

Annual UNEDF Meeting, MSU, 6/21/2011

Treatment of HFB Resonances

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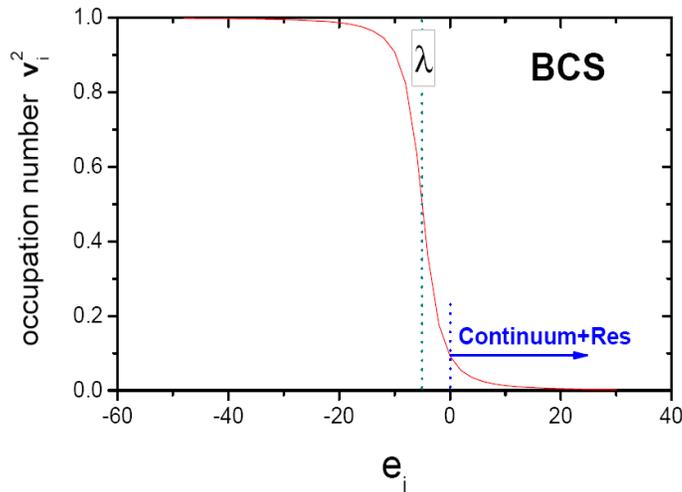
University of Tennessee

Oak Ridge National Lab

The Wavelet-based DFT solver, J. PEI

HFB Quasiparticle spectrum

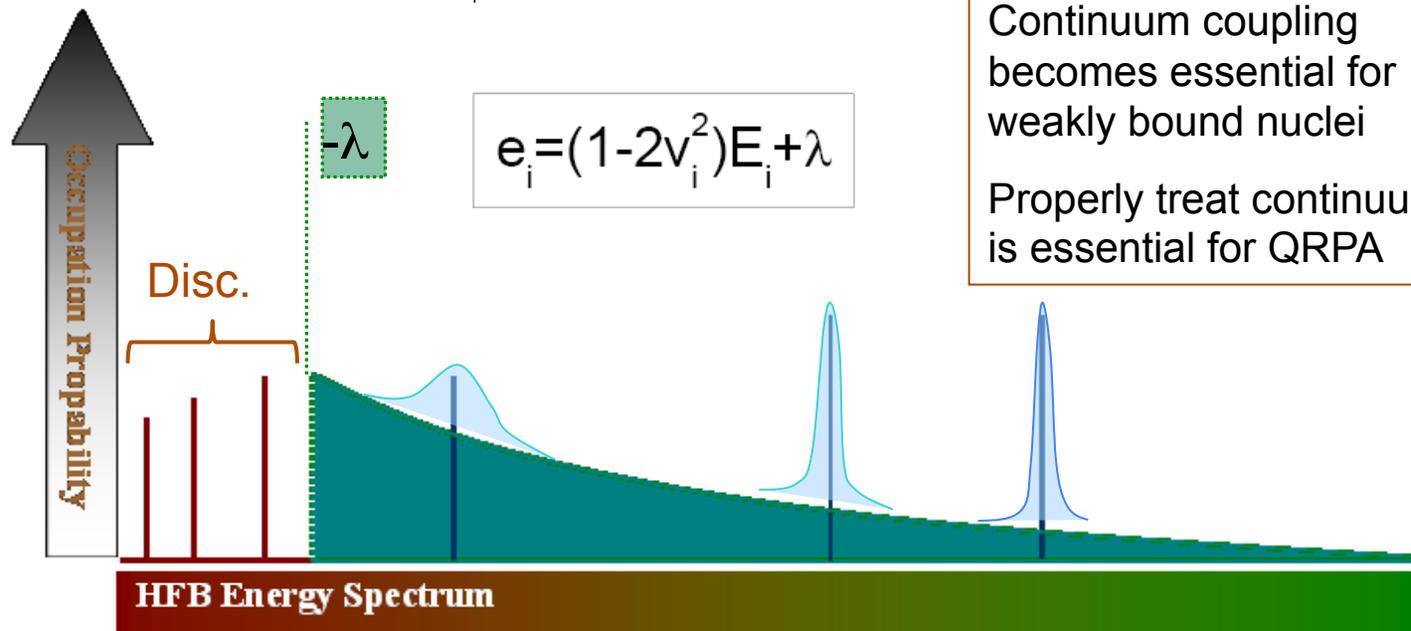
□ BCS



Occupation numbers

$$v_k^2 = \frac{1}{2} \left(1 - \frac{\tilde{\epsilon}_k}{\sqrt{\tilde{\epsilon}_k^2 + \Delta_k^2}} \right)$$

□ HFB



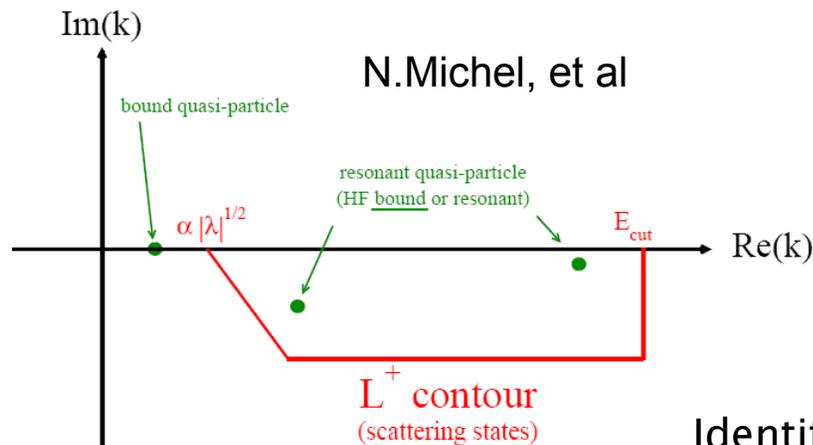
HFB deep-hole states become resonances

Continuum coupling becomes essential for weakly bound nuclei

Properly treat continuum is essential for QRPA

HFB Quasiparticle spectrum

- In the complex k plane



Identify resonance states that have the complex energy: $E - i\Gamma/2$ (widths); and purely scattering states are integrated over the contour.

