Beyond Conventional RPA

Basis Optimization, Uncertainty Quantification and IM-SRG

Laura Mertes

TRIUMF Workshop 2023

Motivation

- strength distributions
  - provide information about nucleus
  - accessible in **experiments**
- use standard **approximate** methods such as (S)RPA

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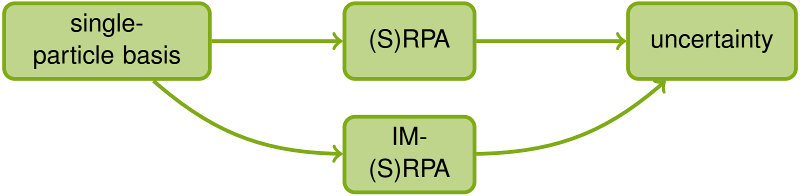
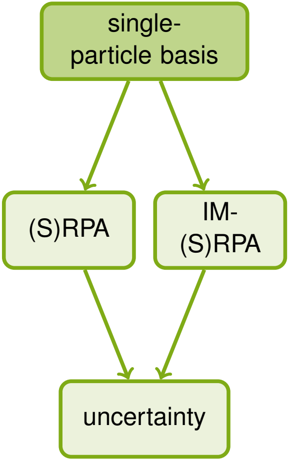


Single-Particle Basis



single-particle basis

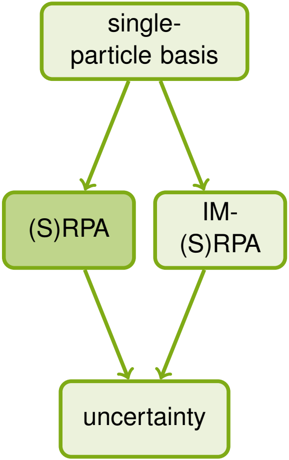
(S)RPA

IM-(S)RPA

uncertainty

- **Hartree-Fock**
- **Natural Orbitals**
  - HF calculation + low-order perturbation theory → one-body density matrix
  - NATs are eigenstates of this matrix

Random-Phase-Approximation (RPA)



single-particle basis

(S)RPA

IM-(S)RPA

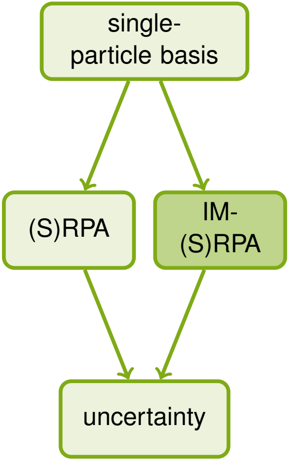
uncertainty

- ground state $|\mathrm{RPA}\rangle$: **ph** excitations of basis state
- $\left(Q_\lambda^{\mathrm{RPA}}\right)^\dagger = \sum_{p_1,h_1}\left(X^\lambda_{p_1 h_1} a^\dagger_{p_1} a_{h_1} - Y^\lambda_{p_1 h_1} a^\dagger_{h_1} a_{p_1}\right)$
- excited states: linear combinations of **ph** and **hp** excitations of $|\mathrm{RPA}\rangle$
- SRPA: includes additional **2p2h** excitations

→ derive equations of motion

→ solve matrix eigenvalue problem

In-Medium (S)RPA



single-particle basis

(S)RPA

IM-(S)RPA

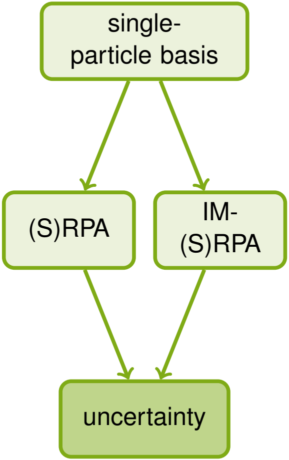
uncertainty

- decouples reference state from ph excitations
- pathological behavior of SRPA: **energy shift** to lower energies
- IM-(S)RPA reduces to (S)TDA which allows ph but **no hp** excitations

