Methods to deal with an effective pairing in the continuum: real and complex energy representations

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FRIB-Theory Alliance workshop
"From bound states to the continuum: Connecting bound state calculations with scattering and reaction theory"

11-22 June 2018

Goal:

Study the many-body properties in open shell nuclei with Fermi level close to the continuum threshold or embedded in it

Outline

- **About representation**
  - Single particle representation
  - Single particle level density
  - Single particle complex energy
- **Model interaction:** pairing
- **Model solutions**
  - Richardson (Exact)
  - Bardeen-Cooper-Schrieffer (BCS)
  - Lipkin-Nogami (LN)
- **Applications:** open shell nuclei (constant pairing)

ABOUT RESONANCES

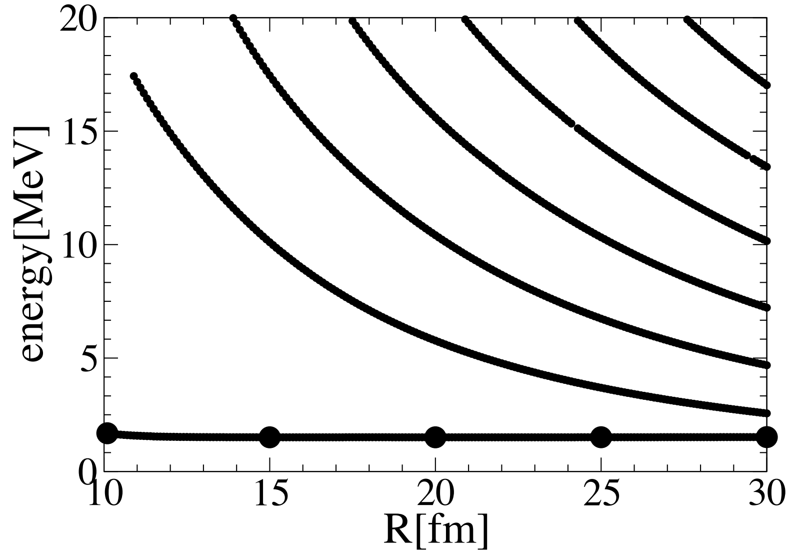
- Signature in box representation

- Signature in real energy representation

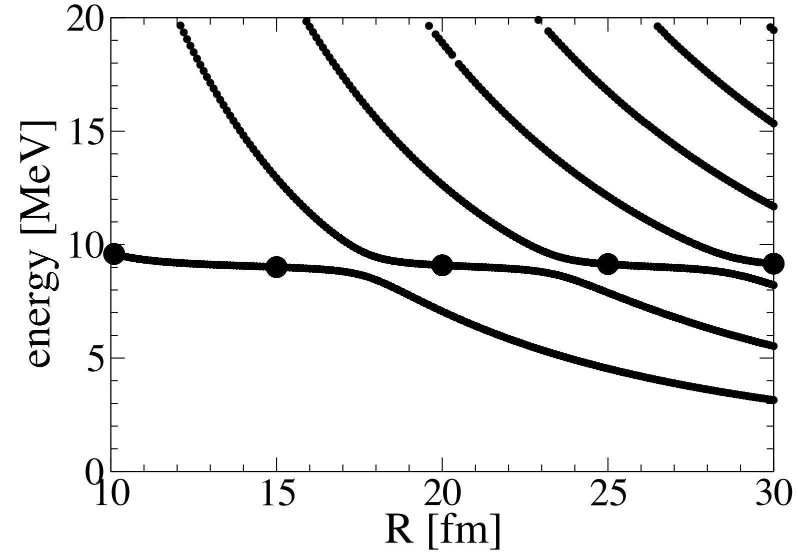
- Signature in complex energy representation

- Resonances as basis states

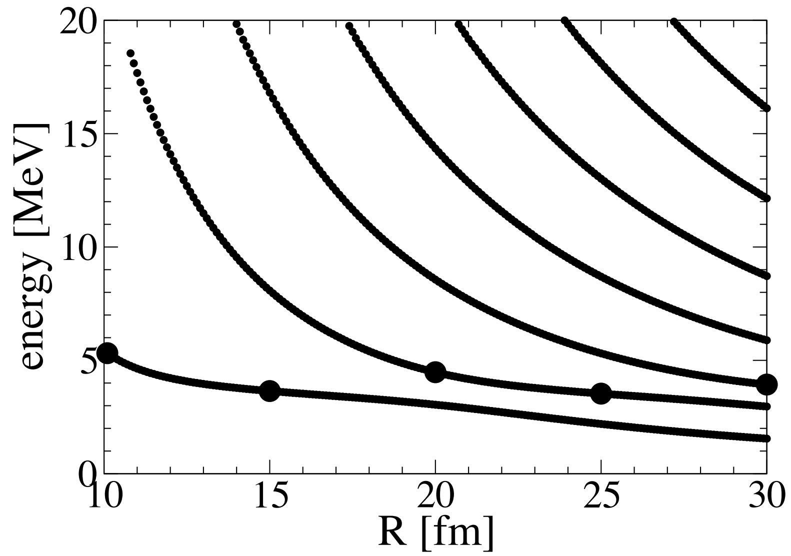
Signature of resonances in the box representation



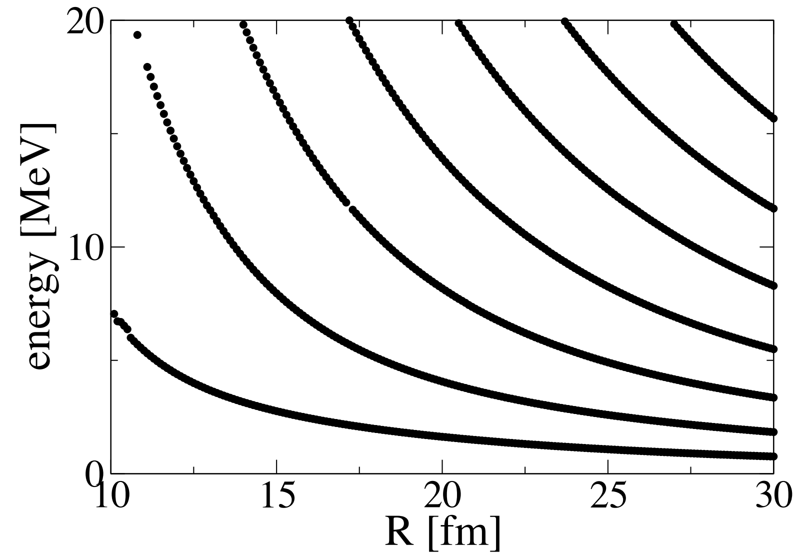
$\epsilon = 1.452 - i\, -0.225 \times 10^{-4}$ MeV