- These resonances are observable in experiments; widths depend very much on the pairing interaction; unique in HFB theory beyond BCS description

HFB Strategy

- ❑ Diagonalization on single-particle basis
- ❑ Direct diagonalization on box lattice (e.g. B-spline)
Very expensive; so many discretized continuum states
- ❑ Madness-HFB strategy:
 - > initial HO basis
 - > Hamiltonian matrix
 - > diagonalization
 - > new eigenvalues and vectors
 - > Convolution(update basis)
 - > box boundary(mask)

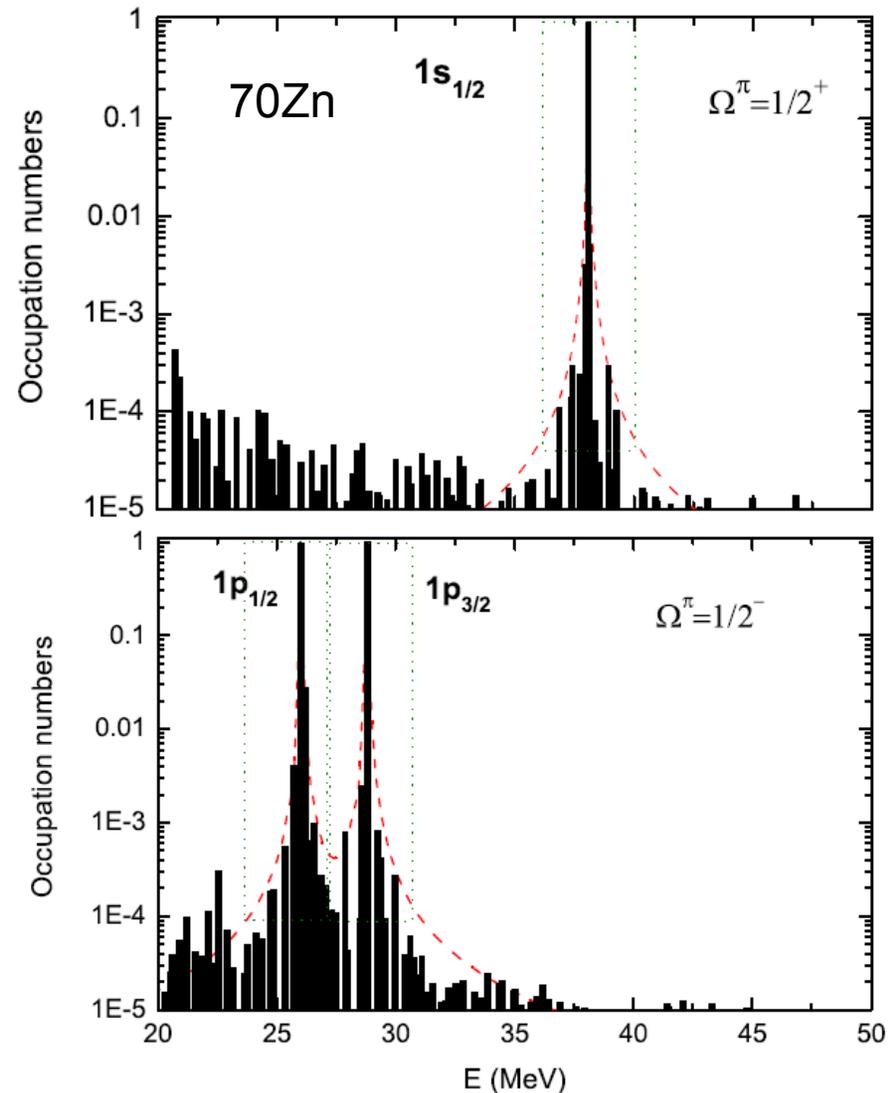
Hybrid-HFB strategy:

box solutions+deep-hole resonances+high energy continuum states

Box solutions

- ❑ In the box solution, also called L^2 discretization, the continuum is discretized into finite states, with very good accuracy compared to exact treatments.
- ❑ Even with this method the resonance widths can be calculated precisely, compared to the complex scaling method.
- ❑ HFB-AX generates very dense quasiparticle spectrum, provides a high resolution for continuum and resonance states.

For example, about 7000 states in a 40×40 fm box.



High energy continuum states

- High-energy approximation (local density approximation)

$$u(\mathbf{r}) \rightarrow u(\mathbf{p}, \mathbf{r})e^{i\hbar\phi(\mathbf{r})}, \quad v(\mathbf{r}) \rightarrow v(\mathbf{p}, \mathbf{r})e^{i\hbar\phi(\mathbf{r})}$$

- This approximation works for HFB-popov equation for Bose gas; works for Bogoliubov de Gennes equations for Fermi gas.

J. Reidl, A. Csordas, R. Graham, and P. Szepfalusy, Phys. Rev. A 59, 3816 (1999)

X.J. Liu, H. Hu, P.D. Drummond, Phys. Rev. A 76, 043605 (2007)

- We follow this approximation for Skyrme HFB.

$$\begin{aligned} \left(\frac{\hbar^2 p^2}{2M^*} + V(\mathbf{r}) - \lambda\right)u(\mathbf{p}, \mathbf{r}) + \Delta(\mathbf{r})v(\mathbf{p}, \mathbf{r}) &= \epsilon(\mathbf{p}, \mathbf{r})u(\mathbf{p}, \mathbf{r}) \\ \left(\frac{\hbar^2 p^2}{2M^*} + V(\mathbf{r}) - \lambda\right)v(\mathbf{p}, \mathbf{r}) - \Delta(\mathbf{r})u(\mathbf{p}, \mathbf{r}) &= -\epsilon(\mathbf{p}, \mathbf{r})v(\mathbf{p}, \mathbf{r}) \end{aligned}$$

$$\epsilon(\mathbf{p}, \mathbf{r}) = \sqrt{\varepsilon_{\text{HF}}^2(\mathbf{p}, \mathbf{r}) + \Delta(\mathbf{r})^2} \quad \text{quasiparticle spectrum}$$

$$\varepsilon_{\text{HF}}(\mathbf{p}, \mathbf{r}) = \frac{\hbar^2 p^2}{2M^*(\mathbf{r})} + V(\mathbf{r}) - \lambda \quad \text{HF energy}$$

