Particle vibration coupling in superfluid nuclei with axial deformation

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Western Michigan University

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Outline

❑ **Introduction**:

Energy scales and and relevant degrees of freedom for low-energy nuclear physics
Covariant energy density functional theory:

❑ **Beyond the mean-field: quasiparticles coupled to vibrations**

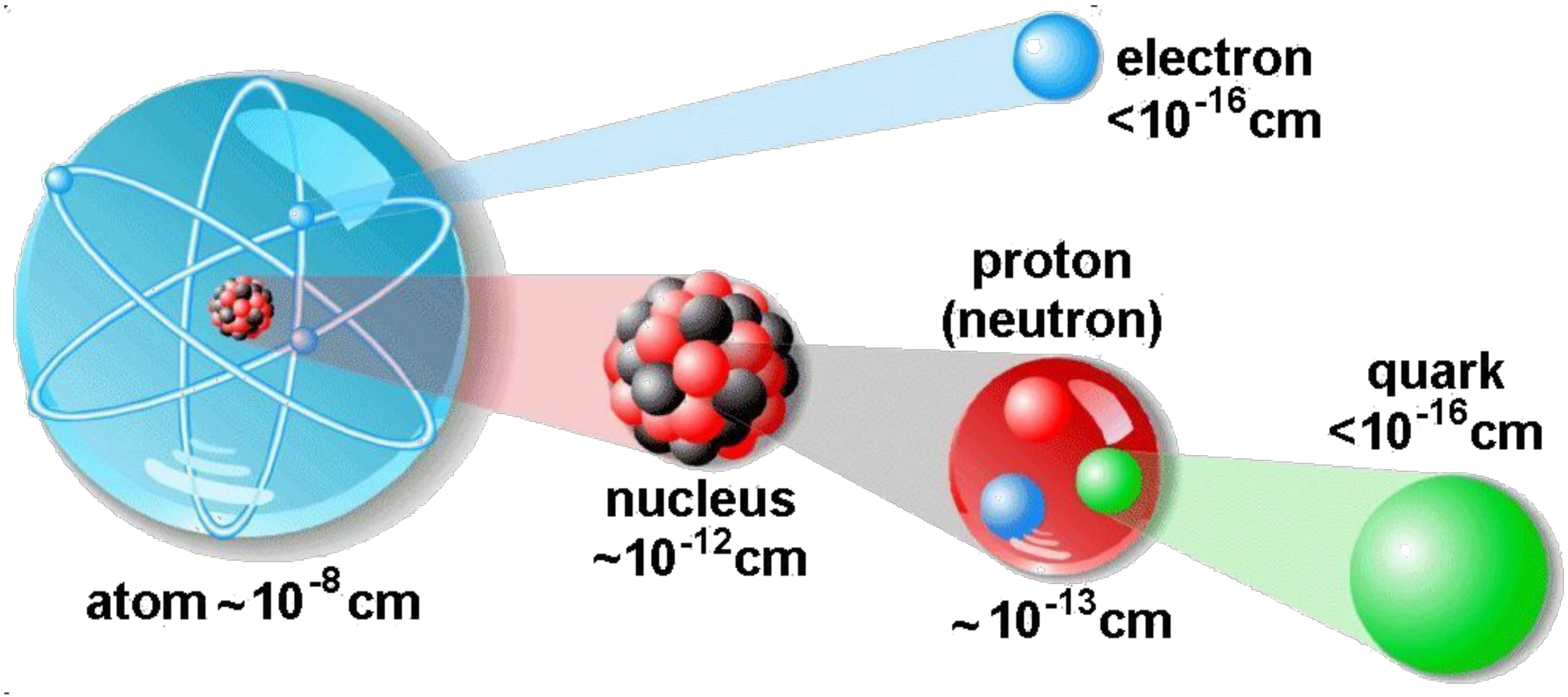
Formalism and numerical scheme

❑ **Application to axially deformed nuclei**

Benchmark to ^{208}Pb
Medium-mass neutron rich nucleus ^{38}Si
Heavy nucleus ^{250}Cf

❑ **Summary & perspectives**

Energy scales and relevant degrees of freedom



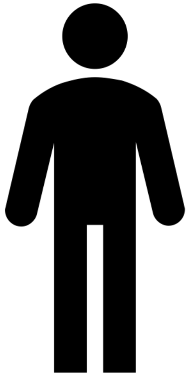
Atoms:
Electromagnetic
Quantum mechanics

Nuclei:
Nuclear interaction
Test ground for different theorical tools

Quarks:
Strong interaction
QCD/standard model

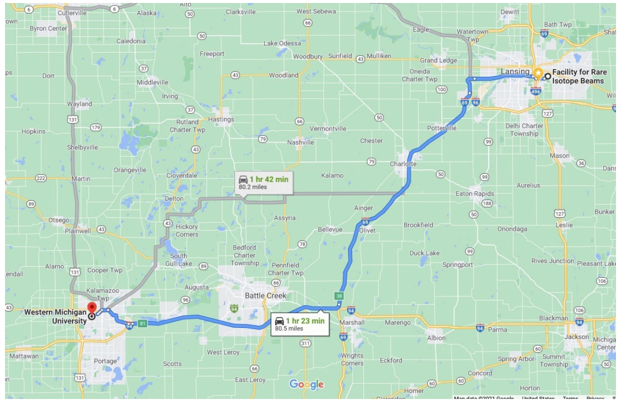
Energy scales and relevant degrees of freedom

Human height



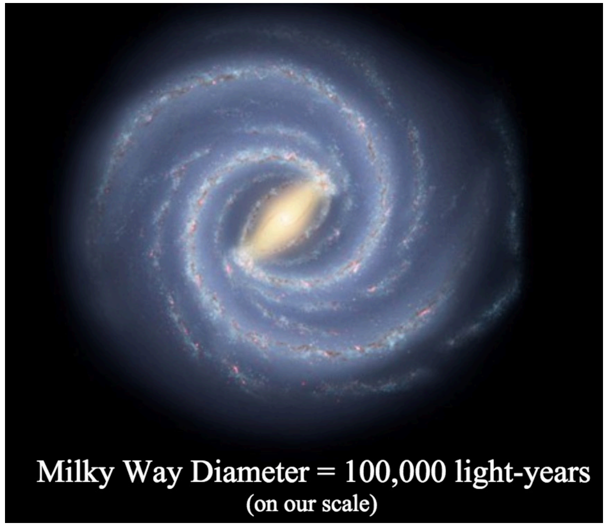
~ 6 feet
~ 1-2 m

Distance to MSU

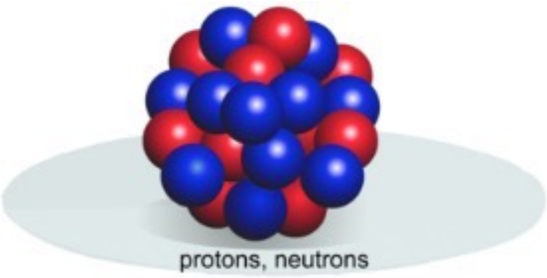


~ 80 miles
~ 10^5 m

The milky way



~ 10^{20} m

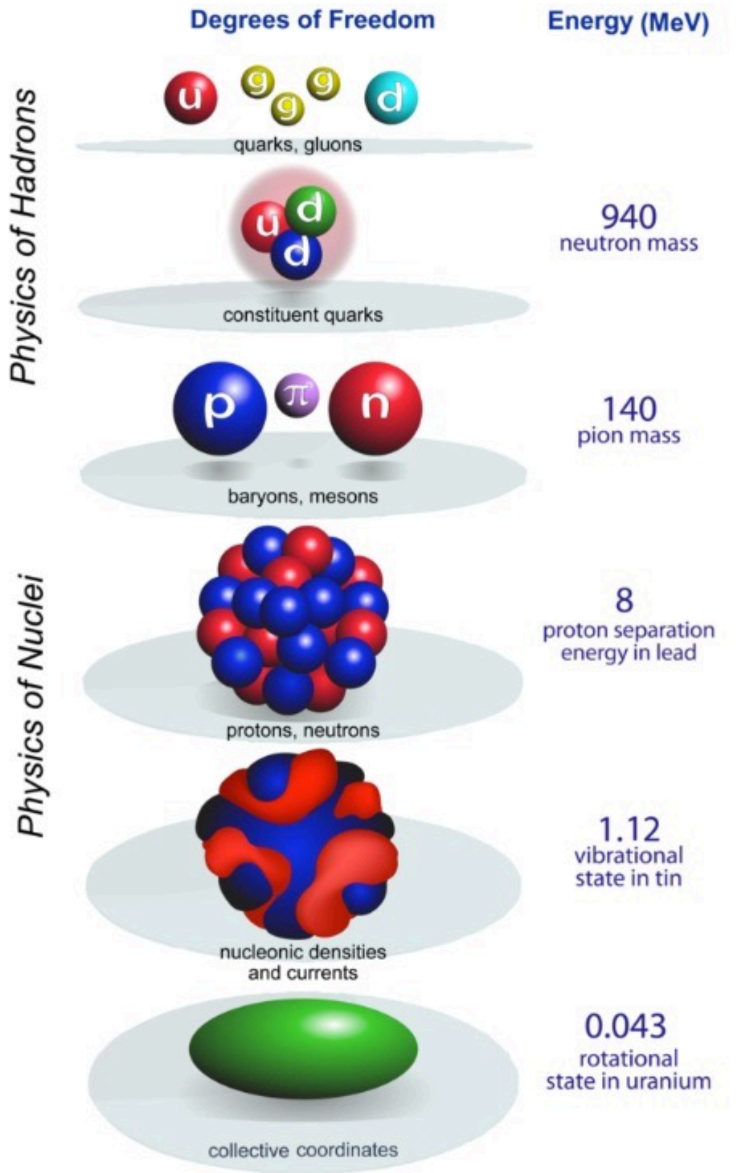


~ fm
~ 10^{-15} m

$$E = \frac{\hbar c}{\lambda}$$

Weinberg's third law of Progress in theoretical Physics:
"You may use any degrees of freedom you like to describe a physical system, but if you use the wrong ones, you'll be sorry!"

Energy scales and relevant degrees of freedom



Energy or Resolution

Standard model

Lattice QCD

ab initio

CI

DFT

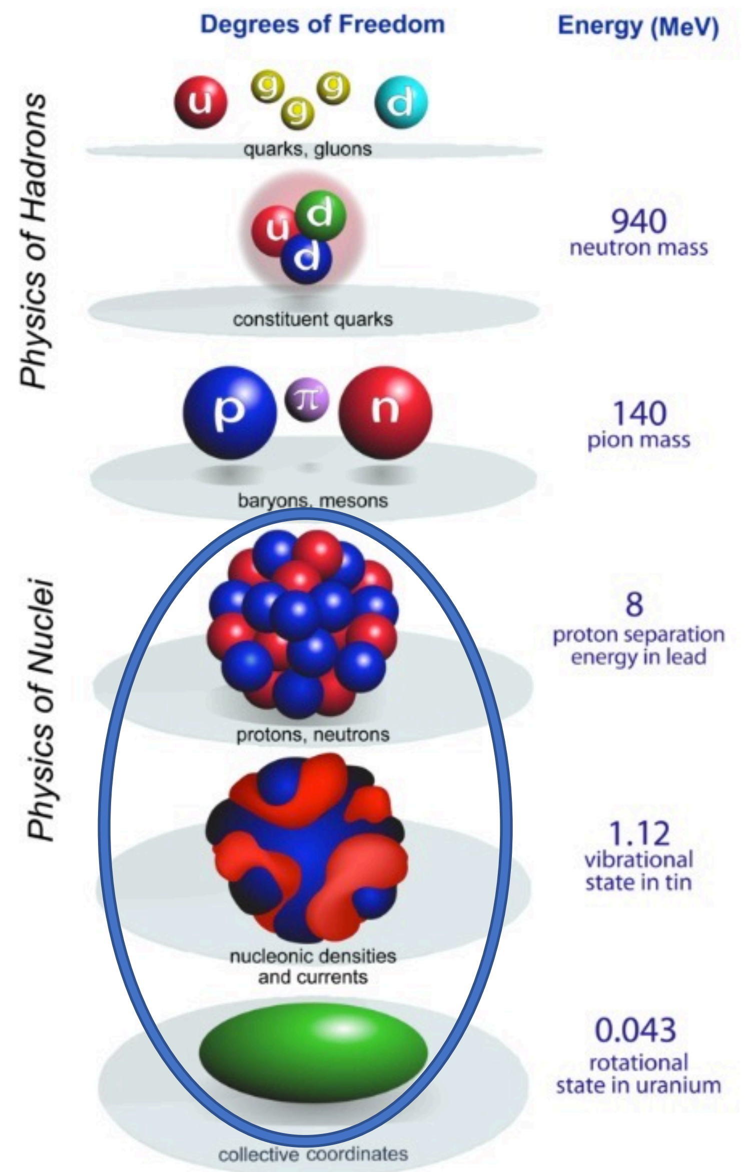
Collective models

Low energy nuclear physics

Energy scales
From keV to GeV~10^6
At different degrees of freedom, we have different quantum many-body methods

Freedom is not free!

