



Particle vibration coupling in superfluid nuclei with axial deformation

Yinu Zhang

Collaboration with Elena Litvinova, Herlik Wibowo
Western Michigan University

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Outline

□ **Introduction:**

Energy scales 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**

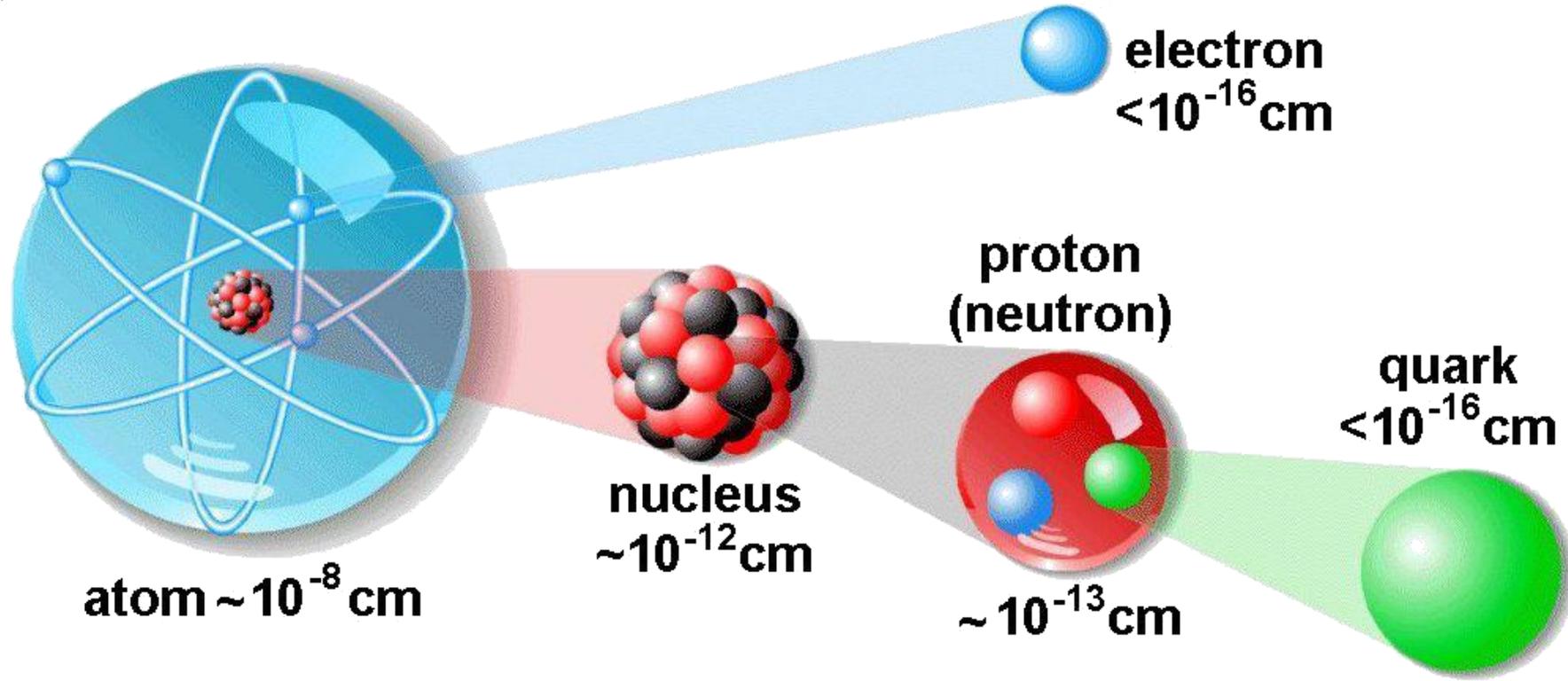
Benchmark to ^{208}Pb

Medium–mass neutron rich nucleus ^{38}Si

Heavy nucleus ^{250}Cf

□ **Summary & perspectives**

Energy scales and relevant degrees of freedom



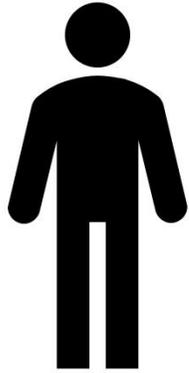
Atoms:
Electromagnetic
Quantum mechanics

Nuclei:
Nuclear interaction
Test ground for
different theoretical tools

Quarks:
Strong interaction
QCD/standard
model

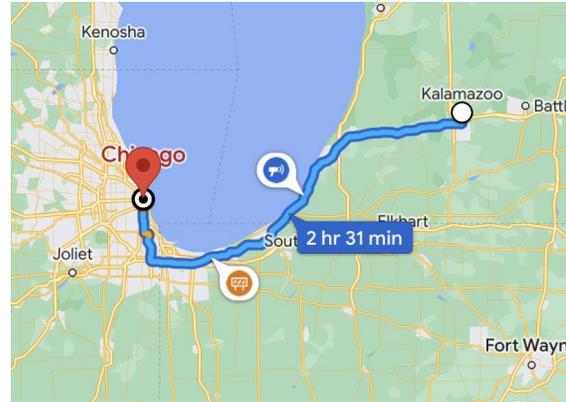
Energy scales and relevant degrees of freedom

Human height



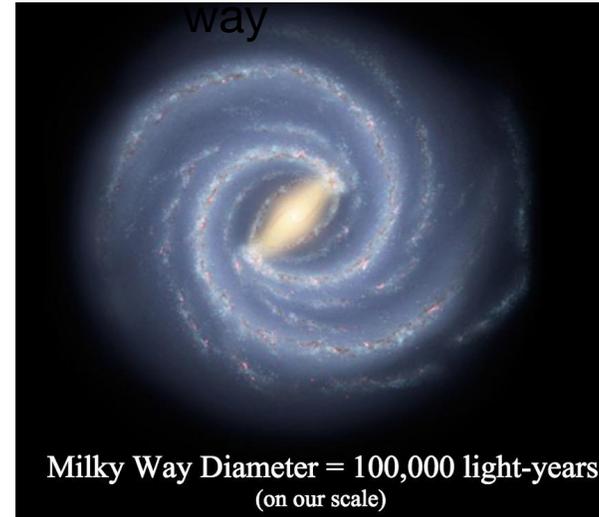
~ 1-2 m

Distance from Kalamazoo to Chicago



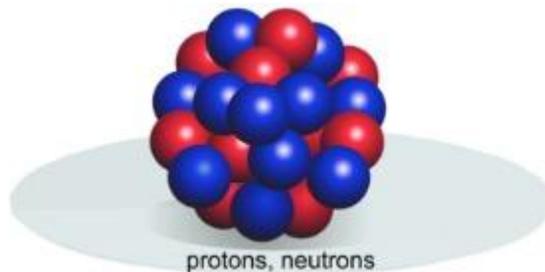
~ 10^5 m
~ 200 km

The milky way



Milky Way Diameter = 100,000 light-years
(on our scale)

~ 10^{20} m

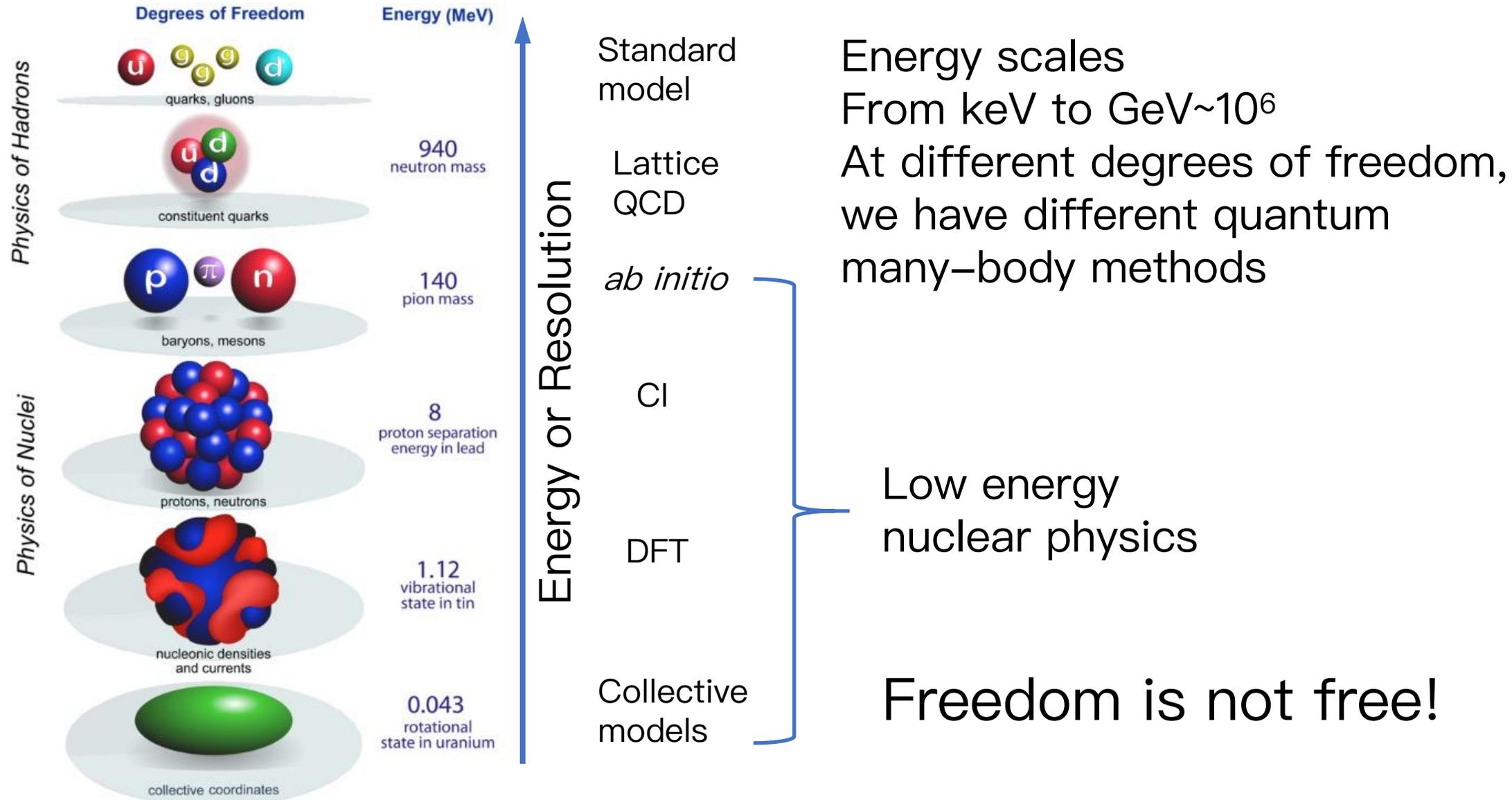


~ fm
~ 10^{-15} m
$$E = \frac{\hbar c}{\lambda}$$

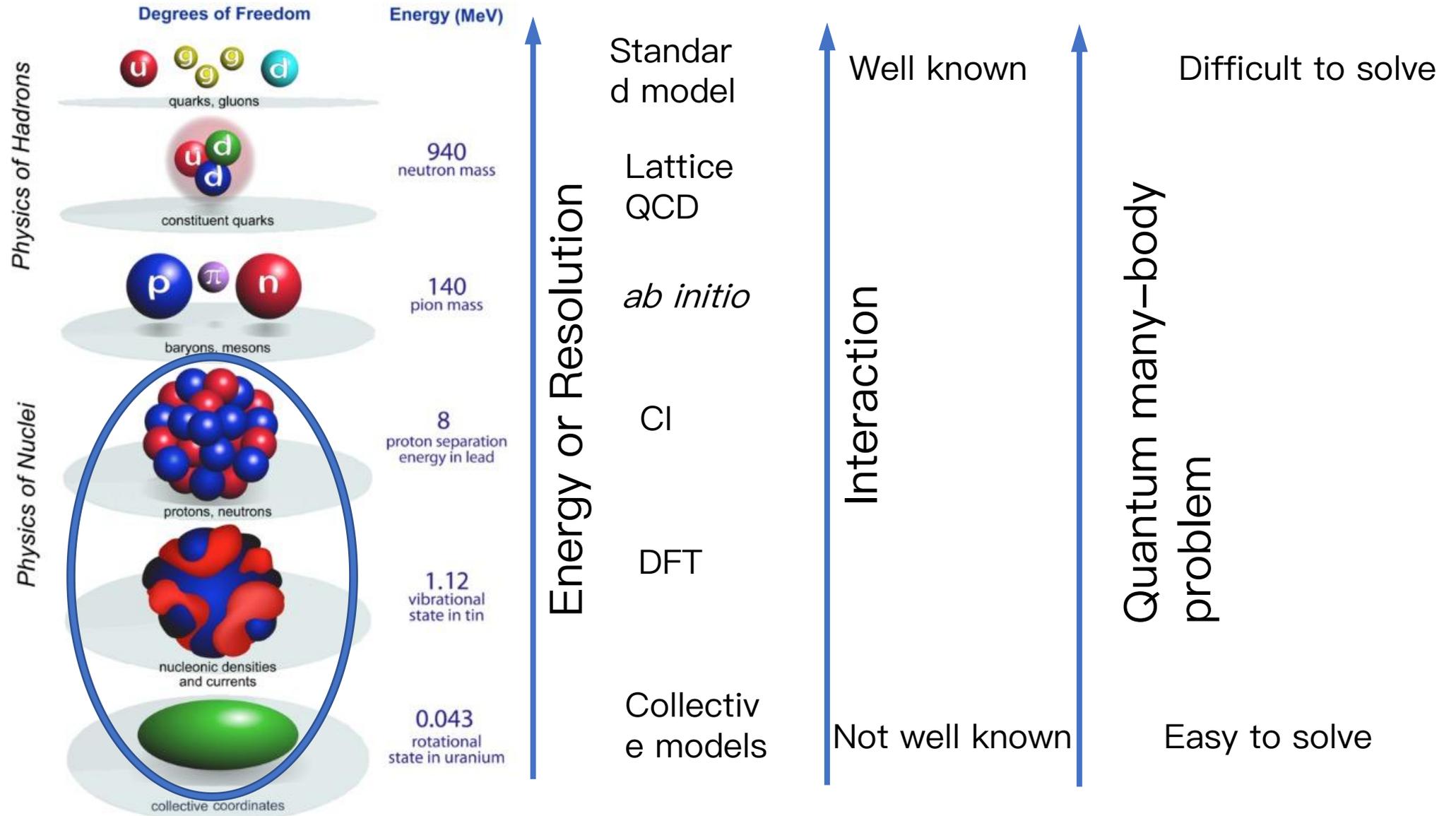
Weinberg's third law of Progress in theoretical Physics:

“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!”

