Low-lying spectroscopy of medium-mass deformed nuclei with the in-medium similarity renormalization group and generator coordinate method

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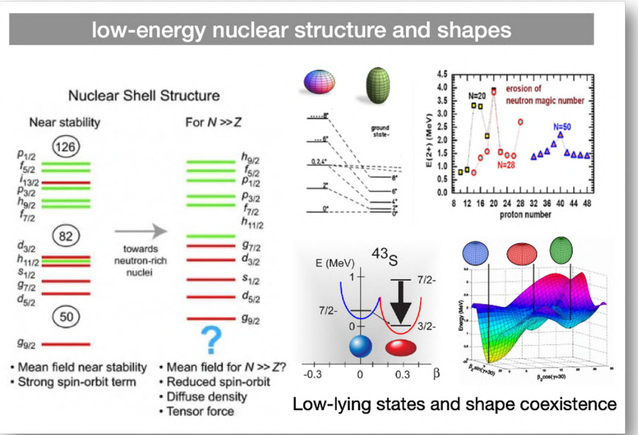
Outline

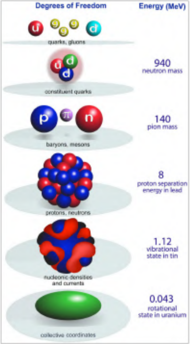
Probing nuclear structure with low-lying spectroscopy

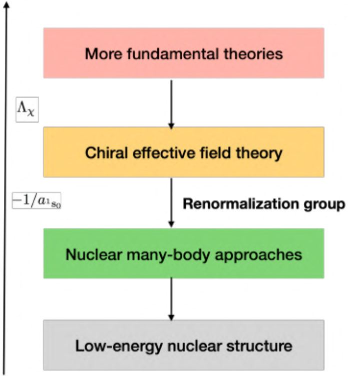
The shell structure of single-nucleon energy spectrum is indicated from the systematic behaviors of binding energies and low-lying spectroscopic properties and is of importance to the stability of certain atomic nuclei.

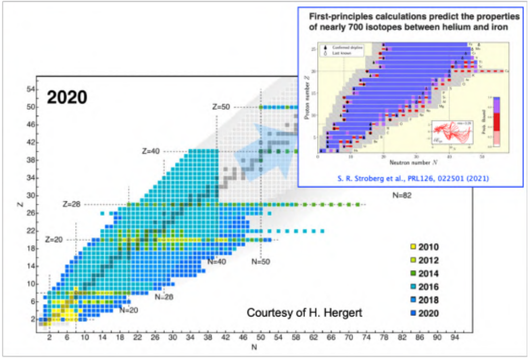


- Onset (erosion) of large nucleon shell gaps from stable to dripline nuclei can be inferred from high (low) excitation energy of 2_1^+ state in even-even nuclei.
- Low-energy structure in odd-mass nuclei is enriched by shape coexistence and interplay of single-particle and collective motions.

Modeling nuclear structure with high-resolution nuclear forces







- Energy scale of nuclear collective excitations: $0.1 - 1.0$ MeV, usually studied with collective models, ISM and MR-EDF approaches.
- Challenge and inefficient to model nuclear collective excitations starting from chiral nuclear forces, bridging the energy scales from 10^2 MeV to 10^{-1} MeV.

Processing the chiral interaction with SRG

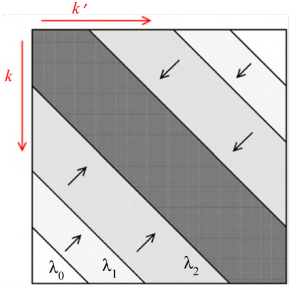
- Apply unitary transformations to decouple the coupling between high and low-momentum states

$$H_s = U_s H U_s^\dagger \equiv T_{\rm rel} + V_s$$

from which one finds the flow

equation

$$\frac{dH_s}{ds} = [\eta_s, H_s], \quad \eta_s = [T_{\rm rel}, H_s]$$



The flow parameter s is usually replaced with $\lambda = s^{-1/4}$ in units of fm^{-1} (a measure of the spread of off-diagonal strength).

