J-matrix analysis of resonant states in the shell model

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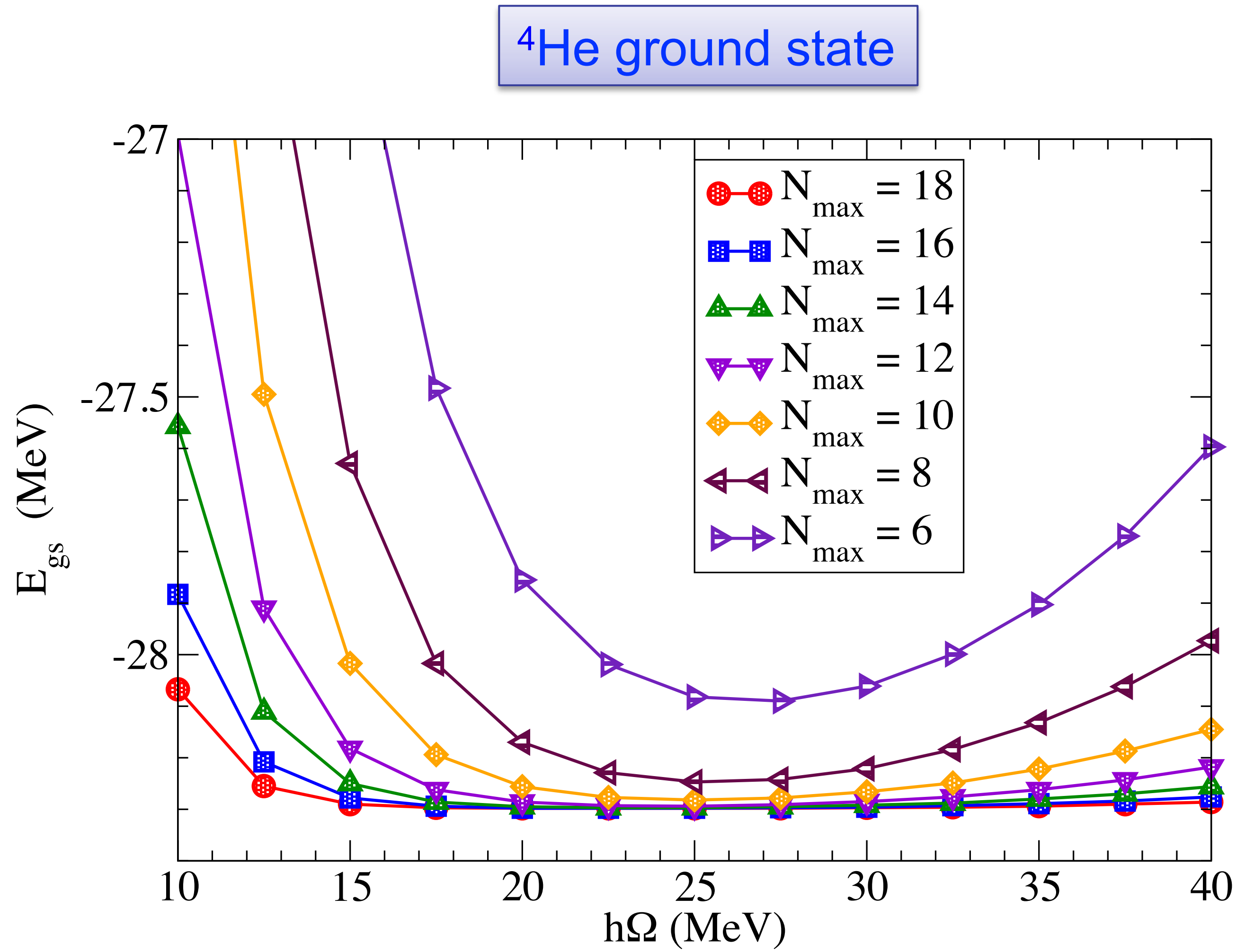
Highlights

some general properties for oscillator basis calculations; this is the only relevance to NCSM