$\epsilon = 9.019 - i\, 0.126$ MeV

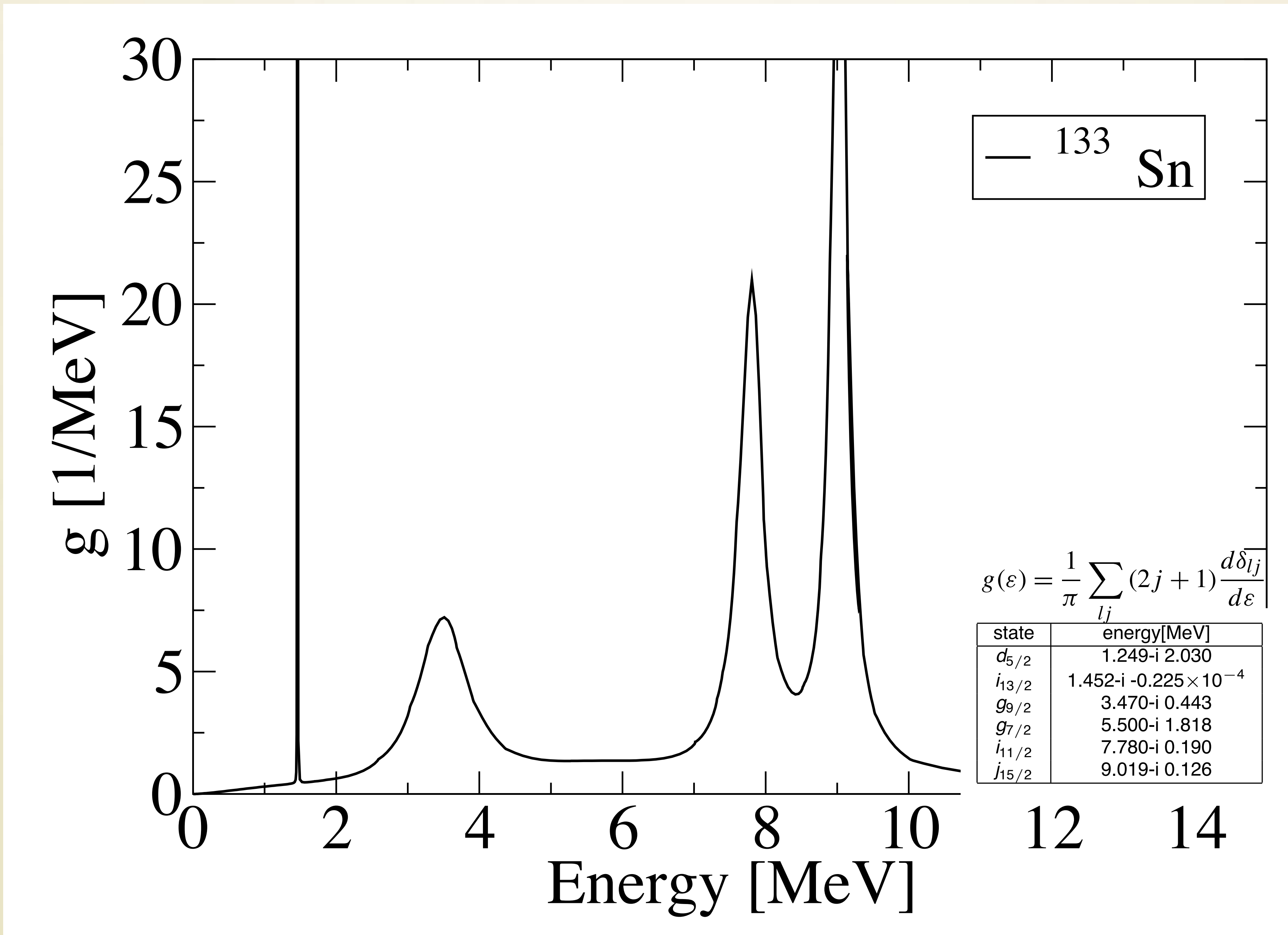


$\epsilon = 3.470 - i\, 0.443$ MeV



$\epsilon = 1.249 - i\, 2.030$ MeV

Signature of resonances in the real energy representation



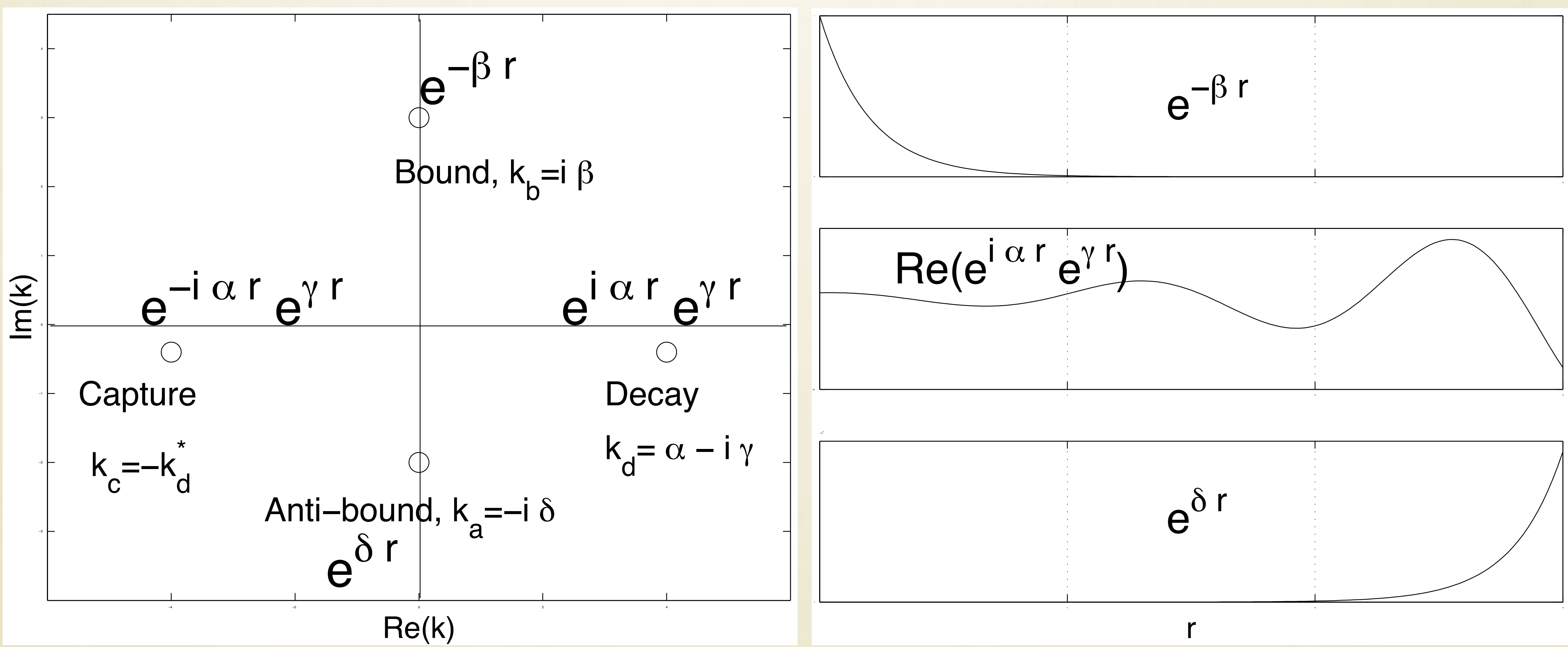
$$g(\varepsilon) = \frac{1}{\pi} \sum_{lj} (2j+1) \frac{d\delta_{lj}}{d\varepsilon}$$

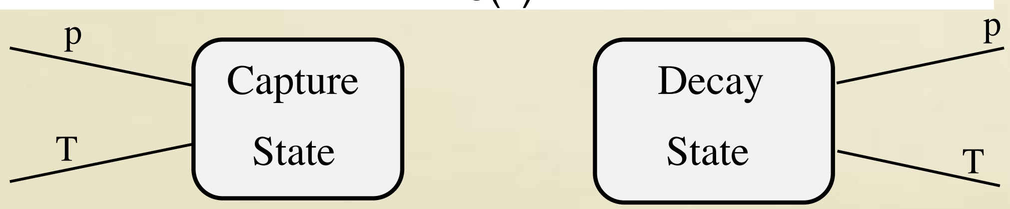
state	energy[MeV]
$d_{5/2}$	1.249-i 2.030
$i_{13/2}$	1.452-i -0.225×10^{-4}
$g_{9/2}$	3.470-i 0.443
$g_{7/2}$	5.500-i 1.818
$i_{11/2}$	7.780-i 0.190
$j_{15/2}$	9.019-i 0.126

Signature of resonances in the complex energy representation

$$\varphi_{lj}(k,r) = \frac{i}{2} k^{-(l+1)} \left[f_{lj}(-k) f_{lj}(k,r) - (-)^l f_{lj}(k) f_{lj}(-k,r) \right] \qquad f_{lj}(\pm k, r \to \infty) \longrightarrow e^{\mp ikr}\, e^{\frac{\pi}{2} l}$$

$$S_{lj}(k) = \frac{f_{lj}(k)}{f_{lj}(-k)} \qquad S_l^R(E) = e^{i2\delta_l^R(E)} = 1 - \frac{i\Gamma}{E - (E_R - i\Gamma/2)}$$

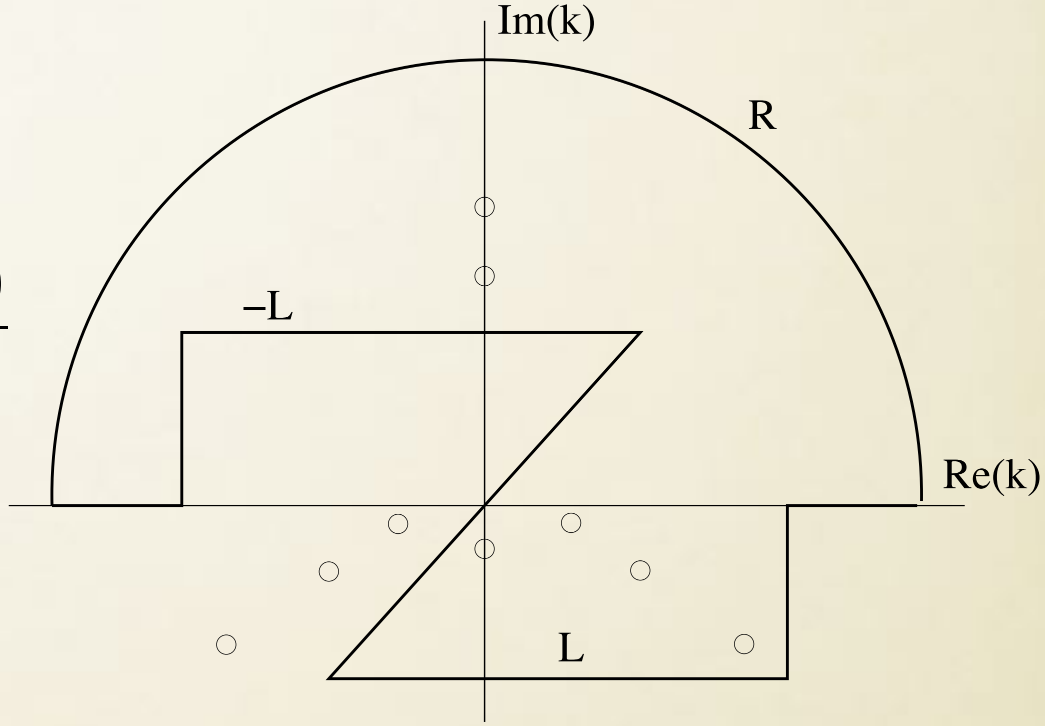




Continuum states as basis expansion

T. Berggren, Nuclear Physics A **109**, 265 (1968)

$$G_{lj}(k;r,r') = (-)^{l+1}\, k^l\, \frac{\varphi_{lj}(k,r_<)\, f_{lj}(-k,r_>)}{f_{lj}(-k)}$$



$$\delta(r-r') = \sum_{n=n_b,n_a,n_d} u_n(r)\, u_n(r') + \int_L dk\, u(k,r)\, u(k,r')$$

$$f(r) = \int f(r')\,\delta(r-r')\,dr'$$

$$f(r) = \sum_{n=n_b,n_a,n_d} c_n\, u_n(r) + \int_L c(k)\, u(k,r)\, dk$$

MODEL INTERACTION
For the
Many-body calculation in open shells

- Single particle basis

- Model interaction: pairing

- Correlations between continuum states

How to Introduce the Single Particle Basis in Many-Body Calculations

$$H = \sum_{i=1}^{A} \left[-\frac{\hbar^2}{2m_i} \right] \nabla^2_{\boldsymbol{r}_i} + \sum_{i<j=1}^{A} v(\boldsymbol{r}_i, \boldsymbol{r}_j)$$

$$H = \left\{ \sum_{i=1}^{A} \left[-\frac{\hbar^2}{2m_i} \right] \nabla^2_{\boldsymbol{r}_i} + \sum_{i=1}^{A} v(\boldsymbol{r}_i) \right\} + \left\{ \sum_{i<j=1}^{A} v(\boldsymbol{r}_i, \boldsymbol{r}_j) - \sum_{i=1}^{A} v(\boldsymbol{r}_i) \right\}$$

$$H = \sum_{i=1}^{A} h(\boldsymbol{r}_i) + V$$

$$h(\bar{r}) = -\frac{\hbar^2}{2\mu}\nabla^2 + v(r)$$

$$h(\boldsymbol{r})\phi_\alpha(\boldsymbol{r}) = \varepsilon_\alpha \phi_\alpha(\boldsymbol{r})$$

$$\delta(r - r') = \sum_{n_b, n_v, n_r} u_{nlj}(r)\, u_{nlj}(r') + \int_L dk\, u_{lj}(k, r)\, u_{lj}(k, r')$$

Computer Code: ANTI

L. Gr. Ixaru, M. Rizea, T. Vertse, Comp. Phys. Comm. **85**, 217 (1995)

Model Interaction

$$H = \sum_{am_a} \varepsilon_a c^\dagger_{am_a} c_{am_a} + \sum_{JM} \sum_{b \le a} \sum_{d \le c} \langle ab, JM | V | cd, JM \rangle A^\dagger_{JM}(ab) A_{JM}(cd)$$

$$\langle cd, JM | V | ab, JM \rangle = -\frac{G}{2} \sqrt{(2j_c + 1)(2j_a + 1)} \delta_{J0} \delta_{cd} \delta_{ab}$$