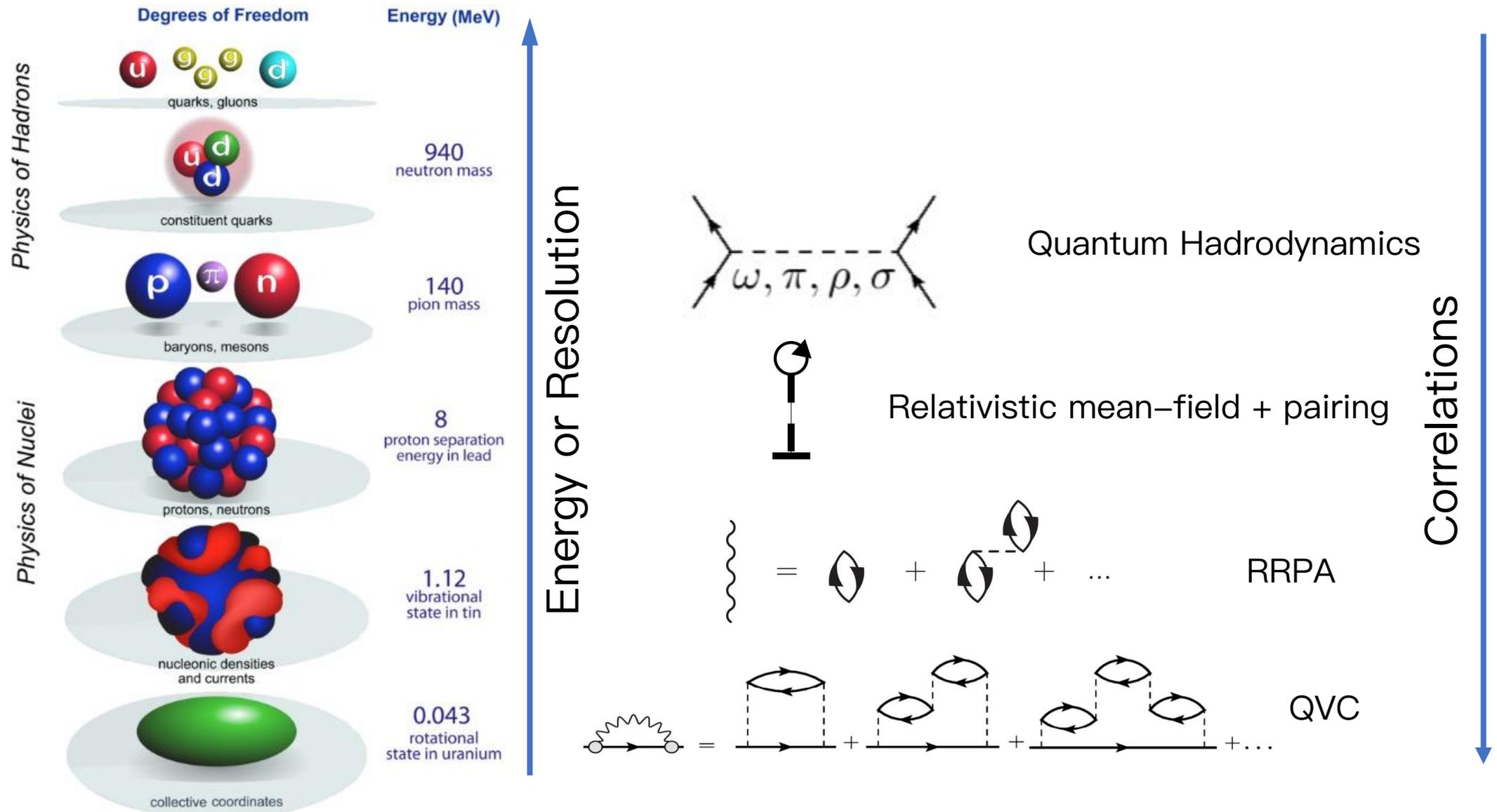
Energy scales and relevant degrees of freedom



Energy scales and relevant degrees of freedom



Energy scales and relevant degrees of freedom



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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

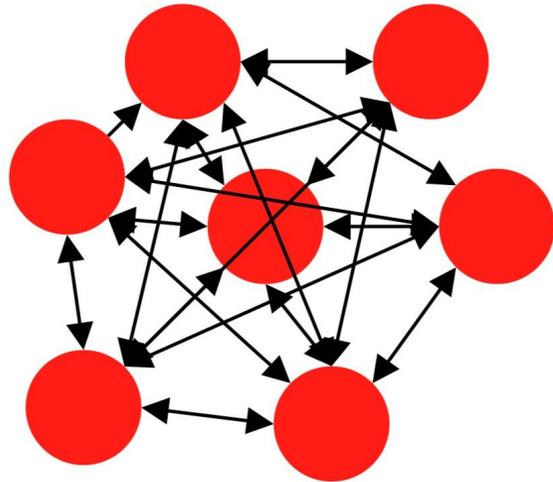
Medium–mass neutron rich nucleus ^{38}Si

Heavy nucleus ^{250}Cf

□ Summary & perspectives

Independent Particle Approximation

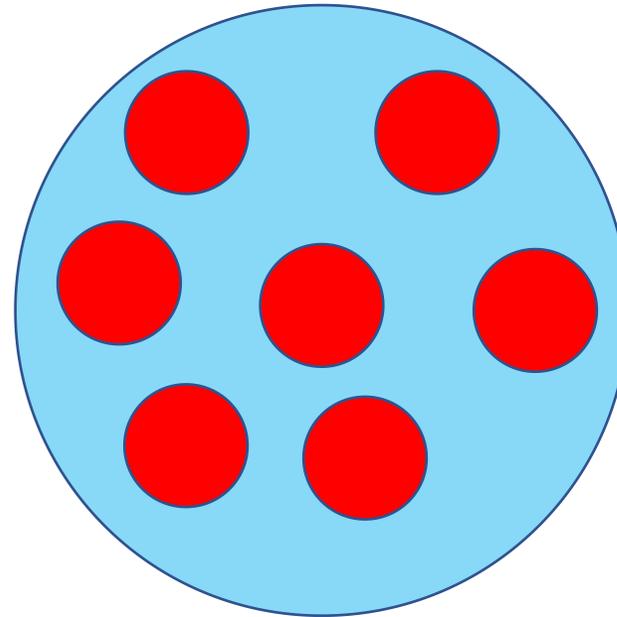
Many body systems



$$\Psi(\vec{x}_1, \vec{x}_2, \dots, \vec{x}_N)$$

Common feature of ab-initio: find the fully correlated nuclear wave-function

Independent particles



$$\varphi(\vec{x}_1) \varphi(\vec{x}_2) \dots \varphi(\vec{x}_N)$$

Mean-field theory: the nucleus as a set of independent protons and neutrons moving in an effective potential

Density function theory

Hohenberg–Hohn theorem(1964):

1998 Nobel price in Chemistry

The exact energy of a quantum mechanical many body system is a functional of the local density $\rho(r)$.

$$E = \langle \Psi | H | \Psi \rangle \approx \langle \Phi | \hat{H}_{eff}(\hat{\rho}) | \Phi \rangle = E[\hat{\rho}]$$

This functional is universal. It does not depend on the system, only on the interaction.

Kohn–Sham theory:

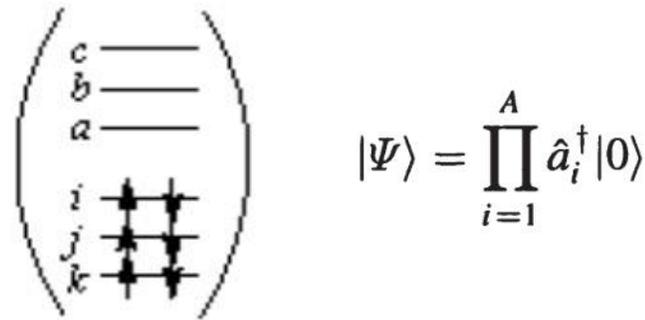
In order to reproduce shell structure Kohn and Sham introduced a single particle potential $V_{eff}(r)$, which is defined by the condition, that after the solution of the single particle eigenvalue problem

$$\left\{ -\frac{\hbar^2}{2m} \Delta + V_{eff}(\mathbf{r}) \right\} \varphi_k(\mathbf{r}) = \varepsilon_k \varphi_k(\mathbf{r})$$

Density function theory

The mean-field approximation

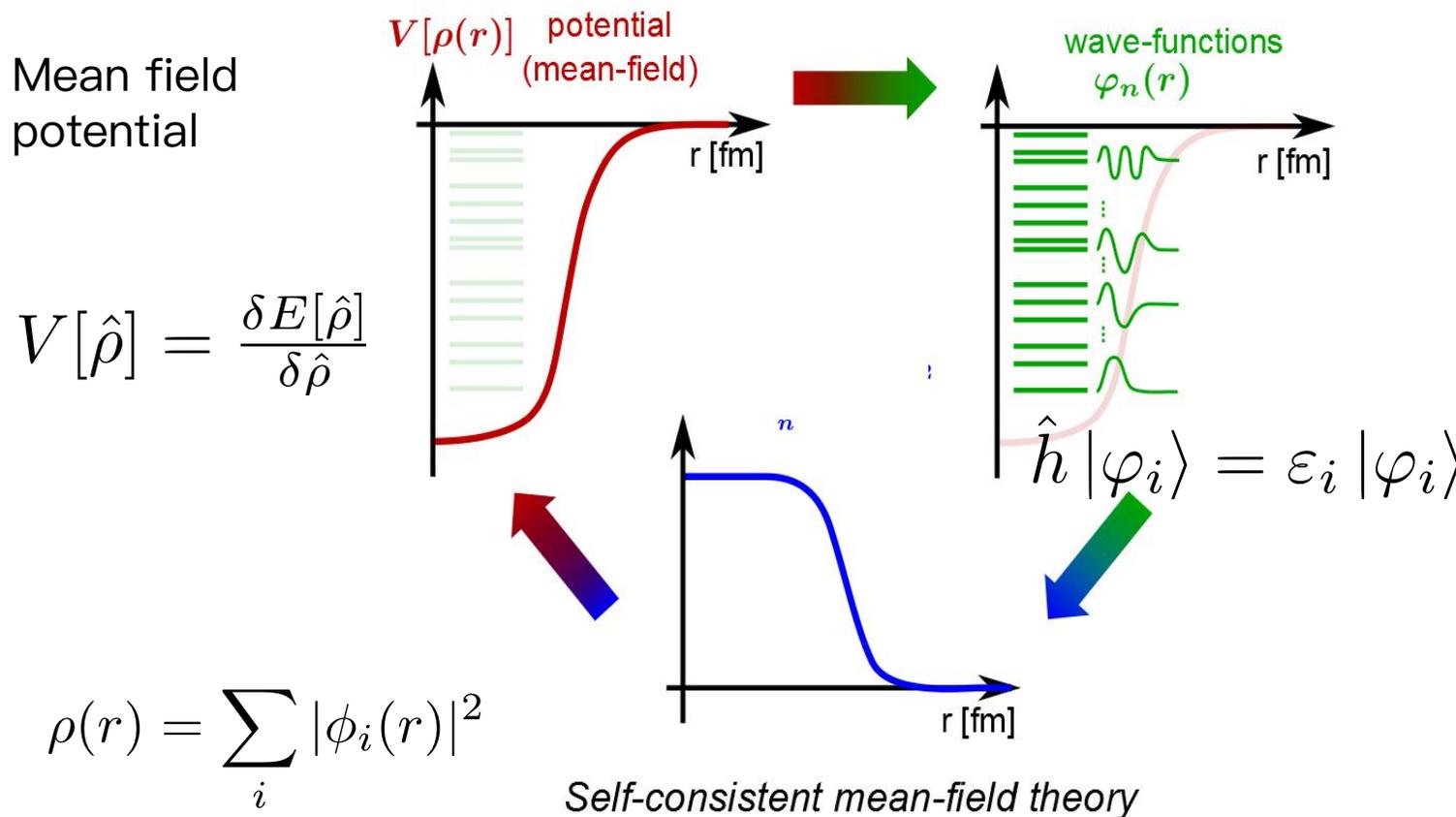
- The wavefunction is restricted by a single Slater determinant


$$|\Psi\rangle = \prod_{i=1}^A \hat{a}_i^\dagger |0\rangle$$

- Nucleon wave-functions $\Psi(r)$ obey the Schrödinger equation, where the potential $V(r)$ is the effective mean-field $V_{\text{eff}}(r)$
- Basic degree of freedom: the (one-body) density of particles $\rho(r)$
Reduce 3N-dimensional problem to a 3-dimensional one

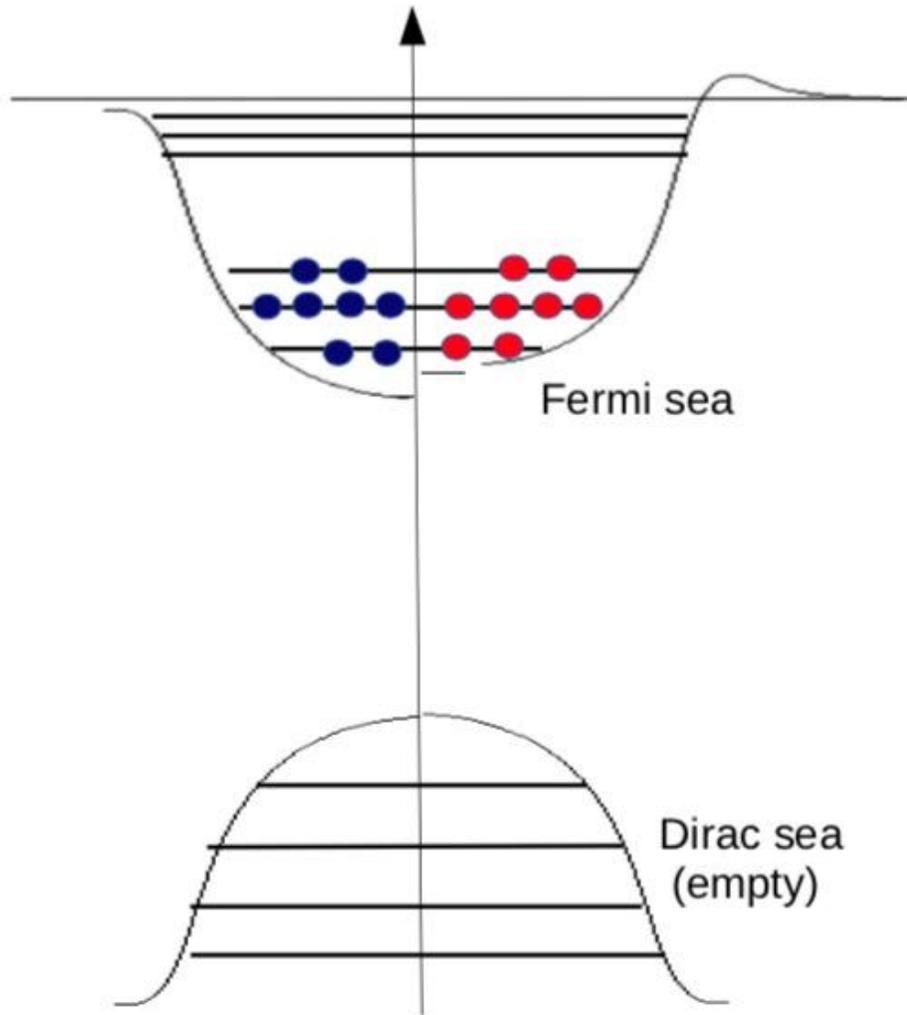
$$\rho(r) = \sum_i |\phi_i(r)|^2$$

Density function theory



- Starting points:
 - A nuclear interaction $v(r_1, r_2)$ (known)
 - A Slater determinant for the nucleus (to be determined)
- Goal: find the Slater determinant, (equivalently, the density ρ)
- Method: Minimize the energy defined as the expectation value of the Hamiltonian on the Slater determinant
- Resulting equations are non-linear: V depends on ρ which depends on the $\phi_i(r)$ which depend on V

