Exotic halos and collective excitations in weakly-bound deformed nuclei



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Physics and motivations

- Radioactive Beam Facilities can provide great opportunities and challenges for study of extremely unstable nuclei
- FRIB(U.S), HIAF(China recently approved); supercomputing
- Exotics: threshold effects, continuum coupling vs pairing anti-halo, exotic surfaces (dilute halos/deformed halos, vibrations/new modes, few-body vs many-body, BEC-BCS---low density superfluity, decoupling, clustering)





Continuum effects

- Continuum coupling: pairing induced; angular-momentum dependence
- Weakly-bound s.p. states coupled with continuum: resonances
- Near-threshold non-resonant continuum is important for halos (Pei 2013)
- High energy continuum: Thomas-Fermi approximation (Pei 2011)
- Enhance stability; enhance halo features; enhance collectivity?







Continuum effects





Continuum coupling in HFB theory

- Current progress: particularly difficult for deformed nuclei
 - Diagonalization on single-particle basis :HO, woods-saxon, PTG, Gamow...
 - Direct diagonalization on coordinate-space lattice
 - Outgoing boundary condition: *difficult for deformed cases*

*******H. Oba, M. Matsuo, PRC, 2009,* self-consistent calculations are still missing

 Coordinate-space HFB has advantages for describing weakly-bound systems and large deformations

Bound states, continuum and embedded resonances are treated on an equal footing; L² discretization leads to a very large configuration space
 Computing resources and capabilities are increasing exponentially



Does continuum discretization work?

• Non-resonant continuum check with Thomas-Fermi approximation



- 2. Calculate the HFB resonance widths with box stabilization Pei, Kruppa, Nazarewicz, PRC, 2011
- Problem: broad resonance is expensive (CDCC also surfers)



Large coordinate-space HFB calculations

- Conventionally, HFB solvers were benchmarked by energies, this is not sufficient for detailed properties of soft weakly-bound nuclei.
- Subtle interplay among surface deformations, surface diffuseness, and continuum needs precise HFB solutions.
- Large coordinate-space resulted in a vast number of continuum states and provides good resolutions for resonances and continuum (proportional L³)
- Small box may not be sufficient for describing pairing properties.
 M. Grasso, N. Sandulescu, Nguyen Van Giai, R. Liotta, PRC, 2001.
 H. Oba and M. Matsuo, PRC, (2009)
- Small box may be not good for broad resonances.
- Small box may cause false peaks in QRPA



Hybrid parallel HFB calculations



Large boxes calculations are crucial for describing halo densities, large deformation and discretized continuum

From 20 fm to 40 fm, the estimated computing cost increased by 40 times.

• Calculations performed in Tianhe-1A; Tianhe-2 (TOP 1)

advantage: take into account deformation, pairing, and weak-binding effects simultaneously.



Exotic egg-like halo structure

- Self-consistent calculations: SLy4 force + density dependent pairing
- 38Ne, (a) neutron density; (b) n pairing density
- About 2 neutrons in the halo
- Deformations: beta2 = 0.24, beta2_pair=0.48
- Mainly contributed by near-threshold continuum



New exotic "egg"-like halo structure obtained; accurate approach is^zessential

J.P., Y.N. Zhang, F.R. Xu, PRC (R) 87, 051302(2013)





Near-Threshold Continuum

- Different box calculations to distinguish resonances and continuum states
- Near threshold non-resonant continuum is responsible for halo and surface deformations
- No halo in ⁴⁰Mg since no near-threshold continuum contributions (*N*=28)





Phase-space decoupling

- Non-resonant continuum states gradually grows and decouples in heavy nuclei
- sparse negative-parity level density is crucial; deformed halos in medium-mass nuclei is possible, e.g. in ¹¹⁰Ge. Heavy halos are hindered due to denser levels.
- Core-halo decoupling is related to the phase space decoupling in quasiptaricle spectrum





Systematics of deformed halos

- Halo hindered by deformed cores? (seems correct) F. Nunes, NPA, 2005(3-body model)
- Halo and surface deformations are mainly contributed by near-threshold continuum
- Heavy halos not likely existed; decoupling effect decreased





Coordinate-space vs Basis expansion

Basis expansion HFB fails in describing weakly-bound nuclei!