→ strengths from IM-RPA at higher energies

→ instabilities are removed

Uncertainty Quantification

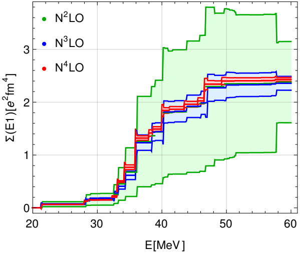

single-particle basis

(S)RPA

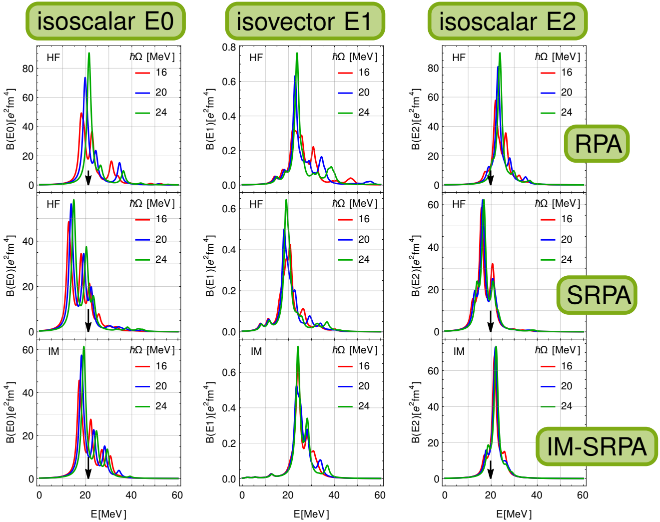
IM-(S)RPA

uncertainty

- different chiral orders Q^i of interaction
- observable X in terms of Q^i
- applying Bayes' theorem for uncertainty quantification



Basis Optimization for ^{16}O



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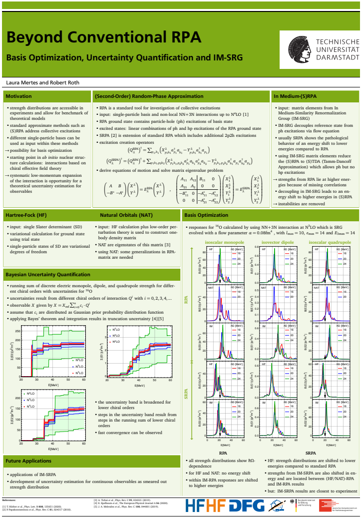
- Thank you for your attention!



Beyond Conventional RPA

Basis Optimization, Uncertainty Quantification and IM-SRG

Laura Mertes and Robert Roth

Motivation

- strength distributions are accessible in experiments and allow for benchmark of theoretical models
- standard approximate methods such as (S)RPA address collective excitations
- different single-particle bases can be used as input within these methods

→ possibility for basis optimization

- starting point in *ab initio* nuclear structure calculations: interactions based on chiral effective field theory

→ systematic low-momentum expansion of the interaction is opportunity for a theoretical uncertainty estimation for observables

(Second-Order) Random-Phase Approximation

- RPA is a standard tool for investigation of collective excitations
- input: single-particle basis and non-local NN+3N interactions up to N^{4}LO [1]
- RPA ground state contains particle-hole (ph) excitations of basis state
- excited states: linear combinations of ph and hp excitations of the RPA ground state
- SRPA [2] is extension of standard RPA which includes additional 2p2h excitations
- excitation creation operators

$$(Q_\lambda^{\mathrm{RPA}})^\dagger = \textstyle\sum_{p_1h_1}\left(X^\lambda_{p_1h_1} a^\dagger_{p_1} a_{h_1} - Y^\lambda_{p_1h_1} a^\dagger_{h_1} a_{p_1}\right)$$

$$(Q_\lambda^{\mathrm{SRPA}})^\dagger = (Q_\lambda^{\mathrm{RPA}})^\dagger + \textstyle\sum_{p_1h_1,p_2h_2}\left(X^\lambda_{p_1h_1,p_2h_2} a^\dagger_{p_1} a_{h_1} a^\dagger_{p_2} a_{h_2} - Y^\lambda_{p_1h_1,p_2h_2} a^\dagger_{h_1} a_{p_1} a^\dagger_{h_2} a_{p_2}\right)$$