Covariant Energy Density Functionals



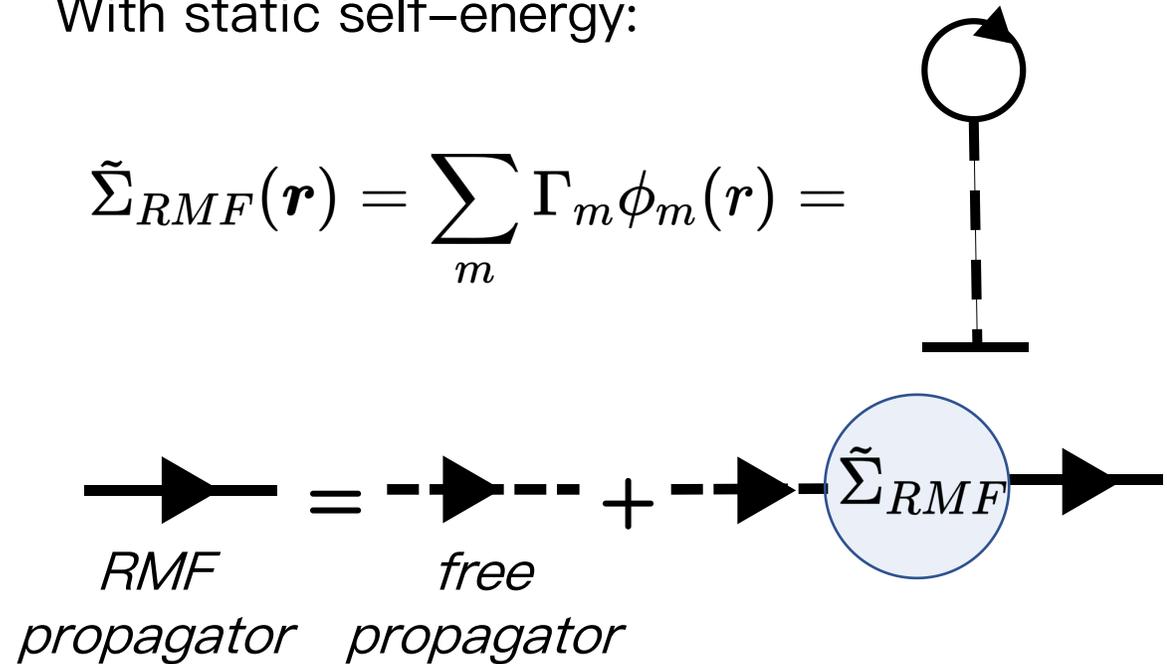
Mean-field approximation

Dirac Hamiltonian:

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

With static self-energy:

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



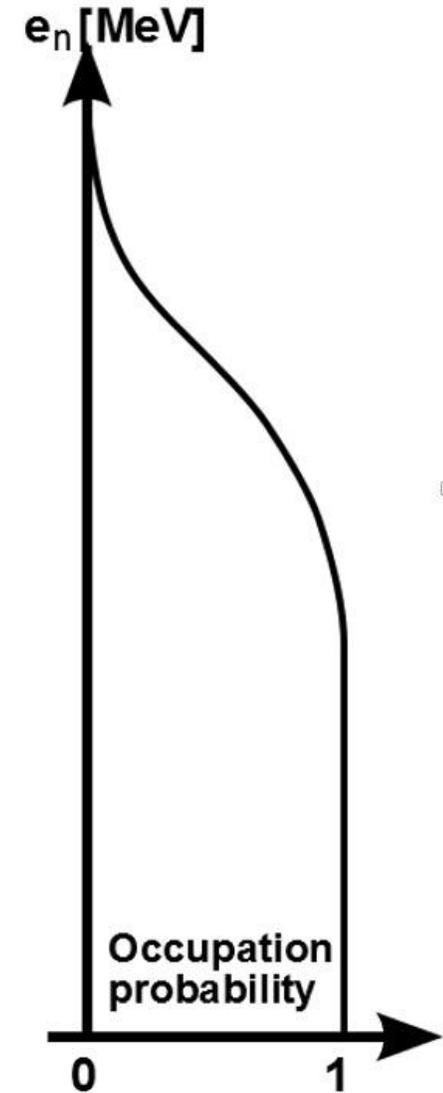
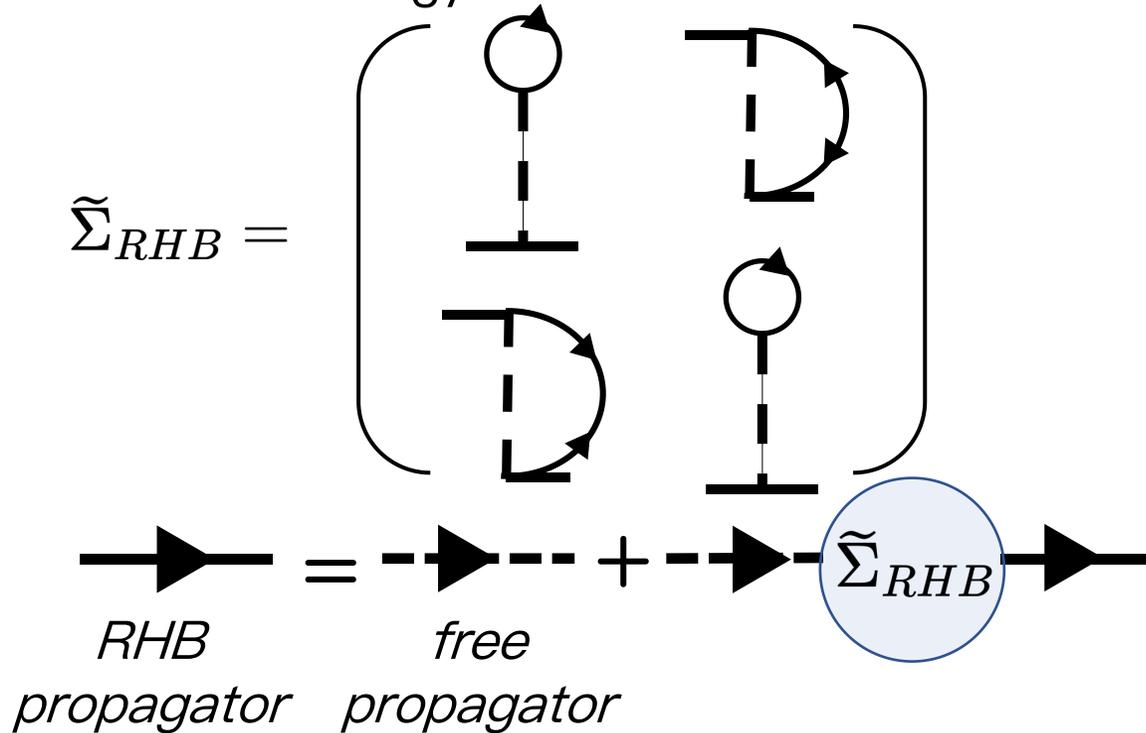
Covariant Energy Density Functionals

+ Superfluid pairing correlations in open-shell nuclei

RHB Hamiltonian:

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

RHB Self-energy:

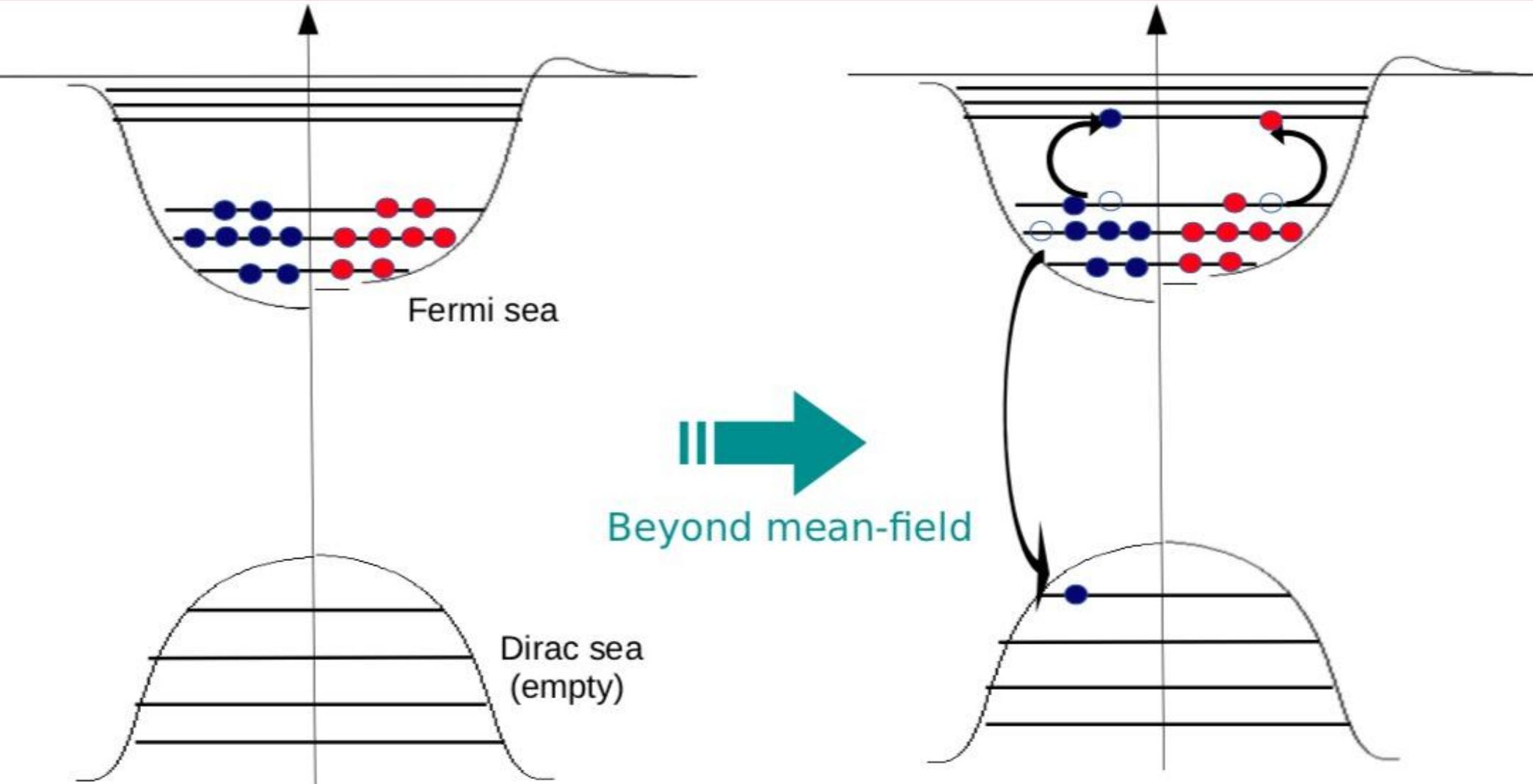


Ways to improve present EDFs

Beyond phenomenological mean field and extension

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

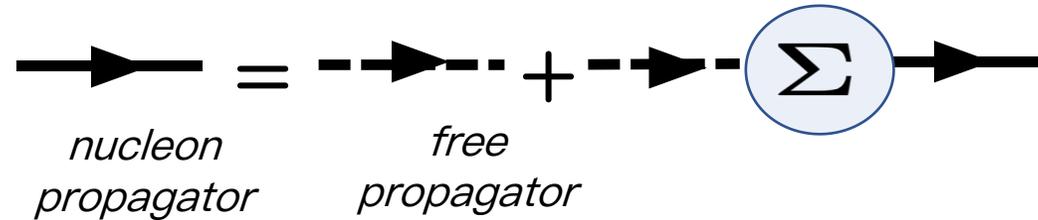
Beyond the mean-field: quasiparticles coupled to vibrations



Beyond the mean-field: quasiparticles coupled to vibrations

The Dyson equation for nucleon

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



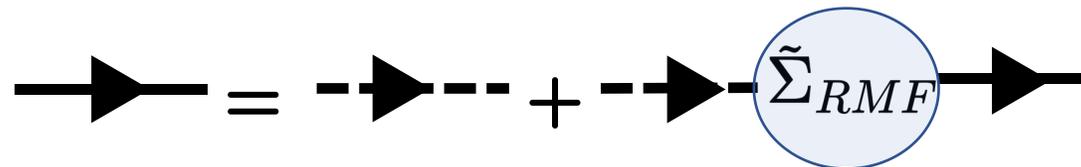
In general, the self-energy can be written as sums of the stationary local and energy dependent nonlocal terms:

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

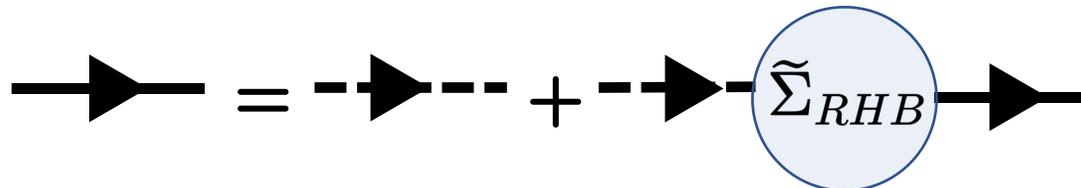
static dynamic

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

RMF:

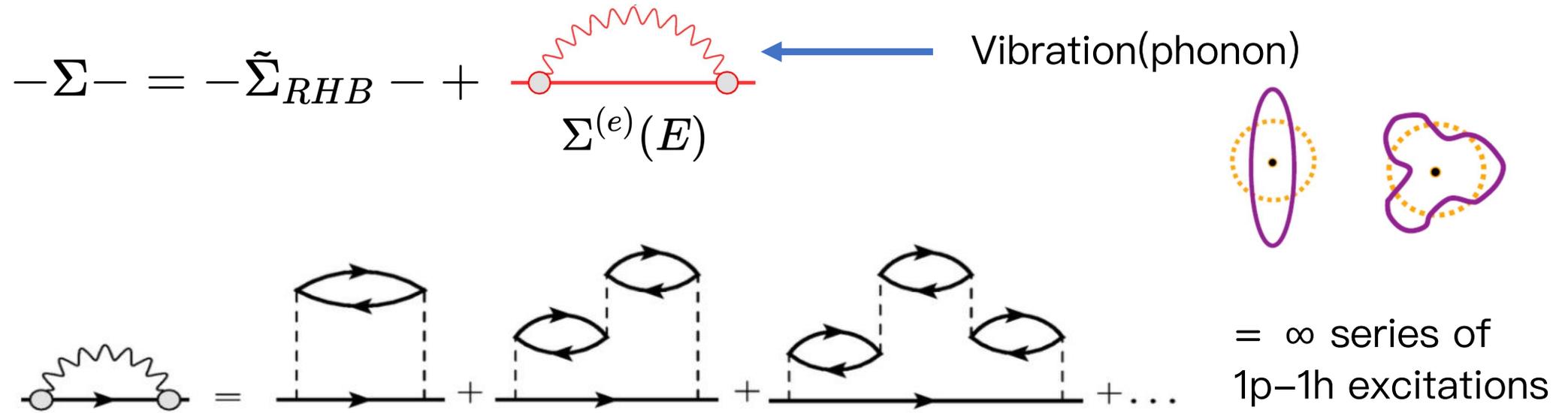


RHB:



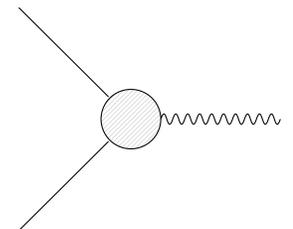
Beyond the mean-field: quasiparticles coupled to vibrations

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



Allows a non perturbative treatment of the NN interaction

QVC vertex $\gamma_{kl}^{\mu} = \sum_{k'l'} V_{kl'lk'} \delta\rho_{k'l'}^{\mu}$



Beyond the mean-field: quasiparticles coupled to vibrations

Quasiparticle propagator:



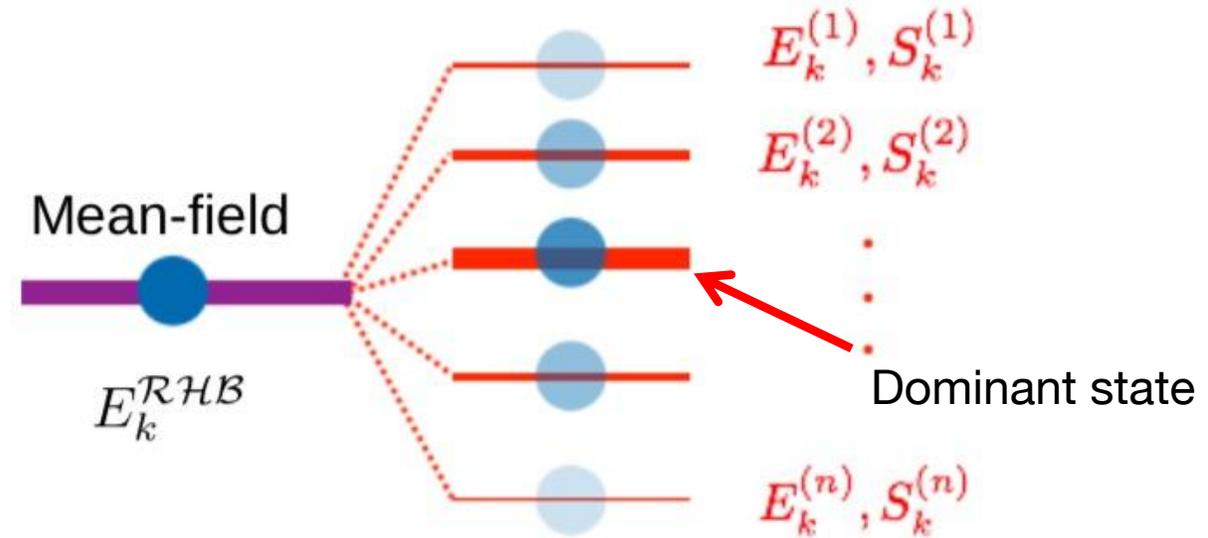
$$G(E) = \left(\varepsilon - \mathcal{H}_{RHB} - \underbrace{\Sigma^{(e)}(E)}_{\text{Introduces new poles}} \right)^{-1}$$

Energy dependent term

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

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

Fragmentation of single (quasi) particle states:



With fractional occupation numbers

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

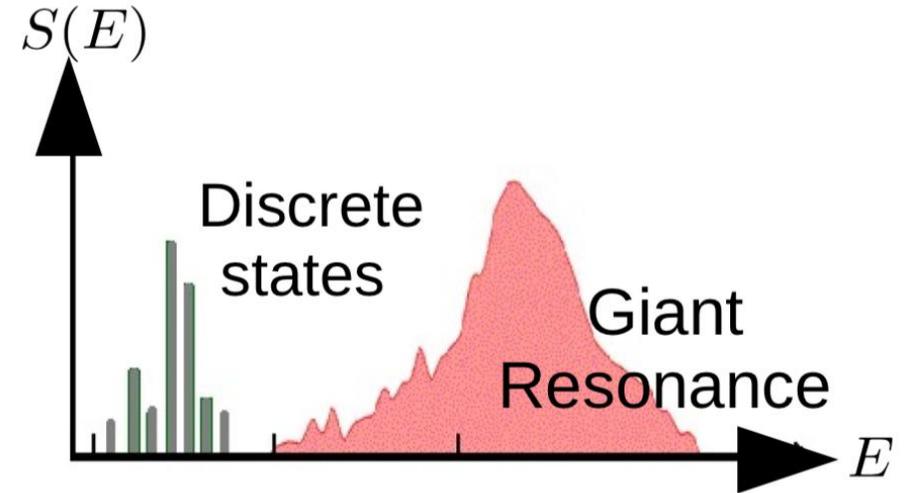
$$E_k^{RHB} = \sum_{\nu} S_k^{(\nu)} E_k^{(\nu)}$$

Excited states: nuclear response theory

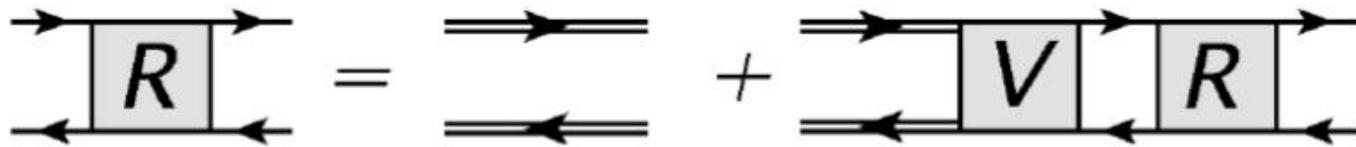
Response of the nucleus to an external field :
Transition strength:

$$S(E) = \sum_f \left| \langle \Psi_f | \hat{F} | \Psi_i \rangle \right|^2 \delta(E - E_f + E_i)$$

$$= -\frac{1}{\pi} \lim_{\Delta \rightarrow 0^+} \text{Im} \langle \Psi_i | \hat{F}^\dagger R(E + i\Delta) \hat{F} | \Psi_i \rangle$$



Response function (2-body propagator)
Solution of the Bethe-Salpeter equation



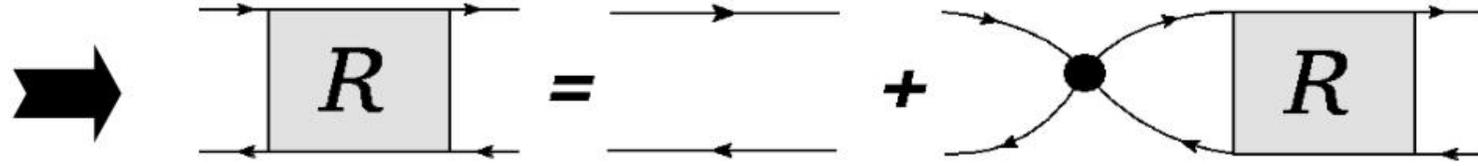
$$V(E) = i \frac{\delta \tilde{\Sigma}_{RHB}}{\delta G} + i \frac{\delta \Sigma^e(E)}{\delta G}$$

Effective interaction induced by the nuclear medium

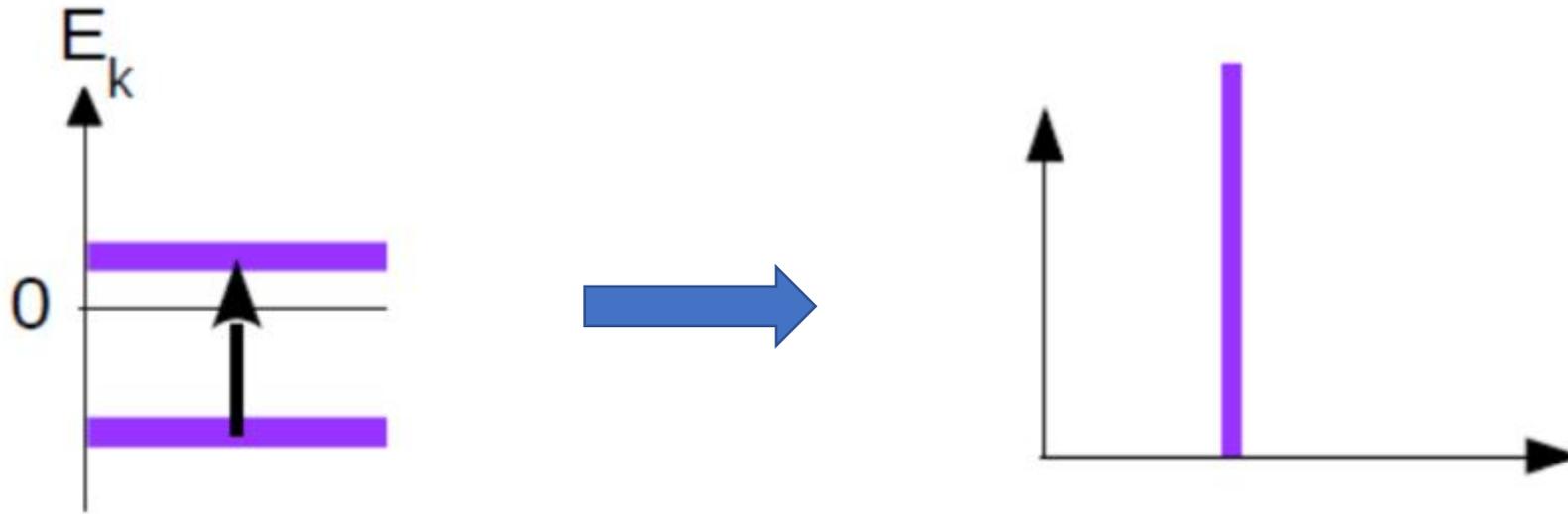
Static interaction + pairing

Energy-dependent phonon exchange

Excited states: nuclear response theory



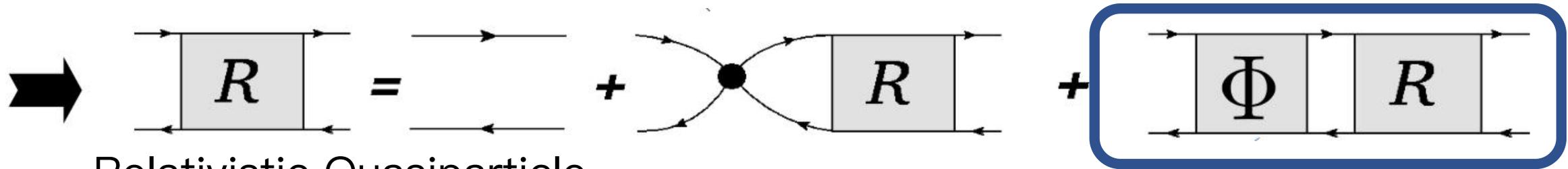
Relativistic Quasiparticle
Random Phase Approximation
(RQRPA)



Single-particle states

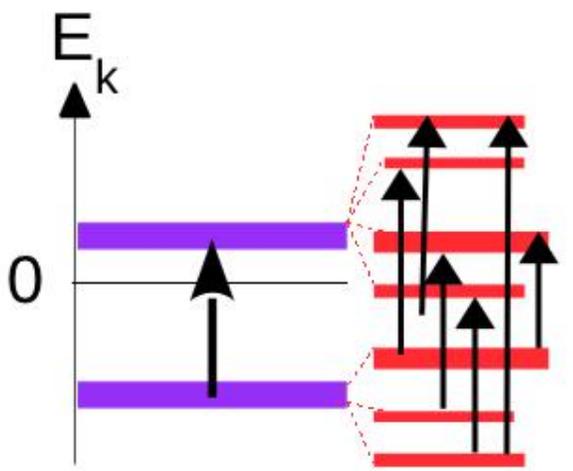
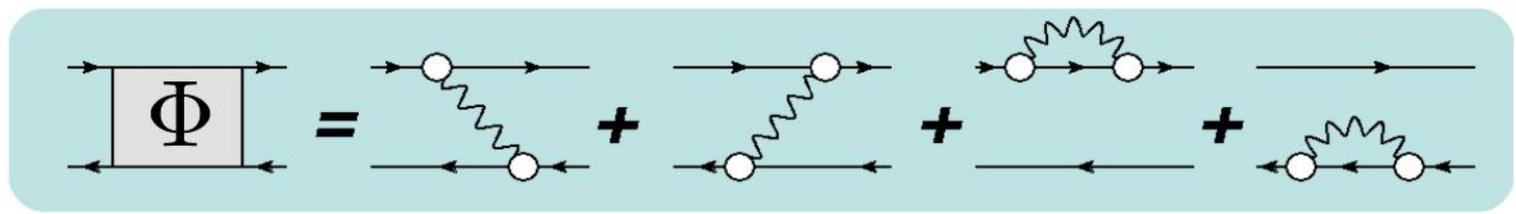
Many-body states
 $1(q)p-1(q)h$