Density and pairing density at surfaces



HFB solvers and Continuum effects------J.C. Pei

Quasiparticle spectrum near thershold



Box size dependence of energies

• Total energy is not sensitive to box size, however (pairing, deformation, stability)....

38	246	070	2005	266
Ne	24fm	27fm	30fm	36fm
E_{tot}	-220.29	-220.29	-220.35	-220.33
E_{c}	18.94	18.95	18.95	18.96
E_{pair}	-68.10	-67.77	-67.41	-67.43
E_{kin}^p	138.34	138.46	138.51	138.56
E_{kin}^{n}	444.84	443.48	442.85	442.10
β_{2p}	0.00	0.00	0.00	0.00
β_{2n}	0.13	0.19	0.24	0.34
R_{rms}	9.39	9.38	9.38	9.37
Δ_p	1.46	1.47	1.47	1.46
Δ_n	2.97	2.95	2.93	2.92
λ_p	-23.853	-23.802	-23.784	-23.747
λ_n	-0.079	-0.096	-0.103	-0.116



Y.N. Zhang, J.C. Pei, F.R. Xu, PRC 88, 054305, 2013



Peninsula of stability

• Enhanced stability due to deformations and continuum effects



Y.N. Zhang, J. P., F.R. Xu, PRC 88, 054305, 2013



MADNESS-SHF+BCS solver

• Benchmark for the triaxial deformed nucleus Mo110:

	MADNESS-HF	HFODD(1)	HFODD(2)
E_t	924.77	923.86	924.05
λ_p	-12.743	-12.651	-12.713
λ_n	-5.432	-5.457	-5.459
E_{k}	2005.89	2005.22	2003.33
E_p	-16.01	-17.27	-16.93
E_{c}	251.55	251.29	251.43
R_{rms}	4.656	4.66	4.664
Q_{20}	816.36	864.82	834.3
$ Q_{21} $	0.56	0	0.0
Q_{22}	321.46	314.15	314.78
Q_2	1144.54	1178.97	1149.08





• Next step: full 3D HFB calculations are very expensive.

Pei et al, JPCS, 2012 Bonger et al., CPC, 2013 Pei, G. Fann, W. Nazarewicz, et al. in preparation, 2014



Deformed continuum-QRPA study excited states

- Continuum effects in excited states would be very important: cross threshold
- Exotic collective modes: collectivity, weakly binding increase collectivity? different modes mixing, astrophysical interests, how to detect
- Study effective interactions: tensor force?
- Sensitive to pairing interactions
- A basic work for further studies: 0v-beta-decay; di-neutron; cold atoms;
 3D-QRPA.....
- Progress in 2013 year: developed code and benchmark (succeed recently for monopole excitations, including time-odd terms)



FAM-QRPA

Motivation

Standard QRPA in the matrix form is extremely expensive for deformed nuclei, even more to include continuum configuration

FAM-QRPA provides alternative way solving QRPA equation iteratively rather than diagonalization (it is popular in other quantum systems: Chemistry)

First application in nuclear physics: T. Nakatsukasa, PRC, 2007

• Current status of FAM-QRPA

Based on HFBRAD (spherical coordinate-space HFB),

(PRC, T. Nakatsukasa, 2011)

Based on deformed relativistic HB (T. Nikšić, Phys. Rev. C 88, 044327, 2013)

Based on HFBTHO(deformed HO/THO basis),

(M. Stoitsov, PRC 84, 041305(R),2011)

Relativistic FAM-RPA (Liang HZ, PRC, 2013)