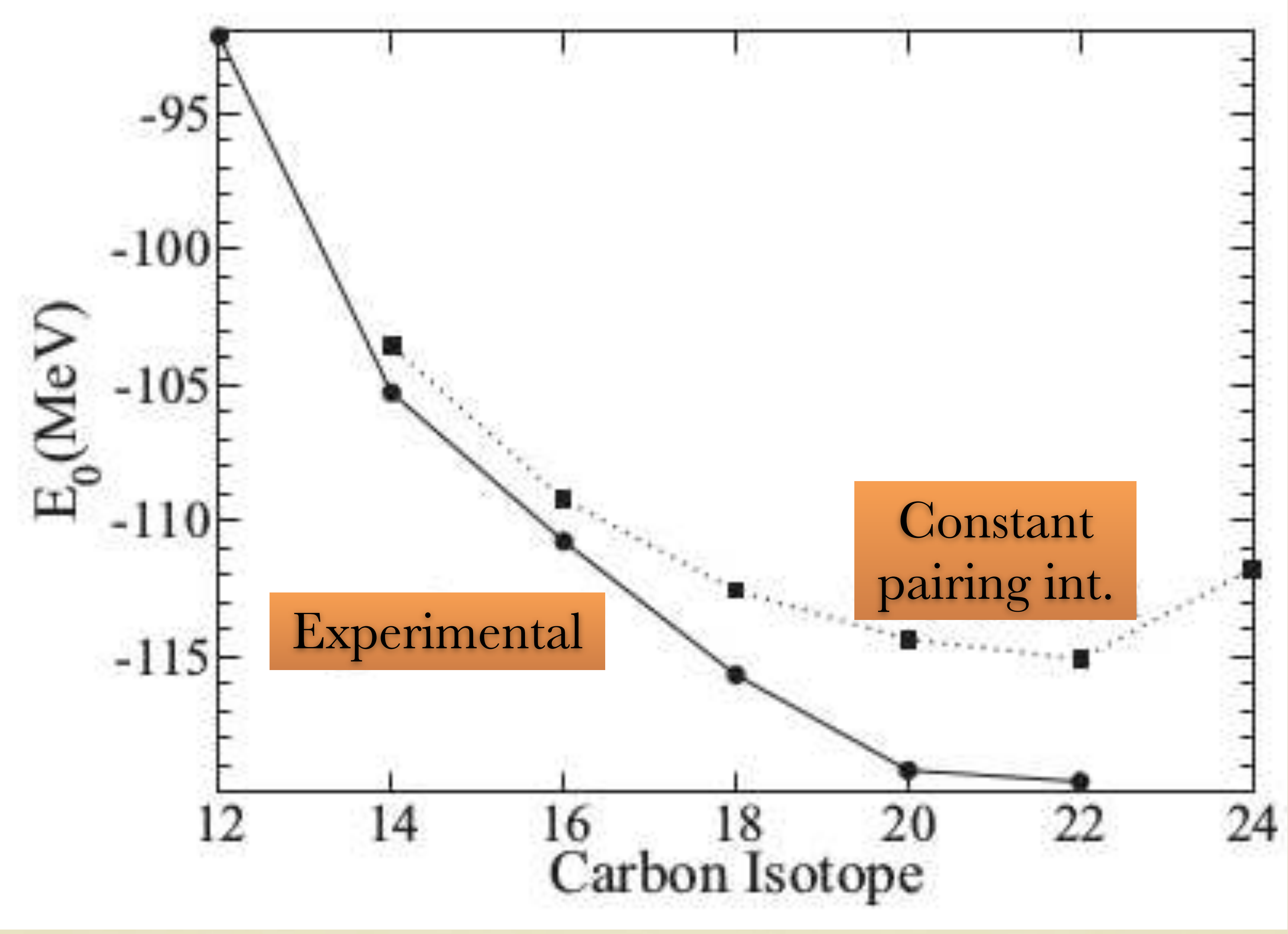
Pairing Hamiltonian

$$H = \sum_{am_a} \varepsilon_a c^\dagger_{am_a} c_{am_a} - G P^\dagger P$$

$$P^\dagger = \sum_{am_a > 0} c^\dagger_{am_a} c^\dagger_{a\bar{m}_a}$$

About the limitations of the pairing interaction

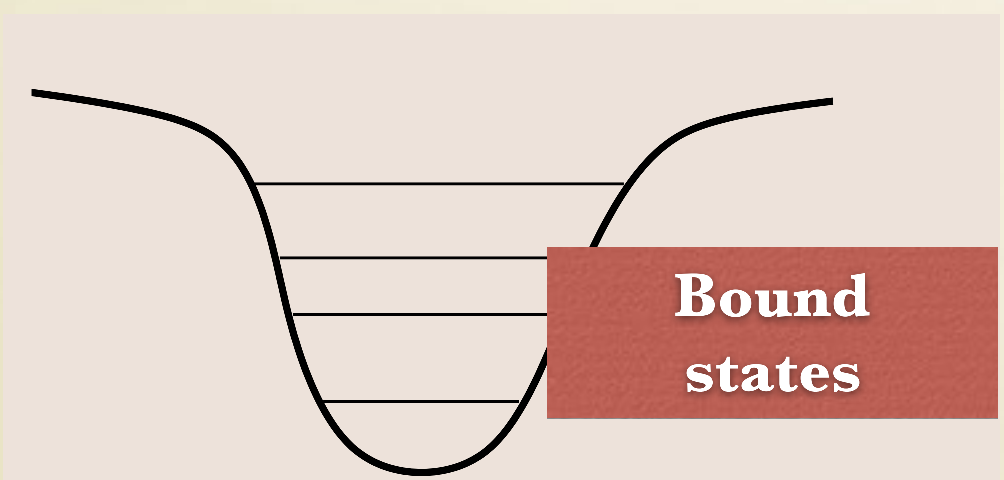
Missing correlations $\langle cd, JM | V | ab, JM \rangle$

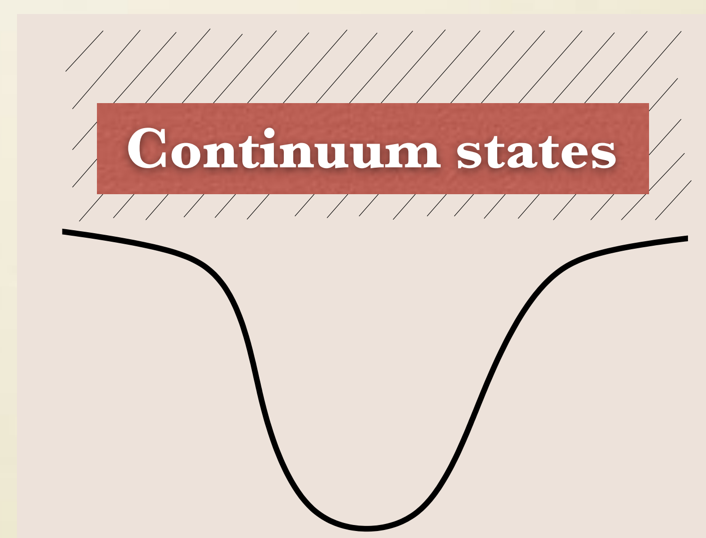


Classification of the Two Body Correlations

- Bound-Bound
- Bound-Continuum
- Continuum-Continuum

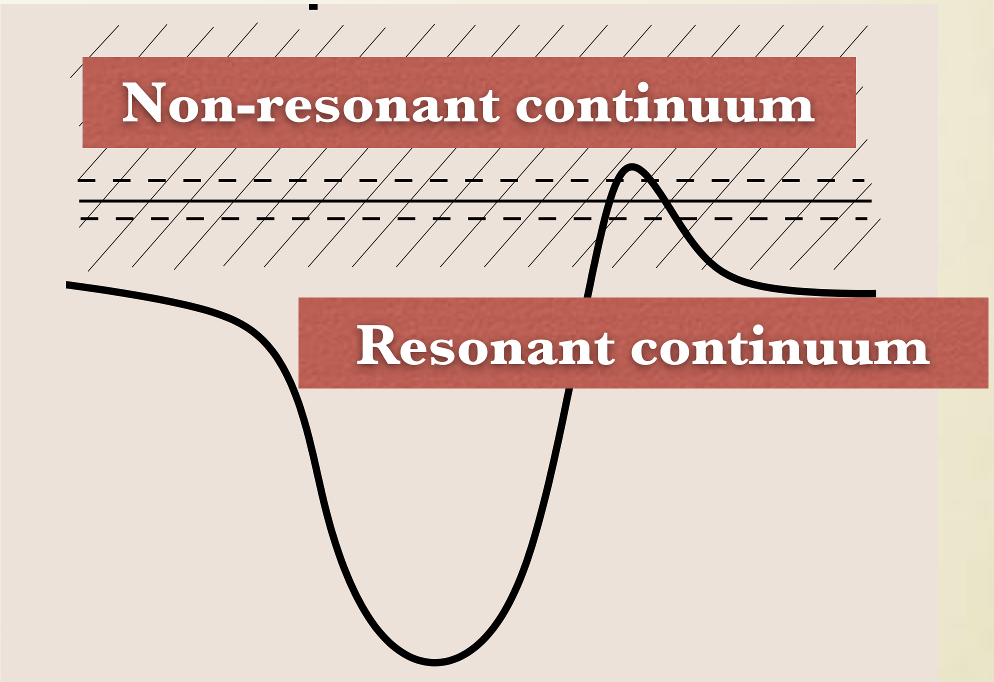
$$\langle cd, JM | V | ab, JM \rangle$$





Classification of Continuum-Continuum Correlations

CONTINUUM



- Resonant-Resonant
- Resonant-Non Resonant
- Non Resonant-Non Resonant

$$\langle cd, JM|V|ab, JM\rangle$$

CONSERVING PARTICLE NUMBER MODEL SOLUTION

Richardson

- Real energy representation
- Complex energy representation

Conserving particle number solution: Richardson

Richardson ansatz

$$|\Psi\rangle = \prod_{i=1}^{N_{pair}} \left(\sum_a \frac{P_a^\dagger}{2\varepsilon_a - E_i} \right) |0\rangle$$

$$N|\Psi\rangle = (2N_{pair})|\Psi\rangle$$

Pair creation operator

$$P_a^\dagger = \sum_{m_a>0} c_{am_a}^\dagger c_{a\bar{m}_a}^\dagger$$

Many-body eigenvalue

$$H|\Psi\rangle = E\,|\Psi\rangle$$

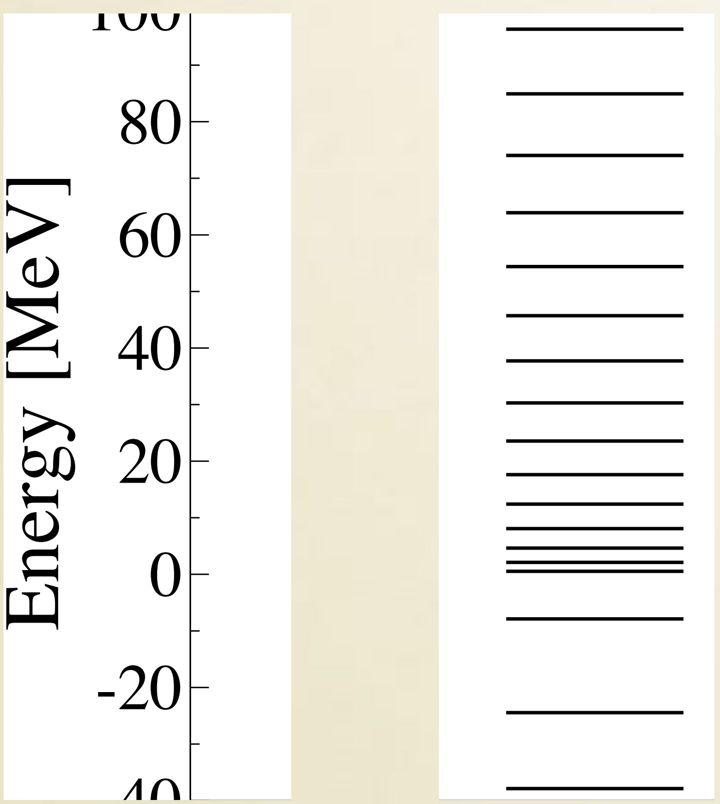
$$E = \sum_{i=1}^{N_{pair}} E_i$$

Richardson equations

$$1 - \frac{G}{2} \sum_a \frac{2j_a + 1}{2\varepsilon_a - E_i} + 2G \sum_{j\neq i}^{N_{pair}} \frac{1}{E_j - E_i} = 0$$