- ✓ Motivation
- ✓ *J*-matrix formalism
- ✓ resonance information from E_ν

J-matrix ⟷ *NCSM: Nα scattering*

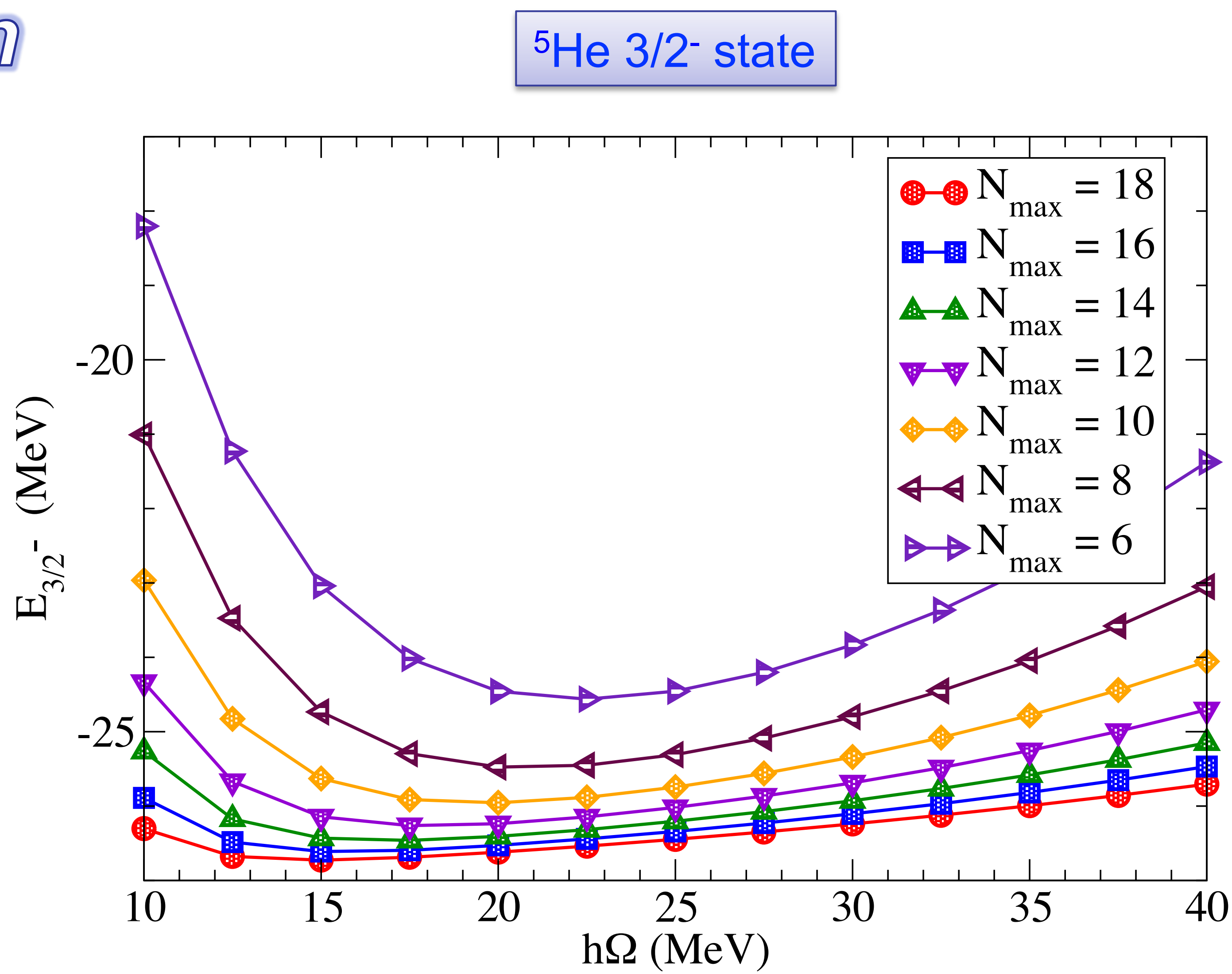
Motivation



Conventional:

bound state energies are associated with variational minimum in shell model calculations

Motivation



Can we extract resonance energy and width from calculations with oscillator basis?

J-matrix

Schrödinger equation: $$H^l u_l(E,r) = E u_l(E,r).$$

Expansion: $$u_l(E,r) = \sum_{n=0}^{\infty} a_{nl}(E) R_{nl}(r).$$

$$R_{nl}(r) = (-1)^n \sqrt{\frac{2n!}{r_0 \Gamma(n+l+3/2)}} \left(\frac{r}{r_0}\right)^{l+1} \exp\left(-\frac{r^2}{2r_0^2}\right) L_n^{l+1/2}\left(\frac{r^2}{r_0^2}\right)$$

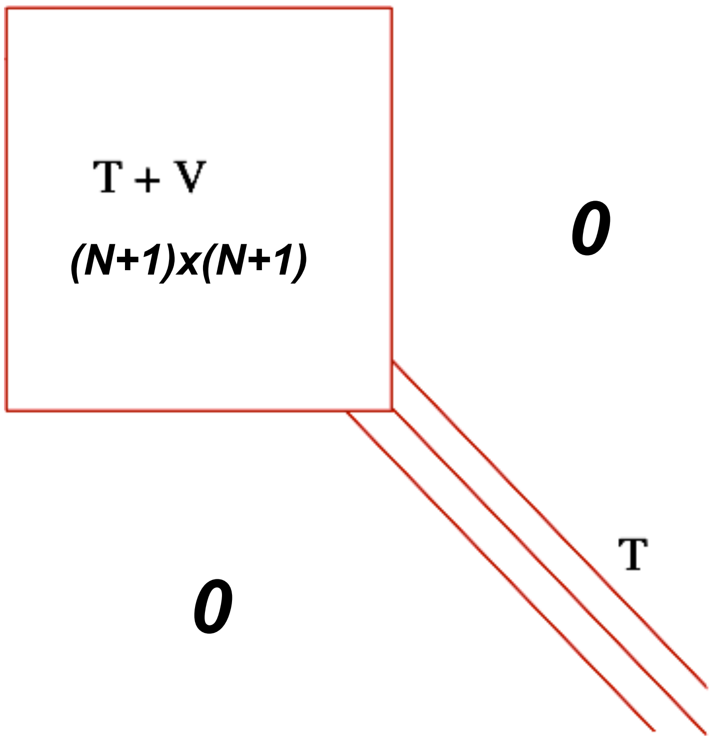
$r_0 = \sqrt{\hbar / m\Omega}$, $\hbar\Omega$ ***is oscillator parameters, m is reduced mass.***