Evolution of the potential

$$\frac{dV_s(k,k')}{ds} = -(k^2 - k'^2)V_s(k,k') + \frac{2}{\pi}\int_0^\infty q^2 dq (k^2 + k'^2 - 2q^2) V_s(k,q) V_s(q,k')$$

With the SRG-evolved $NN + 3N$, the normal-ordered one-body matrix element,

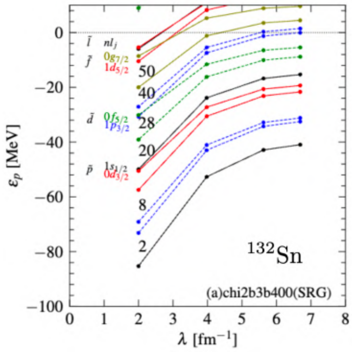
$$f_{pq}(\lambda) \quad = \quad t_{pq} + \sum_{rs} V_{prqs}(\lambda)\rho^r_s + \frac{1}{4}\sum_{rstu} W_{prsqtu}(\lambda)(\rho^r_t\rho^s_u - \rho^r_u\rho^s_t).$$

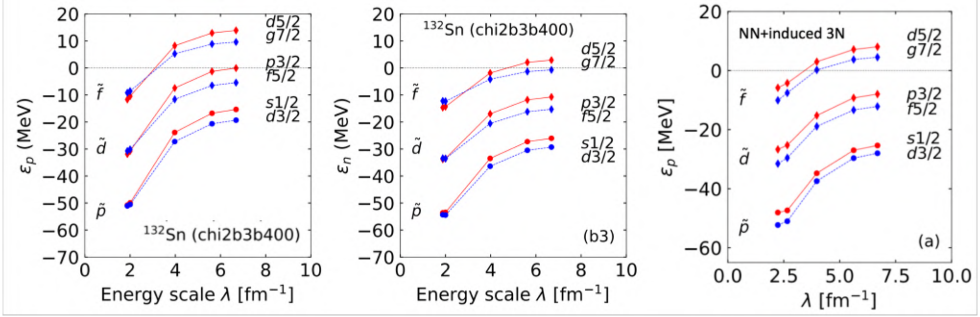
- The effective single-particle energies (ESPE) in HF,

$$[D(\lambda)f(\lambda)D^\dagger(\lambda)]_{kl} = \varepsilon_k(\lambda)\delta_{kl}$$

- The emergence of pseudospin symmetry (Arima, Hecht, 1969) and magic numbers in the ESPE spectra. For the pseudospin doublets ($\tilde{\ell} = \ell + 1, \tilde{j} = \tilde{\ell} \pm 1/2$)

$$\varepsilon_{k=(n,\ell,j=\ell+1/2)} \simeq \varepsilon_{k=(n-1,\ell+2,j=\ell+3/2)}.$$





- The splitting of the pseudospin doublets is decreasing with the resolution scale λ for the $NN + 3N$ interaction.
- However, the degeneracy is not observed in the ESPE spectra by the NN plus induced $3N$ interactions.

JMY, H. Hergert, et al., in preparation

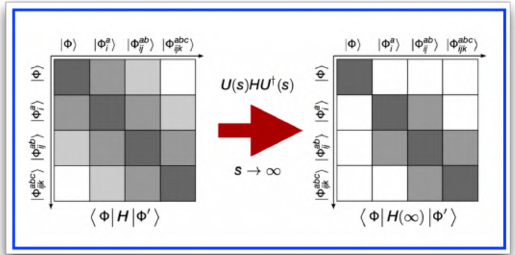
Apply unitary transformations to $\hat{H}$ in the configuration space to obtain ground state

$$\hat{H}(s) = \hat{U}(s)\hat{H}_0\hat{U}^\dagger(s)$$

- Flow equation

$$\frac{d\hat{H}(s)}{ds} = [\hat{\eta}(s), \hat{H}(s)]$$

- The generator $\eta(s)$ is chosen to decouple a given reference state from its excitations.
- Not necessary to construct the whole H matrix in the configuration space.



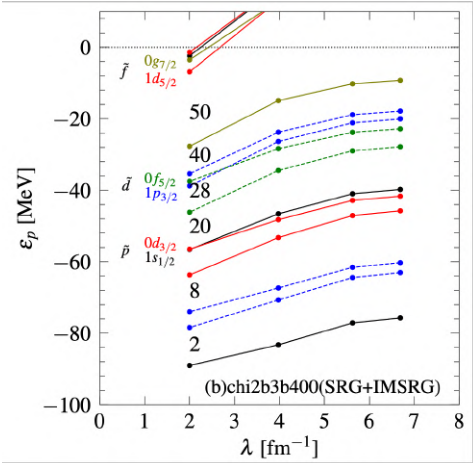
H. Hergert et al., Phys. Rep. 621, 165 (2016)