Conserving particle number solution: Continuum spectrum

Single Particle Level Density Ansatz



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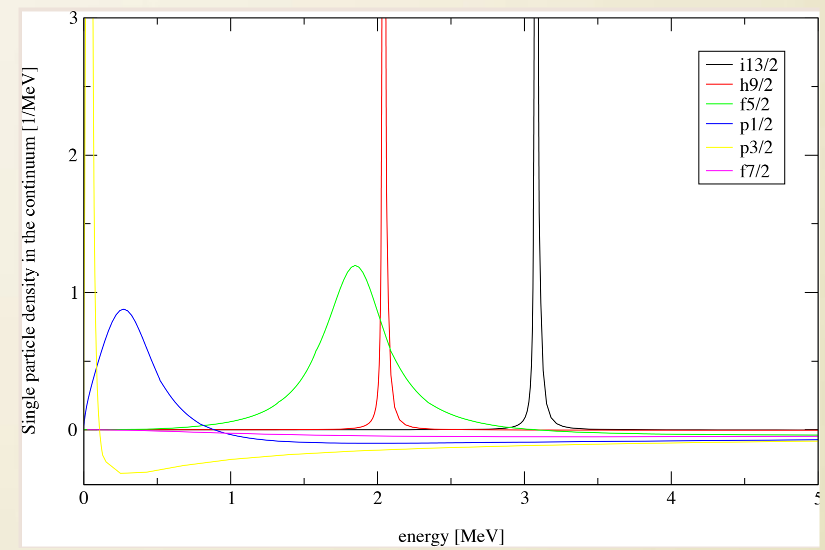


$$\lim_{R\to\infty}\left[\sqrt{\frac{\mu}{2\pi^2\hbar^2\varepsilon}}R + \frac{1}{\pi}\frac{d\delta_{lj}}{d\varepsilon}\right] - \lim_{R\to\infty}\sqrt{\frac{\mu}{2\pi^2\hbar^2\varepsilon}}R = g_{lj}(\epsilon) = \frac{1}{\pi}\frac{d\delta_{lj}}{d\epsilon}$$

$$h(r)\ u(k,r) = \epsilon\ u(k,r)$$

Conserving particle number solution: Continuum spectrum

$$\sum_n f_n \rightarrow \sum\!\!\!\!\!\!\int f = \sum_{n_b} (2j_{n_b}+1) f_{n_b} + \int_0^\infty d\varepsilon\, g(\varepsilon) f(\varepsilon)$$

Richardson equations

Effective pairing in the continuum

$$1 - \frac{1}{2}\sum_b (2j_b+1)\frac{G}{2\varepsilon_b - E_\alpha} - \frac{1}{2}\int_0^\infty d\varepsilon\, \frac{G\,g(\varepsilon)}{2\varepsilon - E_\alpha} + 2G\sum_{\beta\neq\alpha}\frac{1}{E_\beta - E_\alpha} = 0$$

Compare with…

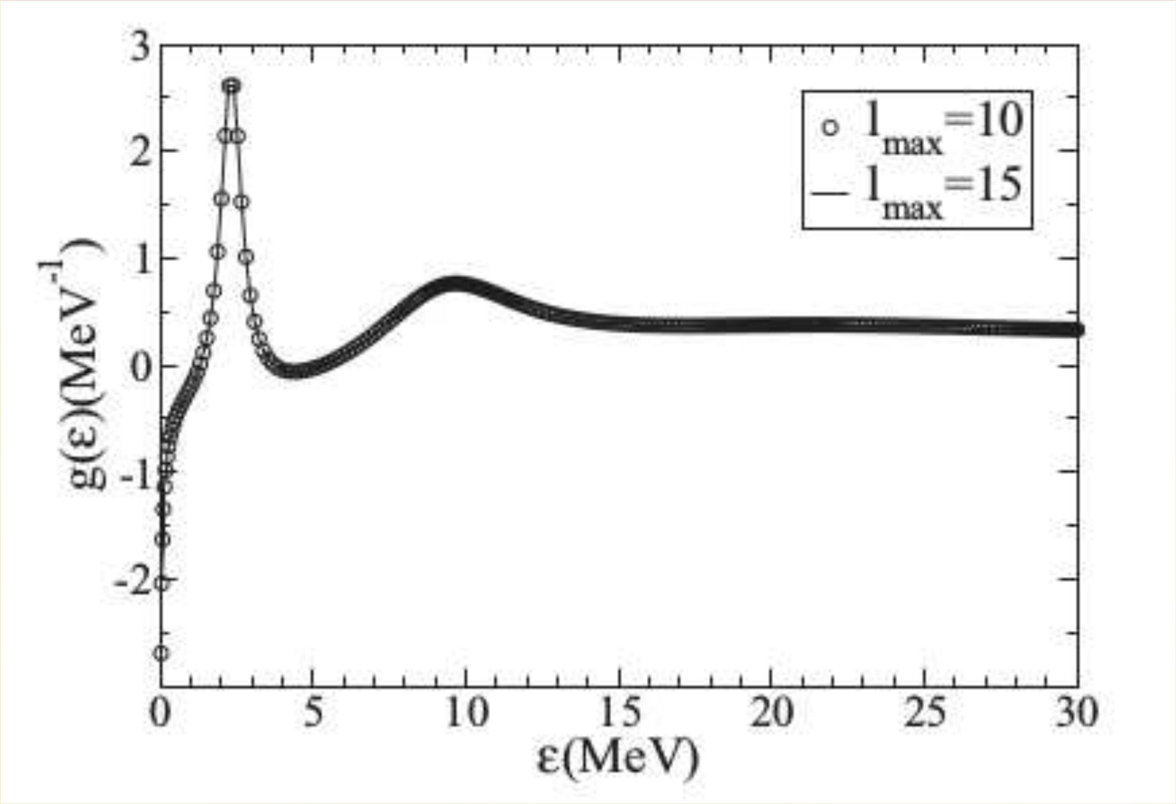
$$1 - \frac{G}{2}\sum_a \frac{2j_a+1}{2\varepsilon_a - E_i} + 2G\sum_{j\neq i}^{N_{pair}} \frac{1}{E_j - E_i} = 0$$

$$g(\varepsilon) = \frac{1}{\pi}\sum_{lj}(2j+1)\frac{d\delta_{lj}}{d\varepsilon}$$