$E = (q^2/2)\hbar\Omega$ – ***c.m. energy,*** $q = kr_0$ – ***dimensionless momentum.***

$$\sum_{n'=0}^{\infty} (H^l_{nn'} - \delta_{nn'} E) a_{n'l}(E) = 0.$$

J-matrix

Structure of Hamiltonian:



parameters: $N,\ \hbar\Omega$

Infinite Hamiltonian matrix:

$$H^l_{nn'} = T^l_{nn'} + V^l_{nn'}$$

Non-zero kinetic energy matrix elements:

$$T^l_{nn} = \frac{\hbar\Omega}{2}(2n + l + 3/2)$$

$$T^l_{nn+1} = T^l_{n+1n} = -\frac{\hbar\Omega}{2}\sqrt{(n+1)(n+l+3/2)}$$

$T^l_{nn'} \sim n$

$V^l_{nn'}$ – *decrease with* $n, n' \to \infty$

Truncated potential matrix:

$$\tilde{V}^l_{nn'} = \begin{cases} V^l_{nn'} & \text{if} \quad n \quad \text{and} \quad n' \le N; \\ 0 & \text{if} \quad n \quad \text{or} \quad n' > N. \end{cases}$$

J-matrix

Phase shift:

$$\tan\delta(E) = -\frac{S_{Nl}(E) - G_{NN}(E)T^{l}_{N,N+1}S_{N+1,l}(E)}{C_{Nl}(E) - G_{NN}(E)T^{l}_{N,N+1}C_{N+1,l}(E)}$$

Regular and irregular oscillator solutions

$$S_{nl}(E) = \sqrt{\frac{2r_0 n!}{\Gamma(n+l+3/2)}}\; q^{l+1}\exp\left(-\frac{q^2}{2}\right)L_n^{l+1/2}(q^2)\ ,$$

$$C_{nl}(E) = \sqrt{\frac{2r_0 n!}{\Gamma(n+l+3/2)}}\;\frac{\Gamma(l+1/2)}{\pi\, q^l}\exp\left(-\frac{q^2}{2}\right)\Phi(-n-l-1/2, -l+1/2; q^2)\ .$$

$$\sum_{n=0}^{\infty} S_{nl}(E)R_{nl}(r) = \sqrt{\frac{2}{\pi}}kr\, j_l(kr),$$

$$\sum_{n=0}^{\infty} C_{nl}(E)R_{nl}(r) \to -\sqrt{\frac{2}{\pi}}kr\, n_l(kr).$$

$$E = \frac{q^2}{2}\hbar\Omega$$

J-matrix

Phase shift:

$$\tan\delta(E) = -\frac{S_{Nl}(E) - G_{NN}(E)T^{l}_{N,N+1}S_{N+1,l}(E)}{C_{Nl}(E) - G_{NN}(E)T^{l}_{N,N+1}C_{N+1,l}(E)}$$

$$G_{NN}(E) = -\sum_{\nu=0}^{N}\frac{\langle N|\nu\rangle^2}{E_\nu - E}$$

$$E_\nu,\ \langle n|\nu\rangle\ \ (\nu = 0,1,\ldots,N)$$

are obtained from

$$\sum_{n'=0}^{N} H^{l}_{nn'}\langle n'|\nu\rangle = E_\nu\langle n|\nu\rangle,\ \ n \le N$$

All NCSM states are needed that is impossible to obtain

J-matrix

S-matrix:

$$S(E) = \frac{C^{(-)}_{N,l}(E) - G_{NN}(E)T^{l}_{N,N+1}C^{(-)}_{N+1,l}(E)}{C^{(+)}_{N,l}(E) - G_{NN}(E)T^{l}_{N,N+1}C^{(+)}_{N+1,l}(E)}$$

$$C^{(\pm)}_{nl}(E) = C_{nl}(E) \pm i\, S_{nl}(E)$$

$$\sum_{n=0}^{\infty} C^{(\pm)}_{nl}(E)R_{nl}(r) \rightarrow \sqrt{\frac{2}{\pi}}kr\, h^{(\pm)}_{l}(kr).$$

J-matrix

$E = E_\nu$:

✔ $$\delta(E_\nu) = -\arctan\left(\frac{S_{N+1,l}(E_\nu)}{C_{N+1,l}(E_\nu)}\right)$$

✔ $$S(E_\nu) = \frac{C^{(-)}_{N+1,l}(E_\nu)}{C^{(+)}_{N+1,l}(E_\nu)}$$

Only one eigenvalue E_ν is an input!

