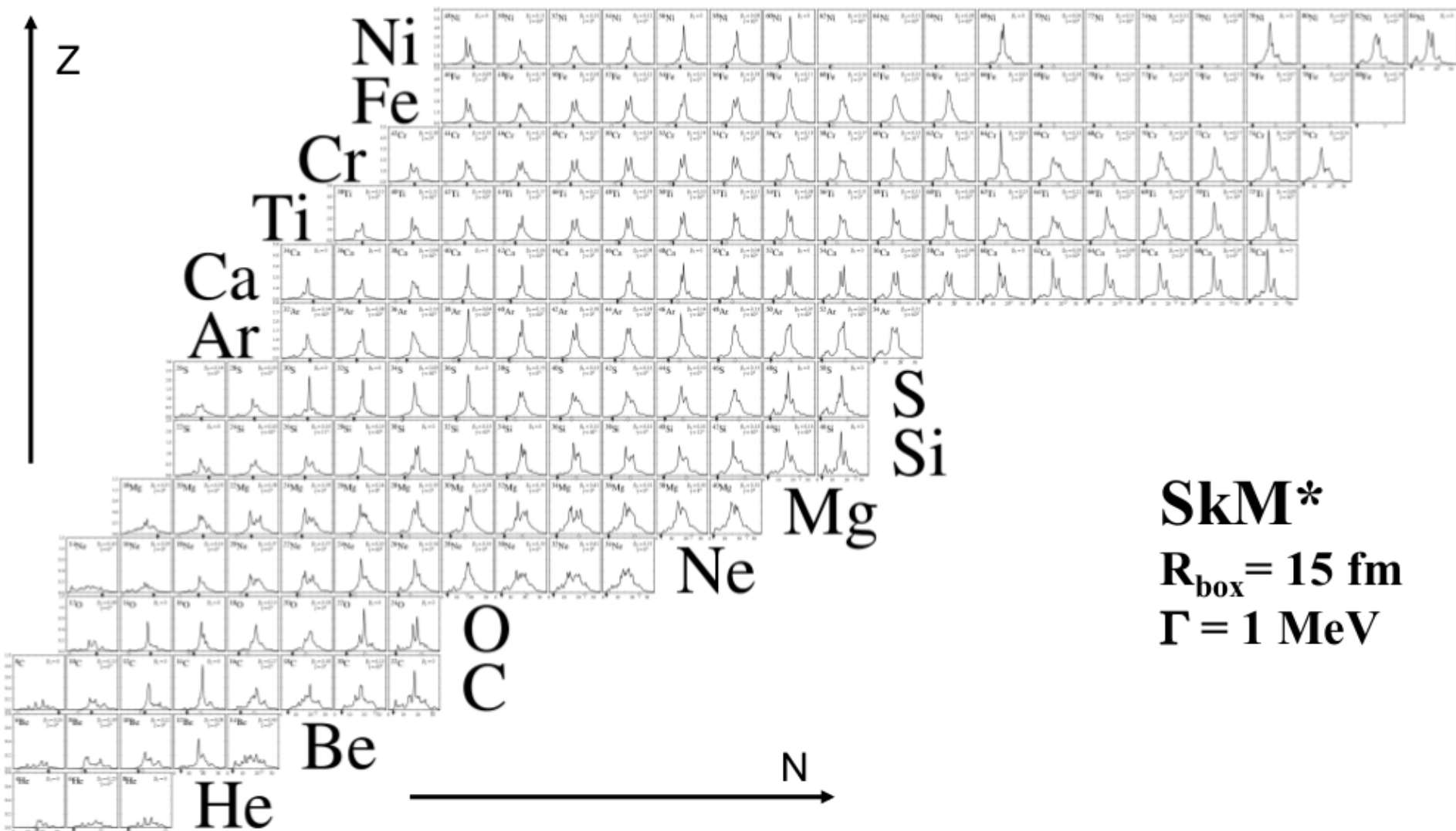
S. Ebata, T. Nakatsukasa, T. Inakura, *Phys. Rev. C* 90, 024303 (2014)

TABLE I. Ground-state properties of even-even isotopes with $Z = 6-20$ obtained by the HF+BCS and HF with SkM* calculation: quadrupole deformation parameters (β_2, γ), pairing gaps for neutrons and protons (Δ_n, Δ_p), and chemical potentials for neutrons and protons (λ_n, λ_p). In the case of normal phase ($\Delta = 0$), we define the chemical potential as the single-particle energy of the highest occupied orbital, $\lambda_n = \epsilon_N^0$ and $\lambda_p = \epsilon_Z^0$. The pairing gaps and chemical potentials are given in units of MeV.