The level density contains the resonant and non resonant continuum

Conserving particle number solution
Application: Carbon isotopes

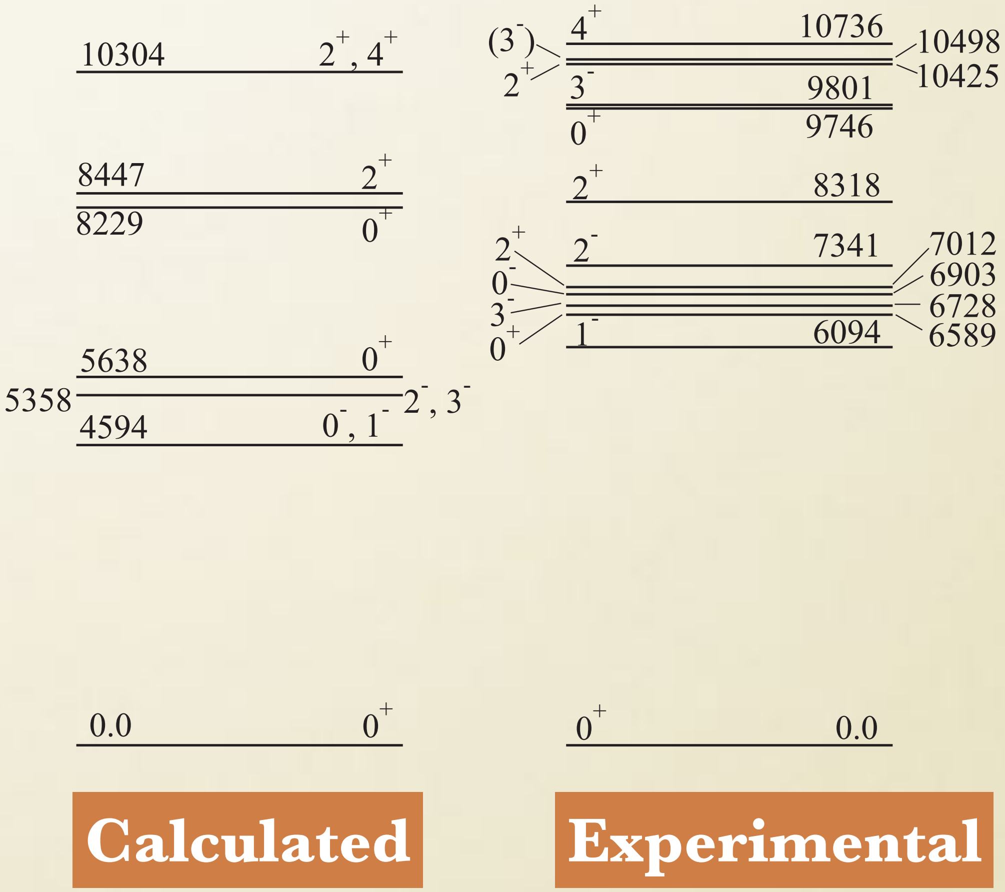
Neutron level density in ^{12}C



bound states : $0p_{1/2}$, $1s_{1/2}$, $0d_{5/2}$

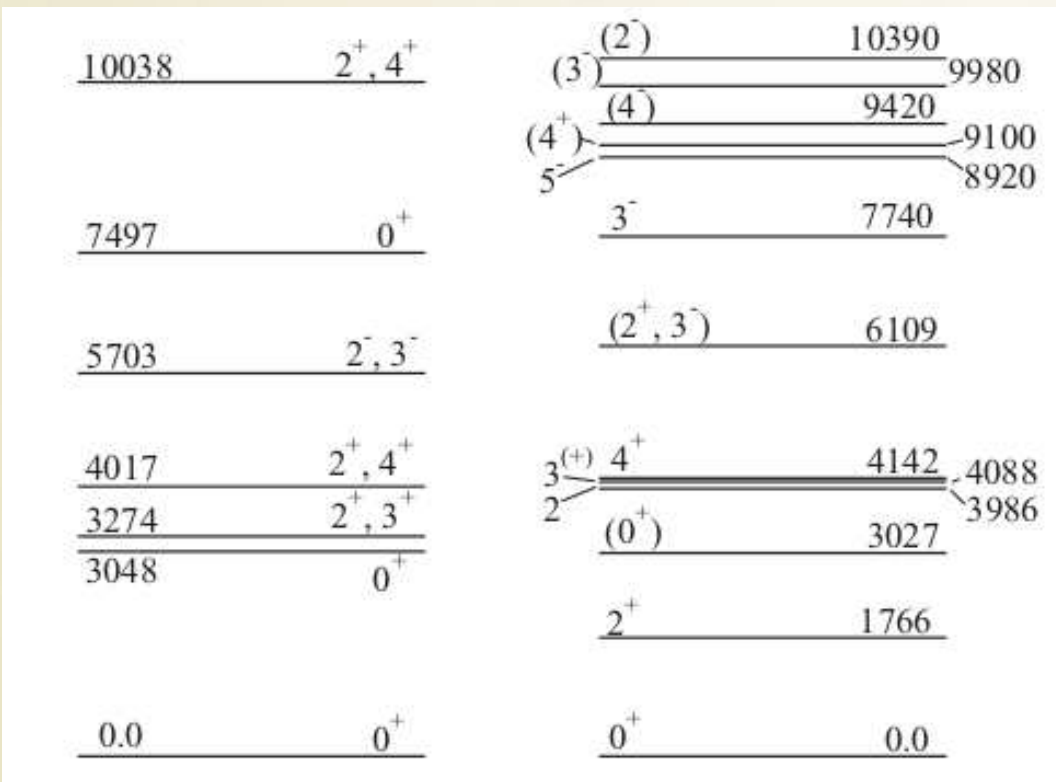
$$G = \frac{10.9}{A} MeV$$

Spectrum of ^{14}C



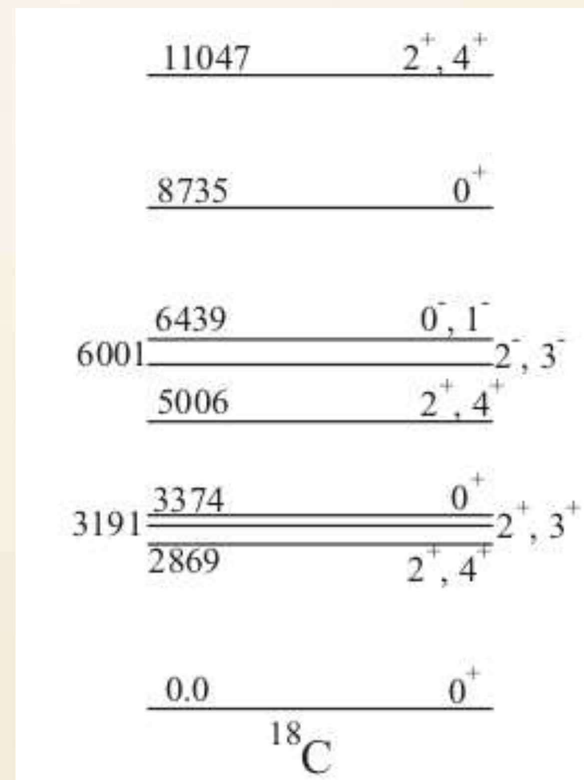
Conserving particle number solution
Application: Carbon isotopes

Spectrum of ^{16}C



Calculated **Experimental**

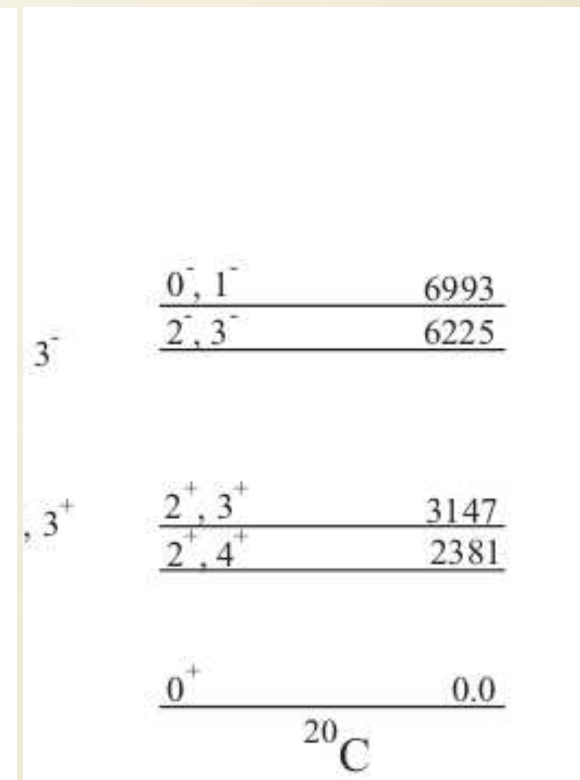
6 particles



Calculated

Exp. (2+) 1.620 MeV

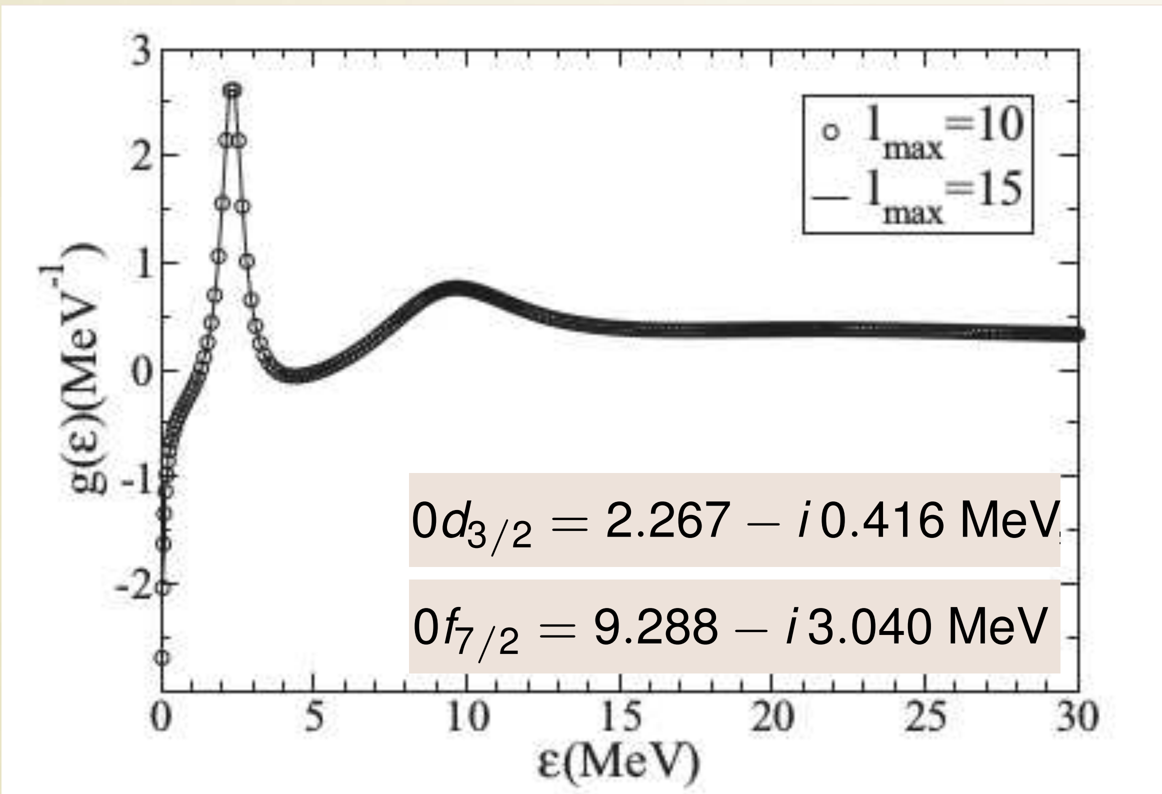
8 particles



Calculated

Conserving particle number solution in the complex energy plane

$$g(\varepsilon) = g_{Res}(\varepsilon) + g_{Bckg}(\varepsilon)$$



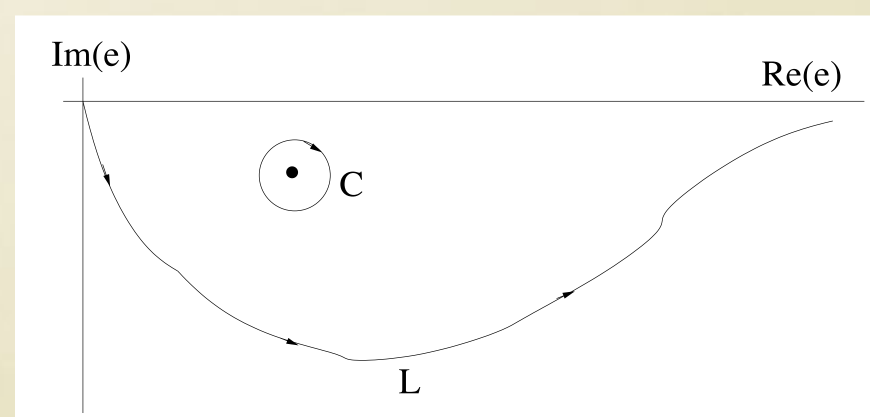
Resonant density

$$g_{Res}(\varepsilon) = \sum_r \frac{2j_r+1}{\pi}\frac{d\delta_r}{d\varepsilon} \cong \sum_r \frac{2j_r+1}{\pi}\frac{\Gamma_r/2}{(\varepsilon-\epsilon_r)^2+(\Gamma_r/2)^2}$$

Continuum part in the Richardson eq.

$$\int_0^\infty d\varepsilon\,\frac{g_{Res}(\varepsilon)}{2\varepsilon-E_k} \cong \sum_r \frac{2j_r+1}{\pi}\left[\int_0^\infty \frac{d\varepsilon}{2\varepsilon-E_k}\frac{\Gamma_r/2}{(\varepsilon-\epsilon_r)^2+(\Gamma_r/2)^2}\right]$$

Analytic deformation



Just to remember

$$1-\frac{1}{2}\sum_b(2j_b+1)\frac{G}{2\varepsilon_b-E_\alpha}-\frac{1}{2}\int_0^\infty d\varepsilon\,\frac{G\,g(\varepsilon)}{2\varepsilon-E_\alpha}+2G\sum_{\beta\neq\alpha}\frac{1}{E_\beta-E_\alpha}=0$$

Separation of resonant and non resonant contributions

Richardson equations in the complex energy plane

$$1 - \frac{G}{2}\sum_b \frac{2j_b+1}{2\varepsilon_b - E_k} - \frac{G}{2}\sum_r \frac{2j_r+1}{2\varepsilon_r - E_k}$$

$$-\frac{G}{2}\int_0^\infty g_{CxBckg}(\varepsilon)\,\frac{d\varepsilon}{2\varepsilon - iE_k} - \frac{G}{2}\int_0^\infty g_{Bckg}(\varepsilon)\,\frac{d\varepsilon}{2\varepsilon - E_k}$$

$$+2G\sum_{l\neq k}\frac{1}{E_l - E_k} = 0$$

with $\varepsilon_r = \epsilon_r - \frac{\Gamma_r}{2}$

(we change $z = -i\varepsilon$)