Excited states: nuclear response theory

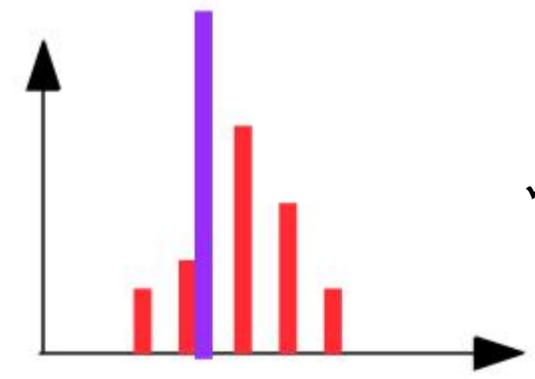


Relativistic Quasiparticle
Random Phase Approximation
(RQRPA)

Quasiparticle-Vibration Coupling amplitude:



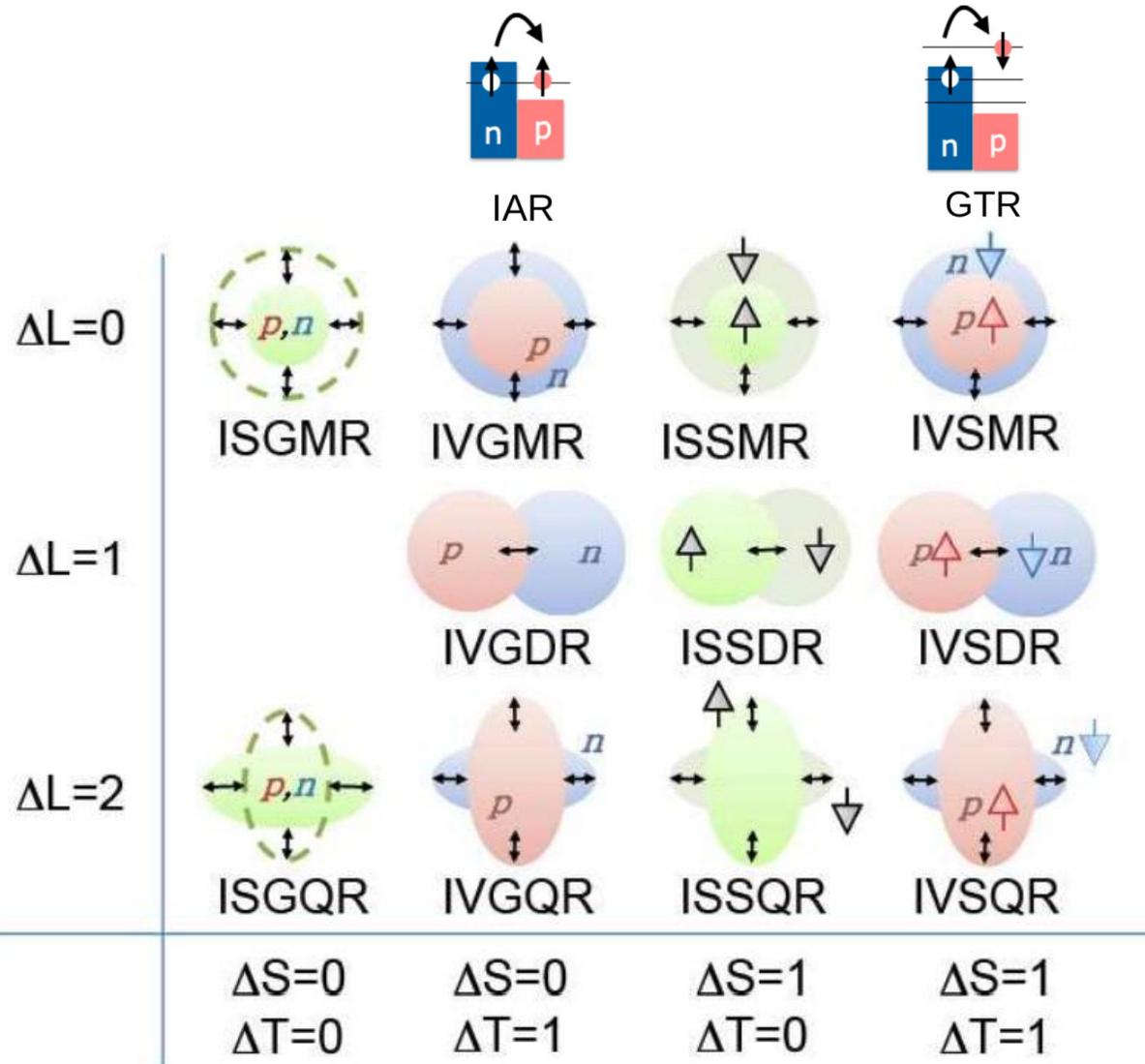
Single-particle states



Many-body states
 $1(q)p-1(q)h \otimes 1$ phonon configurations

✓ Spreading width

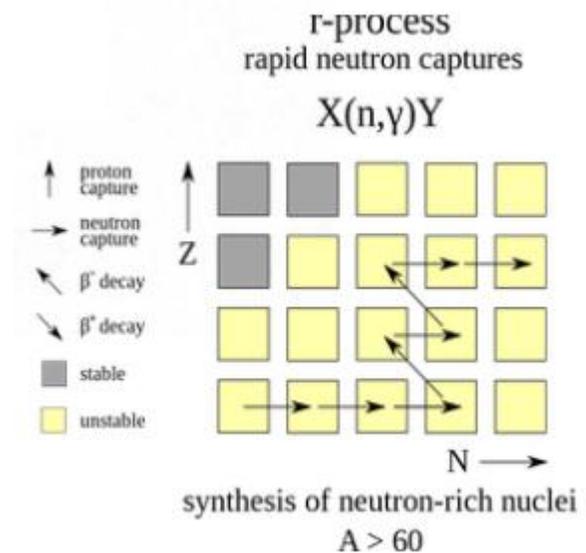
Nuclear Vibrational motions



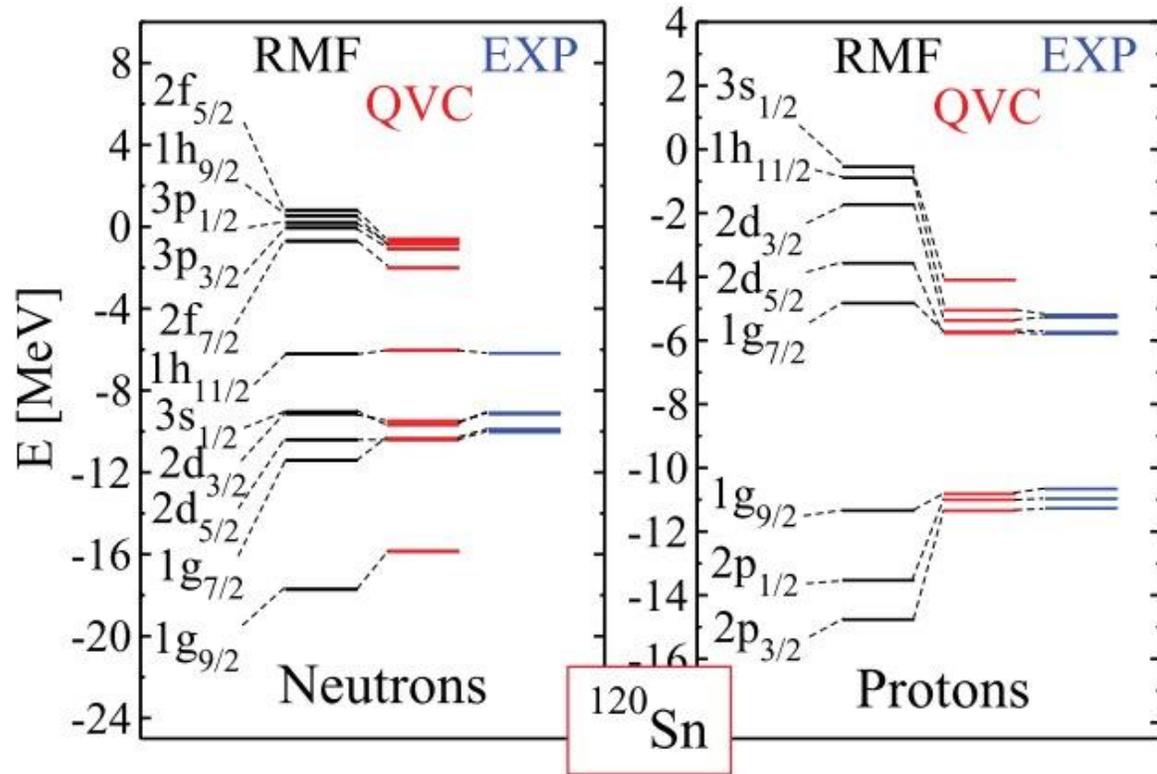
The quanta of vibrational energy are called phonons.

Quadrupole oscillations are the lowest order nuclear vibrational mode.

A quadrupole phonon carries 2 units of angular momentum and has even parity



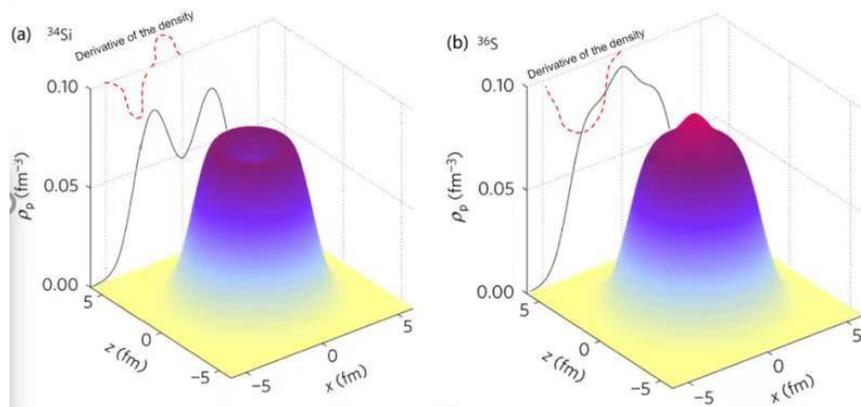
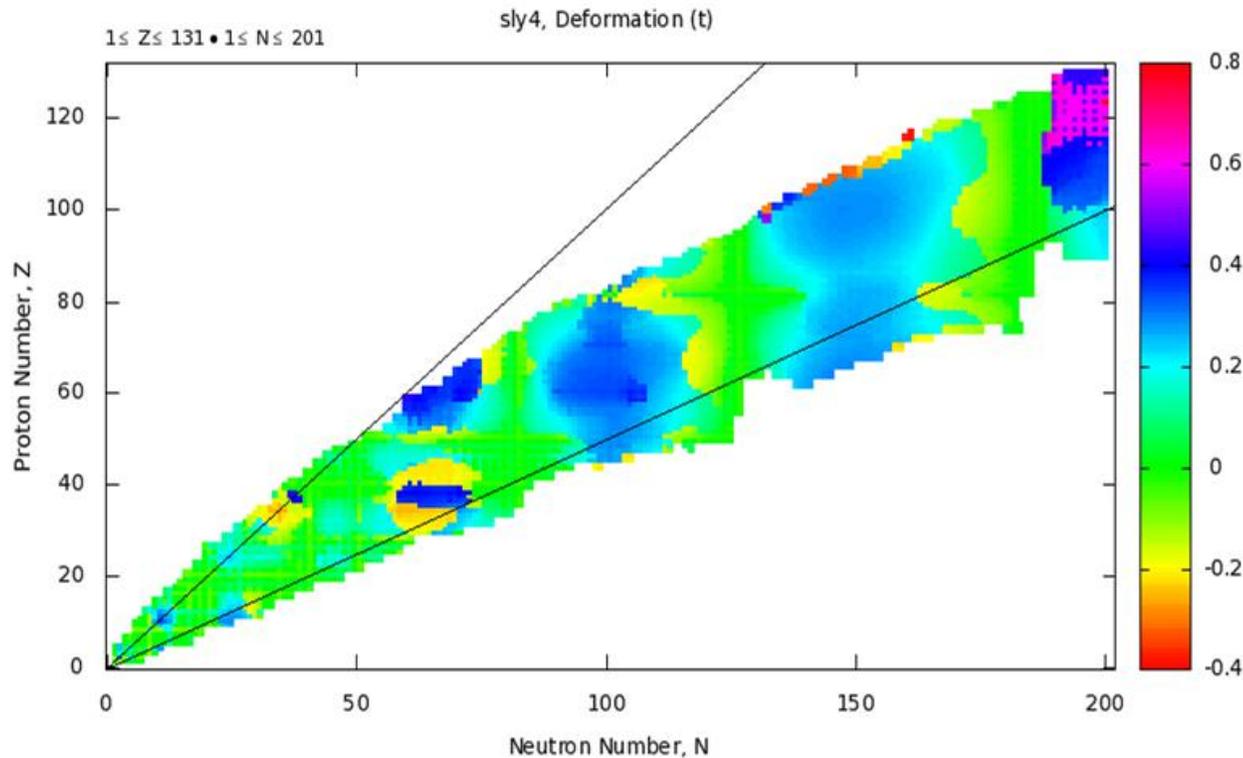
(Quasi)particle–vibration coupling in spherical case



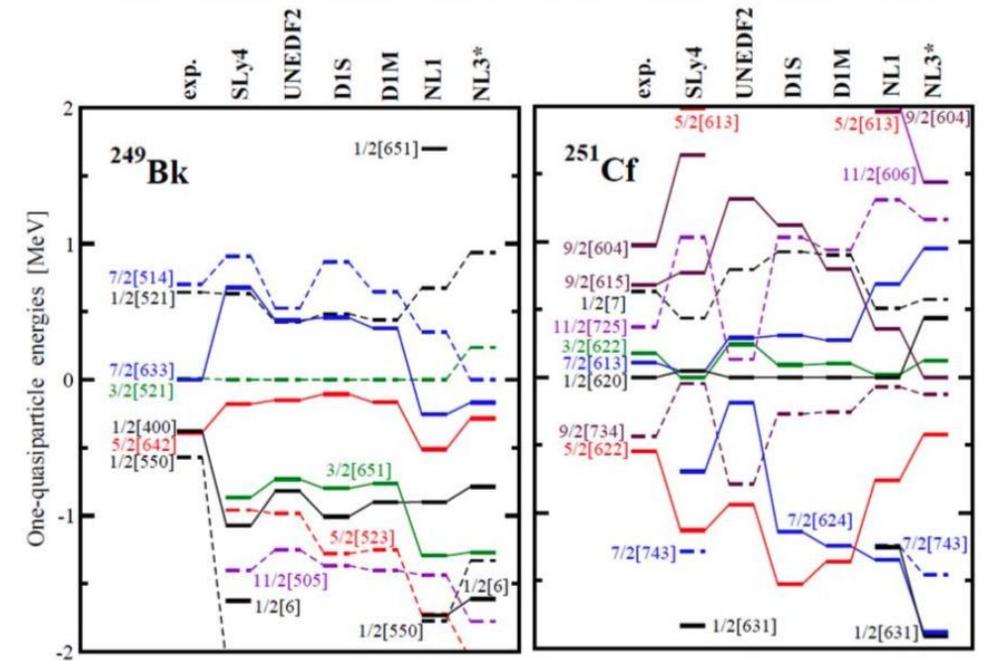
(nlj) v	S^{th}	S^{exp}
$2d_{5/2}$	0.32	0.43
$1g_{7/2}$	0.40	0.60
$2d_{3/2}$	0.53	0.45
$3s_{1/2}$	0.43	0.32
$1h_{11/2}$	0.58	0.49
$2f_{7/2}$	0.31	0.35
$3p_{3/2}$	0.58	0.54