Derivatives of effective mass, spin-orbit terms omitted for high energy states

Continuum to observables

$$\rho_c(\mathbf{r}) = \sum_p \left[1 - \frac{\varepsilon_{\text{HF}}}{\epsilon} \right] \Theta[\epsilon - E_c],$$

$$\rho_c(\mathbf{r}) = \frac{M^*}{2\pi^2 \hbar^2} \int_{\epsilon_c} d\epsilon \left(\frac{\epsilon}{\sqrt{\epsilon^2 - \Delta^2}} - 1 \right) \times \sqrt{\frac{2M^*}{\hbar^2} (\sqrt{\epsilon^2 - \Delta^2} - V(\mathbf{r}) + \lambda)},$$

$$\tau_c(\mathbf{r}) = \sum_p p^2 \left[1 - \frac{\varepsilon_{\text{HF}}}{\epsilon} \right] \Theta[\epsilon - E_c]$$

$$\tau_c(\mathbf{r}) = \frac{M^*}{2\pi^2 \hbar^2} \int_{\epsilon_c} d\epsilon \left(\frac{\epsilon}{\sqrt{\epsilon^2 - \Delta^2}} - 1 \right) \times \left[\frac{2M^*}{\hbar^2} (\sqrt{\epsilon^2 - \Delta^2} - V(\mathbf{r}) + \lambda) \right]^{3/2}$$

$$\tilde{\rho}_c(\mathbf{r}) = - \sum_p v_p u_p = - \sum_p \frac{\Delta}{\epsilon} \Theta[\epsilon - E_c]$$

$$\tilde{\rho}_c(\mathbf{r}) = - \frac{M^* \Delta}{2\pi^2 \hbar^2} \times \int_{\epsilon_c} d\epsilon \frac{\sqrt{\frac{2M^*}{\hbar^2} (\sqrt{\epsilon^2 - \Delta^2} - V(\mathbf{r}) + \lambda)}}{\sqrt{\epsilon^2 - \Delta^2}}$$

Transform from the p -representations to the integral in terms of energy

Continuum to observables

□ Contributions from 40 to 60 MeV

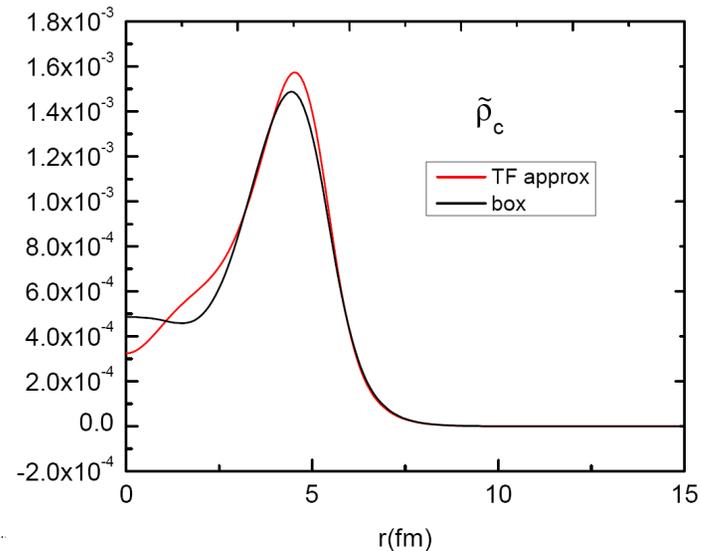
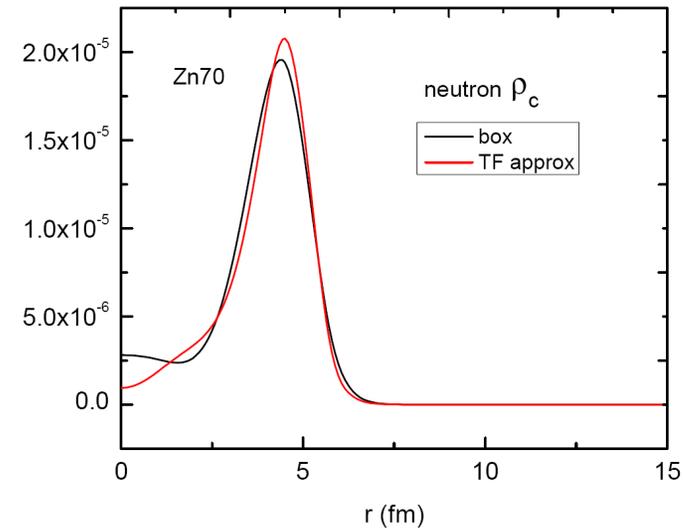
- Local density approximation
- Box solution from HFB-AX

What we see:

Generally the two methods agrees with each other;

The distributions are very similar for the three kind of densities, and this depends on the pairing potential;

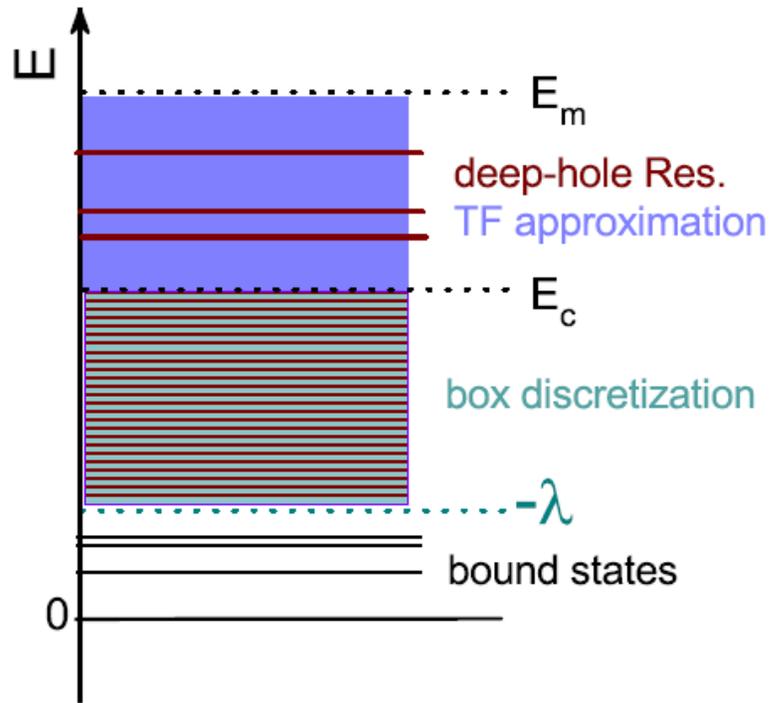
Continuum significantly impacts the pp channel.