Energy scales and relevant degrees of freedom



Energy or Resolution

Standard model

Lattice QCD

ab initio

CI

DFT

Collective models

Interaction

Well known

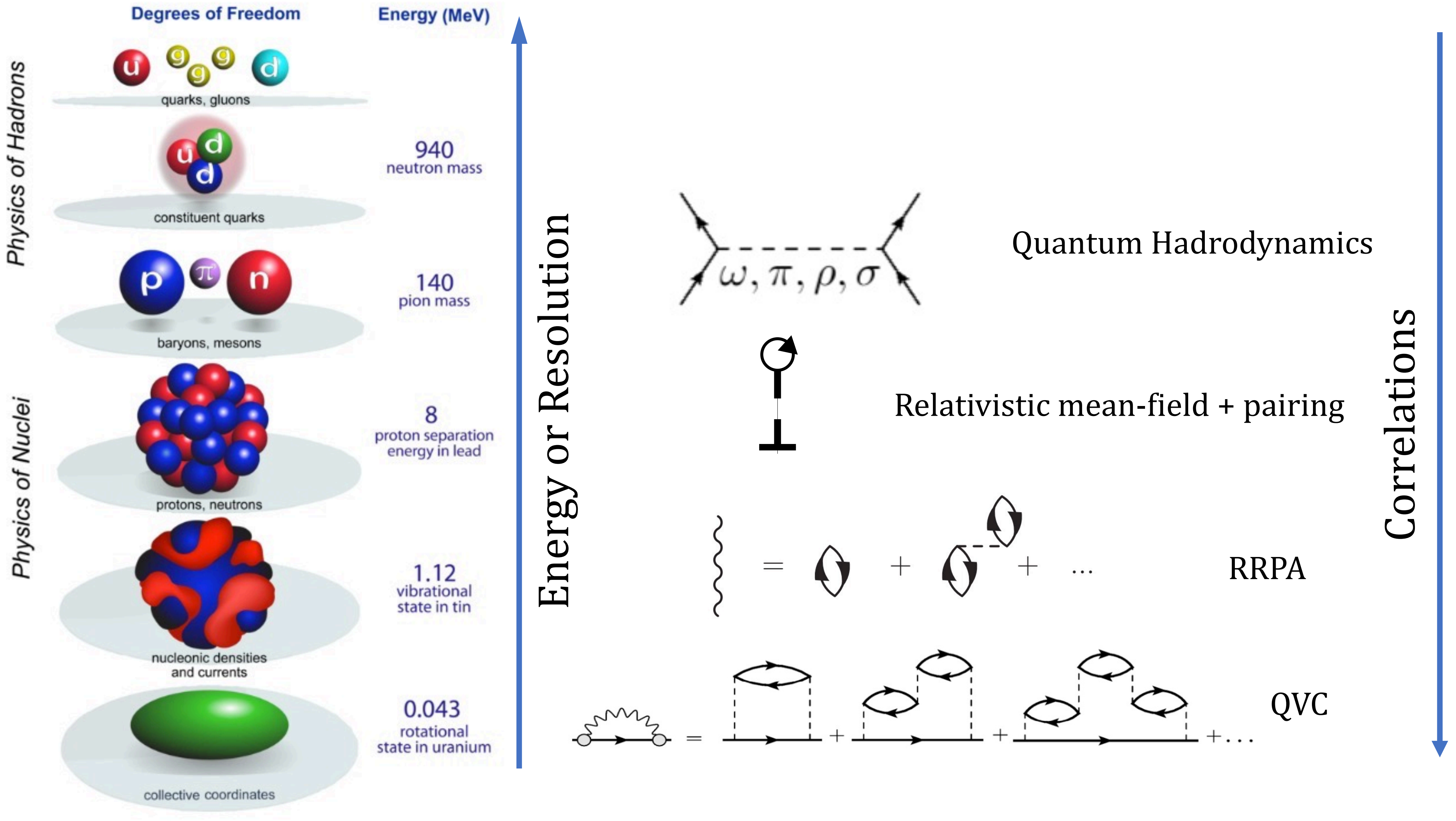
Not well known

Quantum many-body problem

Difficult to solve

Easy to solve

Energy scales and relevant degrees of freedom



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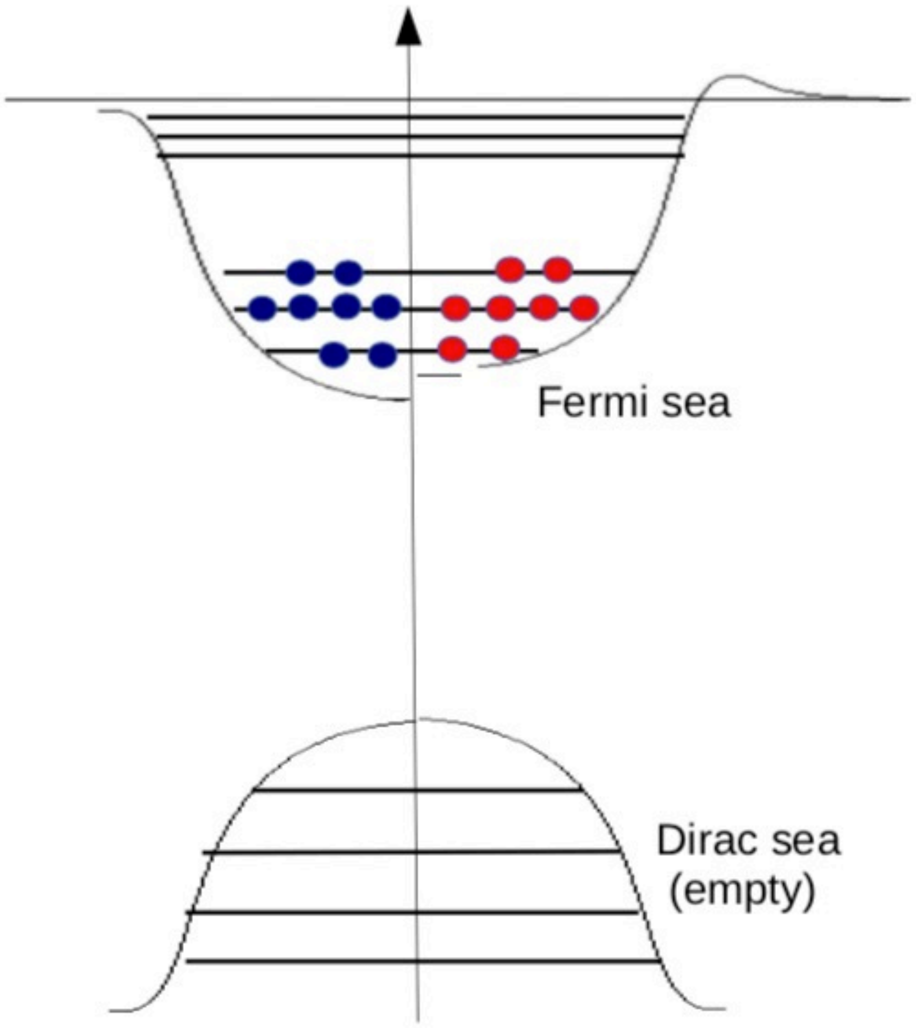
Covariant Energy Density Functionals



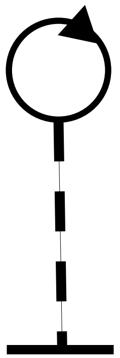
Mean-field approximation

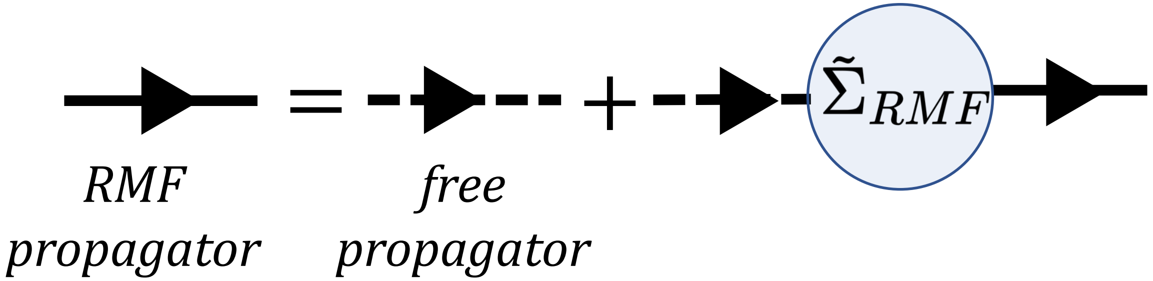
Dirac Hamiltonian:

$$h^{\mathcal{D}} = \boldsymbol{\alpha}\mathbf{p} + \beta(m + \tilde{\Sigma}_{RMF})$$

With static self-energy:

$$\tilde{\Sigma}_{RMF}(\boldsymbol{r}) = \sum_m \Gamma_m \phi_m(\boldsymbol{r}) =$$





Covariant Energy Density Functionals

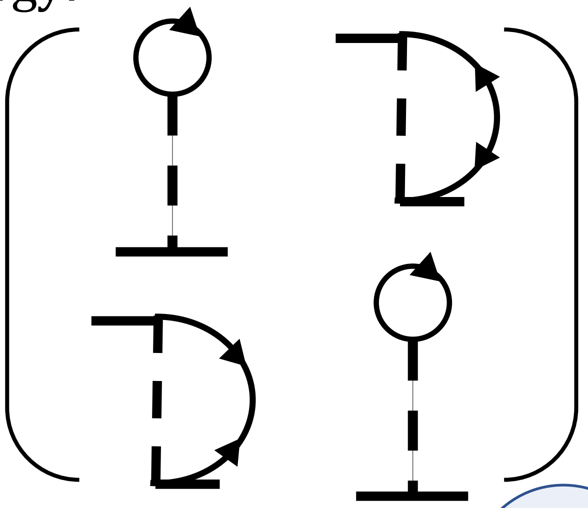
+ Superfluid pairing correlations in open-shell nuclei

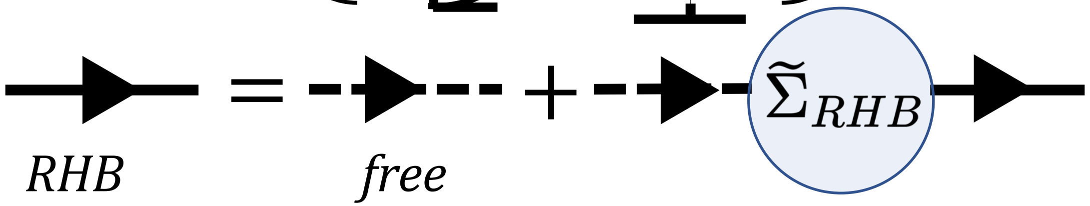
RHB Hamiltonian:

$$\mathcal{H}_{\mathrm{RHB}} = 2\frac{\delta E_{\mathrm{RHB}}}{\delta \mathcal{R}} = \begin{pmatrix} h^{\mathcal{D}} - m - \lambda & \Delta \\ -\Delta^* & -h^{\mathcal{D}*} + m + \lambda \end{pmatrix}$$