Dominant states and spectroscopic factors in ^{120}Sn

Deformed nuclei



Deformed one-quasiparticle states: covariant and non-relativistic DFT description versus experiment



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 traditional method:

Diagonalization the QRPA matrix

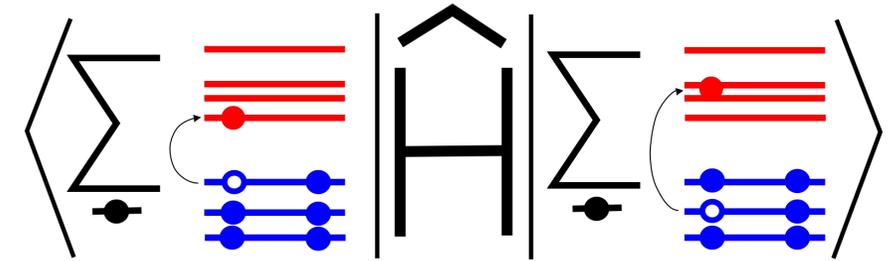
$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \omega \begin{pmatrix} X \\ -Y \end{pmatrix}$$

$\delta\rho_{ph}$ (pointing to X)
 $\delta\rho_{hp}$ (pointing to -Y)

with

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

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



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:

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

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

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

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

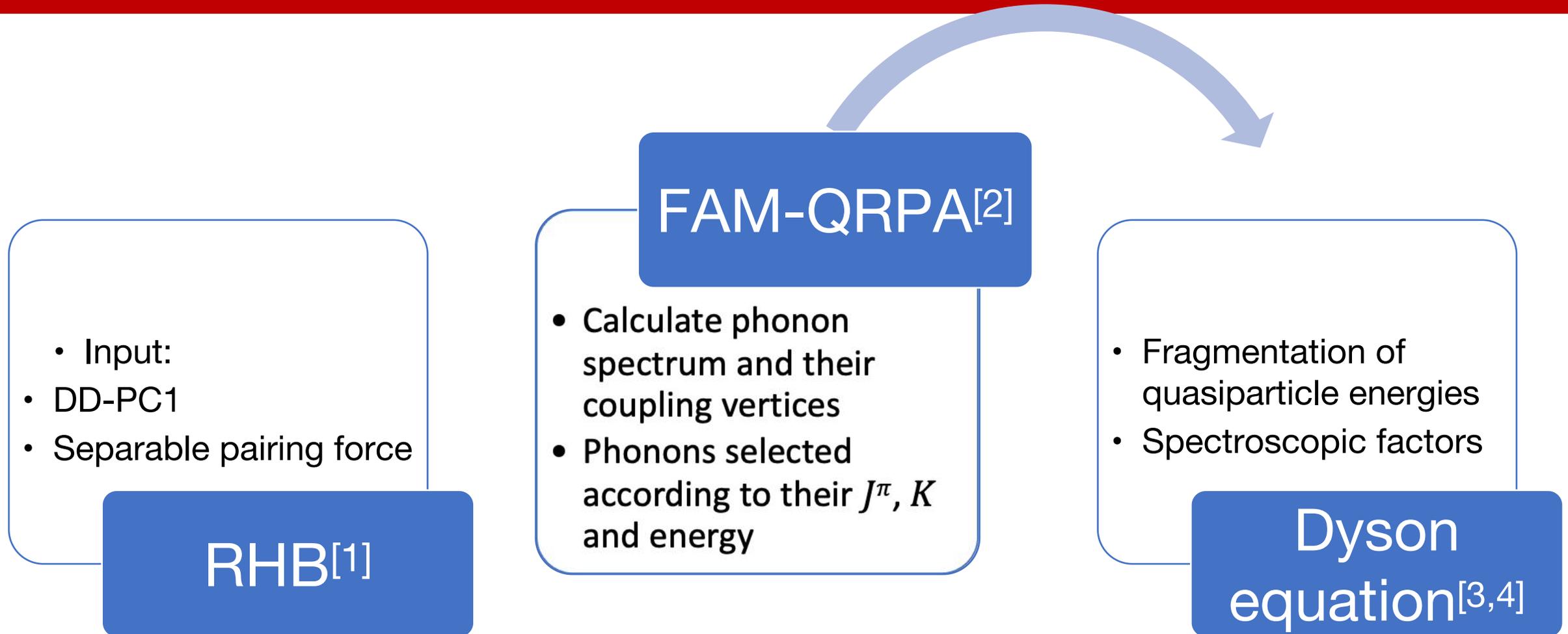
$$\omega |X_i(\omega) \rangle = (h_0 - \varepsilon_i) |X_i(\omega) \rangle + \hat{Q} \{ \delta h(\omega) + V_{\text{ext}}(\omega) \} |\phi_i \rangle$$

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

finite difference method for residual interaction \rightarrow avoid two-body matrix element calculation

iterative method \rightarrow avoid huge matrix diagonalization

Numerical scheme



[1] T. Nikšić D. Vretenar, P. Ring

[2] P. Avogadro T. Nakatsukasa

[3] E. Litvinova and Y Z

[4] Y. Z, E. Litvinova, et al

PRC 78 034318

PRC 84 014314

PRC 104, 044303

PRC 105, 044326

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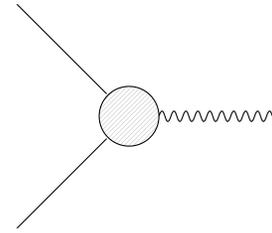
Heavy nucleus ^{250}Cf

□ Summary & perspectives

Calculate quasiparticle phonon coupling vertex for different β_2

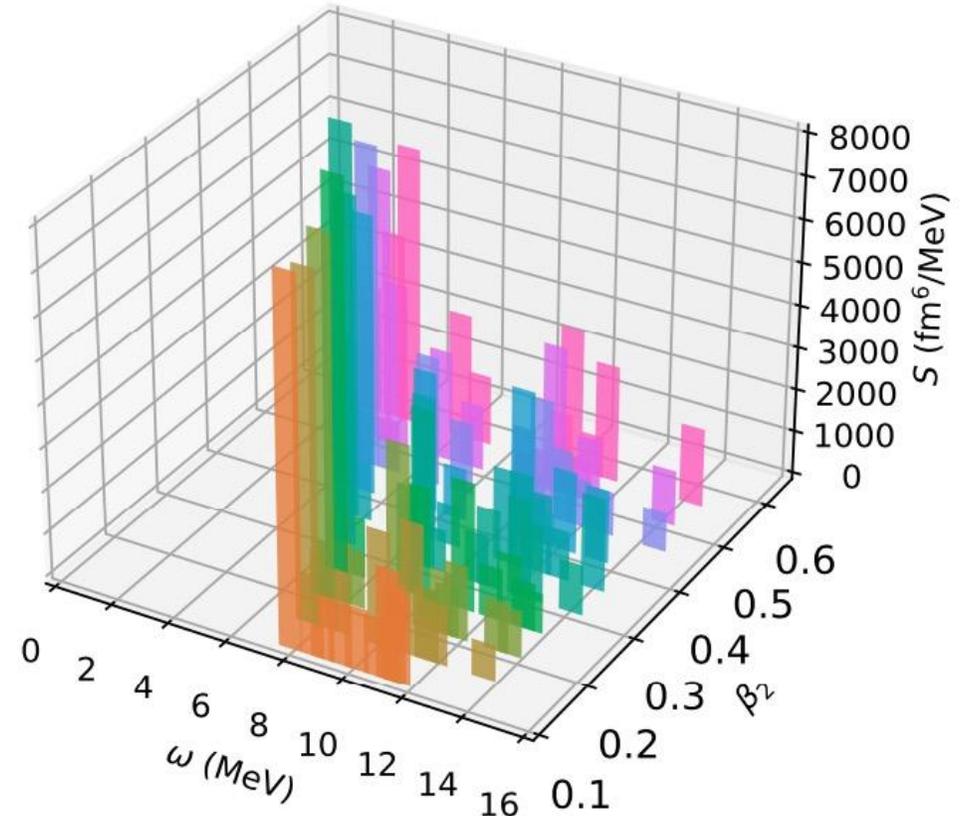
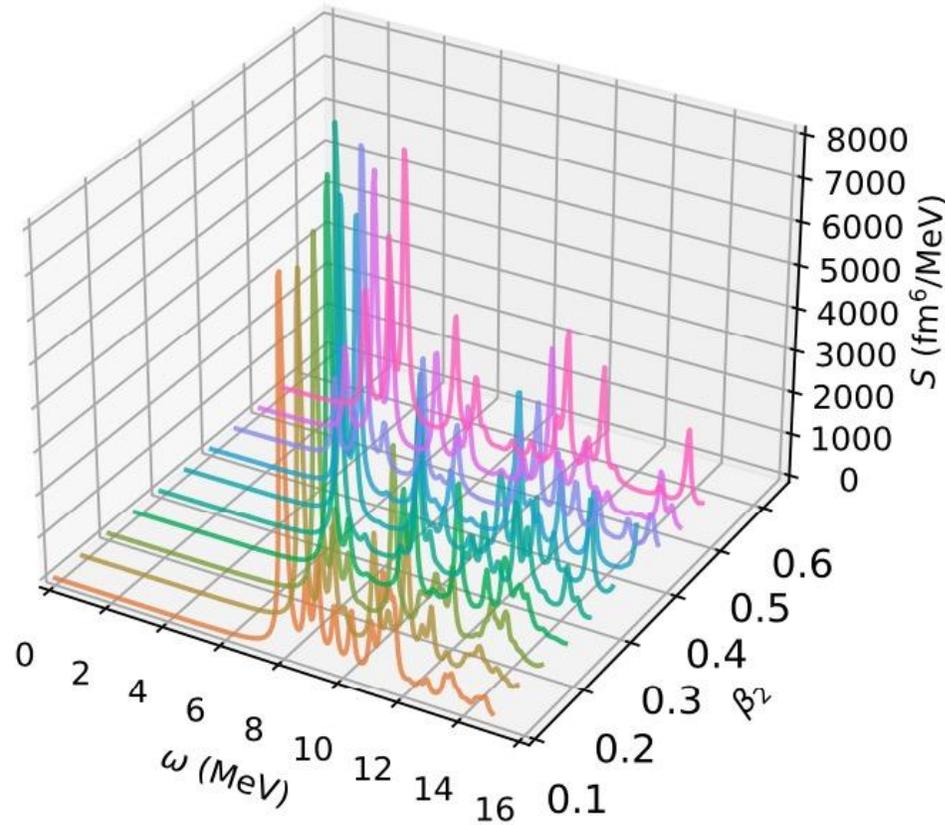
^{38}Si

$$\gamma_{kl}^\mu = \sum_{k'l'} V_{kl'lk'} \delta\rho_{k'l'}^\mu = \frac{\delta H}{\delta \hat{\rho}} \delta\rho$$

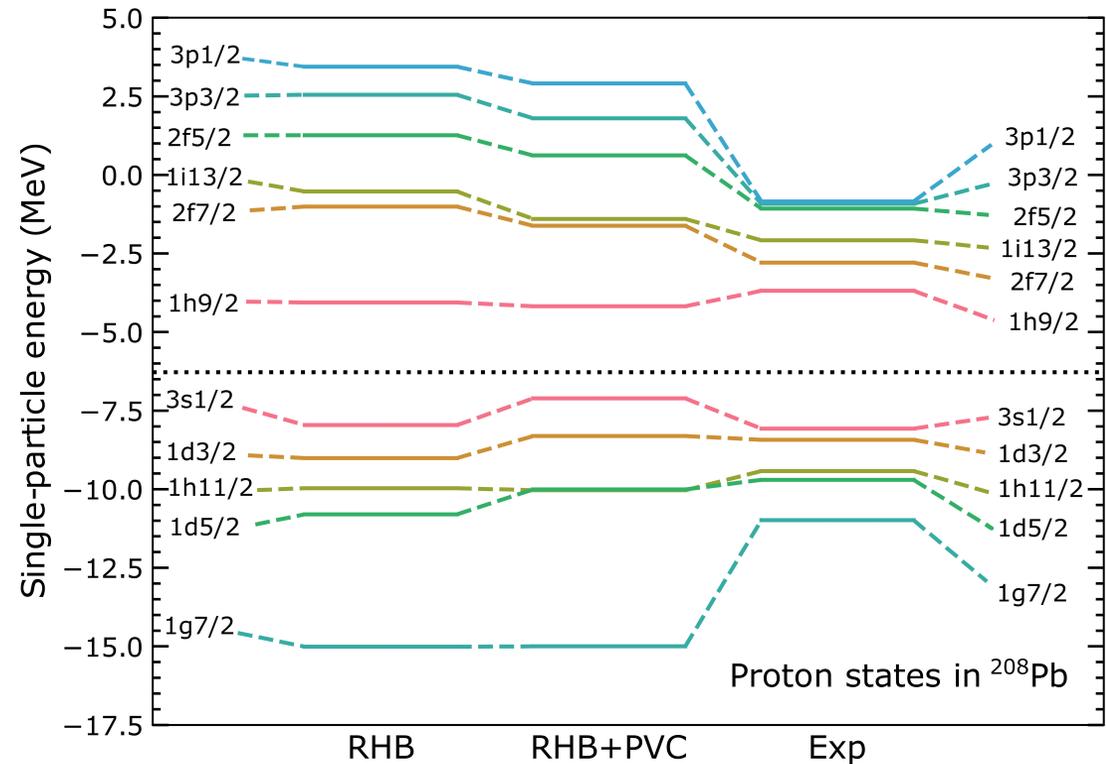
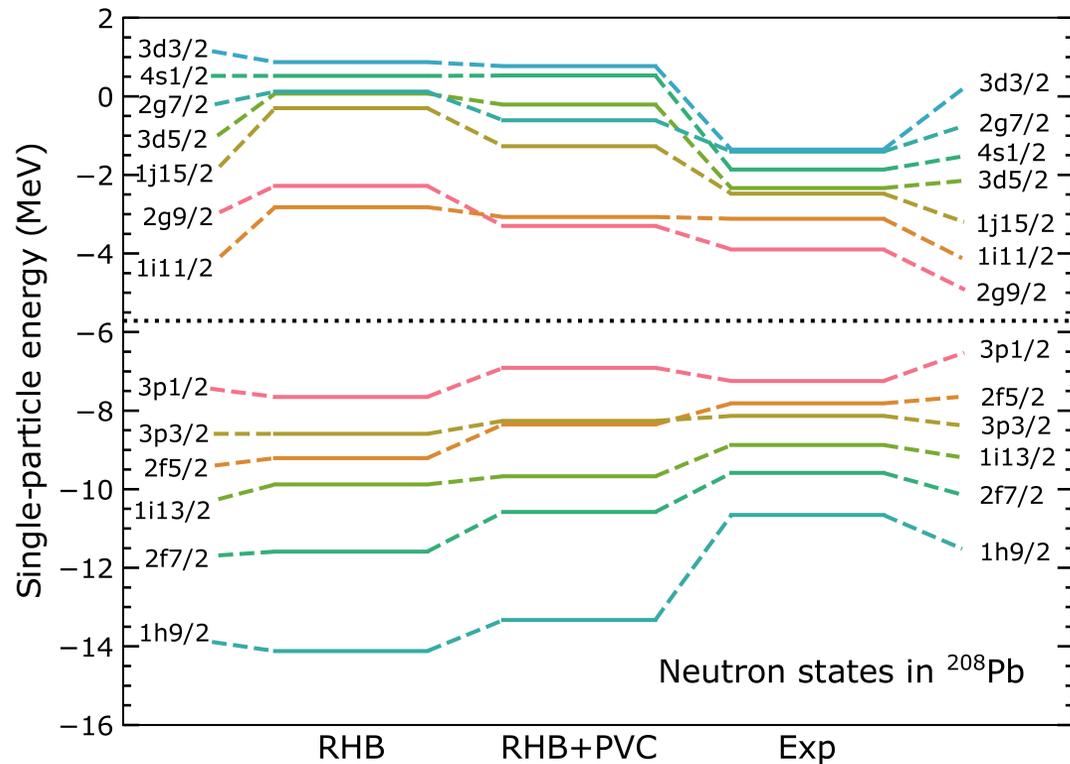