Hybrid HFB

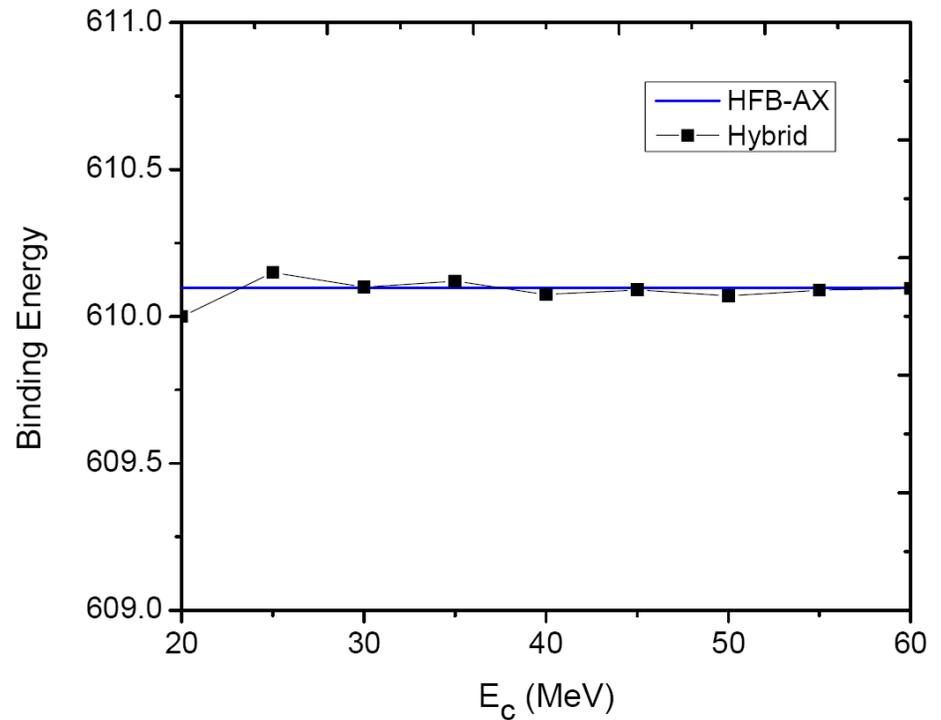
Test the local-density approximation

Assume the continuum coupling is very weak for deep-hole states



$$\rho(\mathbf{r}) = \sum_{\substack{E_i < E_c \\ E_i > 0}} 2|v_i|^2 + \sum_{\text{deep-hole}} 2|v_i|^2 + \rho_c(\mathbf{r}).$$

Test for Zn70 neutrons



Similar to pairing regularization method

HFB resonances

General formulas for resonance widths:

□ Continuum level density

$$\Delta(E) = \text{Tr}[\delta(E - H) - \delta(E - \underbrace{H_0}_{\uparrow})]$$

Hamilton without interaction

With the Green function method:

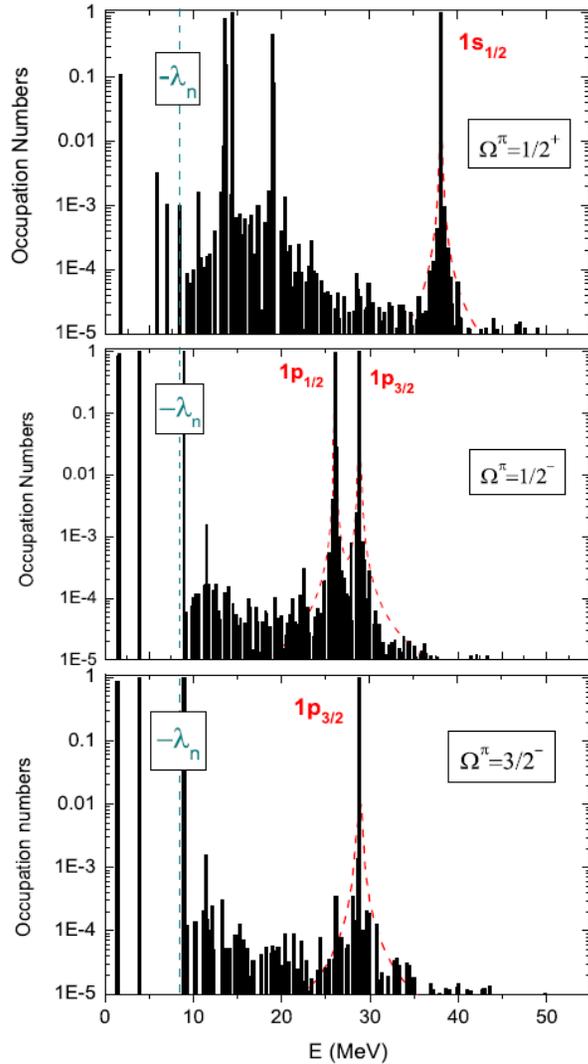
$$\Delta_l(E) = -\frac{1}{\pi} \text{Im}\{\text{Tr}[\hat{G}_l(E + i0) - \hat{G}_l^0(E + i0)]\}$$