- For the Hamiltonian $\hat{H}(s=\infty)$,

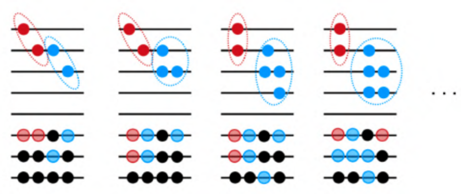
$$\hat{H}(\infty)\,|\Phi_{\rm HF}\rangle = E_0\,|\Phi_{\rm HF}\rangle$$

- The $\hat{H}(\infty)$ serves as an effective Hamiltonian for MF-based approaches.
- Emergence of large spin-orbit splitting and pseudospin symmetry as well in the ESPE spectra of $H_\lambda(\infty)$ at $\lambda = 2.0\ \mathrm{fm}^{-1}$.
- Nuclear shell structure is non-observable, but the energies of low-lying states are observables and should not change with the flow parameter.

T. Duguet, H. Hergert, J. D. Holt, V. Soma, PRC92, 034313 (2015)



many-particle many-hole excitations



challenge for most ab initio methods!

IMSRG(3)

- Computational scaling $O(N^9)$
- memory storage N^6
  computational challenge!

IMSRG(A)

- From a simple HF reference state $|\Phi\rangle$ to exact ground state $|\Psi\rangle$

$$|\Psi\rangle = e^{\hat{\Omega}}|\Phi\rangle,$$

where many-body correlations are built into the correlation operator $\hat{\Omega}$,

$$\hat{\Omega} = \hat{\Omega}^{(1b)} + \hat{\Omega}^{(2b)} + \hat{\Omega}^{(3b)} + \cdots + \hat{\Omega}^{(Ab)}$$

determined from the IMSRG.

Extension of the IMSRG for deformed nuclei

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Multi-reference: Build collective correlations into the reference state (no core methods)

- From a correlated reference state $|\Phi\rangle$ to exact ground state $|\Psi\rangle$

$$|\Psi\rangle = e^{\hat{\Omega}}|\Phi_{\rm Cor}\rangle, \quad \hat{\Omega} = \hat{\Omega}^{(1b)} + \hat{\Omega}^{(2b)} + \cdots$$

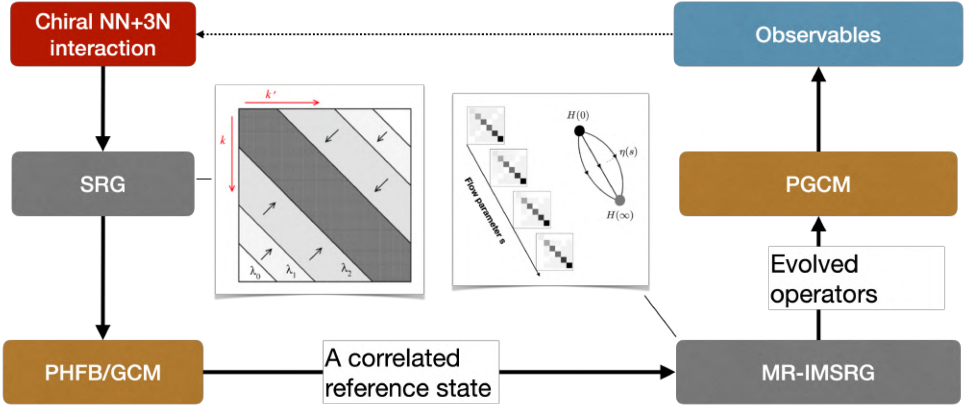
  and the correlated reference state $|\Phi_{\rm Cor}\rangle$ can be chosen as a state with many-particle many-hole excitations relevant for nuclear collective excitations.
- IM-NCSM: reference state from NCSM calculation with a small $N_{\rm max}$