Strength for $J=3$ $K=2$

Phonon for $J=3$ $K=2$

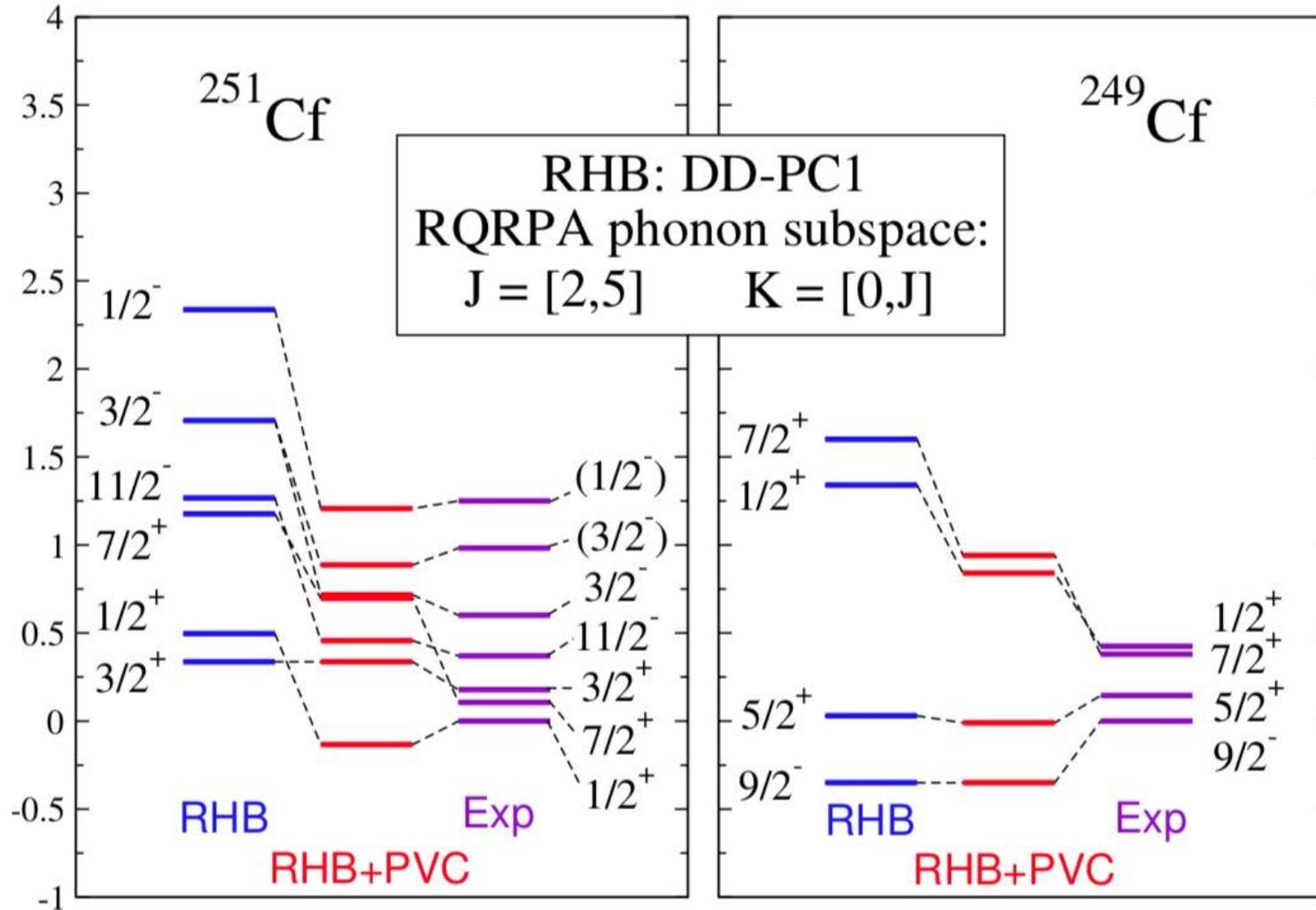


Single particle spectrum in ^{208}Pb



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

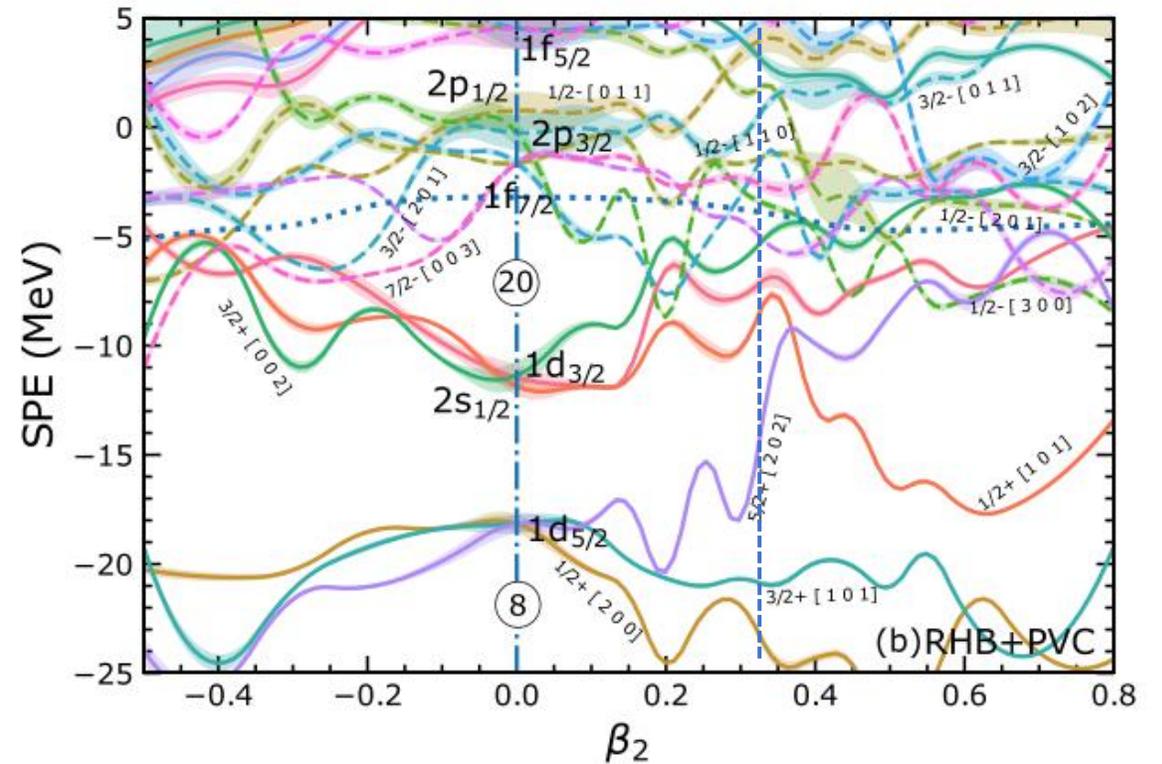
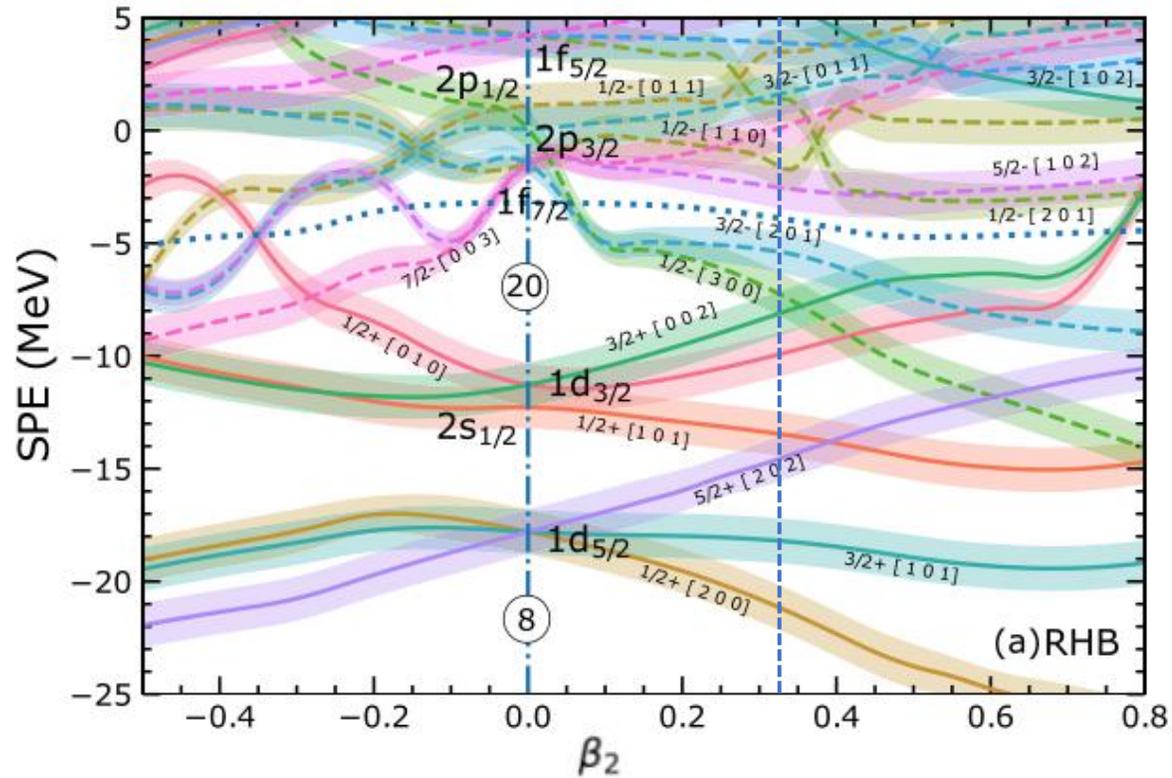
Deformed QVC: heavy ^{249}Cf & ^{251}Cf



