Progress report of development of a Skyrme QRPA code for deformed nuclei

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Quasiparticle random-phase approximation

Introduce a creation operator of an excited state:

$$\hat{O}^{+} = \sum_{ij} X_{ij}\, a_i^{+} a_j^{+} - Y_{ij}\, a_j a_i$$

creation operator of quasiparticle

HFB calculation

X_{ij} and Y_{ij} ⟵ QRPA equation

Eigenvalue equation linear in X_{ij} and Y_{ij} .
eigenvalue = excitation energy

Scheme of system of codes

HFB calculation with HFBTHO, M. Stoitsov et al., Computer Physics Communications **167** (2005) 43.

We use HO basis for our tests.

Interface code to convert output of HFBTHO to input for our code

quasiparticle wave functions,

energies, and auxiliary information

Calculation of interaction matrix elements

Diagonalization of QRPA-Hamiltonian matrix

with ScaLAPACK

Test calculation I

Comparison of interaction energies produced by HFBTHO and those by our code

Our code has subprograms to calculate matrix elements of interactions from quasiparticle wave functions

developed independently of HFBTHO

^{16}O, SkP, 20 spherical HO shells, no deformation, no pairing gap

Components of energy in MeV

	E_{t0}	E_{t1}	E_{t2}	E_{t3}
HFBTHO	–1476.285	83.596	–39.177	1075.713
Our code	–1476.285	83.595	–39.176	1075.713

	E_{SO}	$E_{\mathrm{Coul\text{-}dir}}$	$E_{\mathrm{Coul\text{-}ex}}$	E_{int}
HFBTHO	–0.662	16.261	–2.776	–343.331
Our code	–0.662	16.176	–2.776	–343.415

Test calculation II

Separation of spurious states from real excited states

- Rotation, $K^{\pi}=\pm 1^{+}$ ($J=2$)
- Rotation in a gauge space (particle number), $K^{\pi}=0^{+}$ ($J=0$)
- Translation, $K^{\pi}=0^{-}$, $\pm 1^{-}$ ($J=1$)

Spurious states ($E=0$) appear in solutions of QRPA, and real excited states do not have the spurious components, if

- HFB state breaks symmetries,
- wave-function space conserves the symmetries,
- HFB and QRPA equations are solved accurately with the same H and quasiparticle wave-function space.

Test calculations are in small spaces;
dim. of QRPA Hamiltonian matrix < 700

We can check spurious states with $K^{\pi}=0^{+}$ and $K^{\pi}=\pm 1^{+}$ in spaces of this size.