  E. Gebrerufael et al., PRL118, 152503 (2017)
- IM-GCM: reference state from PHFB/GCM calculation

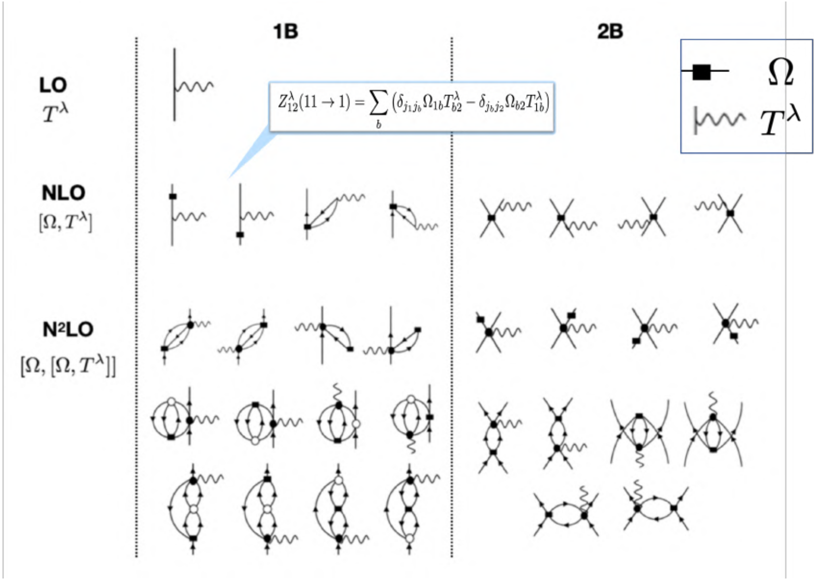
  JMY et al., PRL124, 232501 (2020)

Cons: produce an effective interaction targeted for individual nucleus.

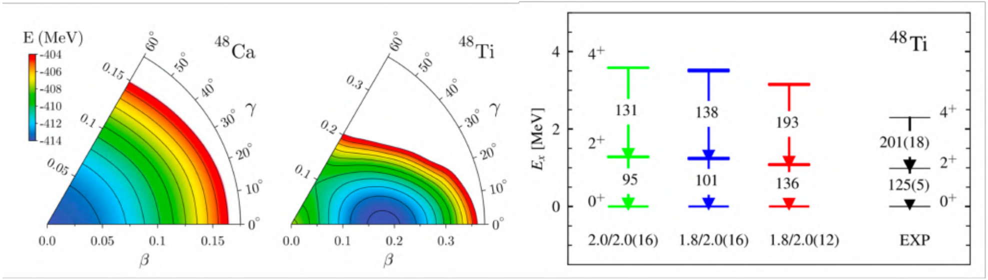
The Framework of IM-GCM



Tensor operators in MR-IMSRG



Application of IM-GCM to ^{48}Ca and ^{48}Ti

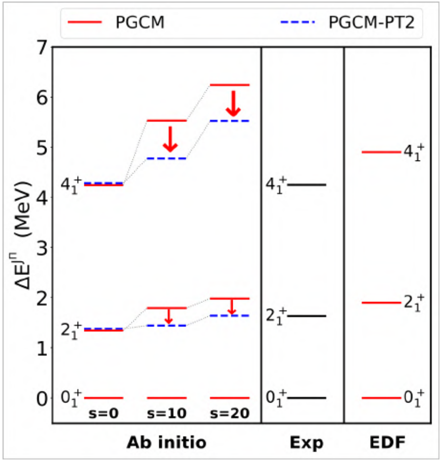


- Using the magic chiral NN+3N interaction EM1.8/2.0 K. Hebeler et al., PRC83, 031301(R) (2011)
- Reference state is chosen as an ensemble of states for ^{48}Ca and ^{48}Ti.
- The above results are given by the IMSRG-evolved Hamiltonian.
- The energy spectrum of ^{48}Ti is reasonably reproduced, even though slightly stretched.

JMY et al., PRL124, 232501 (2020)

Dilation of the energy spectrum

- Since the IMSRG evolution is mainly targeted to the ground state, the energy spectrum by the IMSRG-evolved Hamiltonian is dilated.
- The dilation of the energy spectra can be reduced by including additional correlations with perturbation theory or including cranking frequency as one more generator in the GCM.