Breit-Wigner shape for resonances

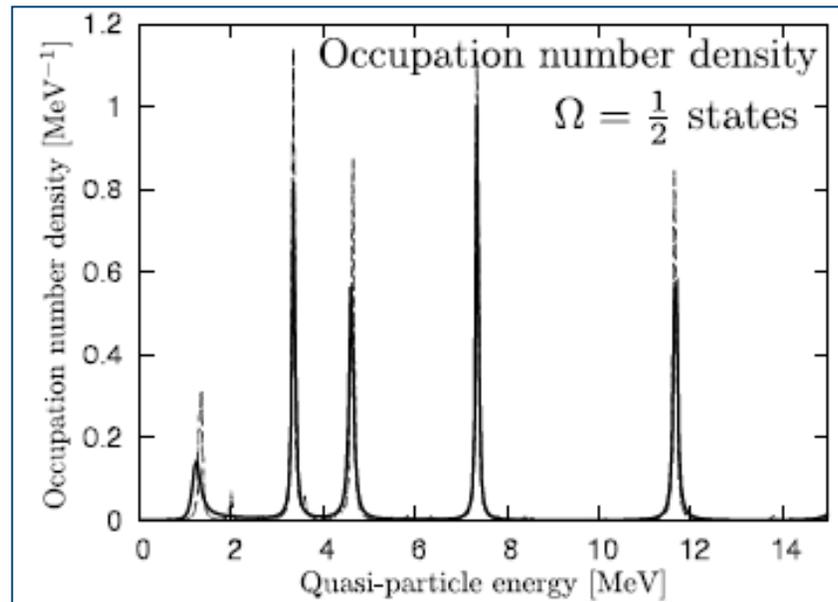
$$\Delta_l^r(E, E_r, \Gamma_r) = \frac{1}{\pi} \frac{\Gamma_r/2}{(E - E_r)^2 + \Gamma_r^2/4}$$

Smoothing-Fitting method

Occupation probability and continuum level density



$$n(E) = \frac{1}{\pi} \text{Im} \sum_{\sigma} \int dr G_{11}(r\sigma, r\sigma, -E - i\epsilon)$$



H. Oba, M. Matsuo, PRC 80, 02430, 2009

Occupation probability is related to the continuum level density, which corresponds to the Breit-Wigner shape

Smoothing-fitting method

□ Straightforward smoothing-fitting method to extract the widths

{ Strutinsky smoothing with a Lorentz function } Then we do fitting:

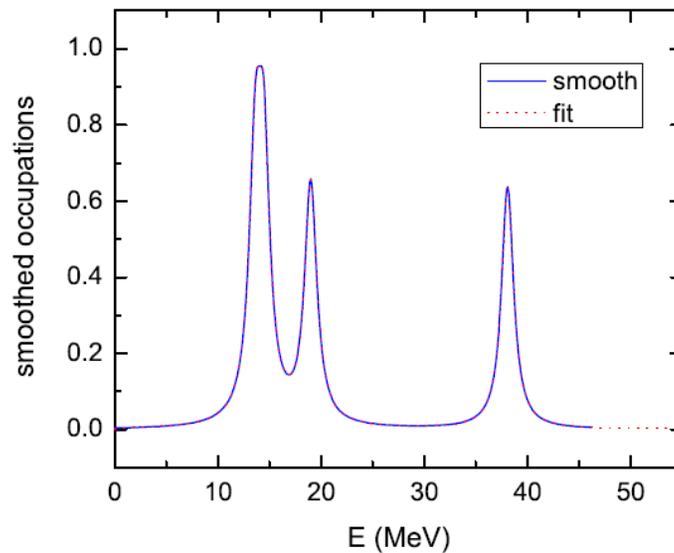
$$\overline{v^2}(E) = \sum_i \frac{v_i^2}{\Gamma} w\left(\frac{E - E_i}{\Gamma}\right)$$

$$\overline{v^2}(E) = v^2 \overline{v_R^2}(E) + v_b^2(E)$$

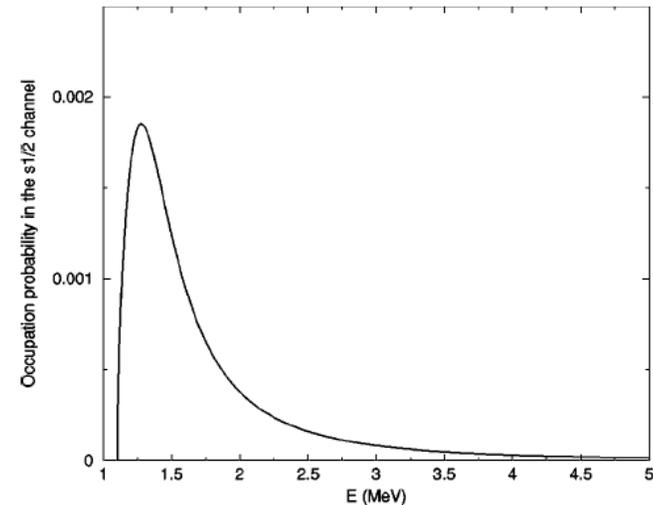
Total occupation

Smoothed B-W

A.T. Kruppa, K. Arai, PRA 59,3556 (1999).



Advantages: Works for resonances in deformed nuclei; precision can be improved using a large box size