Discrete states: N. Hinohara, PRC, 2013



Implementation

- HFB-AX output: 2D wavefunctions and energies, quasiparticle basis
 B-spline lattice transformed to Gauss-Legendre lattice
- FAM-QRPA procedure:
 - 1. Construct transition densities (including time-odd terms):

$$\begin{split} \delta\rho(\omega) &= UXV^T + V^*Y^TU^{\dagger}, \\ \delta\kappa^{(-)}(\omega) &= UXU^T + V^*Y^TV^{\dagger}, \\ \delta\kappa^{(-)}(\omega) &= V^*X^{\dagger}V^{\dagger} + UY^*U^T, \end{split}$$

$$\left\{s_{\phi}, j_{r}, j_{z}, (\nabla \times \mathbf{j})_{\phi}, (\nabla \times \mathbf{s})_{r}, (\nabla \times \mathbf{s})_{z}, (\Delta \mathbf{s})_{\phi}, T_{\phi}\right\}$$

$$\begin{aligned} \mathcal{E}_{t}^{\text{even}} &= C_{t}^{\rho} \left[\rho \right] \rho_{t}^{2} + C_{t}^{\tau} \rho_{t} \tau_{t} + C_{t}^{\Delta \rho} \rho_{t} \Delta \rho_{t} + C_{t}^{\nabla J} \rho_{t} \nabla \mathbf{J} + C^{J} \mathbf{J}_{t}^{2} , \\ \mathcal{E}_{t}^{\text{odd}} &= C_{t}^{s} \left[\rho \right] \mathbf{s}_{t}^{2} + C_{t}^{\Delta s} \mathbf{s}_{t} \cdot \Delta \mathbf{s}_{t} + C_{t}^{T} \mathbf{s}_{t} \cdot \mathbf{T}_{t} + C_{t}^{j} \mathbf{j}_{t}^{2} + C_{t}^{\nabla j} \mathbf{s}_{t} \cdot \nabla \times \mathbf{j}_{t} \\ &+ C_{t}^{\nabla s} \left(\nabla \mathbf{s}_{t} \right) , \end{aligned}$$



Implementation

 (\pm)

2. Calculate H20, H02(including time-odd terms), F20, etc

- 3. Calculate X, Y; and Broyden iteration on X, Y. (30 iterations kept)
- 4. Finally calculate the strength

$$\begin{aligned} X_{\mu\nu} &= -\frac{\delta H_{\mu\nu}^{20}(\omega) - F_{\mu\nu}^{20}}{E_{\mu} + E_{\nu} - \omega}, \quad Y_{\mu\nu} = -\frac{\delta H_{\mu\nu}^{02}(\omega) - F_{\mu\nu}^{02}}{E_{\mu} + E_{\nu} + \omega}, \\ S(F, \omega) &= \frac{1}{2} \sum_{\mu\nu} \left\{ F_{\mu\nu}^{20*} X_{\mu\nu}(\omega) + F_{\mu\nu}^{02*} Y_{\mu\nu}(\omega) \right\}, \end{aligned}$$



Implementation

- Combined parallel calculations in Tianhe-1A for different excitation frequency : MPI distributed parallel for each point in a node: OpenMP multi-thread parallel (12 threads)
- Time-consuming: read wavefunctions (10-20 G) and calculate transiton densities and H20
 cutoff at 65 MeV: 6 hours
 cutoff at 85 MeV: 12 hours
 cutoff at 95 MeV: 20 hours
- Devoted to the monopole modes due to soft incompressibility



Benchmark

• SLy4+volume pairing and surface pairing (100Zr)





Benchmark

- Tests on Cutoff and box sizes
- Spurious modes <= 2 MeV
- Large box is essential





Mg isotopes and soft modes

- Soft mode 4 MeV close to threshold enhanced due to surface pair
- Novel mode 9 MeV novel according to systematics weak in SkM* calculations





Mg isotopes and soft modes

• Earlier calculations by K. Yoshida: SkM*+mixed pairing, 2009





Collectivity and mechanism

- 4 MeV res. collectivity increase
- 1/2⁻ states most important (also for halo)
- Non-resonant continuum (around 2 MeV) pairing halo vibrations

 9 MeV res. is collective no direct relation to cont.
 Most likely pygmy monopole



For experimental detection: around zero degrees (Z.H.Yang, et al., PRL, 2014)



Summary

- Coordinate-space HFB has a very good opportunity to explore new exotic structures and excitations, with the development of supercomputing facilities
- Soft mode due to pairing halo vibrations and threshold continuum
- Collective mode around 8-9 MeV appears

To be done:

• 3D Continuum FAM-QRPA for multipole excitations

Thanks for your attention!