$$E = \sum_{i=1}^{N_{pair}} E_i$$

Before the extension into the complex plane

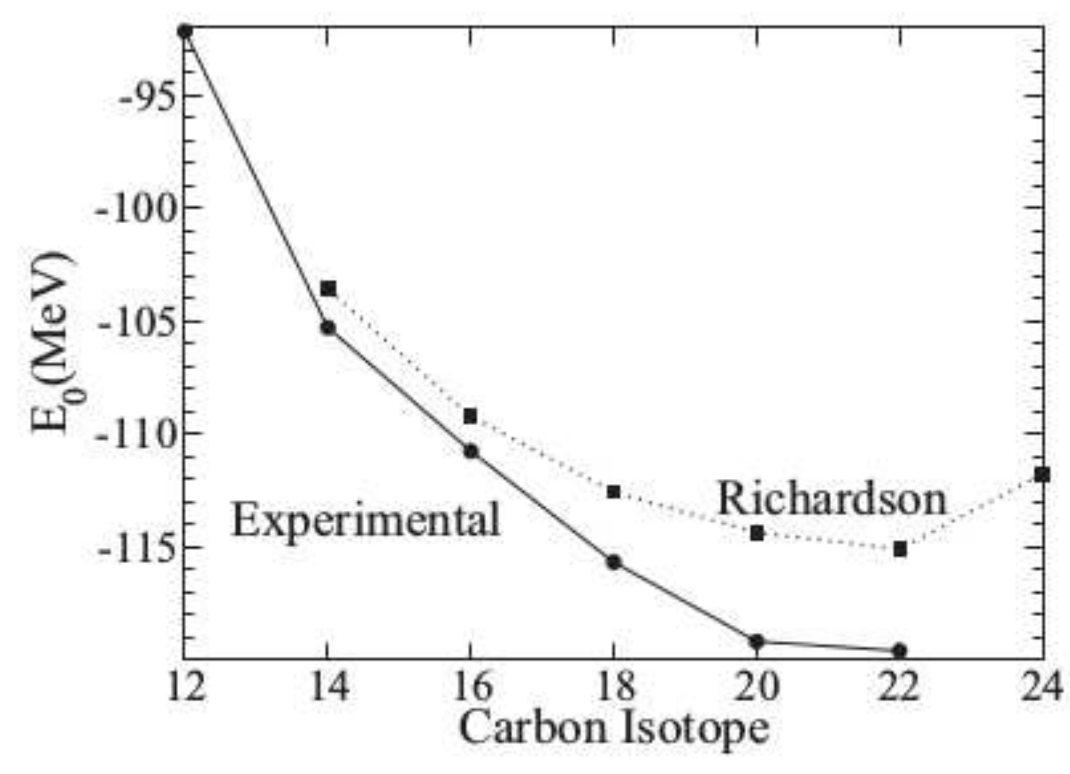
$$1 - \frac{G}{2}\sum_b \frac{(2j_b+1)}{2\varepsilon_b - E_\alpha} -$$

$$-\frac{G}{2}\int_0^\infty d\varepsilon\,\frac{g(\varepsilon)}{2\varepsilon - E_\alpha}$$

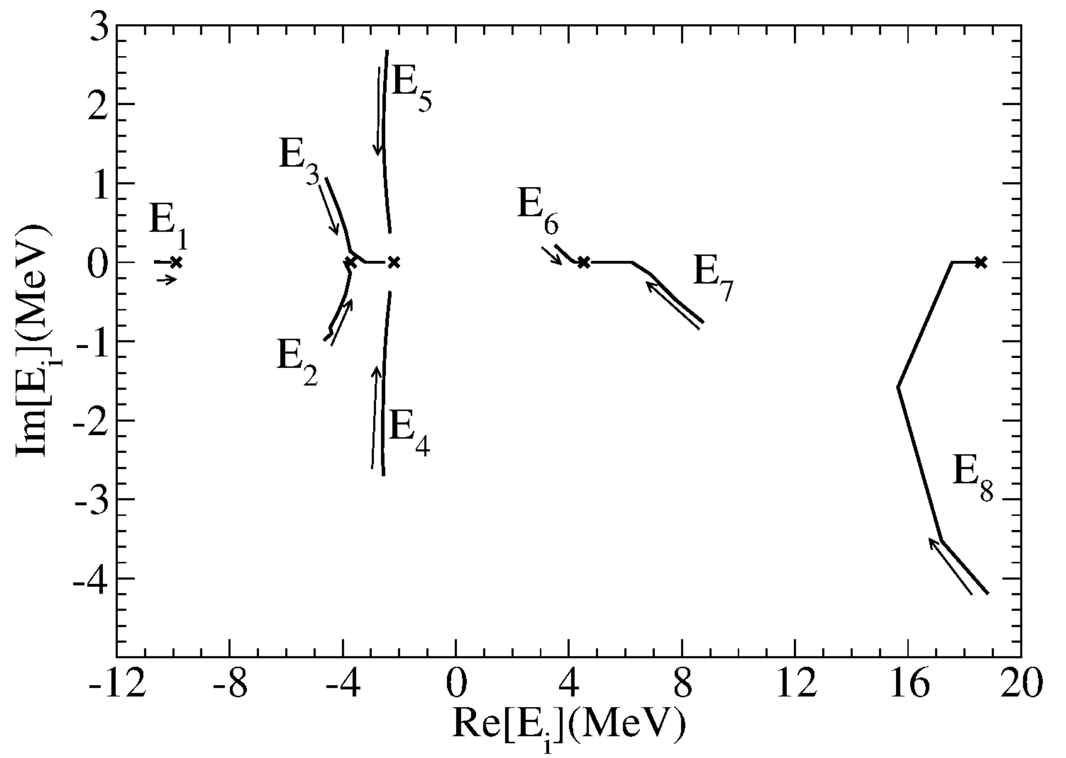
$$+2G\sum_{\beta\neq\alpha}\frac{1}{E_\beta - E_\alpha} = 0$$

Going beyond the drip line

Drip line

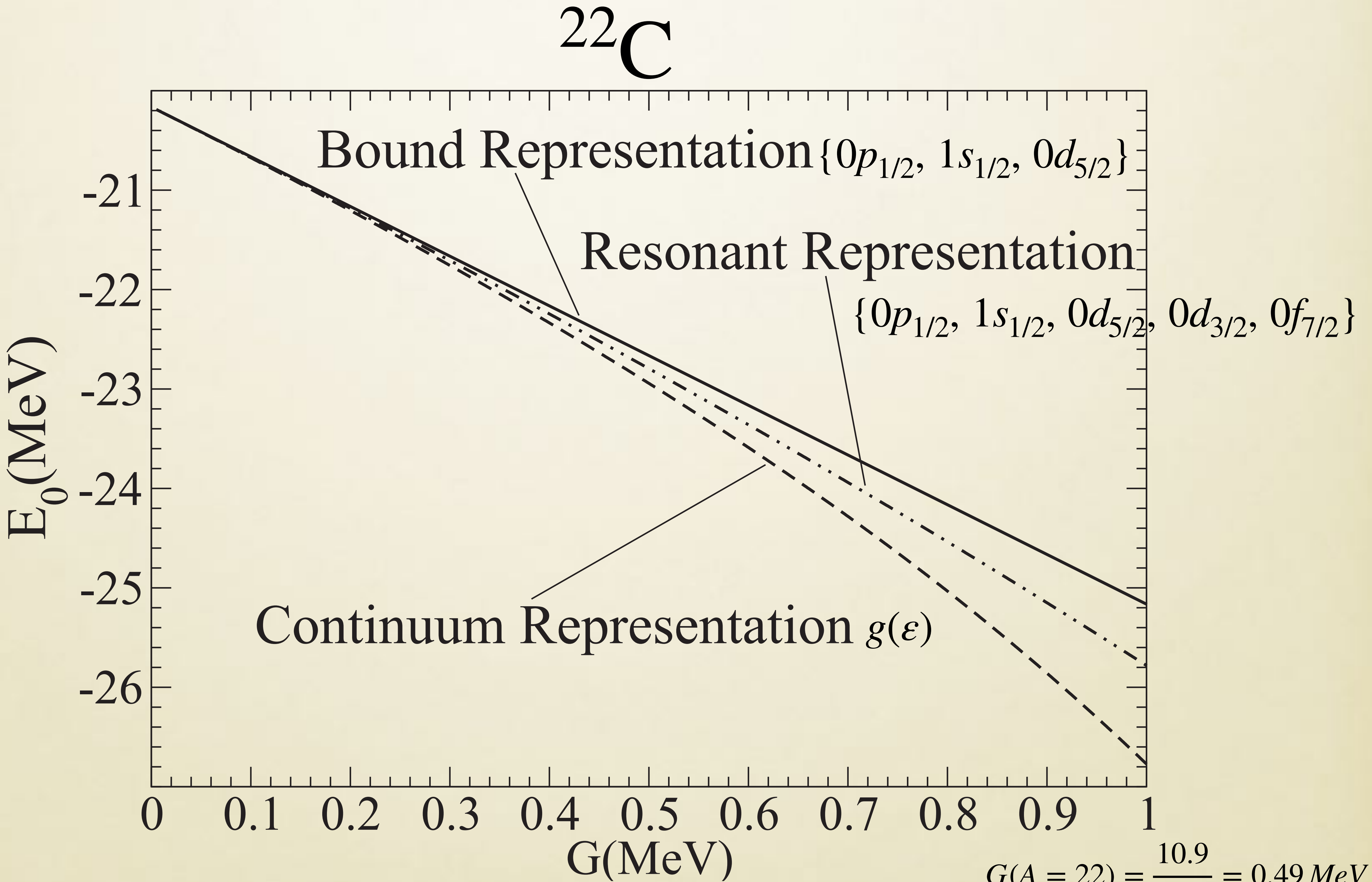


Beyond drip line ^{28}C
16 neutrons



$$E = \sum_{i=1}^{N_{pair}} E_i$$

Assessment of the importance of the resonant and non resonant continuum



$$G(A = 22) = \frac{10.9}{22} = 0.49\,MeV$$

NON CONSERVING PARTICLE MODEL SOLUTION

Bardeen-Cooper-Schrieffer (BCS)
and
Lipkin-Nogami (LN)

- Real energy representation

Non conserving particle number solutions: BCS and LN

BCS and LN ansatz

$$|BCS\rangle = \prod_{a,m_a>0} \left[u_a + (-1)^{a-m_a} v_a\, c^\dagger_{am_a}\, c^\dagger_{a-m_a}\right] |0\rangle$$

BCS Hamiltonian

$$H_{BCS} = H - \lambda N$$

LN Hamiltonian

$$H_{LN} = H - \lambda_1 N - \lambda_2 N^2$$

BCS and LN equations…

$$\frac{4}{G} = \sum_n \frac{1}{E_n} \qquad N = \sum_n v_n^2$$

$$\frac{4\lambda_2}{G} = \frac{\left(\sum_n u_n^3 v_n\right)\left(\sum_n u_n v_n^3\right) - 2\sum_n (u_n v_n)^4}{\left(\sum_n (u_n v_n)^2\right)^2 - 2\sum_n (u_n v_n)^4}$$

$$\langle BCS|H_{LN}\left(\hat{N}^2 - \langle BCS|\hat{N}^2|BCS\rangle\right)|BCS\rangle = 0$$

…in the continuum

$$\sum_n f_n \to \sum\!\!\!\!\!\!\int f$$

$$= \sum_{n_b} (2j_{n_b}+1)\, f_{n_b} + \int_0^\infty d\varepsilon\, g(\varepsilon)\, f(\varepsilon)$$

Non conserving particle number solutions BCS and LN: Aplication in real representation