Different 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

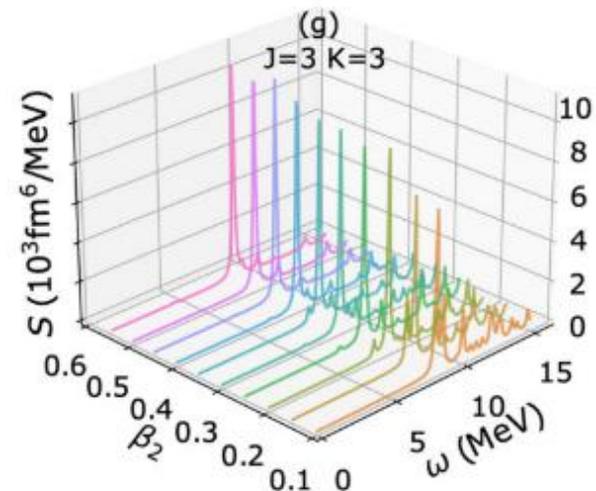
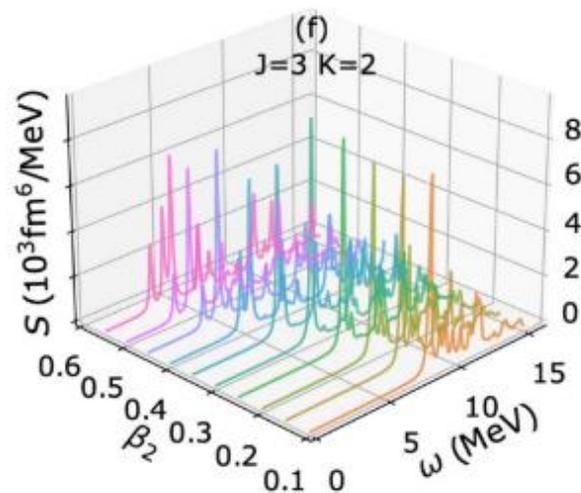
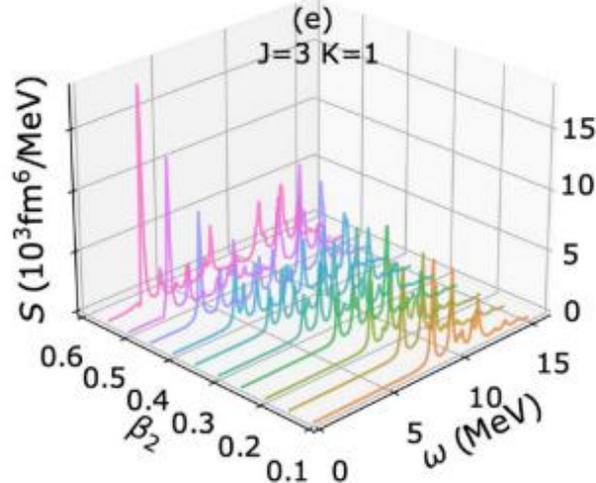
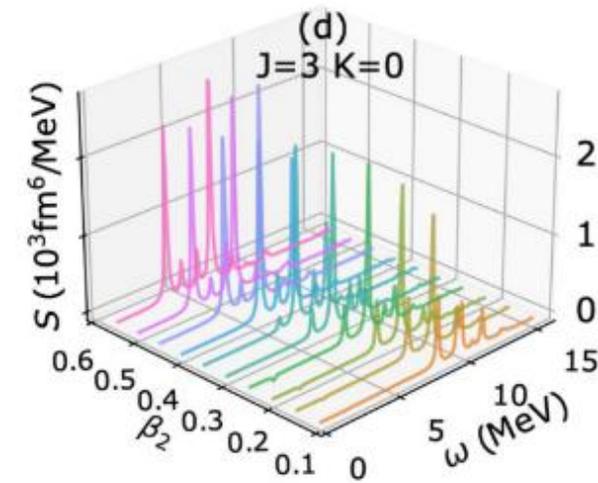
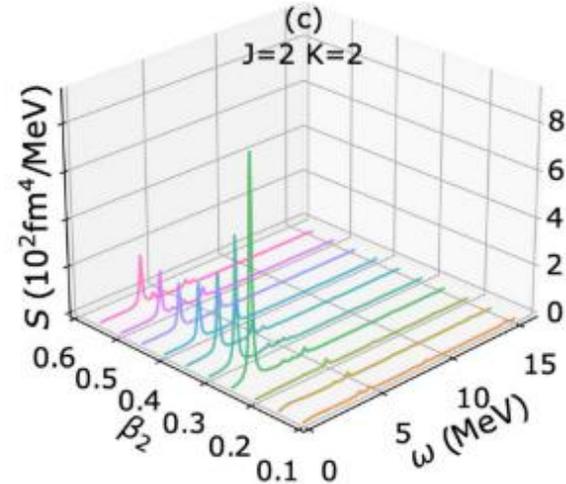
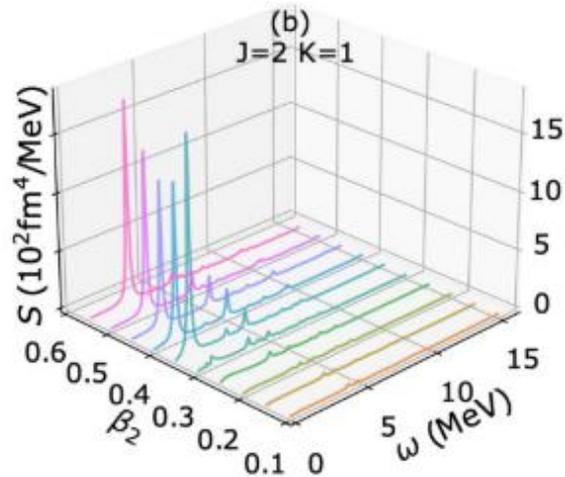
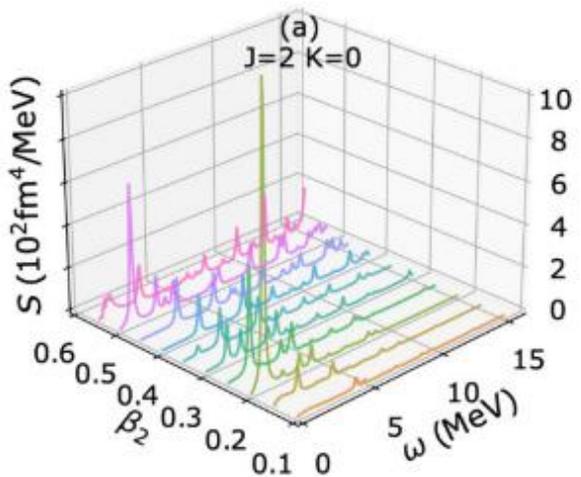
Deformed QVC: neutron rich ^{38}Si



At $\beta_2 = 0$, the degeneracy of the quasiparticle states reproduced, and the occupancies maximized

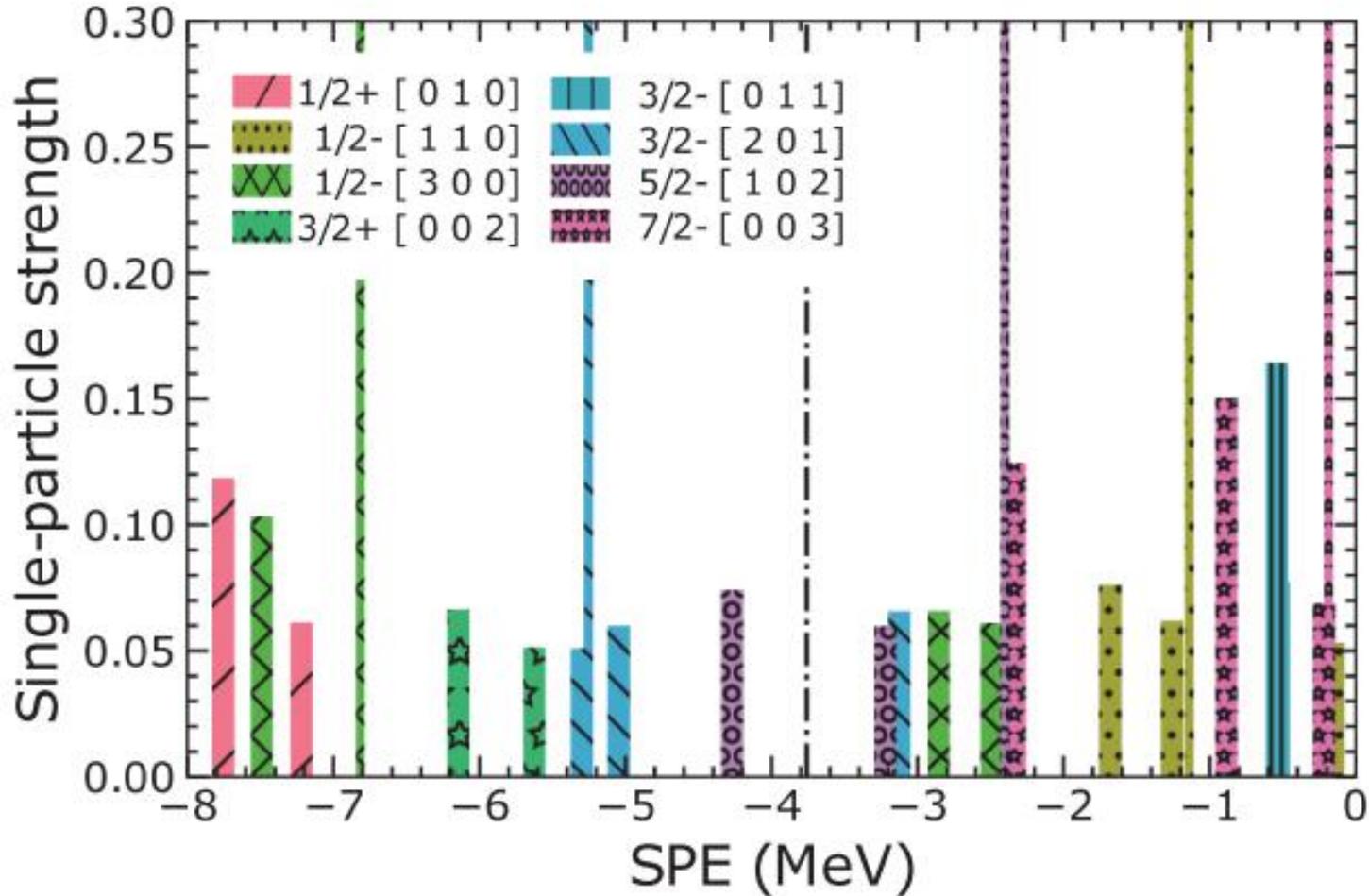
Additional oscillations of the dominant fragments' states due to the evolution of the low-energy collective phonons

Deformed QVC: neutron rich ^{38}Si



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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.



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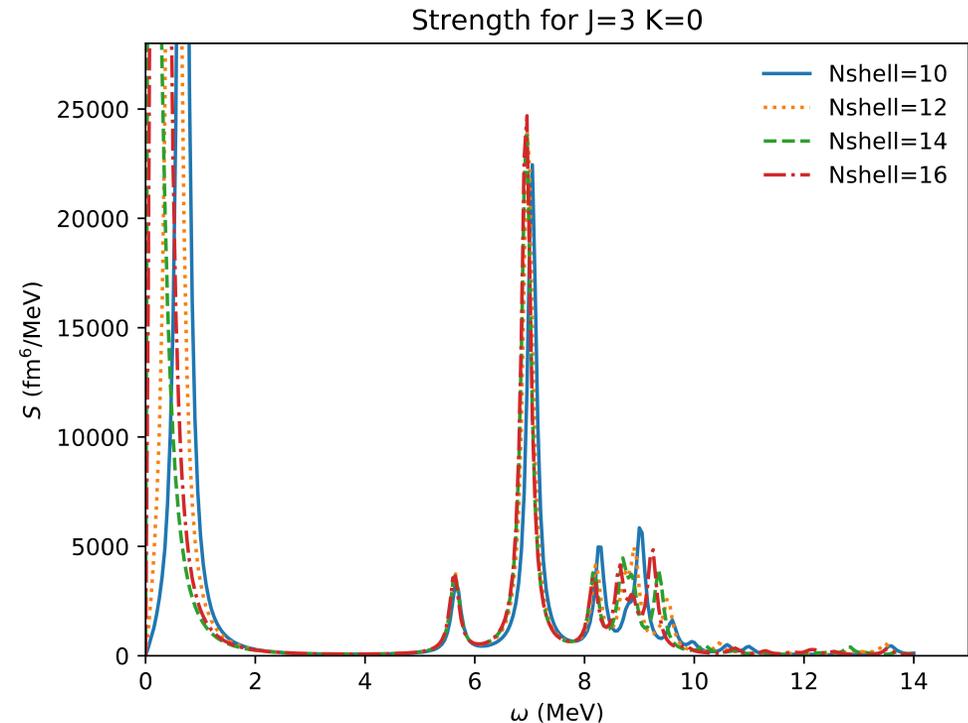
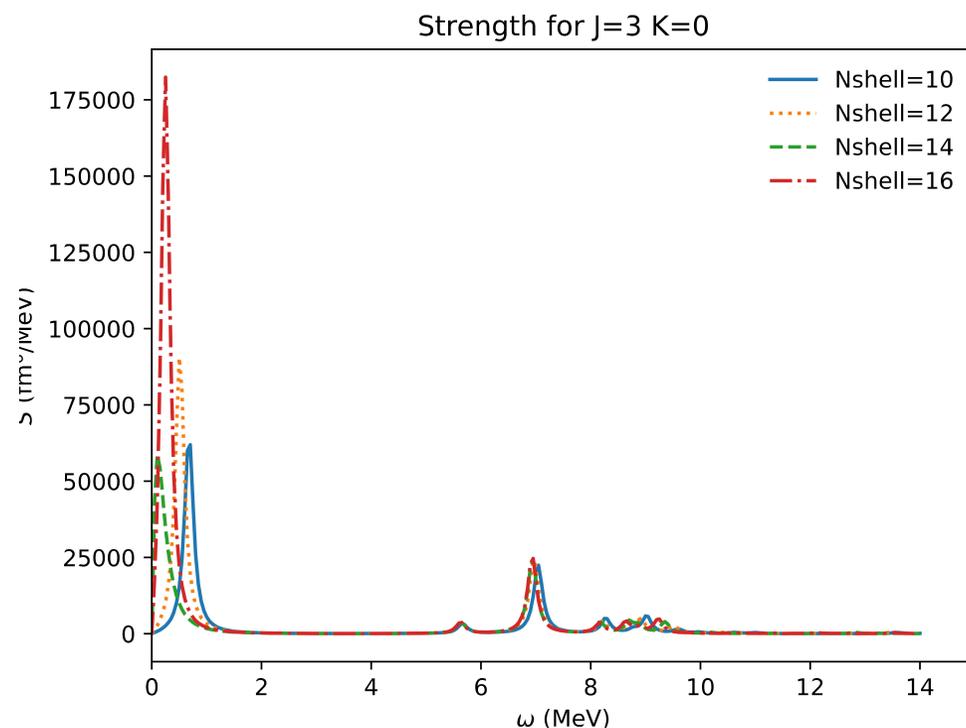
Thank you!

Collaborators:

Elena Litvinova,
Antonio Bjelcic , Tamara Niksic,
Peter Ring,

Western Michigan University
University of Zagreb
The Technical University of Munich

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

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

Derivation of Dirac mean-field

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

Derivation of pairing field

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

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

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

Beyond the mean-field

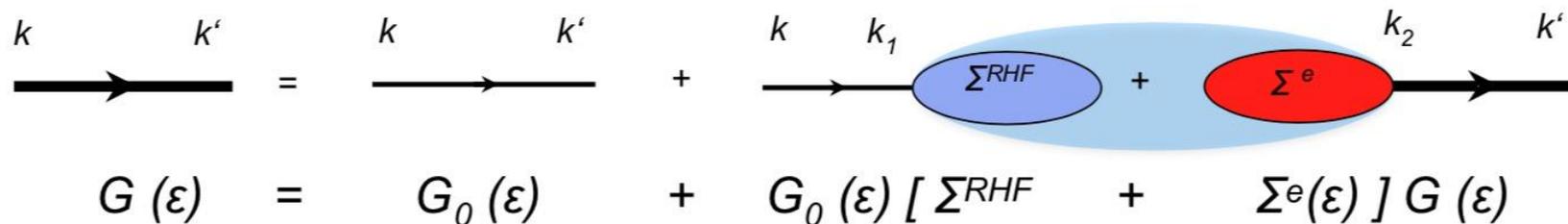
From EDF, we can get nuclear binding energy, radius, deformation etc.
 Plus RPA, we can get giant resonance information
 However, still have limitations

- 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

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

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

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

Particle Vibration Coupling

Model assumptions:

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

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

where the amplitude Γ has the following spectral expansion:

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

and the mean field Green’s function is

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