T. Duguet, J.-P. Ebran, M. Frosini, H. Hergert, V. Somà, EPJA 59, 1 (2023)

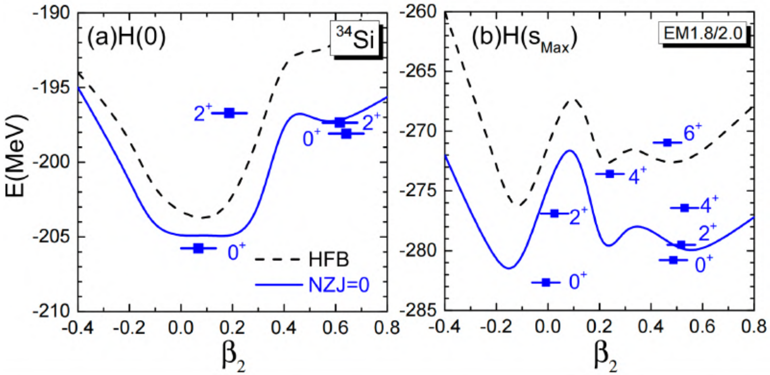
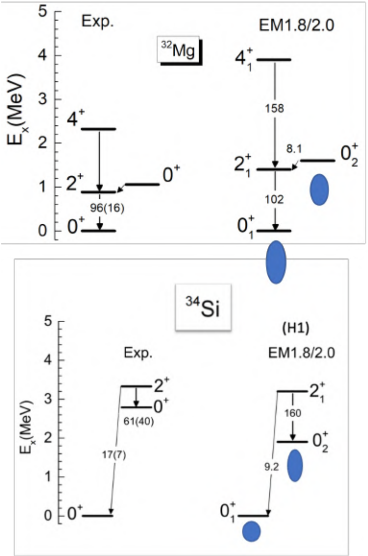
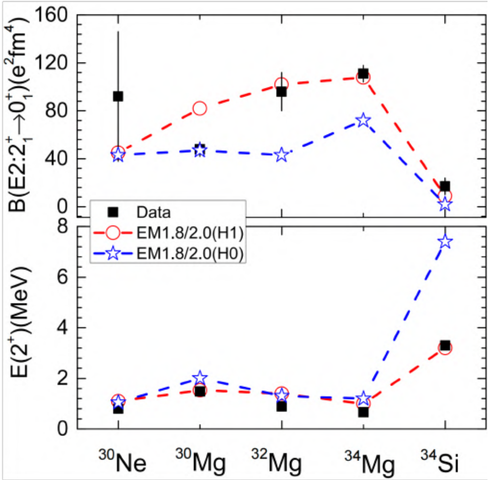


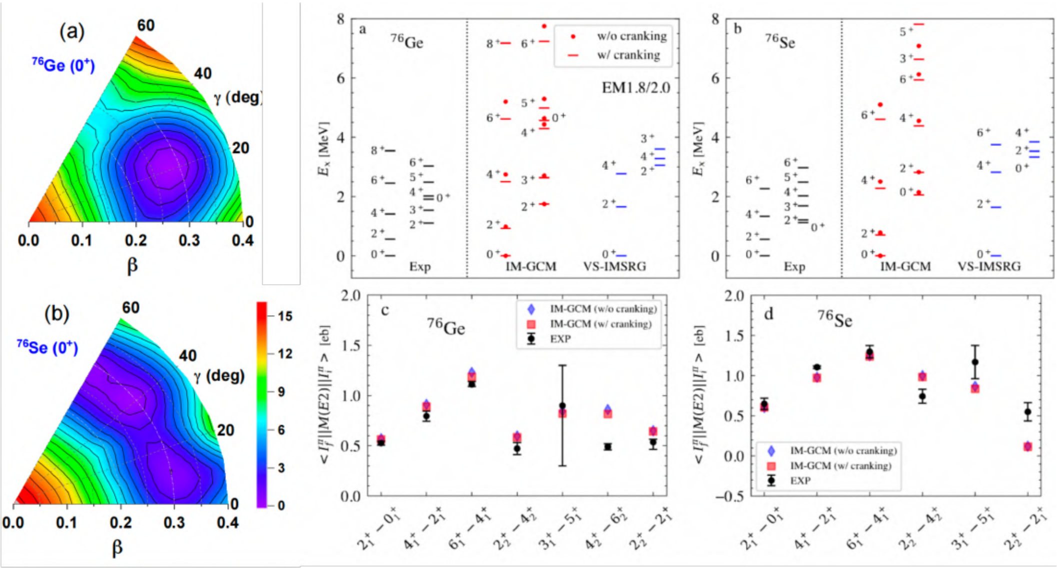
Figure: Mr. Enfu Zhou

- Coexistence of spherical ground state and prolate deformed rotational bands is shown in ^{34}Si, where the ENO turns out to be important.


Exp.
EM1.8/2.0
32Mg
Ex(MeV)
96(16)
158
8.1
102
34Si
(H1)
EM1.8/2.0
61(40)
17(7)
160
9.2


B(E2:2+1→0+1)(e2fm4)
E(2+1)(MeV)
Data
EM1.8/2.0(H1)
EM1.8/2.0(H0)
30Ne
30Mg
32Mg
34Mg
34Si

Application to ^{76}Ge and ^{76}Se



- The wave functions of an odd-mass nucleus

$$\left|\Psi_{\alpha}^{J\pi}\right\rangle = \sum_{c} f_{c}^{J\alpha\pi} \left|NZJ\pi; c\right\rangle,$$

- The basis function with correct quantum numbers $(NZJ\pi)$

$$\left|NZJ\pi; c\right\rangle = \hat{P}^{J}_{MK} \hat{P}^{N} \hat{P}^{Z} \left|\Phi_{\kappa}^{(\mathrm{OA})}(\mathbf{q})\right\rangle,$$