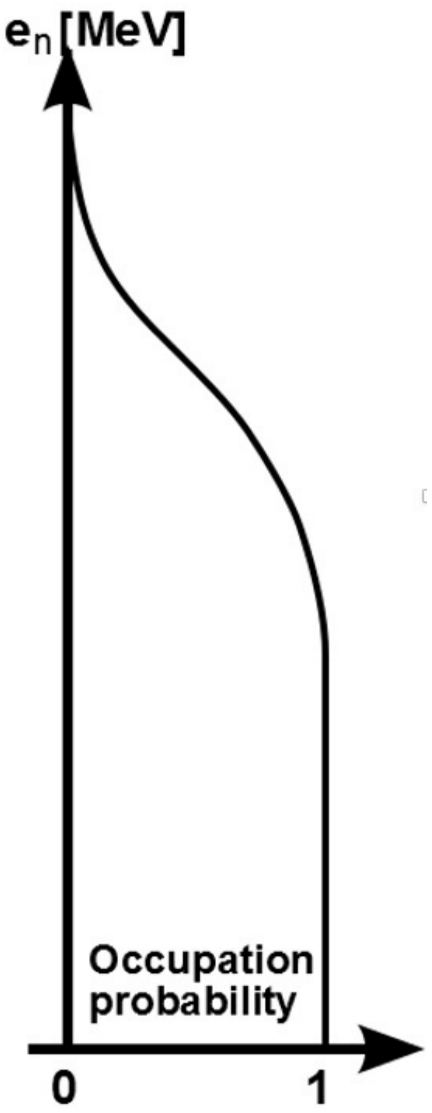
RHB Self-energy:

$\tilde{\Sigma}_{RHB} =$





RHB propagator *free propagator*

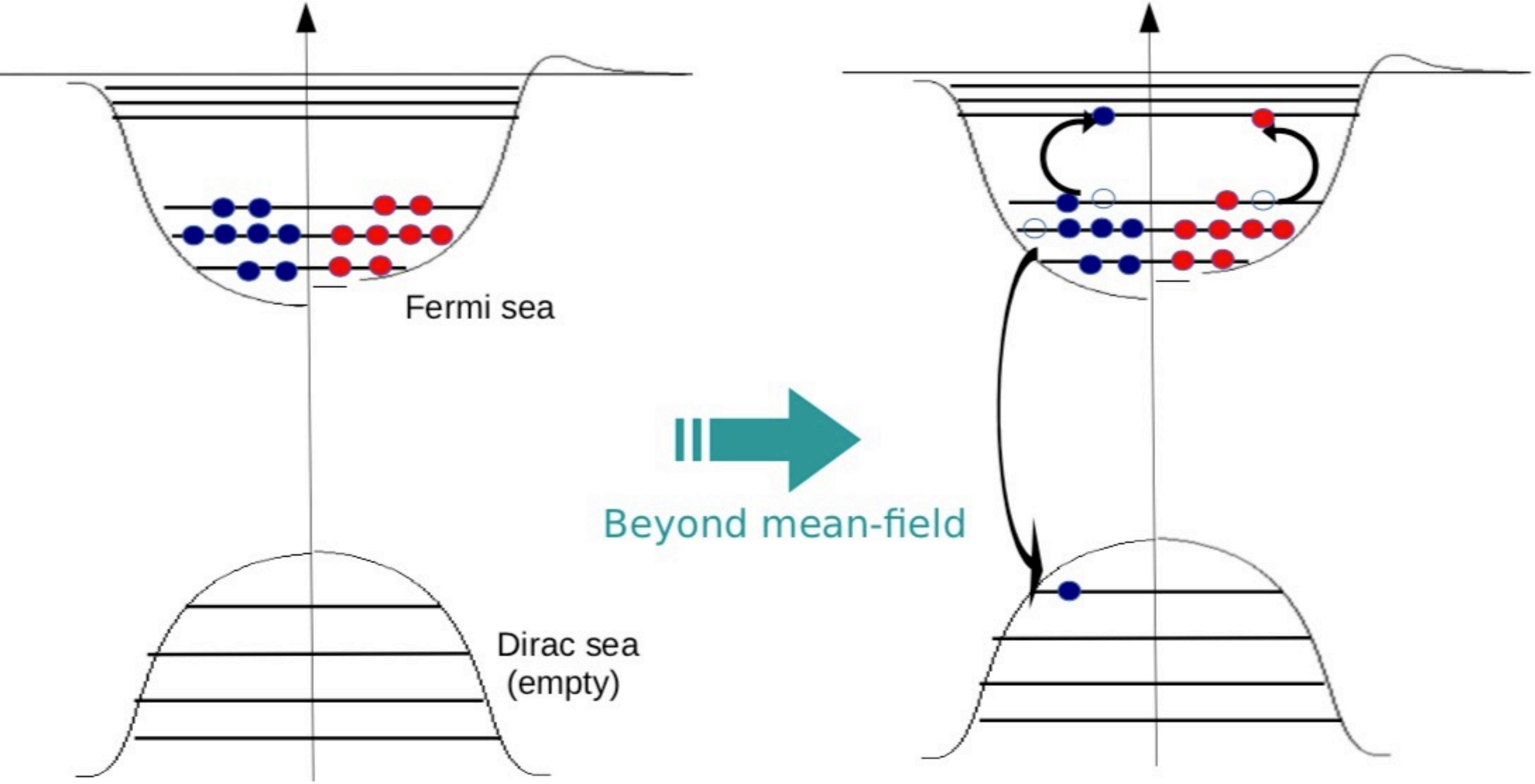


Ways to improve present EDFs

Beyond phenomenological mean field and extension

- Density Matrix Expansions
- Multi-Reference EDFs
- Generator Coordinate Method
- Time-dependent DFT
- Random Phase Approximation
- Particle Vibration Coupling

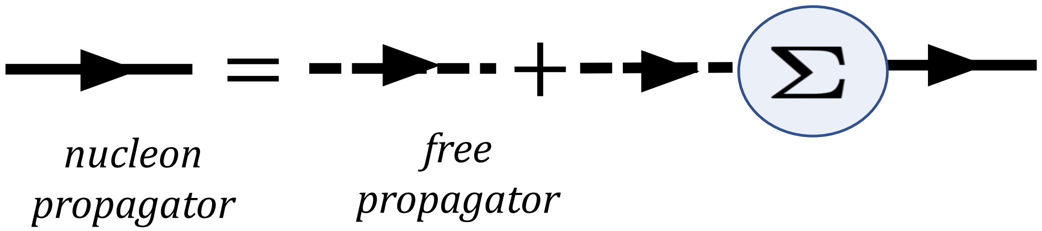
Beyond the mean-field: quasiparticles coupled to vibrations



Beyond the mean-field: quasiparticles coupled to vibrations

The Dyson equation for nucleon

$$G = G^{(0)} + G^{(0)}\Sigma G$$



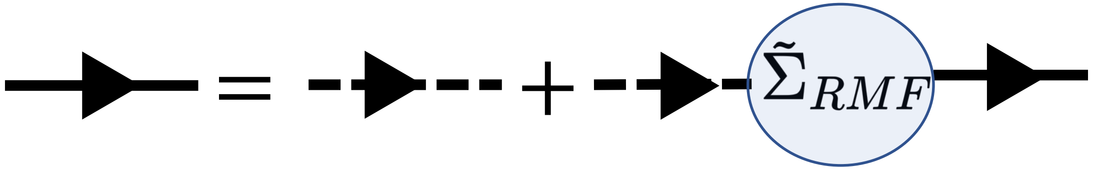
In general, the self-energy can be written as sums of the stationary local and energy dependent nonlocal terms:

$$\Sigma\left(\mathbf{r},\mathbf{r}';\omega\right) = \tilde{\Sigma}(\mathbf{r})\delta\left(\mathbf{r}-\mathbf{r}'\right) + \Sigma^{e}\left(\mathbf{r},\mathbf{r}';\omega\right)$$

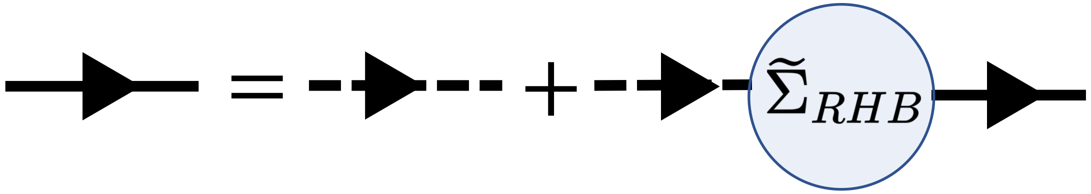
static dynamic

The self-energy Σ can approximately be $\tilde{\Sigma}_{RMF}$ or $\tilde{\Sigma}_{RHB}$

RMF:



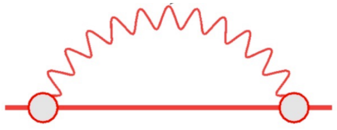
RHB:



Beyond the mean-field: quasiparticles coupled to vibrations

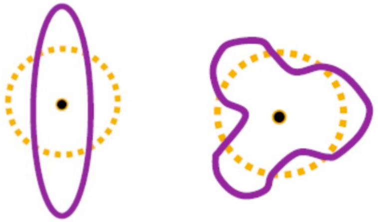
Quasiparticle-Vibration Coupling (QVC) in the nucleonic self-energy

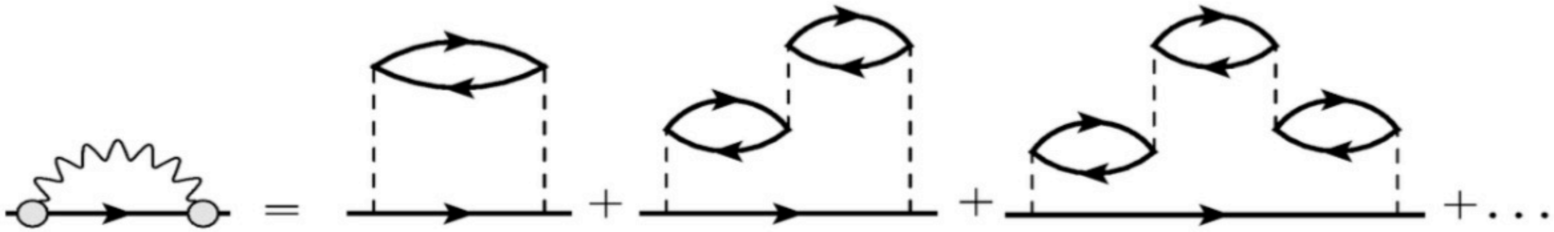
$$-\Sigma- = -\tilde{\Sigma}_{RHB} - +$$



$\Sigma^{(e)}(E)$

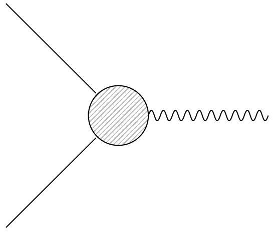
Vibration(phonon)





= ∞ series of 1p-1h excitations

Allows a non perturbative treatment of the NN interaction



QVC vertex $$\gamma^{\mu}_{kl} = \sum_{k'l'} V_{kl'lk'} \delta\rho^{\mu}_{k'l'}$$

Beyond the mean-field: quasiparticles coupled to vibrations

Quasiparticle propagator:

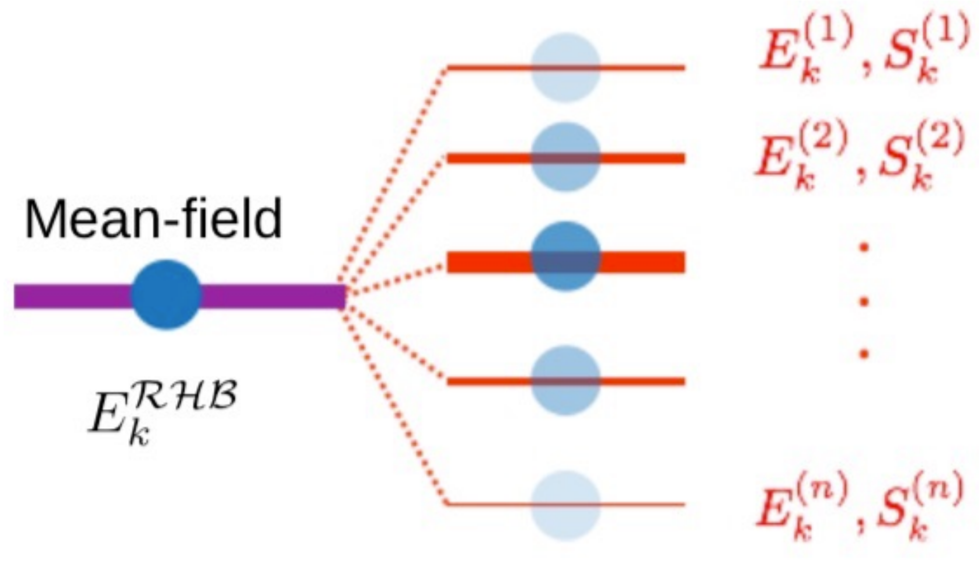
$$G(E) = \left(\varepsilon - \mathcal{H}_{RHB} - \underbrace{\Sigma^{(e)}(E)}_{\text{Introduces new poles}}\right)^{-1}$$

Energy dependent term

$$\Sigma^{(e)}_{k_1 k_2}(\varepsilon) = \sum_{k,\mu} \frac{\gamma_{\mu;k_1 k}\gamma_{\mu;k_2 k}}{\varepsilon - \eta(E_k + \Omega_\mu - i\delta)}$$

$$E_k^{(\nu)} = E_k^{\mathcal{RHB}} + \Sigma_k^{(e)}\left(E_k^{(\nu)}\right)$$

Fragmentation of single (quasi) particle states:

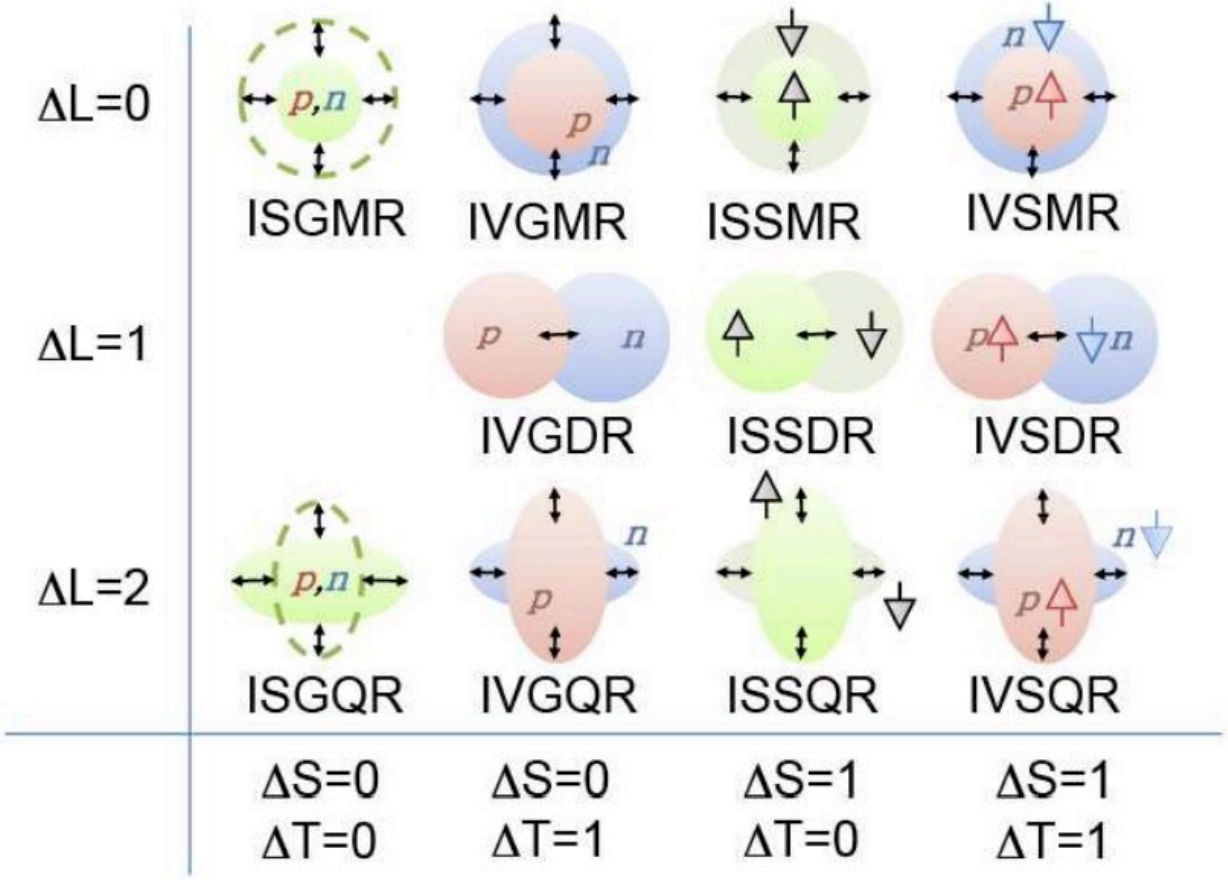


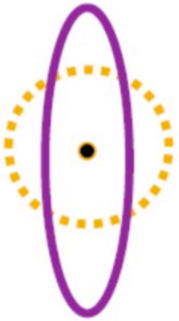
With fractional occupation numbers

$$\sum_\nu S_k^{(\nu)} = 1$$

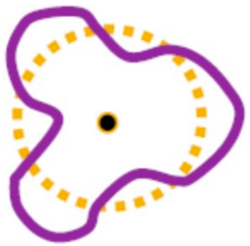
$$E_k^{\mathcal{RHB}} = \sum_\nu S_k^{(\nu)} E_k^{(\nu)}$$

Nuclear Vibrational motions



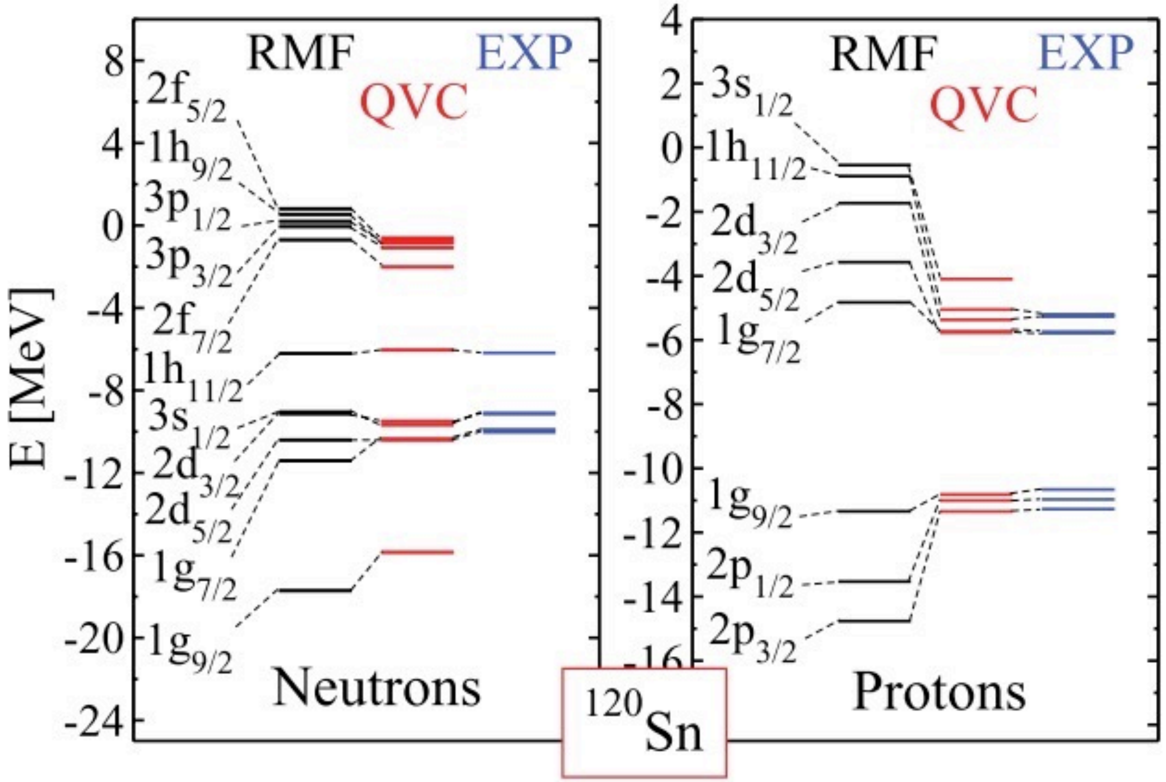


The quanta of vibrational energy are called phonons.
Quadrupole oscillations are the lowest order nuclear vibrational mode.
A quadrupole phonon carries 2 units of angular momentum and has even parity $J^P = 2^+$



An octupole phonon carries 3 units of angular momentum and has odd parity $J^P = 3^-$