$E_\nu(\hbar\Omega),\ \hbar\Omega - continuous\ \ parameter$ → $\delta(E),\ S(E)$

J-matrix

universal function

$$f_{N+1,l}(E) = -\arctan\left(\frac{S_{N+1,l}(E)}{C_{N+1,l}(E)}\right)$$

$$\delta(E_\nu) = f_{N+1,l}(E_\nu)$$

asymptotics $N >> q$ $z \to \infty$

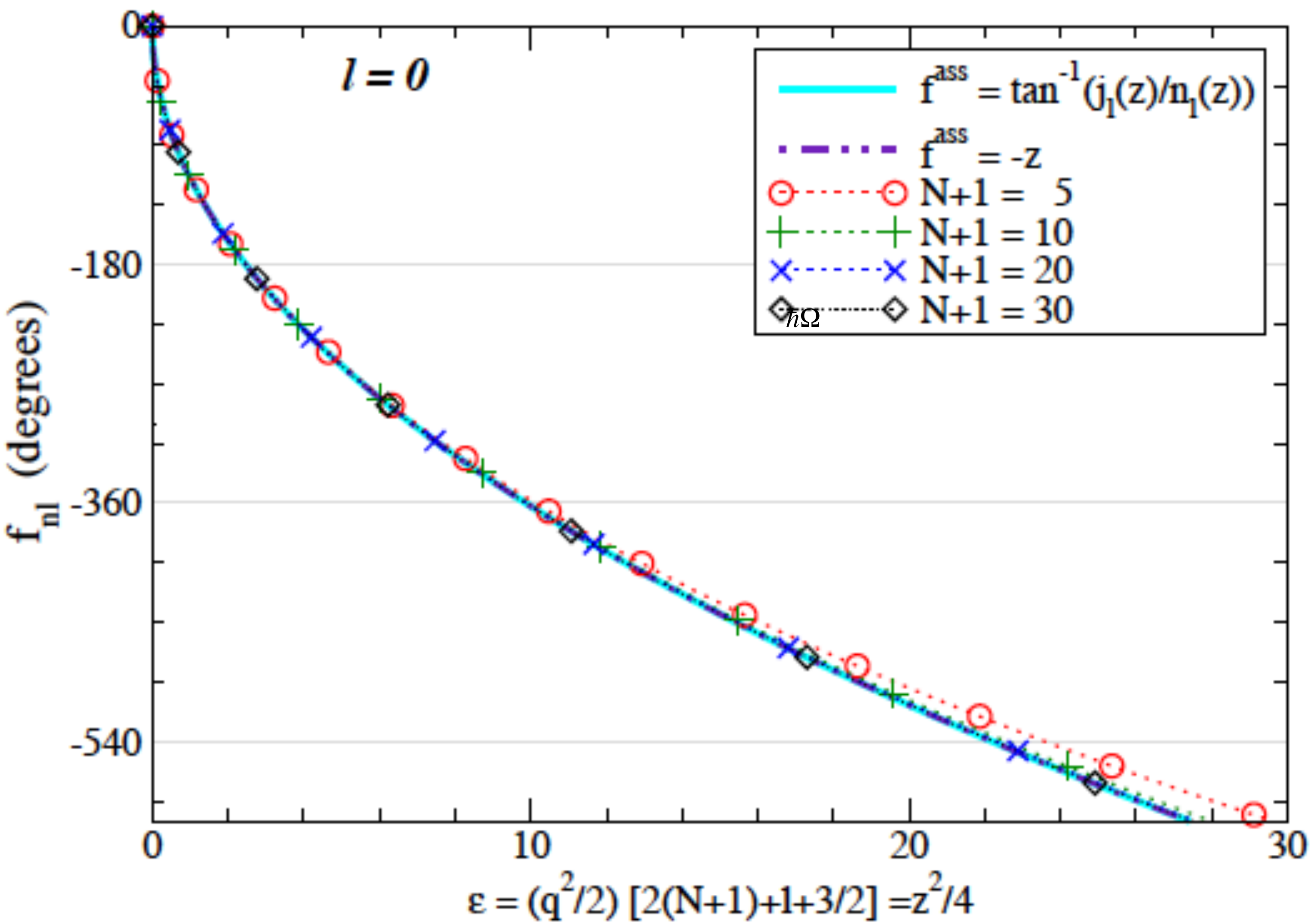
$$f_{N+1,l}(E_\nu) = \delta(E_\nu) \approx \arctan\left(\frac{j_l(z_\nu)}{n_l(z_\nu)}\right) \approx \frac{\pi l}{2} - z_\nu$$