The mean-field configurations $\left|\Phi_{\kappa}^{(\mathrm{OA})}(\mathbf{q})\right\rangle$

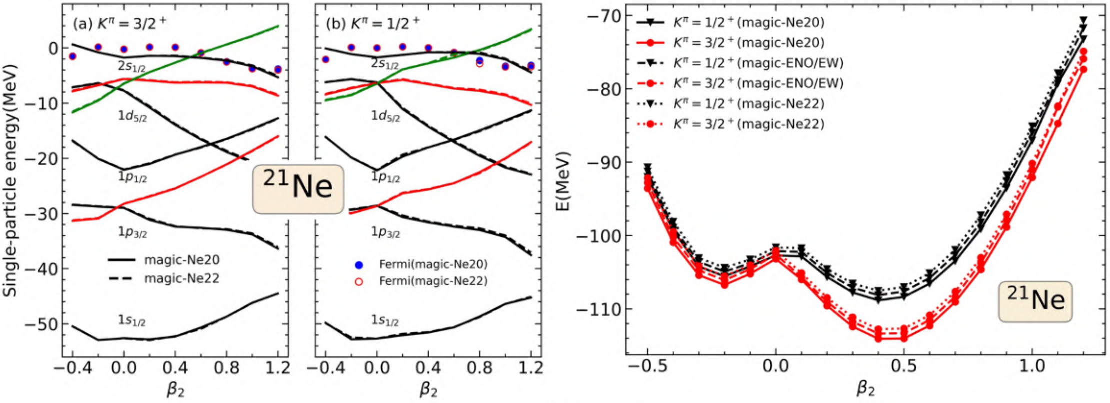
$$\left|\Phi_{\kappa}^{(\mathrm{OA})}(\mathbf{q})\right\rangle = \alpha_{\kappa}^{\dagger} \left|\Phi_{(\kappa)}(\mathbf{q})\right\rangle, \quad \alpha_{\kappa} \left|\Phi_{(\kappa)}(\mathbf{q})\right\rangle = 0,$$

where $\left|\Phi_{(\kappa)}(\mathbf{q})\right\rangle$ is a HFB state with the even-number parity.

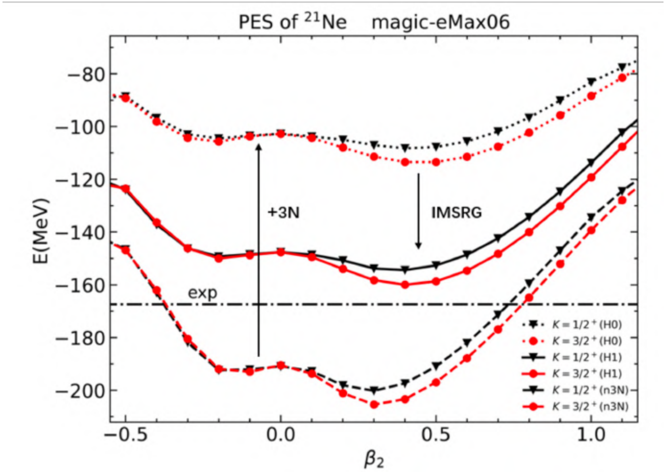
W. Lin, E. F. Zhou, JMY, H. Hergert, arXiv:2403.01177 [nucl-th]

Figure: Mr. Wei Lin

Extension of IM-GCM to odd-mass nuclei

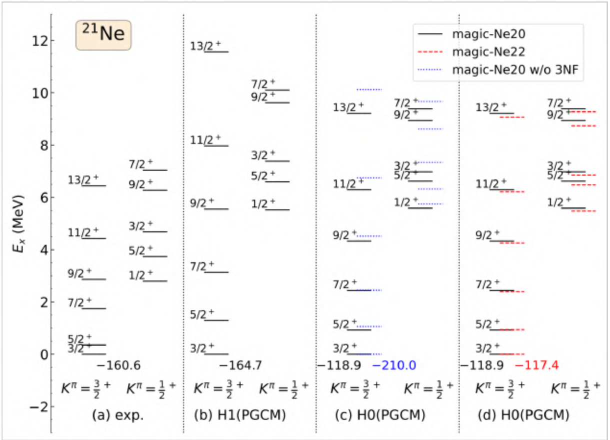


- The ESPEs by choosing the reference state of either ^{20}Ne or ^{22}Ne are similar.
- The different choices of the reference state to which the $3N$ is normal-ordered lead to similar energy curves, except for a systematic shift by about 1 MeV.