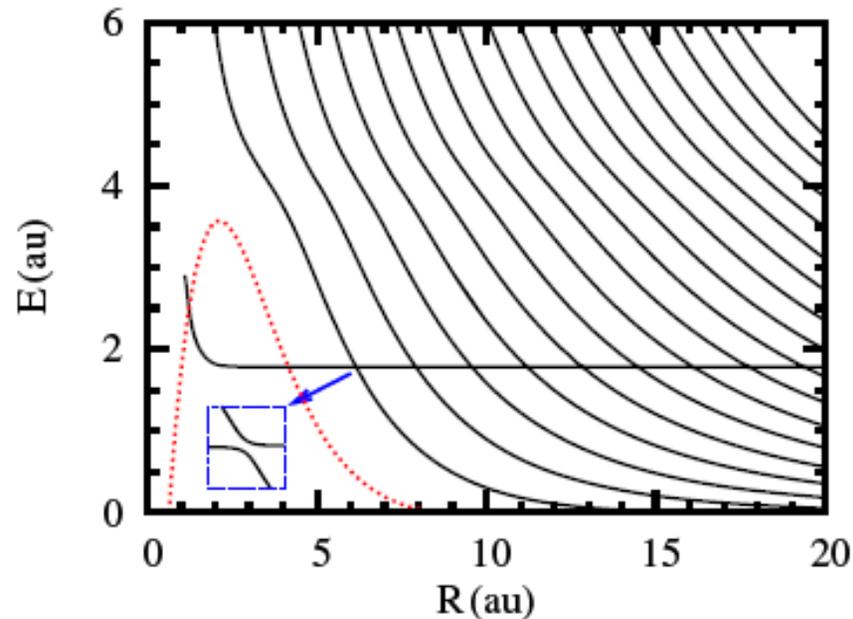


However, resonances near thresholds do not have a B-W shape

M. Grasso, PRC 64, 064321, 2001

Stabilization Method

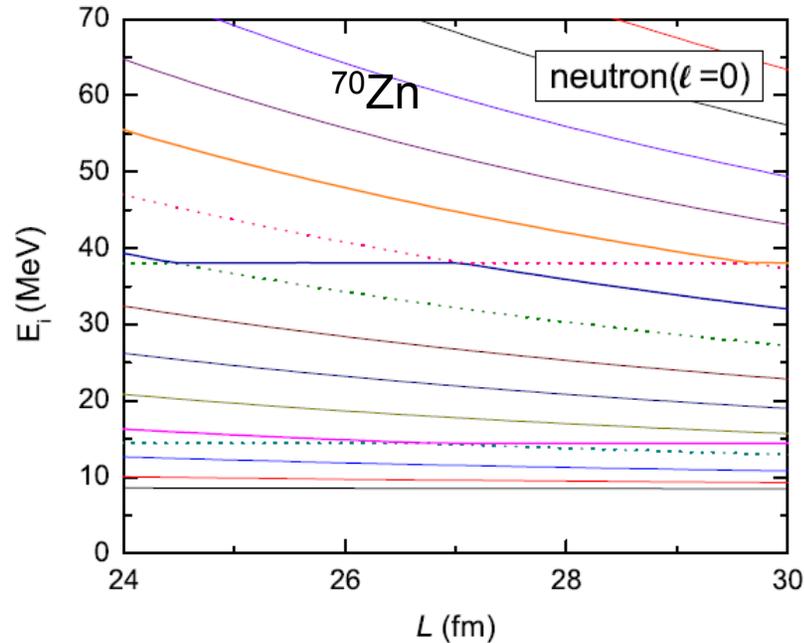
- ❑ Widely used in atomic physics
- ❑ Has been applied to single particle resonances
- ❑ 3-body resonances (A.Kruppa)
- ❑ We applied for the first time to quasiparticle resonances



S.G. Zhou, J. Meng, P. Ring, 2009

Stabilization method

- The main idea is to get resonance widths from the box-size dependence of quasiparticle energies



Spectrum got by HFBRAD solutions with different box sizes

Phase shift: $\eta(E) = \pi \int_0^E \Delta(E') dE'$

Continuum level density: $\Delta(E) = Tr[\delta(E - H) - \delta(E - H_0)]$

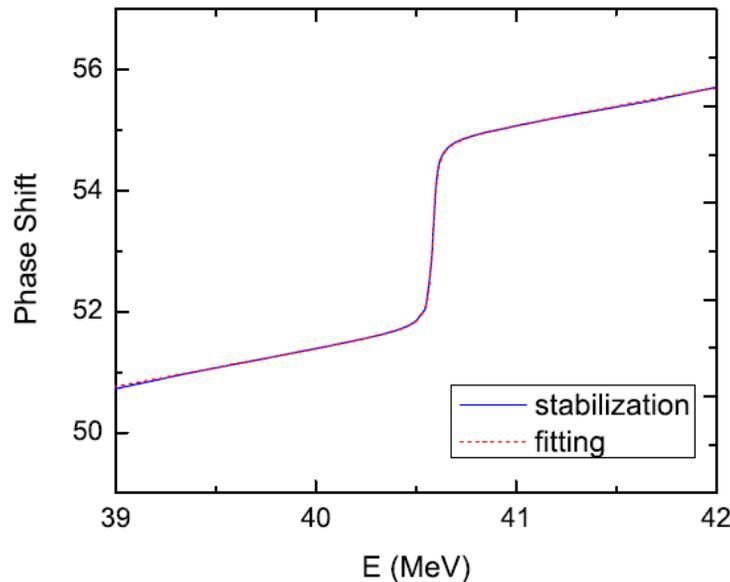
V.A. Mandelshtam, H.S. Taylor, V. Ryaboy and N. Moiseyev, PRA 50, 2764 (1994)

Stabilization method

- Calculate the phase shift

$$L = L_0 + \Delta L, \quad \Delta L = (M - 1)\delta L$$

$$\eta(E) = \pi N(E) + \frac{\pi}{\Delta L} \sum_j (L_0 + \Delta L - L_j(E))$$

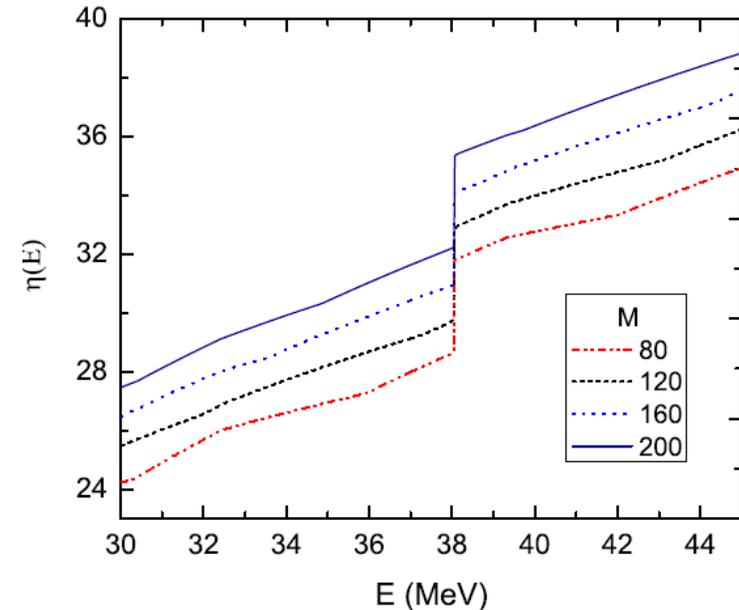


- Fitting with resonance phase shift and background

$$\varphi(E) = \arctan\left(\frac{2(E - E_r)}{\Gamma_r}\right) + \varphi_b(E)$$

Precision depends on two things:

The step size and the step numbers M



$$\delta L \rightarrow 0 \quad \text{and} \quad \Delta L \rightarrow \infty$$

In principle, we can get very accurate results, but it can be expensive

Fermi Golden rule

- Assume the pairing coupling can be treated perturbatively

$$\Gamma = 2\pi | \langle u_{0E} | \Delta(r) | \psi_0 \rangle |^2$$

$$\left[\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right] \frac{\psi_0(r)}{r} Y_{lm} = (-E + \lambda) \frac{\psi_0(r)}{r} Y_{lm}$$

$$\left[\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right] \frac{u_{0E}(r)}{r} Y_{lm} = (E + \lambda) \frac{u_{0E}(r)}{r} Y_{lm}$$

Solve the scattering
wavefunction

$$u_{0E} = \sqrt{\frac{2m}{\hbar^2 \pi k}} (\cos \delta_l F_l(\eta, kr) + \sin \delta_l G_l(\eta, kr))$$

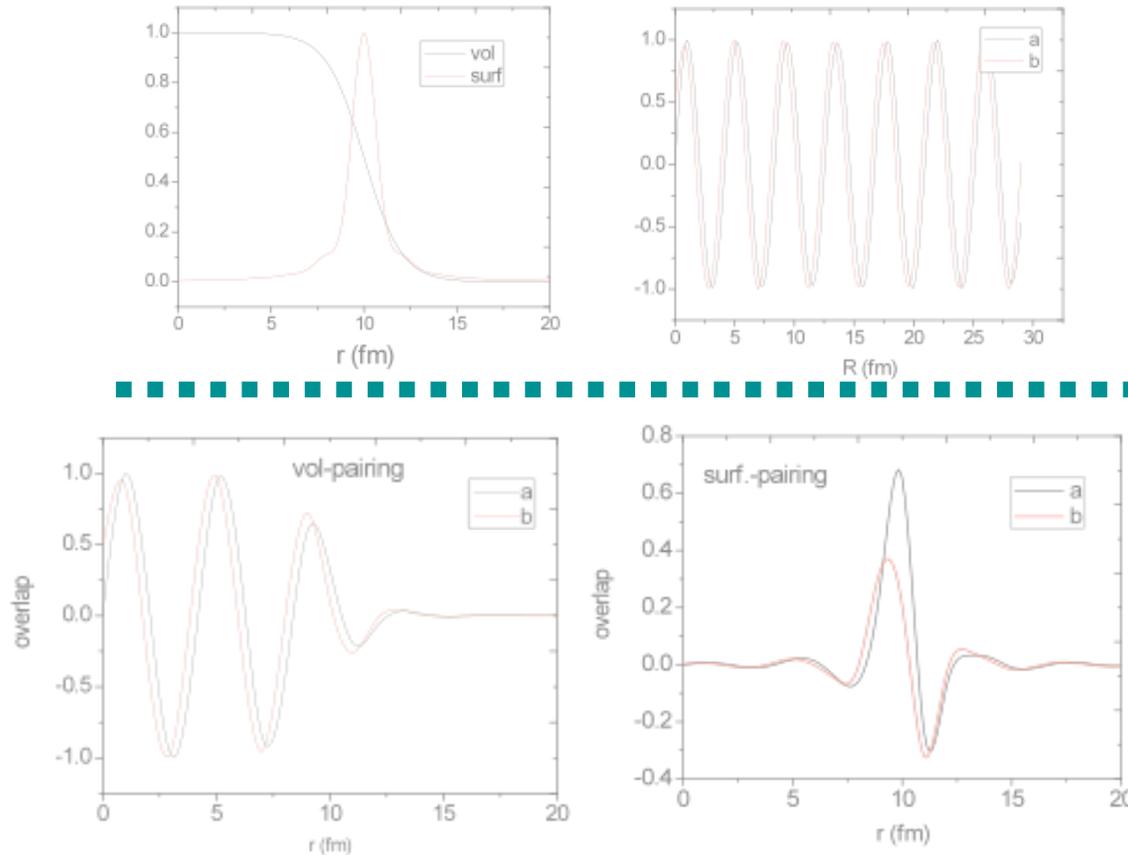
Asymptotic form at large
distances

A. Bulgac, Preprint FT-194-1980; nucl-th/9907088

However, in some calculations, the FG rule is not precise.

Inapplicability of FG rule

- With the volume and surface pairing, two scattering functions a , b



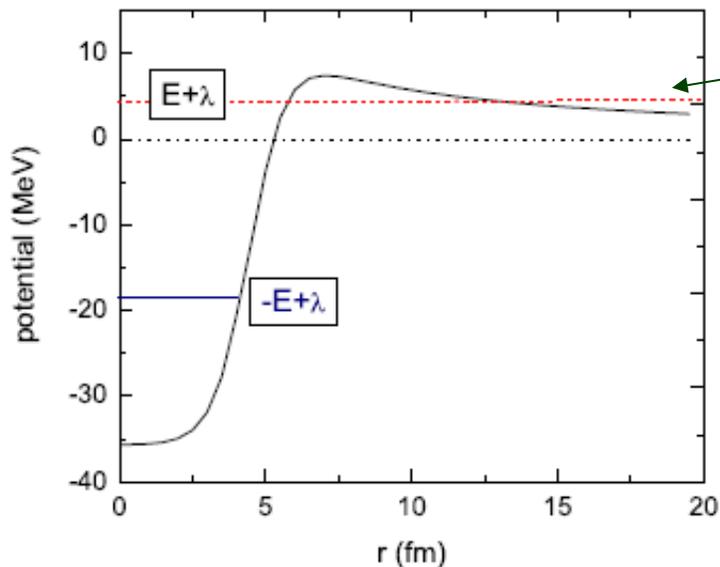
- The overlap is too sensitive to the small changes in u_{0E} to give reliable widths, in the case of surface pairing.