(Quasi)particle-vibration coupling in spherical case

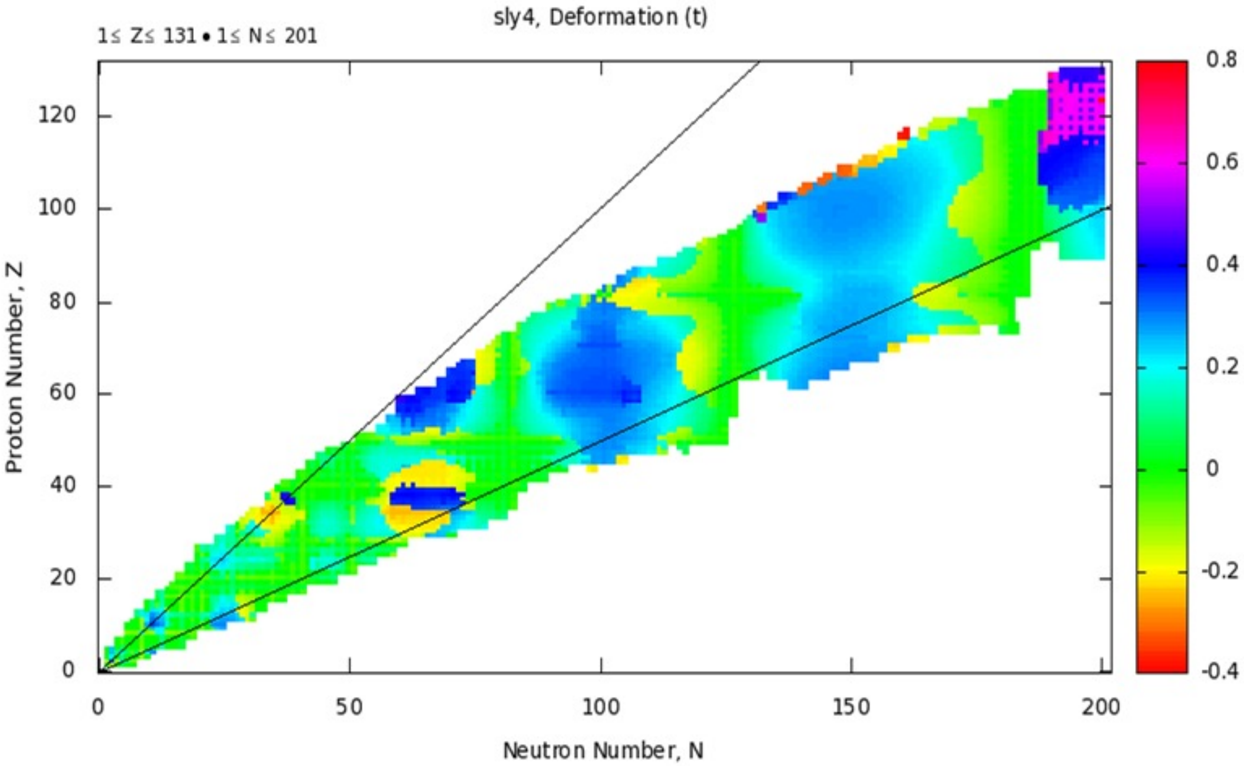


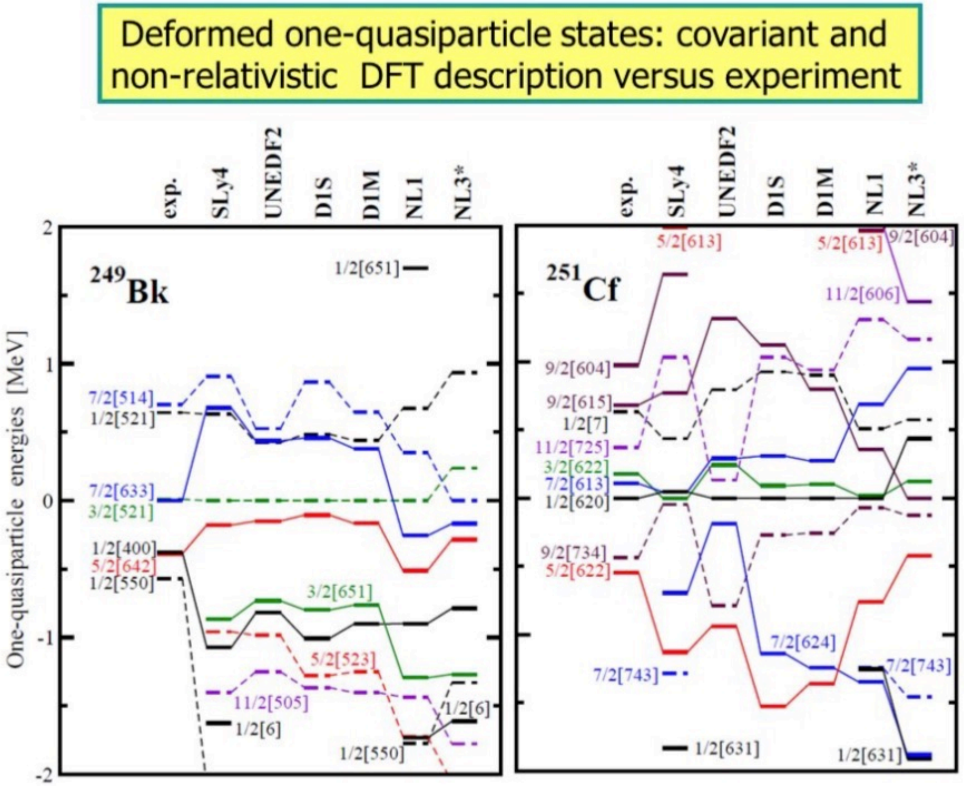
(nlj) ν	S^{th}	S^{exp}
$2d_{5/2}$	0.32	0.43
$1g_{7/2}$	0.40	0.60
$2d_{3/2}$	0.53	0.45
$3s_{1/2}$	0.43	0.32
$1h_{11/2}$	0.58	0.49
$2f_{7/2}$	0.31	0.35
$3p_{3/2}$	0.58	0.54

Dominant states and spectroscopic factors in ^{120}Sn

Elena Litvinova *PRC 85, 021303(R) (2012)*

Deformed nuclei





Private discussion with A. V. Afanasjev

Allow density to break rotational invariance of original interaction → Spontaneous symmetry breaking
Nuclei become deformed and are characterized by several collective coordinates q_i representing the nuclear shape

Quasiparticle Random Phase Approximation for deformed nuclei

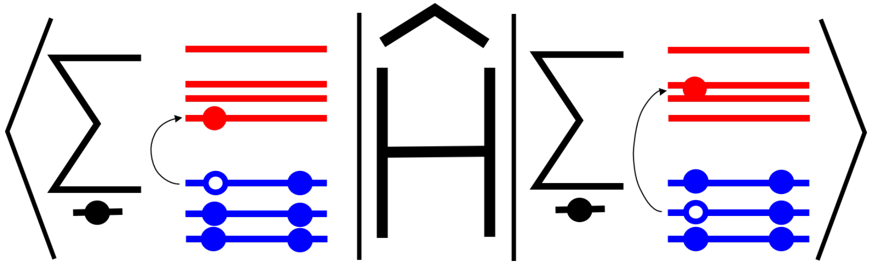
- The tradition method:

Diagonalization the QRPA matrix

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

$\delta\rho_{\mathrm{ph}}$

$\delta\rho_{hp}$



with

$$A_{mi,nj} = (\varepsilon_m - \varepsilon)\delta_{mn}\delta_{ij} + \left\langle \phi_m \left| \frac{\partial h}{\partial \rho_{nj}} \right|_{\rho_0} \middle| \phi_i \right\rangle$$

$$B_{mi,nj} = \left\langle \phi_m \left| \frac{\partial h}{\partial \rho_{jn}} \right|_{\rho_0} \middle| \phi_i \right\rangle$$

the same effective interaction determines the RHB quasiparticle spectrum and the residual interaction

Tremendous computational costs

- Tedious calculation of residual interactions
- Huge matrix dimension for deformed systems.

Finite Amplitude Method for deformed nuclei

Residual interaction can be estimated by the finite difference method:

$$\delta h(\omega) = \frac{1}{\eta}\left(h[\langle\psi'|, |\psi\rangle] - h_0\right)$$

$$|\psi_i\rangle = |\phi_i\rangle + \eta|X_i(\omega)\rangle, \quad \langle\psi_i'| = \langle\phi_i| + \eta\langle Y_i(\omega)|$$

$$\rho_0 + \delta\rho(\omega) = \sum_i |\psi_i\rangle\langle\psi_i'| = (|\phi_i\rangle + \eta|X_i(\omega)\rangle)(\langle\phi_i| + \eta\langle Y_i(\omega)|)$$

Starting from initial amplitudes $X^{(0)}$ and $Y^{(0)}$, we can use an iterative method to solve the following linear-response equations.

$$\omega|X_i(\omega)\rangle = (h_0 - \varepsilon_i)|X_i(\omega)\rangle + \hat{Q}\{\delta h(\omega) + V_{\text{ext}}(\omega)\}|\phi_i\rangle$$

$$\omega\langle Y_i(\omega)| = -\langle Y_i(\omega)|(h_0 - \varepsilon_i) - \langle\phi_i|\{\delta h(\omega) + V_{\text{ext}}(\omega)\}\hat{Q}$$

finite difference method for residual interaction → avoid two-body matrix element calculation
iterative method → avoid huge matrix diagonalization

T. Nakatsukasa, I., Yabana, PRC76 (2007) 024318.
A. Bjelčić, T. Nikšić CPC 253 (2020) 107184

Numerical scheme

Input:
- DD-PC1
- Separable pairing force

RHB

FAM-QRPA

- Calculate phonon spectrum and their coupling vertices
- Phonons selected according to their J^{π}, K and energy

- Fragmentation of quasiparticle energies
- Spectroscopic factors

Dyson equation

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  Heavy nucleus ^{250}Cf

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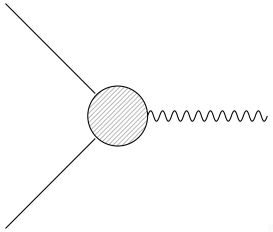
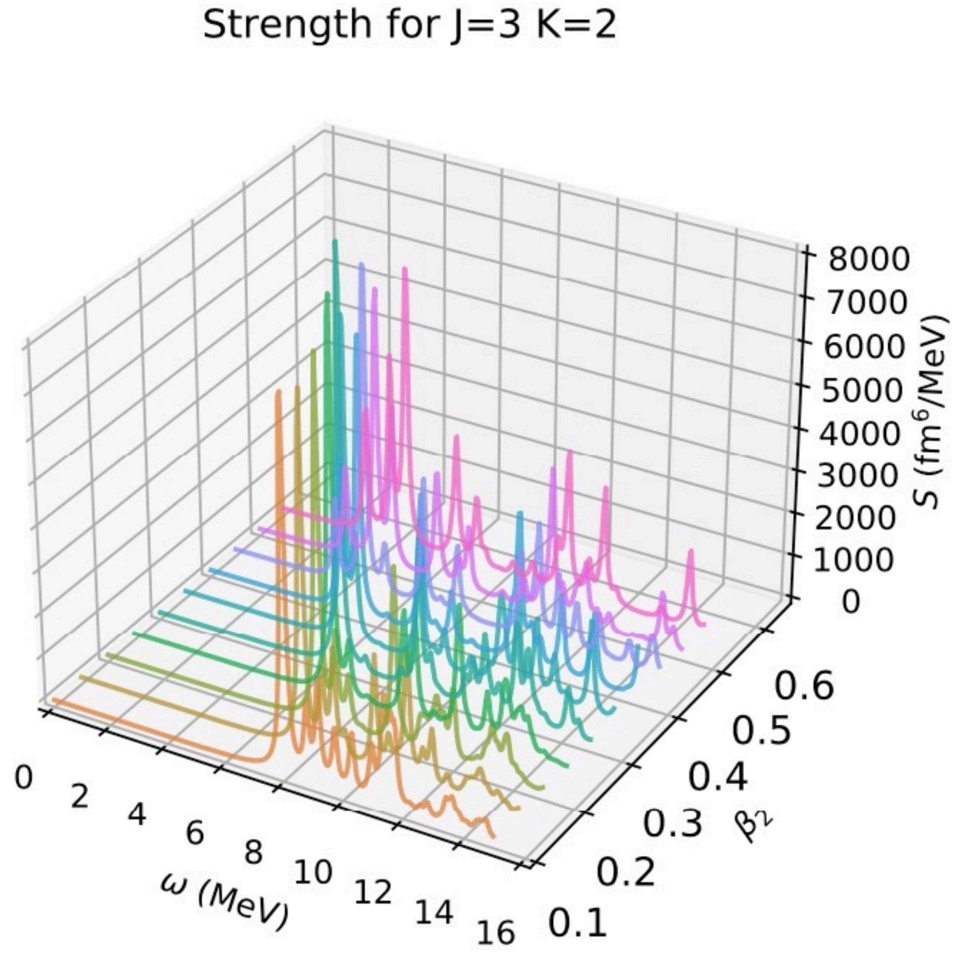
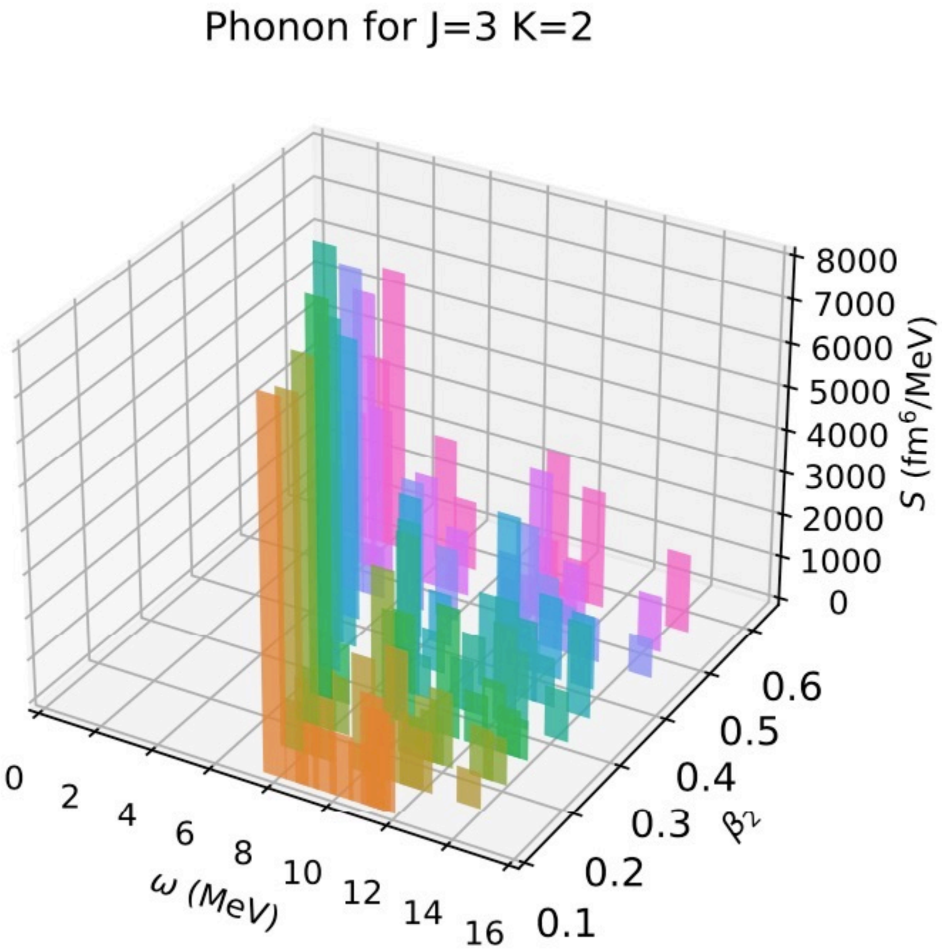
Calculate quasiparticle phonon coupling vertex for different β_2