Tin isotopes from A=102 to A=176

Single particle representation

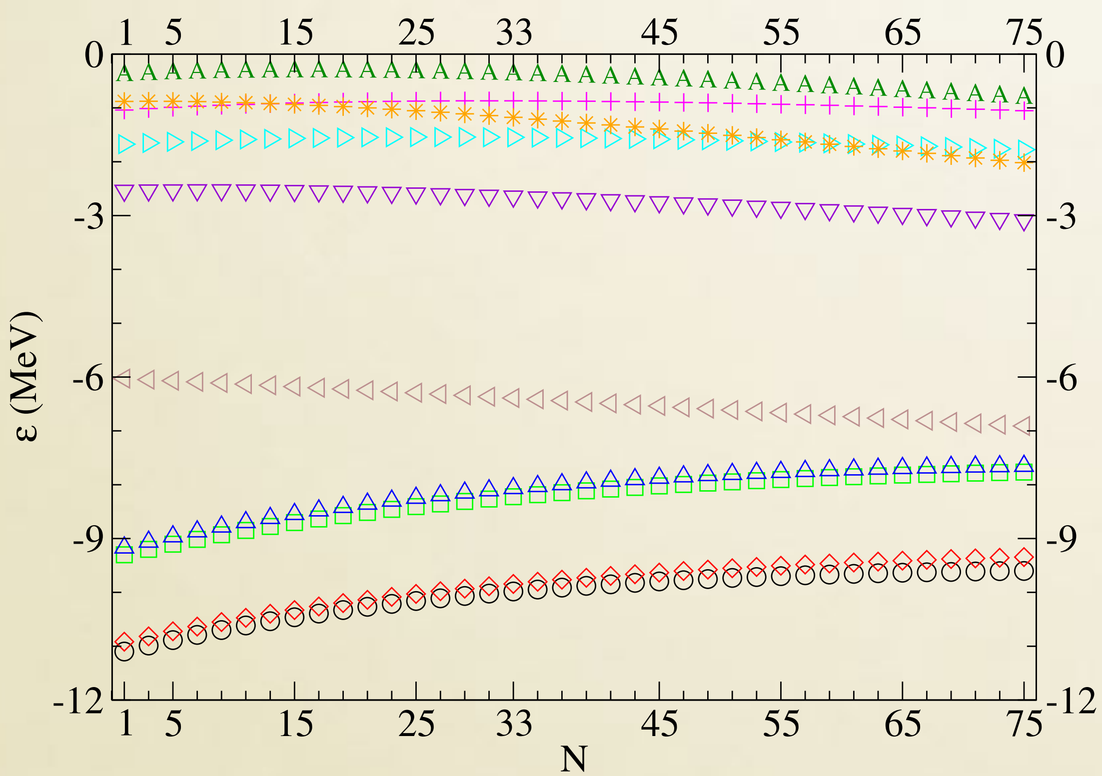
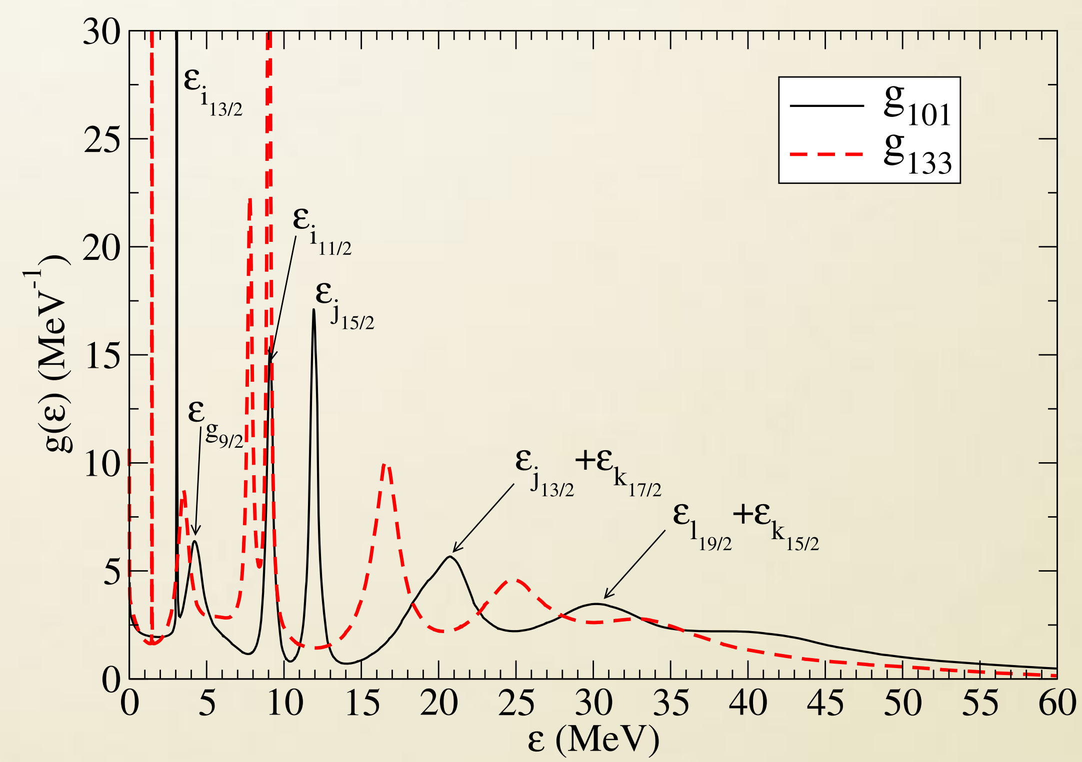


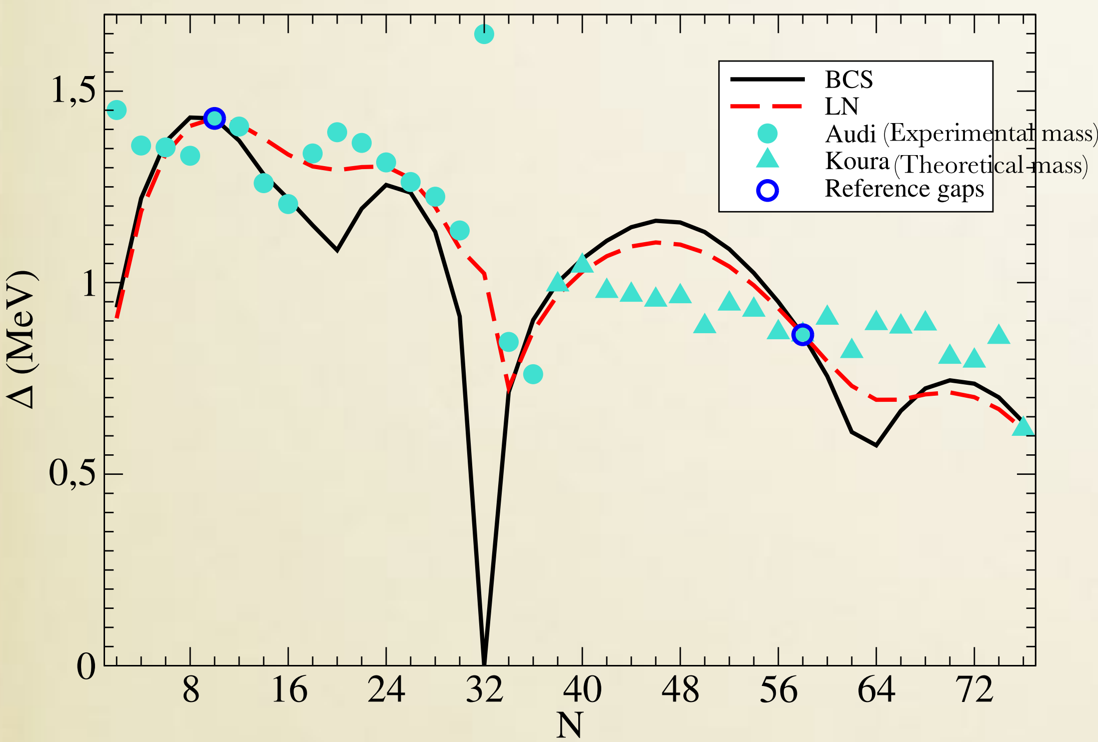
Fig. 1. (Color online.) Evolution of the single particle energies in the core ^{100}Sn as a function of the number of the valence neutrons. The following labels ○ $g_{7/2}$, ◇ $d_{5/2}$, □ $s_{1/2}$, △ $d_{3/2}$, ◁ $h_{11/2}$, ▽ $f_{7/2}$, ▷ $p_{3/2}$, + $p_{1/2}$, * $h_{9/2}$, A $f_{5/2}$ identify each single particle state.



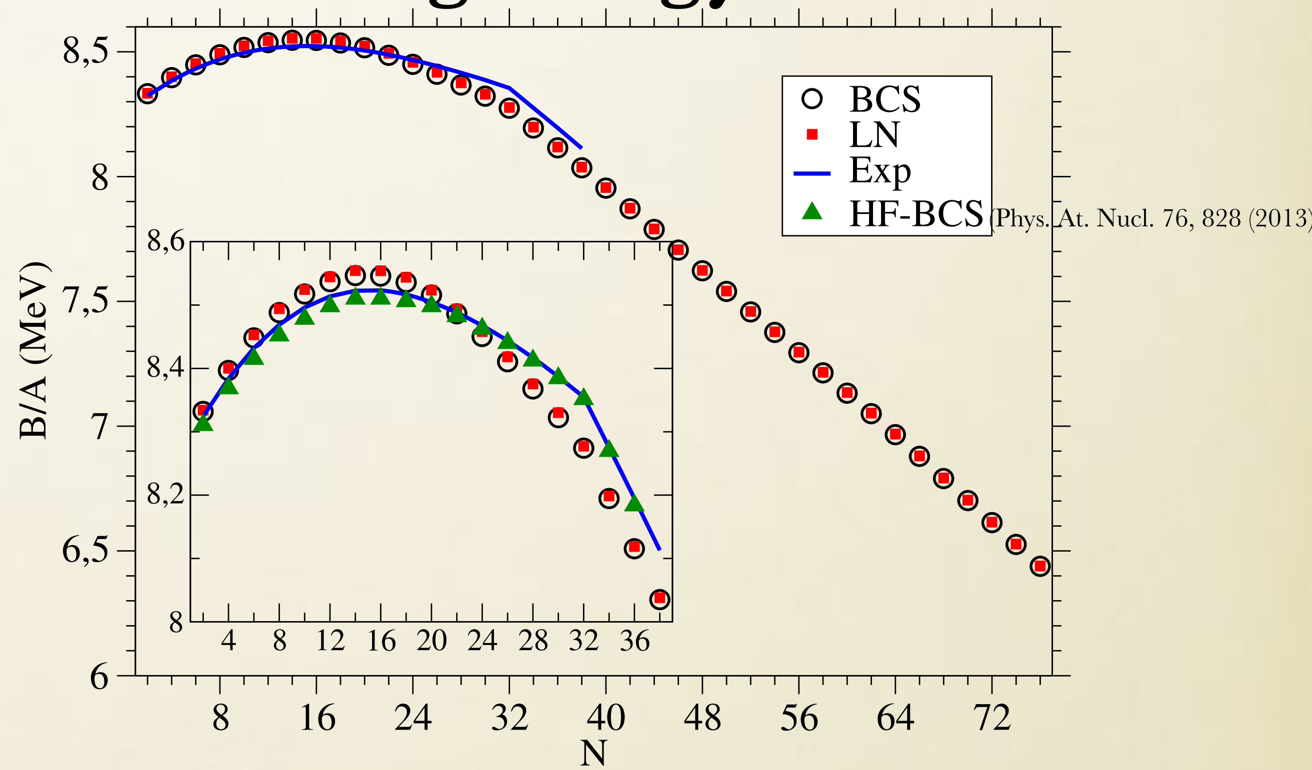
BCS and LN in real representation

Tin isotopes from A=102 to A=176

Gap

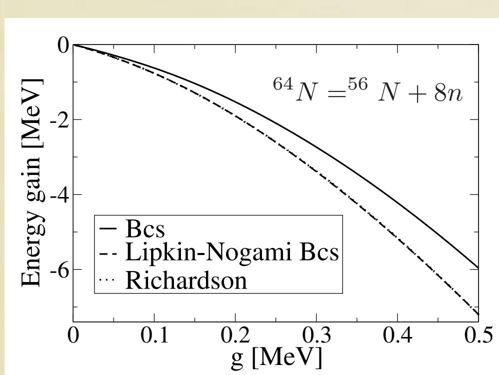


Binding energy



$$\frac{B}{A} = \frac{B(^{100}\mathrm{Sn}) - E_{\mathrm{BCS/LN}}(N)}{50 + N}$$

$$E_{\mathrm{BCS/LN}}(N) = \sum_n v_n^2 \left(\varepsilon_n - \frac{G}{2} v_n^2 \right) - \frac{\Delta^2}{G} - \lambda_2 \sum_n 2 u_n^2 v_n^2$$