$$z_\nu = 2q_\nu\sqrt{(N+1)+l/2+3/4}$$

J-matrix

universal function

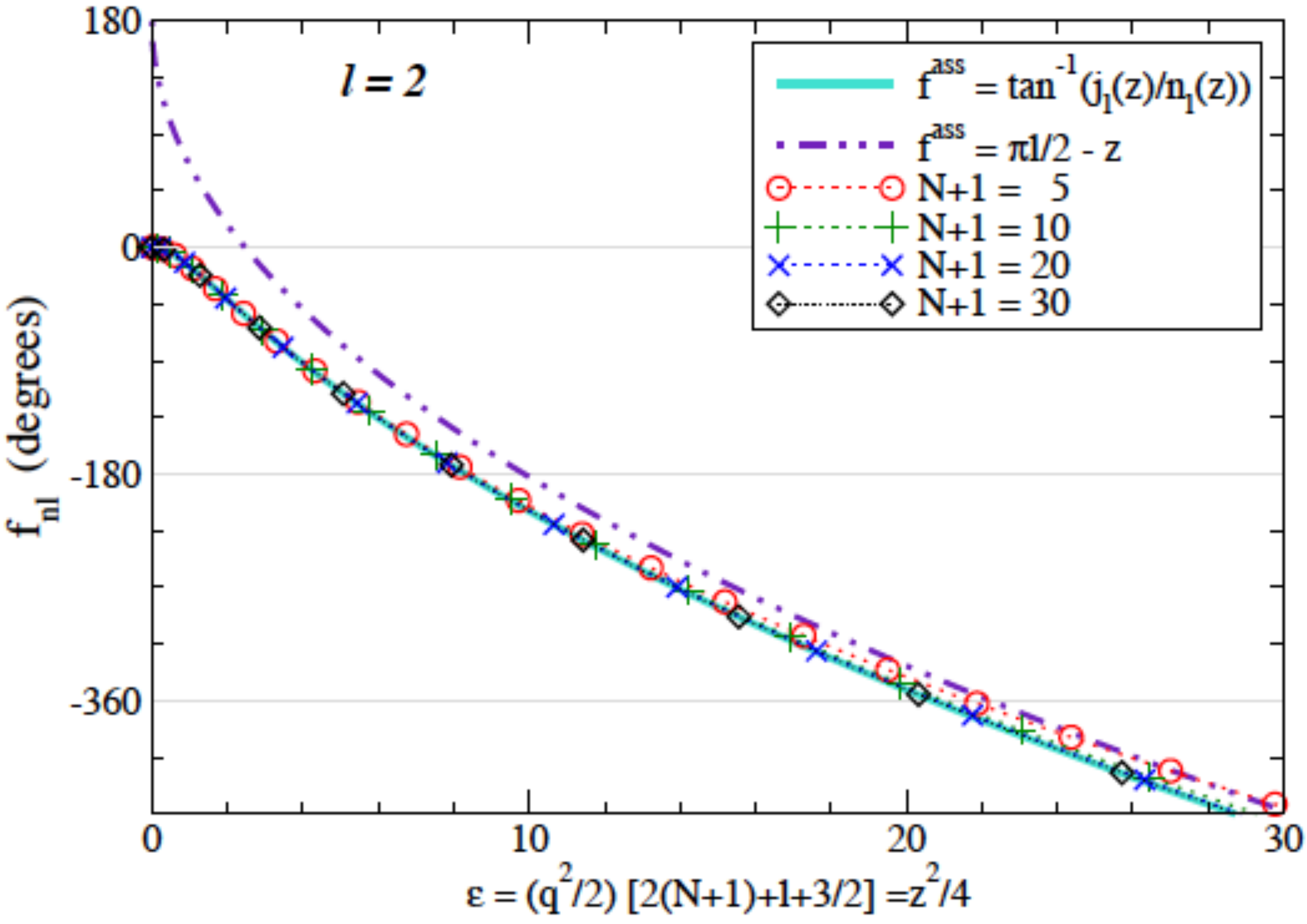
$$f_{N+1,l} = -\arctan\left(\frac{S_{N+1,l}(E)}{C_{N+1,l}(E)}\right)$$