^{38}Si

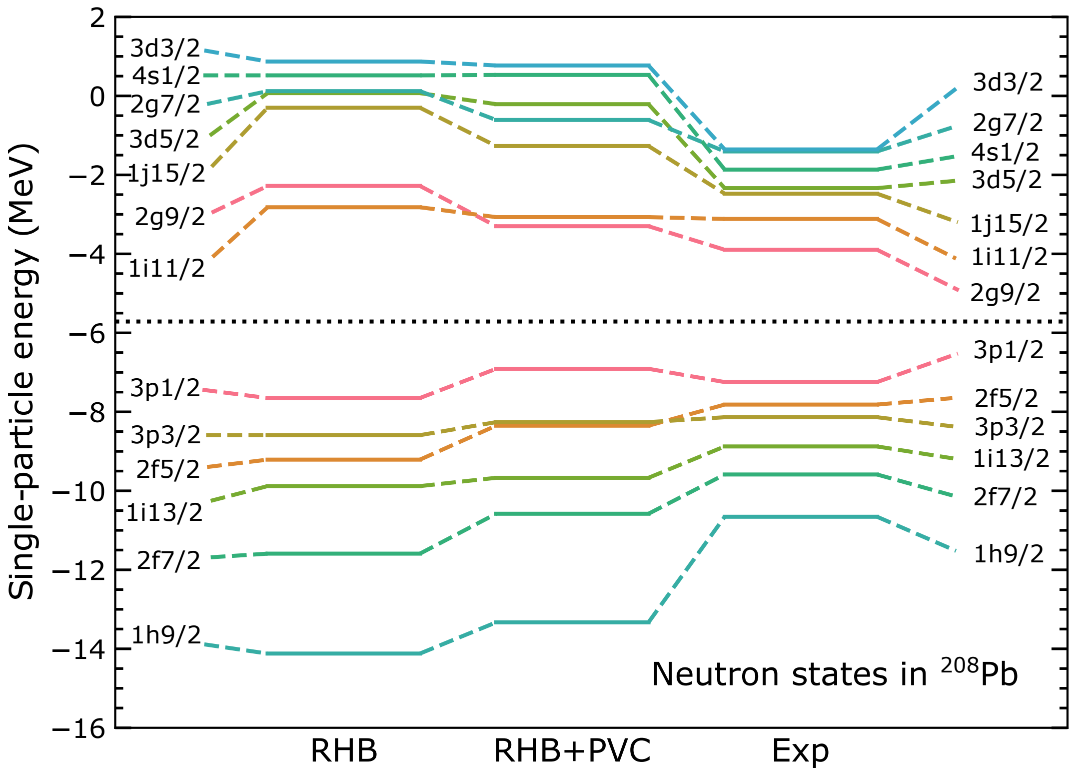
$$\gamma^{\mu}_{kl} = \sum_{k'l'} V_{kl'lk'}\,\delta\rho^{\mu}_{k'l'} = \frac{\delta H}{\delta\hat{\rho}}\delta\rho$$

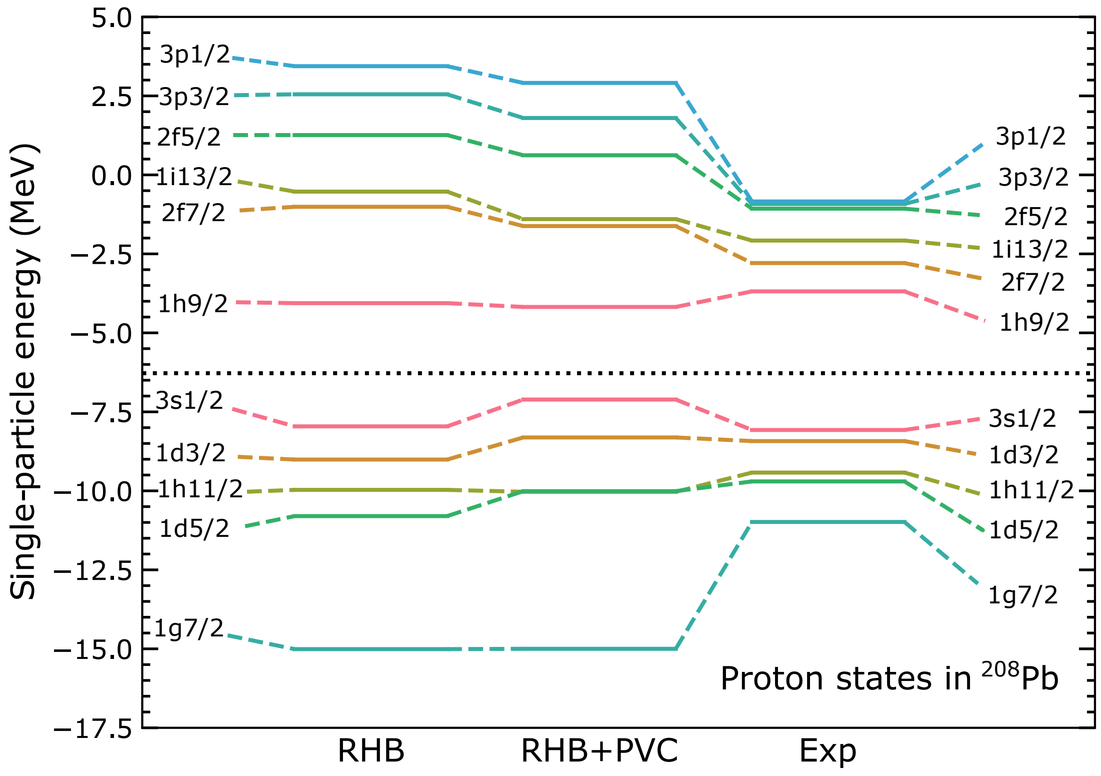






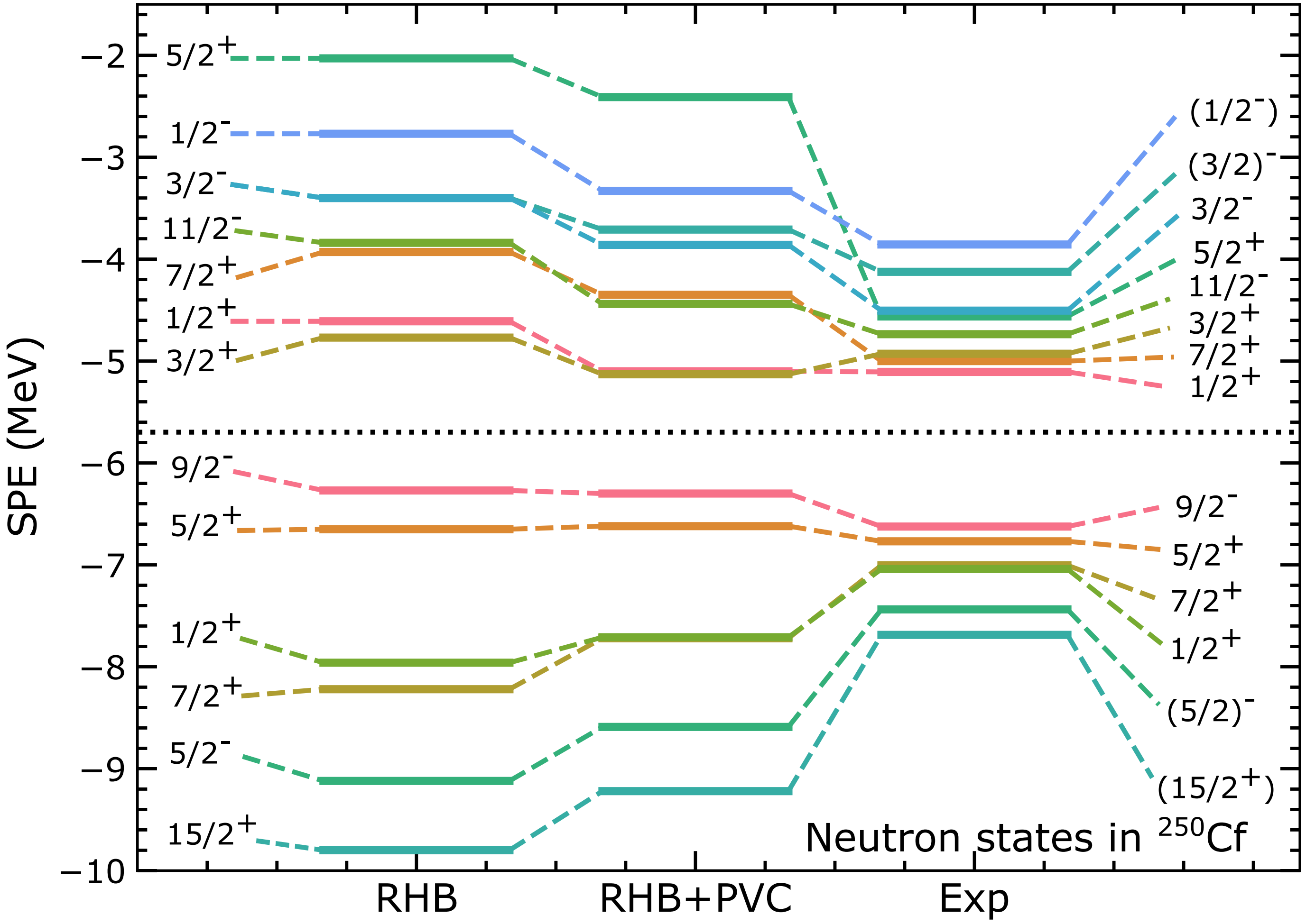
Single particle spectrum in ^{208}Pb





The single-particle energy $\lambda \pm E_n$ above (below) the RHB Fermi energy if their RHB occupancies are smaller (greater) than 0.5