- The $3N$ interaction softens the energy curves along the β_2 direction.

Extension of IM-GCM to odd-mass nuclei

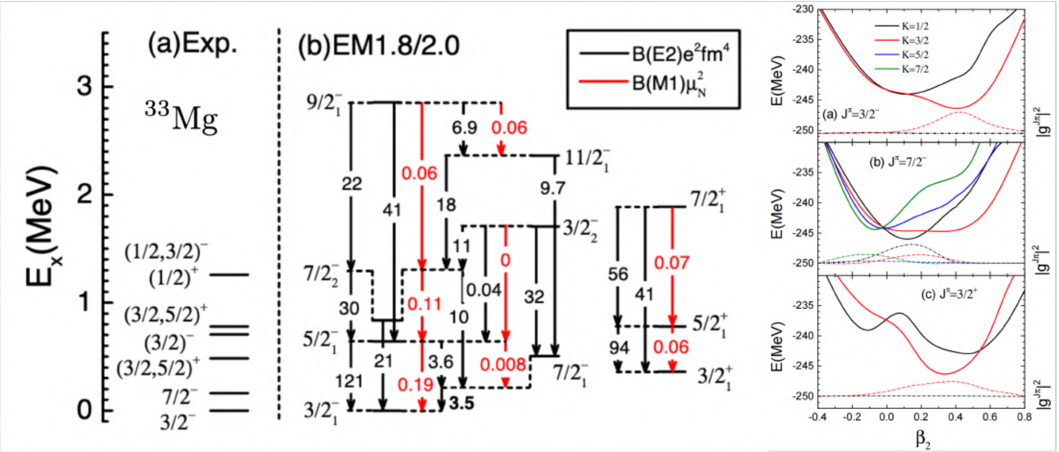


	Exp	H1(bare) (Ne20/eMax6)
$\mu(3/2^+)$	-0.66	$-0.88(-0.72)$
$\mu(5/2^+)$	$+0.49(4)$	$-0.06(+0.05)$
$\mu(7/2^+)$	-	$0.34(0.66)$
$\mu(9/2^+)$	-	$1.12(1.23)$
$\mu(11/2^+)$	-	$1.28(1.77)$
$Q^s(3/2^+)$	$+10.3(8)$	$+8.1(+8.2)$
$Q^s(5/2^+)$	-	$-3.0(-3.0)$
$Q^s(7/2^+)$	-	$-7.9(-7.9)$
$Q^s(9/2^+)$	-	$-10.5(-10.5)$
$Q^s(11/2^+)$	-	$-11.2(-11.2)$
$B(E2;5/2^+)$	$83.6(61)$	$55.1(55.2)$
$B(E2;7/2^+)$	$37.8(137)$	$32.7(32.7)$
$B(E2;9/2^+)$	$31.0(172)$	$19.2(19.3)$
$B(E2;11/2^+)$	$20.6(130)$	$11.3(11.3)$
$B(M1;5/2^+)$	$0.1275(25)$	$0.310(0.320)$
$B(M1;7/2^+)$	$0.2615(21)$	$0.440(0.420)$
$B(M1;9/2^+)$	$0.43(5)$	$0.364(0.452)$
$B(M1;11/2^+)$	$0.36(7)$	$0.478(0.466)$

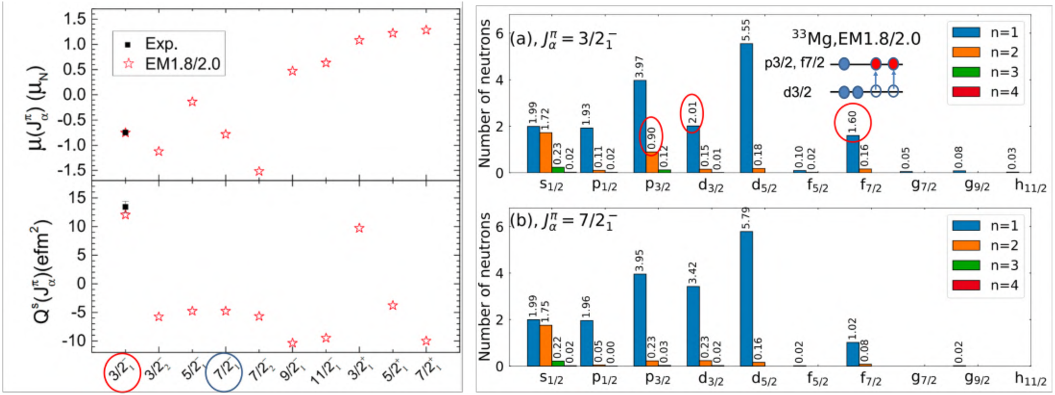
$B(EM\lambda; J \to J-1)$

- The energy spectrum becomes stretched and quadrupole collectivity is reduced when the $3N$ interaction is turned off.