J-matrix

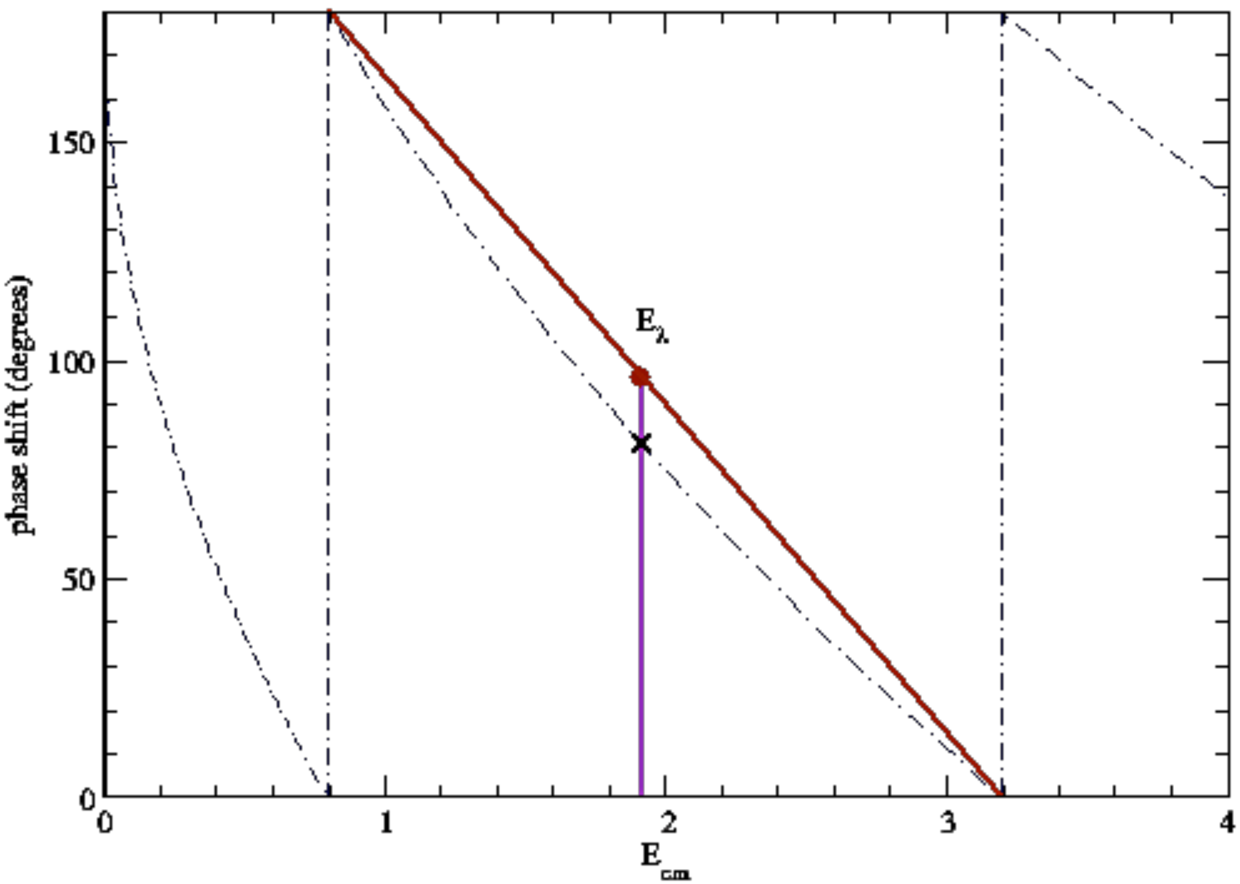
universal function

$$f_{N+1,l} = -\arctan\left(\frac{S_{N+1,l}(q)}{C_{N+1,l}(q)}\right)$$



compare J-matrix with Lifshitz

- I. M. Lifshitz (1947).
- O. Rubtsova, V. Kukulin, V. Pomerantsev,
  JETP Lett. 90, 402 (2009);Phys. Rev. C 81, 064003 (2010).



Lifshitz:

$$H = H^0 + V$$

$$\delta(E_\lambda) = -\pi \frac{E_\lambda - E_j^0}{D_j}$$

$$D_j = E_{j+1}^0 - E_j^0$$

J-matrix:

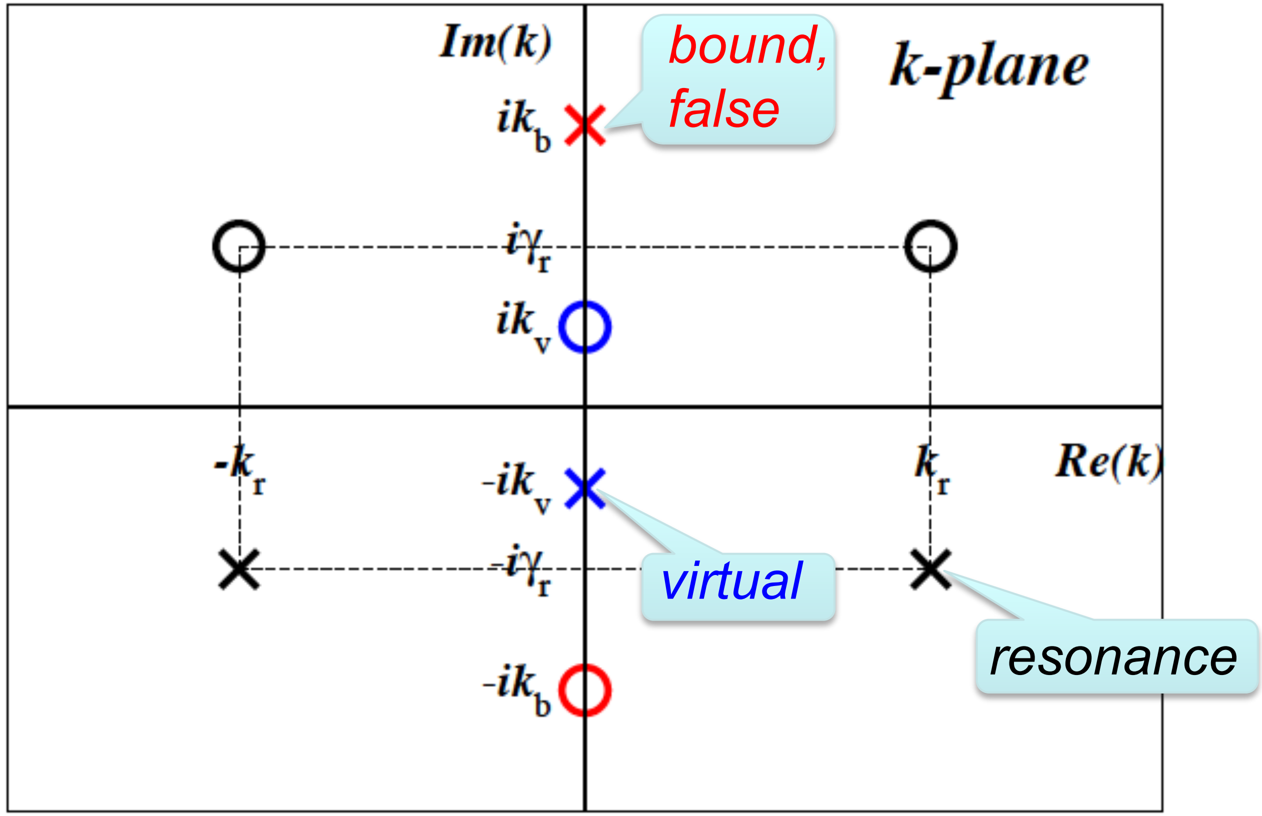
$$\delta(E_\lambda) = -\arctan\left(\frac{S_{N+1,l}(E_\lambda)}{C_{N+1,l}(E_\lambda)}\right)$$