Deformed QVC: heavy ^{250}Cf



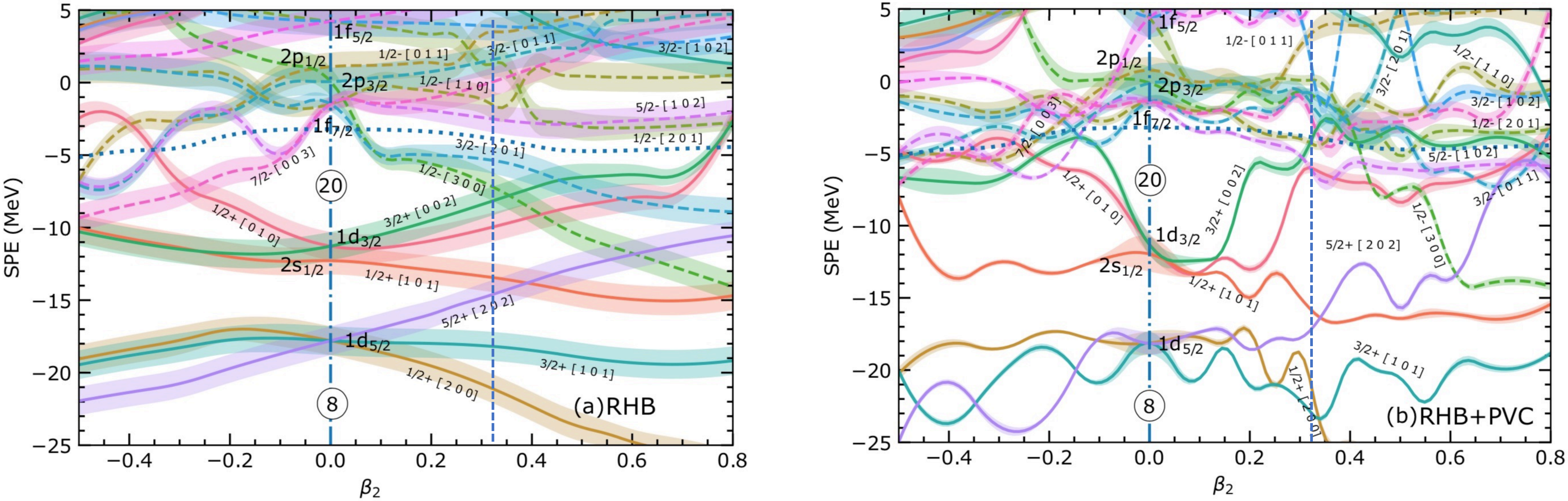
$J^P = 2^+ \quad J^P = 3^-$

$0 \leq K \leq J$

Quadrupole and octupole channels couple to the RHB states with considerable strength

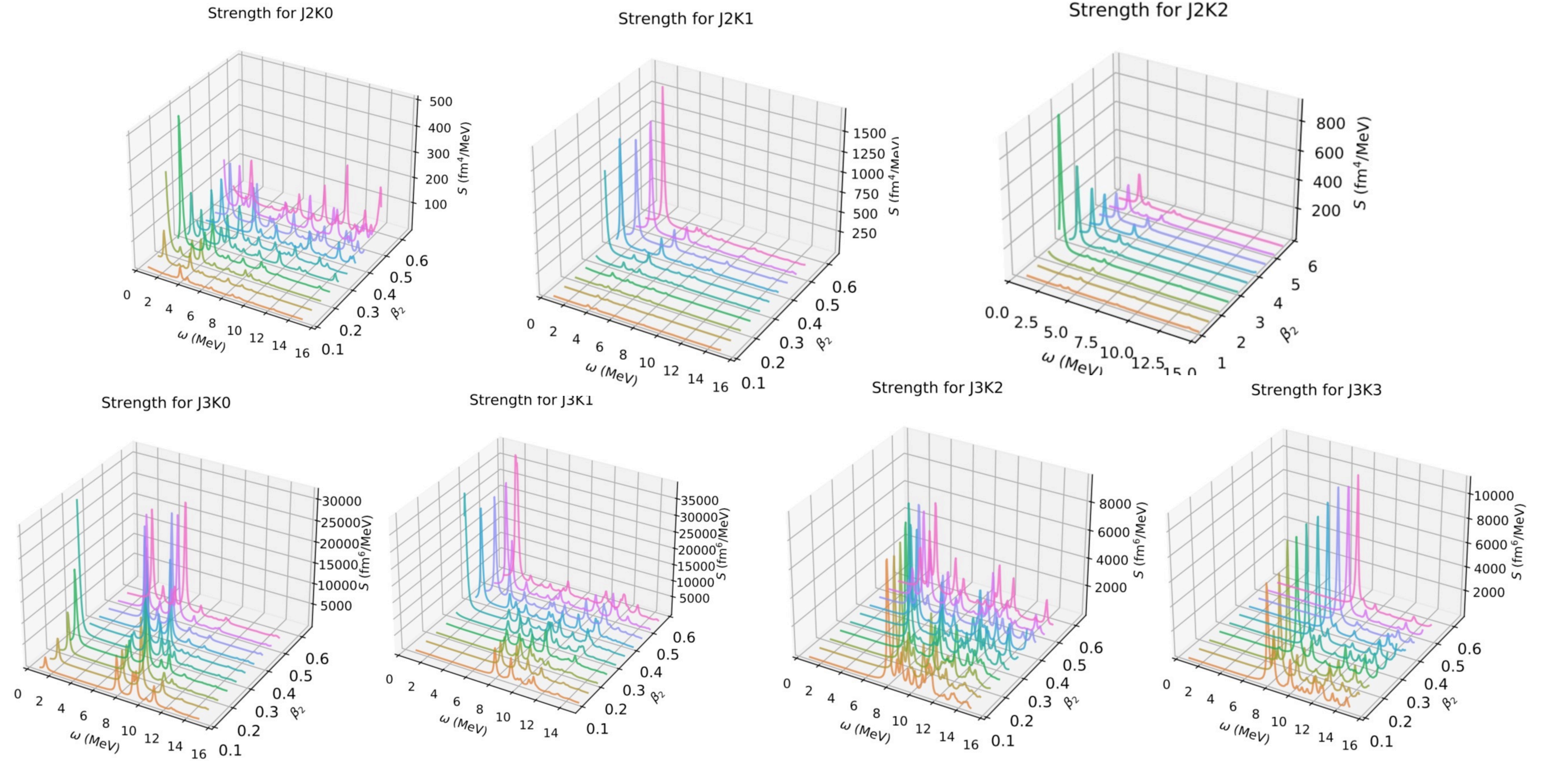
Compare them to the band-head levels in ^{251}Cf and ^{249}Cf from experiment data

Deformed QVC: neutron rich ^{38}Si



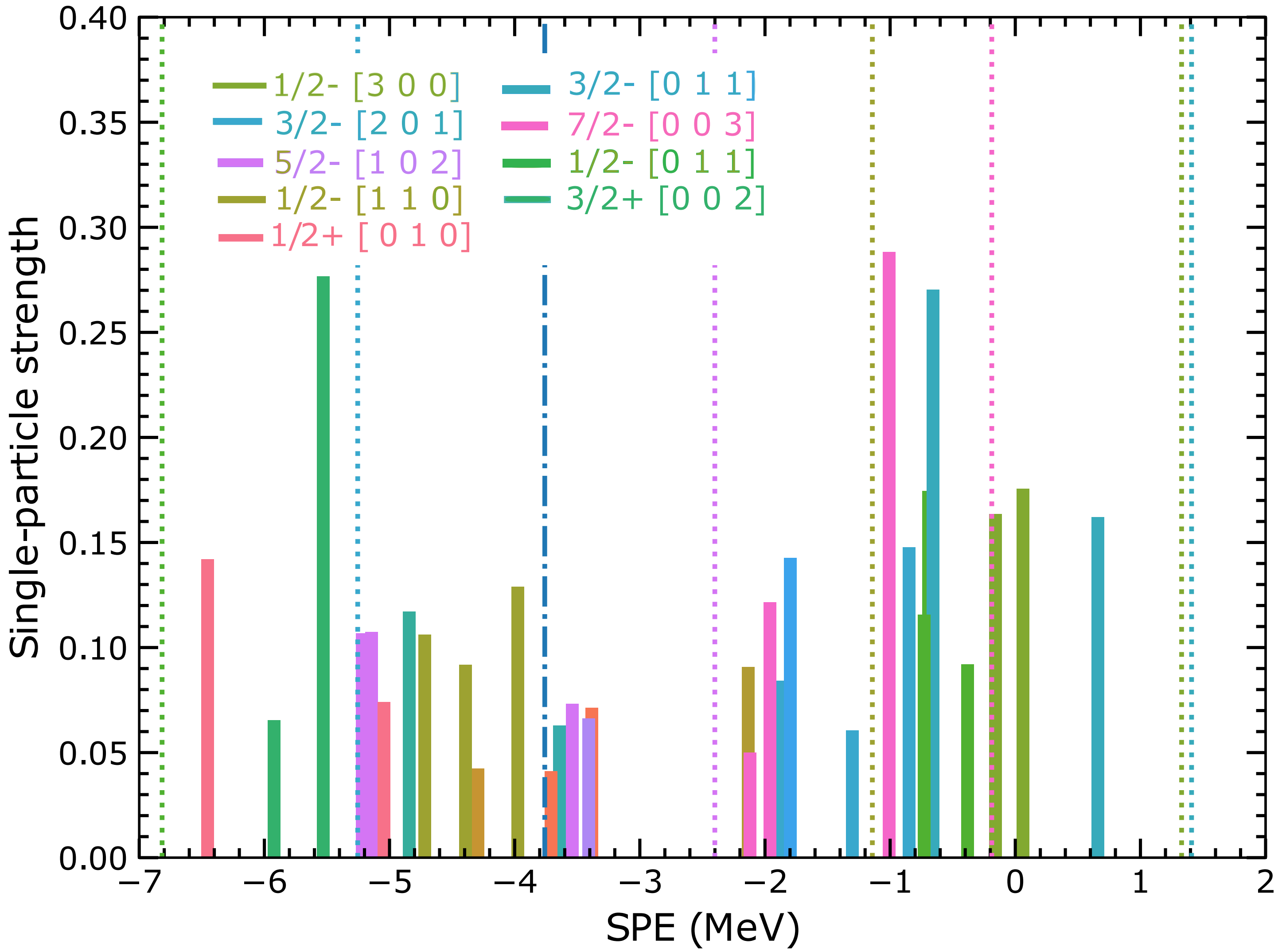
At $\beta_2 = 0$, the degeneracy of the quasiparticle states reproduced, and the occupancies maximized
Additional oscillations of the dominant fragments' states due to the evolution of the low-energy collective phonons
Formation of the new shell closure at the neutron number N = 16

Deformed QVC: neutron rich ^{38}Si



Deformed QVC: neutron rich ^{38}Si

Potential energy surface minimum $\beta_2 = 0.31$



Remarkable fragmentations

- Deformation
- Pairing

Lead to a few competing fragments
Major fragments is moving toward the Fermi energy

Summary

Beyond mean-field in the particle-vibration coupling scheme:

Provide a formal of extension of EDF to include many-body correlation

Degrees of freedom:

- Quasiparticle states
- phonons

Implemented for open-shell nuclei with axial deformations

For the medium-mass and heavy nuclei

- a significant fragmentation of the quasiparticle states around the Fermi surface
- an increase of the level densities in both neutron and proton subsystems

Improves agreement with experimental data compared to the mean-field approximation

Perspectives:

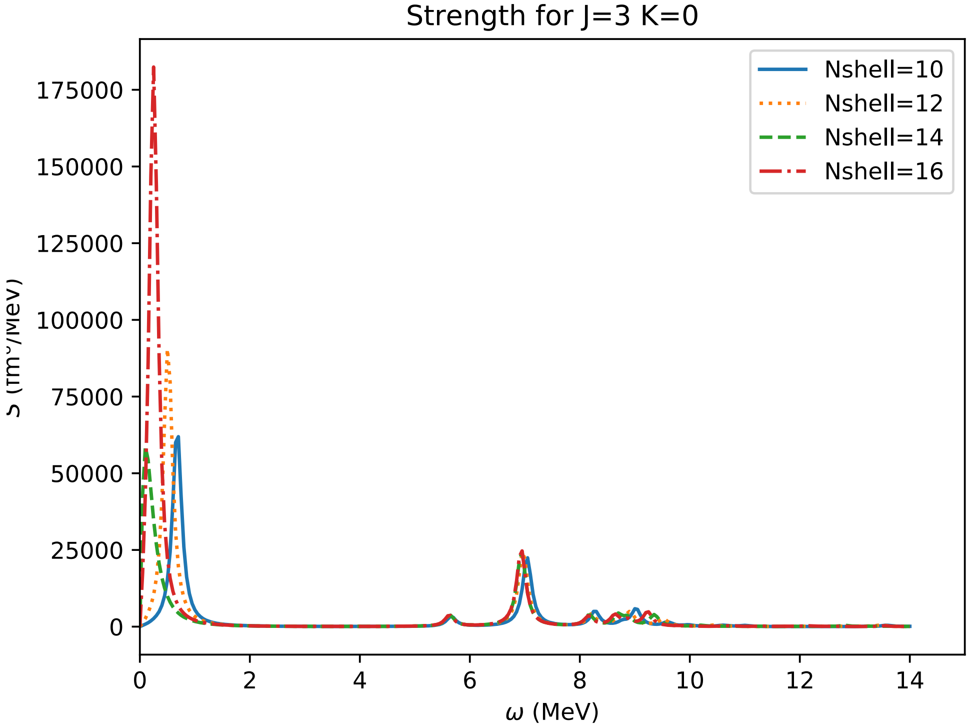
- Introduce the energy-dependent potential in the response function.
  It should lead to a fragmentation of the giant resonance spectrum due to complex configurations such as 2p-2h excitations and to a considerable increase of the width.
- Start from chiral interaction, see the PVC effects.