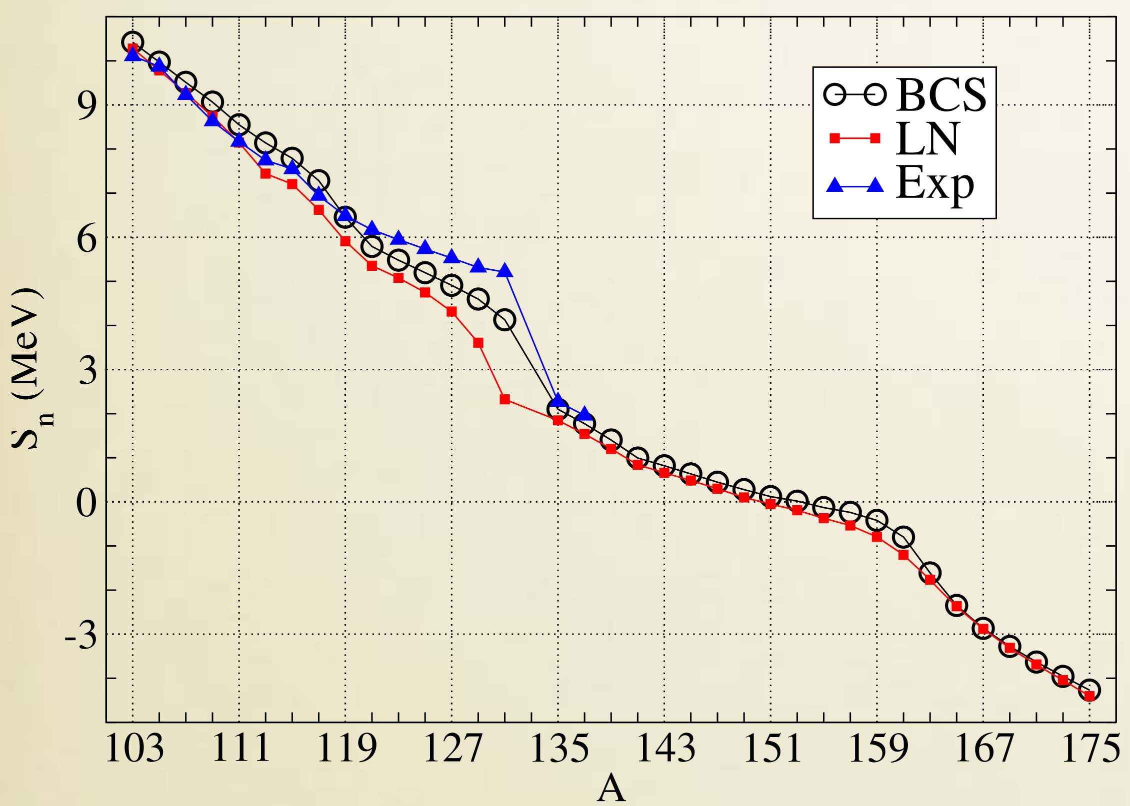


Bound representation

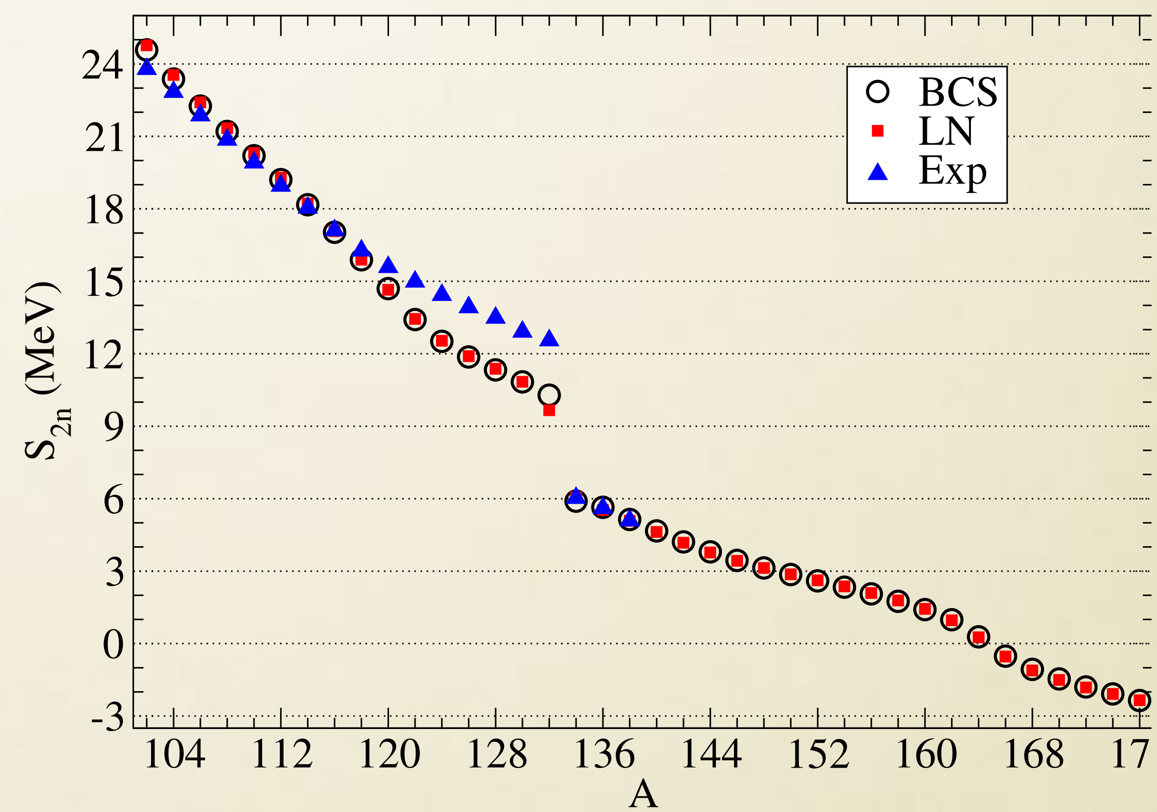
BCS and LN in real representation

Tin isotopes
From proton drip line to neutron drip line

Drip line



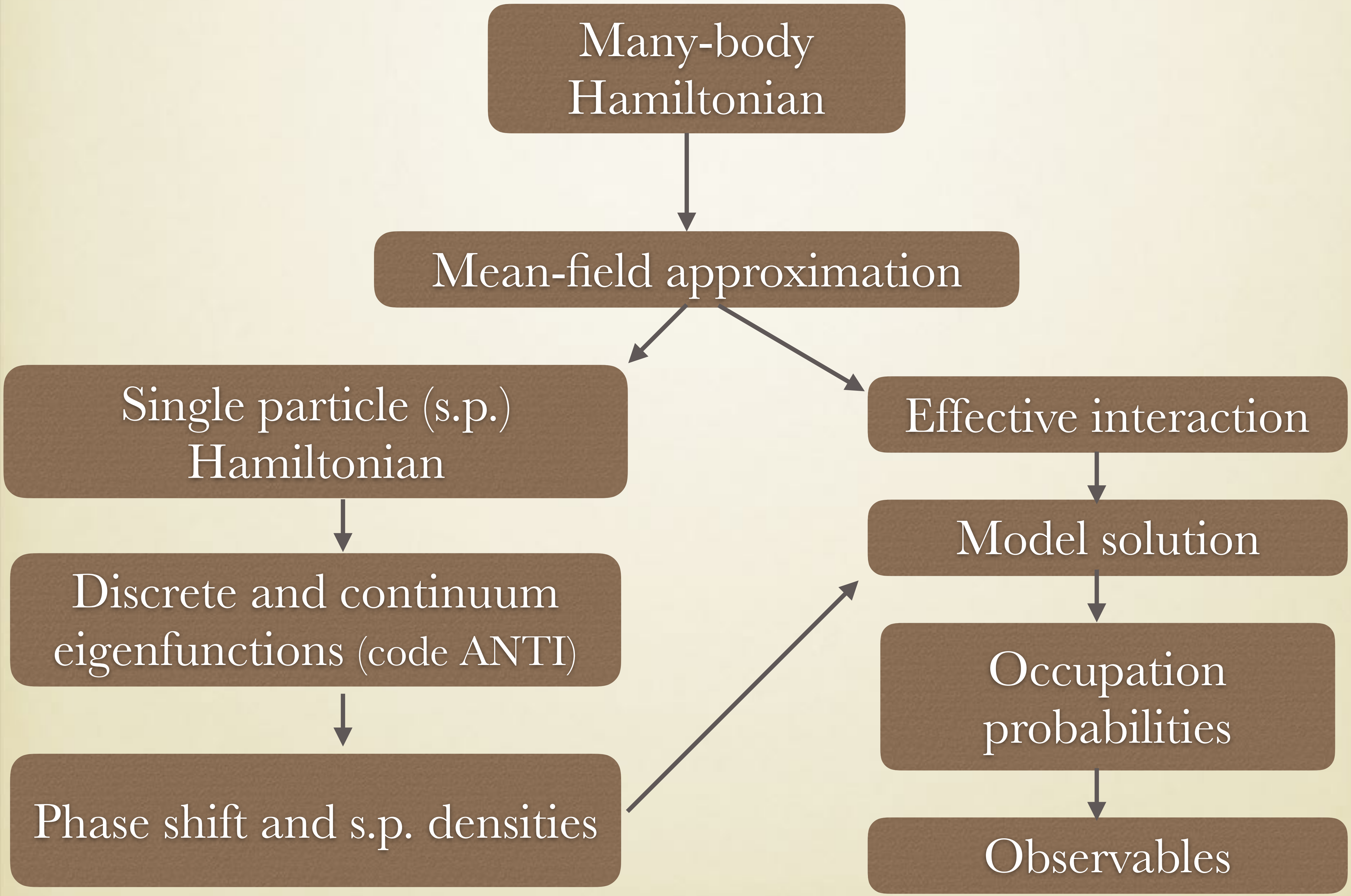
Two-neutron separation energy



Discussion and Outlook

- **PRO:** *fast/manageable dimensions*
- **CONS:** *losses of correlations*
- **Improvements (pairing):**
  - Separable interaction
  - Effective interaction
  - Realistic interaction

Workflow for practitioners



THANK YOU

FOR YOUR ATTENTION