Application to ^{33}Mg



- Very weak EM transitions from $7/2_1^-$ to ground state.
- The $7/2_1^-$ is likely a shape isomer state, according to the distribution of wave function.

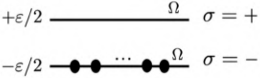


- Magnetic dipole moment and spectroscopic quadrupole moment of the ground state are reasonably reproduced, and the spin parity is $3/2^-$, which is a $2p$-$2h$ excitation compared to the $7/2^-_1$ state, according to average neutron natural orbital occupations.

Test of EC+GCM for the Lipkin model

Mr. Qingyang Luo

- The Hamiltonian of the Lipkin model



$$\hat{H} = \frac{\varepsilon}{2}\sum_{\sigma m}\sigma \hat{c}^{\dagger}_{\sigma m}\hat{c}_{\sigma m} - \frac{V}{2}\sum_{mm'\sigma}\hat{c}^{\dagger}_{\sigma m}\hat{c}^{\dagger}_{\sigma m'}\hat{c}_{-\sigma m'}\hat{c}_{-\sigma m}$$

$$= \varepsilon \hat{K}_0 - \frac{V}{2}(\hat{K}_+\hat{K}_+ + \hat{K}_-\hat{K}_-), \qquad \chi = \frac{V}{\varepsilon}(\Omega - 1)$$

- GCM wave function

$$|\Psi^{\kappa}_{\rm GCM}(\chi)\rangle = \sum_{\mathbf{q}=1}^{N_q} f^{\kappa}(\chi;\mathbf{q})\,|\Phi(\mathbf{q})\rangle$$

$$|\Phi(\alpha,\varphi)\rangle = \prod_{m=1}^{\Omega} a^{\dagger}_{0m}(\alpha,\varphi)|-\rangle$$

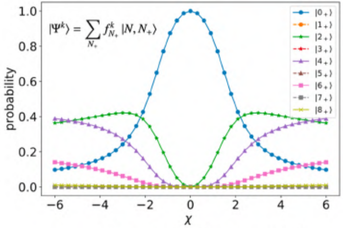
- EC+GCM wave function

$$|\Psi^{k}_{\rm EC}(\chi_{\odot})\rangle = \sum_{\kappa=1}^{k_{\max}\geq k}\sum_{t=1}^{N_t} g^{k}(\kappa,\chi_t)\,|\Psi^{\kappa}_{\rm GCM}(\chi_t)\rangle$$

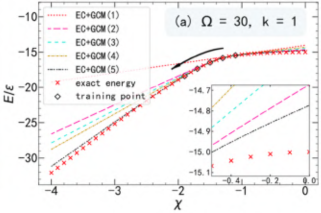
Generalized eigenvalue equation

$$\sum_{\kappa'=1}^{k_{\max}}\sum_{t'=1}^{N_t}\left[\mathcal{H}^{\kappa\kappa'}_{tt'}(\chi_{\odot}) - E^{k}_{\chi_{\odot}}N^{\kappa\kappa'}_{tt'}\right]g^{k}(\kappa',\chi_{t'}) = 0,$$

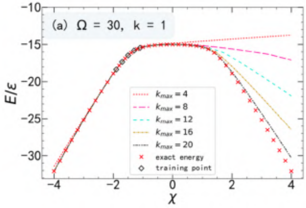
QY Luo, X Zhang, LH Chen, JMY, arXiv:2404.08581



Diagonalization method



EC_1 +GCM



EC_{kmax} +GCM

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- Remarkable advances have been achieved in ab initio studies of nuclear structure and decays. However, the low-lying states of medium mass deformed nuclei are still challenging for most ab initio methods.
- The IM-GCM, a combination of IMSRG and GCM, stands out as a promising approach for the low-lying states of nuclei with complicated shapes. It has been successfully applied to describe the low-lying states of ^{48}Ti, ^{76}Ge, ^{76}Se, and nuclei around $N = 20$ with shape coexistence, even though the energy spectra are generally more stretched than data.

Next steps

- Extension to odd-mass nuclei with octupole correlations.
- Uncertainty quantification with the EC+GCM method.

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Collaborators

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