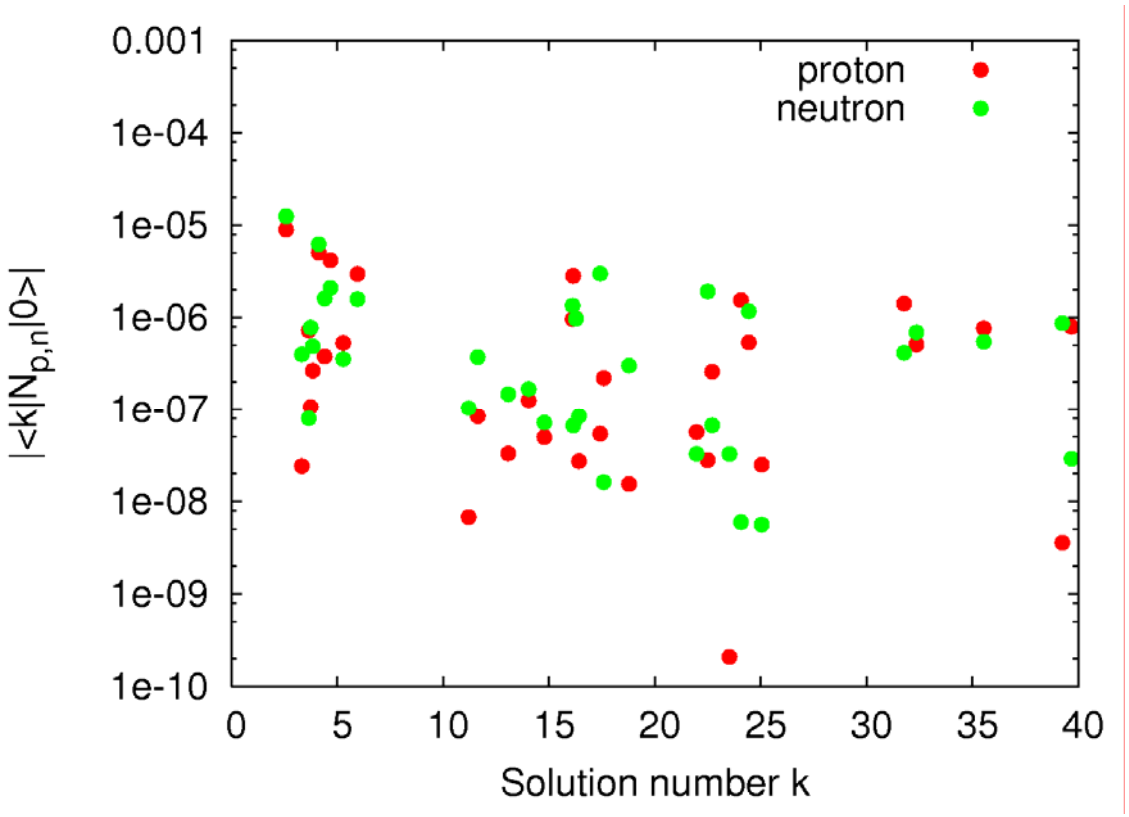
^{26}Mg, SkP, volume-type pairing, 3 spherical HO shells
β=0, Δ_p=1.681 MeV, Δ_n= 1.426 MeV

$K^\pi = 0^+$

Eigenvalues of QRPA (MeV)

0.008
0.024
2.582
3.330
3.444
3.649
…

"Particle-number transition strength"



^{24}Mg, SkP, volume-type pairing, 5 spherical HO shells
β=0.28, Δ_p=0.034 MeV, Δ_n= 0.131 MeV

$K^\pi=1^+$
Eigenvalues of QRPA (MeV)
0.045
2.672
2.696
2.877
3.359
4.119
…

Strength function not quite ready

Code passes all these tests.

Plan for rest of year

- Parallelize calculation of interaction matrix elements

  Dimension of QRPA Hamiltonian matrix for ^{24}Mg, $K^{\pi}=1^{+}$ was 700, and it took 24 hours to get interaction matrix elements with a single processor.

- Implement calculation of strength functions.

- Prepare systematic calculations of even-even nuclei across the entire table of isotopes.

  Is it possible without sacrificing accuracy?

After that

See talk by M. Horoi

A computational question

QRPA equation

$$\sum_{\varsigma\xi}\begin{pmatrix} A & B \\ B^T & A' \end{pmatrix}_{\mu\nu,\varsigma\xi}\begin{pmatrix} X \\ Y \end{pmatrix}_{\varsigma\xi} = \hbar\omega \sum_{\varsigma\xi}\begin{pmatrix} I & O \\ O & -I \end{pmatrix}_{\mu\nu,\varsigma\xi}\begin{pmatrix} X \\ Y \end{pmatrix}_{\varsigma\xi}$$

A and *A´* are Hermitian; all are real.

ScaLAPACK diagonalization subroutine *pdsygvx* solves

$$\mathscr{A}\,\boldsymbol{x} = \lambda\,\mathscr{B}\,\boldsymbol{x}$$

$\mathscr{A}$: symmetric matrix

$\mathscr{B}$: symmetric and positive definite matrix

We use this subroutine with

$$\mathscr{A} = \begin{pmatrix} I & O \\ O & -I \end{pmatrix}.$$

We would like a better method.