Width results

comparison (widths: keV)

states	Neutron				Proton			
	E	Γ_{box}	Γ_{smf}	Γ_{per}	E	Γ_{box}	Γ_{smf}	Γ_{per}
$1s_{1/2}$	38.075	1.23	0.80	0.98	35.147	0.64	0.54	0.40
$1p_{3/2}$	28.801	3.42	4.1	0.04	25.424	3.22	2.04	2.27
$1p_{1/2}$	26.043	6.01	7.0	0.19	22.851	2.04	1.57	1.26
$1d_{5/2}$	18.987	13.1	10.6	22.7	15.320	-	0.12	0.09

Special narrow reonance ($1d_{5/2}$)



Fermi-golden rule doesn't work

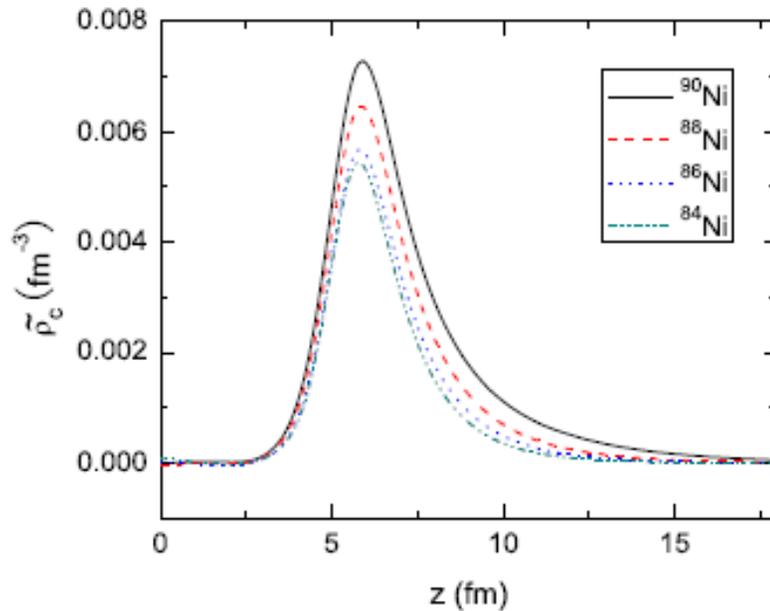
Resonance-like solution for the upper component

It is difficult for the stabilization method to calculate widths of extremely narrow resonances

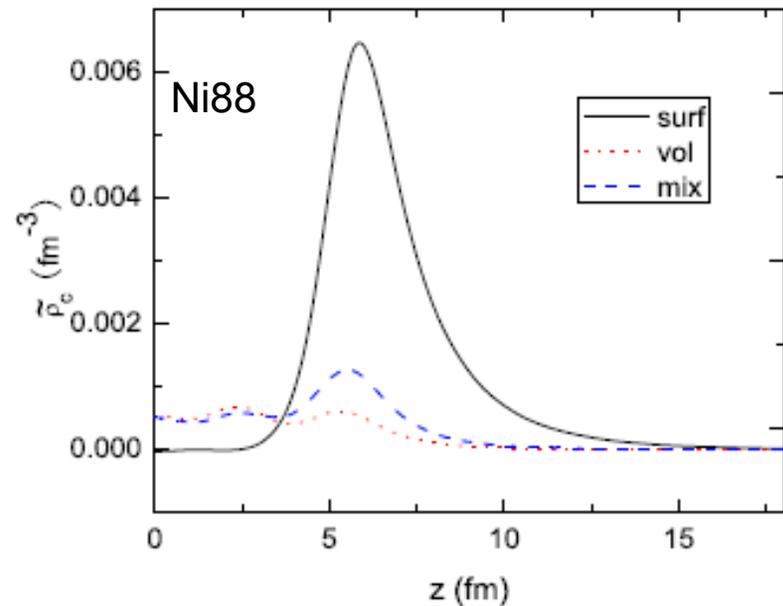
Also happens in neutron states with centrifugal barrier

Weakly-bound Ni isotopes

- continuum contribution from 30 to 60 MeV



Continuum contribution increases as nuclei close to the drip line



Continuum contribution depends very much on the pairing interaction

Weakly-bound Ni isotopes

□ Resonance widths (keV) of ^{90}Ni

states	E_r	Γ_{bcox}	Γ_{smf}	$\Gamma_{GA}[12]$
$1s_{1/2}$	51.419	-	1.1e-3	1.09e-3
$1p_{3/2}$	40.588	30.84	20.17	27.28
$1p_{1/2}$	38.770	32.26	34.67	27.14
$1d_{5/2}$	29.039	1.31	1.37	0.78
$1d_{3/2}$	25.017	25.44	23.08	22.57
$2s_{1/2}$	24.319	50.36	40.87	46.00
$1f_{7/2}$	17.554	401.79	413.04	397.37
$2p_{3/2}$	12.538	499.98	471.22	490.56
$1f_{5/2}$	10.981	672.44	651.12	645.64
$2p_{1/2}$	10.816	440.76	376.19	404.30
$1g_{9/2}$	6.519	1.56	0.52	0.81
$2d_{5/2}$	3.270	221.08	105.17	194.18
$2d_{3/2}$	2.310	611.50	643.88	560.61
$1g_{7/2}$	3.348	69.09	75.13	63.61
$1h_{11/2}$	5.527	162.46	173.66	131.78

□ For example, $1p_{3/2}$ in Ni isotopes: 25.9 keV ($N=58$), 28.2 keV ($N=60$), 30.8 keV ($N=62$)

Widths increase as nuclei close to the drip line

Summary

- local-density approximation:

Works for high energy continuum states. Hybrid HFB strategy can greatly reduce computational costs; will be very useful for optimizing Madness-HFB. It also demonstrates that box solutions have very good precision, and can be used for continuum-QRPA.

- Stabilization method:

Produce reliable widths except for very narrow resonances, slightly overestimate the widths by 10%. Provides an alternative way to study continuum and resonances without solving the scattering wavefunctions

- Drip-line isotopes:

HFB resonance widths are increasing as nuclei close to drip-lines, which is consistent with that high-energy continuum contributions are also increasing.

**Thanks for your
attention!**