	β_2	γ	Δ_n	Δ_p	$-\lambda_n$	$-\lambda_p$	β_2^{HF}	γ^{HF}	$-\lambda_n^{\text{HF}}$	$-\lambda_p^{\text{HF}}$
⁸ C	0.00		0.00	0.00	31.22	2.96	0.00		31.19	2.95
¹⁰ C	0.23	0°	0.00	0.00	17.00	7.86	0.23	0°	16.99	7.84
¹² C	0.00		0.00	0.00	16.82	14.07	0.00		16.80	14.06
¹⁴ C	0.00		0.00	0.00	8.94	18.24	0.00		8.94	18.23
¹⁶ C	0.14	0°	1.00	0.00	4.56	21.22	0.27	0°	5.25	20.52
¹⁸ C	0.27	0°	0.57	0.00	3.90	23.71	0.30	0°	4.69	23.53
²⁰ C	0.23	60°	0.00	0.00	4.84	27.53	0.23	60°	4.83	27.50
²² C	0.00		0.00	0.00	3.41	30.25	0.00		3.42	30.21
¹⁴ O	0.00		0.00	0.00	20.81	5.69	0.00		20.80	5.68
¹⁶ O	0.00		0.00	0.00	13.54	10.26	0.00		13.53	10.25
¹⁸ O	0.00		1.06	0.00	7.94	13.91	0.15	0°	7.75	13.58
²⁰ O	0.00		1.10	0.00	7.45	17.34	0.18	0°	7.80	16.81
²² O	0.00		0.00	0.00	8.06	20.66	0.00		8.04	20.65
²⁴ O	0.00		0.00	0.00	5.17	22.63	0.00		5.17	22.61
²⁶ O	0.00		0.80	0.00	1.13	24.87	0.07	60°	1.26	24.79
¹⁶ Ne	0.25	0°	0.00	0.54	23.06	0.91	0.29	0°	22.81	1.48
¹⁸ Ne	0.00		0.00	1.07	17.16	4.01	0.16	0°	16.82	3.86
²⁰ Ne	0.37	0°	0.00	0.00	13.07	9.19	0.37	0°	13.07	9.18
²² Ne	0.37	0°	0.00	0.00	11.03	12.38	0.37	0°	11.03	12.37
²⁴ Ne	0.17	60°	0.00	0.74	10.57	13.04	0.20	60°	10.62	13.51
²⁶ Ne	0.00		0.00	1.00	7.17	14.92	0.14	0°	6.95	14.92
²⁸ Ne	0.00		0.79	1.01	3.22	17.05	0.16	0°	3.77	17.41
³⁰ Ne	0.00		0.00	1.01	3.79	19.09	0.35	0°	4.14	21.35
³² Ne	0.36	0°	0.95	0.00	2.16	23.61	0.41	0°	2.92	24.28
¹⁸ Mg	0.31	0°	0.00	0.00	25.59	0.20	0.31	0°	25.56	0.19
²⁰ Mg	0.00		0.00	1.13	20.53	2.83	0.18	0°	19.99	3.18
²² Mg	0.38	0°	0.00	0.00	16.31	6.42	0.38	0°	16.30	6.42
²⁴ Mg	0.39	0°	0.00	0.00	14.12	9.51	0.39	0°	14.12	9.50
²⁶ Mg	0.20	54°	0.00	0.86	13.08	11.23	0.24	8°	11.37	11.67

Fully self-consistent calculation of E1 strength distribution

Inakura, Nakatsukasa, Yabana, in preparation



Fully self-consistent calculation of E1 strength distribution

Inakura, Nakatsukasa, Yabana, in preparation