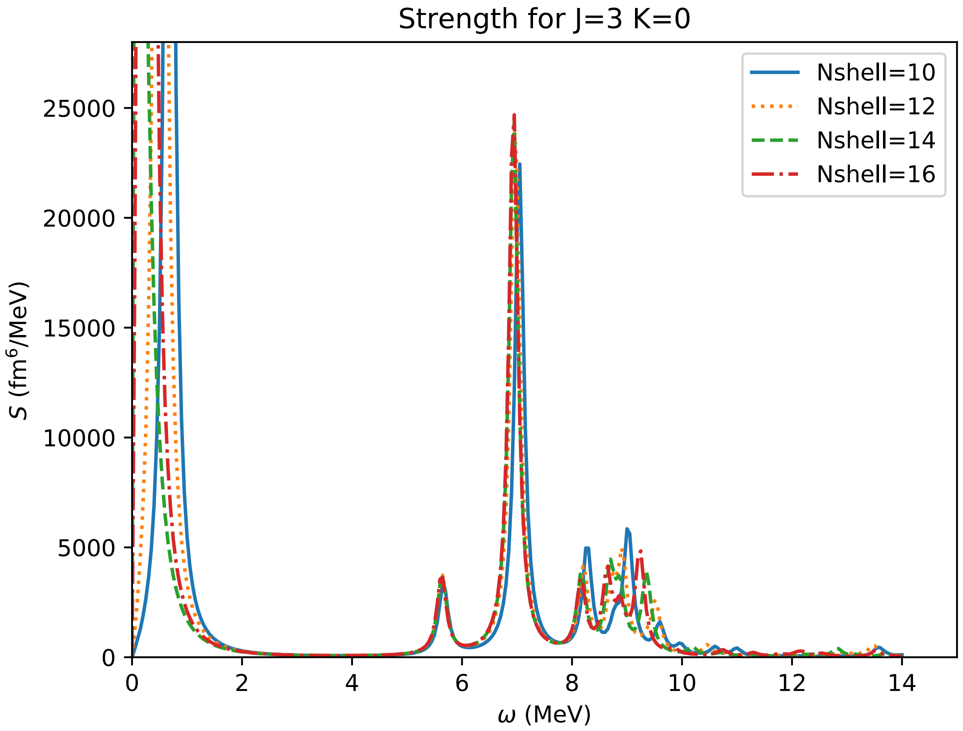
Thank you!

Collaborators:

Elena Litvinova,	Western Michigan University
Antonio Bjelcic , Tamara Niksic,	University of Zagreb
Peter Ring,	The Technical University of Munich
Peter Schuck,	Paris-Sud University

Problem: Spurious states in FAM





Implementation of the method proposed to separate the spurious response related to the breaking of the translation symmetry from the physical response. In practice there is always some mixing mostly due to the finite size of the oscillator basis used in the calculation. However, because the spurious states are due to the finite size of the harmonic oscillator basis, we can change the parameter of the harmonic oscillator. The physical states will remain stable, and the spurious states will heavily rely on harmonic oscillator parameters.

Phonon Calculation

Induced Hamiltonian

$$\delta\mathcal{H}(\omega) = \begin{pmatrix} \delta\mathcal{H}^{11}(\omega) & \delta\mathcal{H}^{20}(\omega) \\ -\delta\mathcal{H}^{02}(\omega) & -\left[\delta\mathcal{H}^{11}(\omega)\right]^T \end{pmatrix}$$
$$= \mathcal{W}^\dagger \begin{pmatrix} \delta h(\omega) & \delta\Delta^{(+)}(\omega) \\ -\delta\Delta^{(-)}(\omega)^* & -\delta h^T(\omega) \end{pmatrix} \mathcal{W}$$

Derivation of Dirac mean-field

$$\delta h_D = \begin{pmatrix} \delta V + \delta S & -\sigma \cdot \delta\Sigma \\ -\sigma \cdot \delta\Sigma & \delta V - \delta S \end{pmatrix}$$

$$\begin{aligned}
\delta\Sigma_s &= \left\{\alpha_s'\left(\rho_v^0\right)\rho_s^0\right\}\delta\rho_v + \left\{\alpha_s\left(\rho_v^0\right)\right\}\delta\rho_s + \delta_s \triangle \delta\rho_s, \\
\delta\Sigma^0 &= \left\{\alpha_v'\left(\rho_v^0\right)\rho_v^0 + \alpha_v\left(\rho_v^0\right) + \tau_3\alpha_{tv}'\left(\rho_v^0\right)\rho_{tv}^0\right\}\delta\rho_v + \left\{\tau_3\alpha_{tv}\left(\rho_v^0\right)\right\}\delta\rho_{tv} \\
\delta\Sigma_R^0 &= \frac{1}{2}\left\{\alpha_s''\left(\rho_v^0\right)\left(\rho_s^0\right)^2 + \alpha_v''\left(\rho_v^0\right)\left(\rho_v^0\right)^2 + \alpha_{tv}''\left(\rho_v^0\right)\left(\rho_{tv}^0\right)^2\right\}\delta\rho_v \\
&\quad + \left\{\alpha_s'\left(\rho_v^0\right)\rho_s^0\right\}\delta\rho_s + \left\{\alpha_v'\left(\rho_v^0\right)\rho_v^0\right\}\delta\rho_v + \left\{\alpha_{tv}'\left(\rho_v^0\right)\rho_{tv}^0\right\}\delta\rho_{tv} \\
\delta\boldsymbol{\Sigma} &= \left\{\alpha_v\left(\rho_v^0\right)\right\}\delta\boldsymbol{j}_v + \left\{\tau_3\alpha_{tv}\left(\rho_v^0\right)\right\}\delta\boldsymbol{j}_{tv}
\end{aligned}$$

Derivation of pairing field

$$\delta\Delta^{(\pm)}(\omega) = \begin{pmatrix} 0 & \delta\Delta_1^{(\pm)}(\omega) \\ -\left[\delta\Delta_1^{(\pm)}(\omega)\right]^T & 0 \end{pmatrix}$$

$$\left(\delta\Delta_1^{(\pm)}(\omega)\right)_{k_1k_2} = -G \times \frac{1+\delta_{K,0}}{2} \times \delta_{|\Lambda_1-\Lambda_2|,K} \times \sum_{N_z'}\sum_{N_r'} W_{k_1,k_2}^{N_z',N_r'} P_{N_z',N_r'}^{(\pm)}(\omega)$$

Beyond the mean-field

From EDF, we can get nuclear binding energy, radius, deformation etc.
Plus RPA, we can get giant resonance information
However, still have limitations

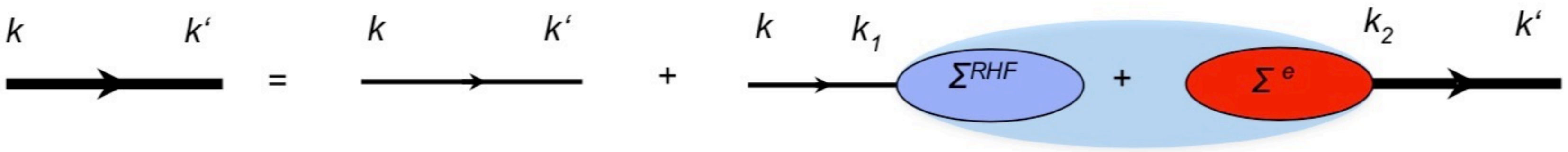
- Single-particle states and their spectroscopic factors

- Width of giant resonance and other excited states

EDF potential is not energy-dependent
Consider the energy-dependent potential

$$\Sigma(\mathbf{r},\mathbf{r}';\omega) = \tilde{\Sigma}(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}') + \Sigma^{e}(\mathbf{r},\mathbf{r}';\omega)$$

One-body propagator G: Dyson equation for Gor'kov Green function



$$G(\varepsilon) = G_0(\varepsilon) + G_0(\varepsilon)\,[\,\Sigma^{RHF} + \Sigma^{e}(\varepsilon)\,]\,G(\varepsilon)$$

Particle Vibration Coupling

The equation of the one-nucleon motion has the form

$$\left(h^D + \beta\Sigma_s^e(\varepsilon) + \Sigma_0^e(\varepsilon)\right)|\psi\rangle = \varepsilon|\psi\rangle$$

h^D denotes the Dirac Hamiltonian with the energy- independent mean field

$$h^D = \boldsymbol{\alpha}\mathbf{p} + \beta(m + \tilde{\Sigma}_s) + \tilde{\Sigma}_0$$

We can get Dirac basis, which diagonalizes the energy-independent part of the Dirac equation

$$h^D|\psi_k\rangle = \varepsilon_k|\psi_k\rangle$$

Define the energy-dependent part

$$\Sigma_{kl}^e(\varepsilon) = \int d^3r d^3r' \psi_k^+(\boldsymbol{r})\left(\beta\Sigma_s^e\left(\boldsymbol{r},\boldsymbol{r}';\varepsilon\right) + \Sigma_0^e\left(\boldsymbol{r},\boldsymbol{r}';\varepsilon\right)\right)\psi_l\left(\boldsymbol{r}'\right)$$

Particle Vibration Coupling

Model assumptions:

In the present work we choose a rather simple particle-phonon coupling model to describe the energy dependence of . Within this model Σ^e is a convolution of the particle-phonon coupling amplitude Σ^e and the exact single-particle Green's function

$$\Sigma^e_{kl}(\varepsilon) = \sum_{k'l'} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi i} \Gamma_{kl'lk'}(\omega) G_{k'l'}(\varepsilon + \omega),$$

where the amplitude Γ has the following spectral expansion:

$$\Gamma_{kl'lk'}(\omega) = -\sum_{\mu} \left(\frac{\gamma^{\mu *}_{k'k} \gamma^{\mu}_{l'l}}{\omega - \Omega^{\mu} + i\eta} - \frac{\gamma^{\mu}_{kk'} \gamma^{\mu *}_{ll'}}{\omega + \Omega^{\mu} - i\eta} \right)$$

and the mean field Green's function is

$$\tilde{G}_{kl}(\varepsilon) = \frac{\delta_{kl}}{\varepsilon - \varepsilon_k + i\sigma_k \eta},$$