- derive equations of motion and solve matrix eigenvalue problem

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix}\begin{pmatrix} X^\lambda \\ Y^\lambda \end{pmatrix} = E^{\mathrm{RPA}}_\lambda \begin{pmatrix} X^\lambda \\ Y^\lambda \end{pmatrix} \quad , \quad \left(\begin{array}{cc|cc} A_{11} & A_{12} & B_{11} & 0 \\ A_{21} & A_{2} & 0 & 0 \\ \hline -B^*_{11} & 0 & -A^*_{11} & -A^*_{12} \\ 0 & 0 & -A^*_{21} & -A^*_{22} \end{array}\right)\begin{pmatrix} X^\lambda_1 \\ X^\lambda_2 \\ Y^\lambda_1 \\ Y^\lambda_2 \end{pmatrix} = E^{\mathrm{SRPA}}_\lambda \begin{pmatrix} X^\lambda_1 \\ X^\lambda_2 \\ Y^\lambda_1 \\ Y^\lambda_2 \end{pmatrix}$$

In Medium-(S)RPA

- input: matrix elements from In Medium-Similarity Renormalization Group (IM-SRG)
- IM-SRG decouples reference state from ph excitations via flow equation
- usually SRPA shows the pathological behavior of an energy shift to lower energies compared to RPA
- using IM-SRG matrix elements reduce the (S)RPA to (S)TDA (Tamm-Dancoff Approximation) which allows ph but no hp excitations

→ strengths from RPA lie at higher energies because of missing correlations

- decoupling in IM-SRG leads to an energy shift to higher energies in (S)RPA

→ instabilities are removed

Hartree-Fock (HF)

- input: single Slater determinant (SD)
- variational calculation for ground state using trial state
- single-particle states of SD are variational degrees of freedom

Natural Orbitals (NAT)

- input: HF calculation plus low-order perturbation theory is used to construct one-body density matrix
- NAT are eigenstates of this matrix [3]
- using NAT: some generalizations in RPA-matrix are needed

Bayesian Uncertainty Quantification

- running sum of discrete electric monopole, dipole, and quadrupole strength for different chiral orders with uncertainties for ^{16}O
- uncertainties result from different chiral orders of interaction Q^i with $i = 0, 2, 3, 4, \ldots$
- observable X given by $X = X_{\mathrm{ref}} \sum_{i=0}^{n} c_i \cdot Q^i$
- assume that c_i are distributed as Gaussian prior probability distribution function
- applying Bayes' theorem and integration results in truncation uncertainty [4][5]

- the uncertainty band is broadened for lower chiral orders
- steps in the uncertainty band result from steps in the running sum of lower chiral orders
- fast convergence can be observed

Basis Optimization

- responses for ^{16}O calculated by using NN+3N interaction at N^{3}LO which is SRG evolved with a flow parameter $\alpha = 0.08\mathrm{fm}^4$, with $l_{\mathrm{max}} = 10$, $e_{\mathrm{max}} = 14$ and $E_{3\mathrm{max}} = 14$

isoscalar monopole

isovector dipole

isoscalar quadrupole

RPA

- all strength distributions show $\hbar\Omega$-dependence
- for HF and NAT: no energy shift
- within IM-RPA responses are shifted to higher energies

SRPA

- HF: strength distributions are shifted to lower energies compared to standard RPA
- strengths from IM-SRPA are also shifted in energy and are located between (HF/NAT)-RPA and IM-RPA results
- but: IM-SRPA results are closest to experiment

Future Applications

- applications of IM-SRPA
- development of uncertainty estimation for continuous observables as smeared out strength distribution

References:

[1] T. Hüther *et al.*, Phys. Lett. B **808**, 135651 (2020).
[2] P. Papakonstantinou *et al.*, Phys. Rev. C **81**, 024317 (2010).
[3] A. Tichai *et al.*, Phys. Rev. C **99**, 034321 (2019).
[4] E. Epelbaum *et al.*, The European Physical Journal A **56** (2020).
[5] J. A. Melendez *et al.*, Phys. Rev. C **100**, 044001 (2019).