S-matrix symmetry

$$S(-k) = \frac{1}{S(k)}$$

$$S(k^*) = \frac{1}{S^*(k)}$$

$$S(-k^*) = S^*(k)$$



$$S(k) = S_r^1 S_r^2 \ldots S_b^1 S_b^2 \ldots S_f^1 S_f^2 \ldots S_v^1 S_v^2 \ldots$$

bound

$$S_b = \frac{(k + ik_b)}{(k - ik_b)}$$

false

$$S_f = \frac{(k + ik_f)}{(k - ik_f)}$$

virtual

$$S_v = \frac{(k - ik_v)}{(k + ik_v)}$$

resonance state

$$S_r = \frac{(k - \kappa_r^*)(k + \kappa_r)}{(k - \kappa_r)(k + \kappa_r^*)}$$

$$\kappa_r = k_r - i\gamma_r$$

Resonance

$$S(k) = S_r^1 S_r^2 \ldots S_b^1 S_b^2 \ldots S_f^1 S_f^2 \ldots S_v^1 S_v^2 \ldots$$

$$\Rightarrow \quad \delta(E) = \delta_r^1 + \delta_r^2 + \ldots + \delta_b^1 + \ldots + \delta_f^1 + \ldots + \delta_v^1 + \ldots$$

resonance phase shift

$$\delta_r = -\arctan\left(\frac{2k\gamma_r}{k^2 - k_r^2 - \gamma_r^2}\right)$$

phase shift behaviour far from resonance

$$\delta_r = \sim \frac{2k\gamma_r}{k_r^2 + \gamma_r^2} \sim c_r\sqrt{E}$$

bound (false)

$$\delta_{b(f)} = \arctan\left(\frac{k_{b(f)}}{k}\right)$$

far from resonance

$$\delta_{b(f)} \sim c_1 - c_2\sqrt{E}$$

virtual

$$\delta_v = -\arctan\left(\frac{k_v}{k}\right)$$

far from resonance

$$\delta_v \sim c_1 + c_2\sqrt{E}$$

Resonance

In vicinity of the resonance with $E_r,\ \Gamma$

$$\delta \approx -\arctan\left(\frac{a\sqrt{E}}{E-b^2}\right)+c\sqrt{E}$$

$$E_r = b^2 - \frac{a^2}{2},\quad \frac{\Gamma}{2} = a\sqrt{b^2-\frac{a^2}{4}},$$

definition of the resonance parameters

$$E = \frac{\hbar^2}{2m}\kappa_r^2 = \frac{\hbar^2}{2m}\left(k_r - i\gamma_r\right)^2 = \frac{\hbar^2}{2m}\left[\left(k_r^2-\gamma_r^2\right)-i2k_r\gamma_r\right]$$

$$\Rightarrow\quad E_r = \frac{\hbar^2}{2m}\left(k_r^2-\gamma_r^2\right),\quad \Gamma/2 = \frac{\hbar^2}{m}k_r\gamma_r$$

+ J-matrix:

$$-\arctan\left(\frac{S_{N+1,l}(E_\nu)}{C_{N+1,l}(E_\nu)}\right) = -\arctan\left(\frac{a\sqrt{E_\nu}}{E_\nu-b^2}\right)+c\sqrt{E_\nu}$$

Resonance

+ *J-matrix:*

$$-\arctan\left(\frac{S_{N+1,l}(E_\nu)}{C_{N+1,l}(E_\nu)}\right) = -\arctan\left(\frac{a\sqrt{E_\nu}}{E_\nu - b^2}\right) + c\sqrt{E_\nu}$$

$$E_r = b^2 - \frac{a^2}{2}, \quad \frac{\Gamma}{2} = a\sqrt{b^2 - \frac{a^2}{4}},$$

How should depend E_ν on $\hbar\Omega$ and N in the vicinity of resonance?

Model 1: s-wave scattering

Model potential

$$V(r) = V_0 \frac{1}{1+\exp\left((r-R)/d_1\right)} + V_s \frac{d_2}{r} \frac{\exp\left((r-R)/d_1\right)}{\left[1+\exp\left((r-R)/d_1\right)\right]^2}$$

$$V_0 = -50\ MeV,\ V_s = 207\ MeV,\ d_1 = 0.53\ fm,\ d_2 = 3.774\ fm,\ R = 3.08\ fm$$

Resonance:

$E_r = 3.403\ MeV$

$\Gamma\ = 0.225\ MeV$

fit:

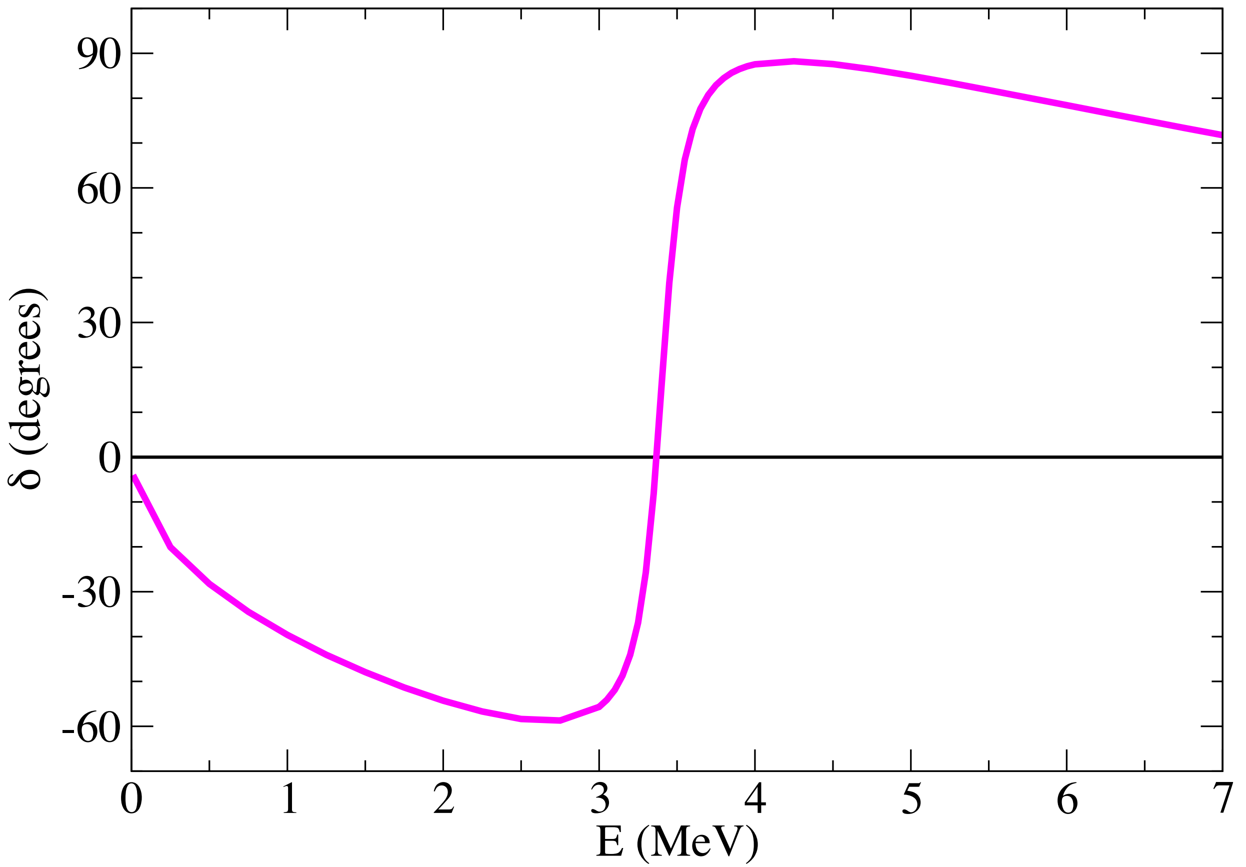
$E_r = 3.404\ MeV$

$\Gamma\ = 0.223\ MeV$

$a\ = 0.0605\ MeV^{1/2}$

$b^2 = 3.4061\ MeV$

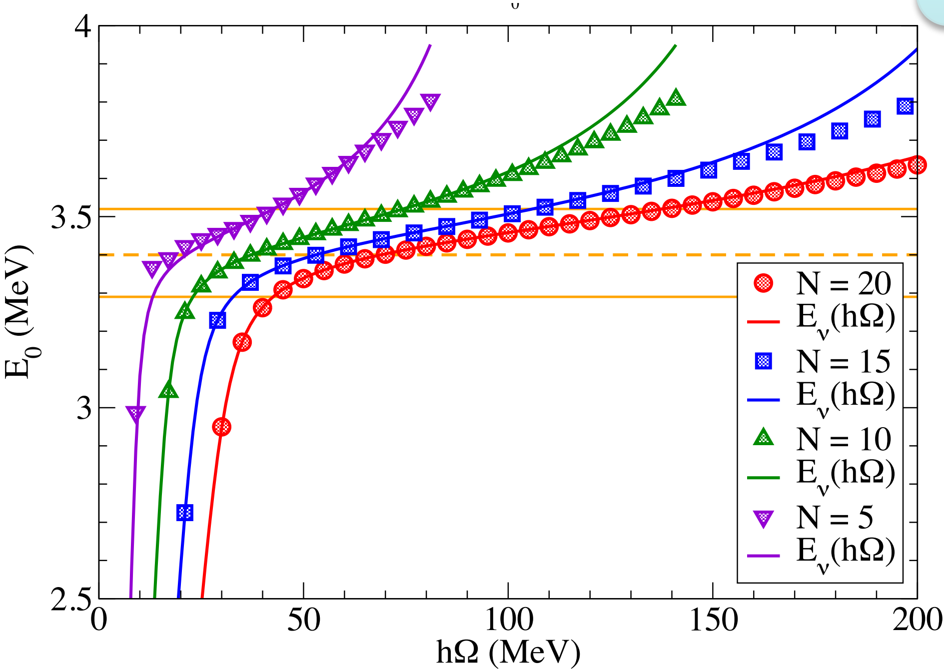
$c\ = -0.7059\ MeV^{-1/2}$



Model 1: s-wave scattering

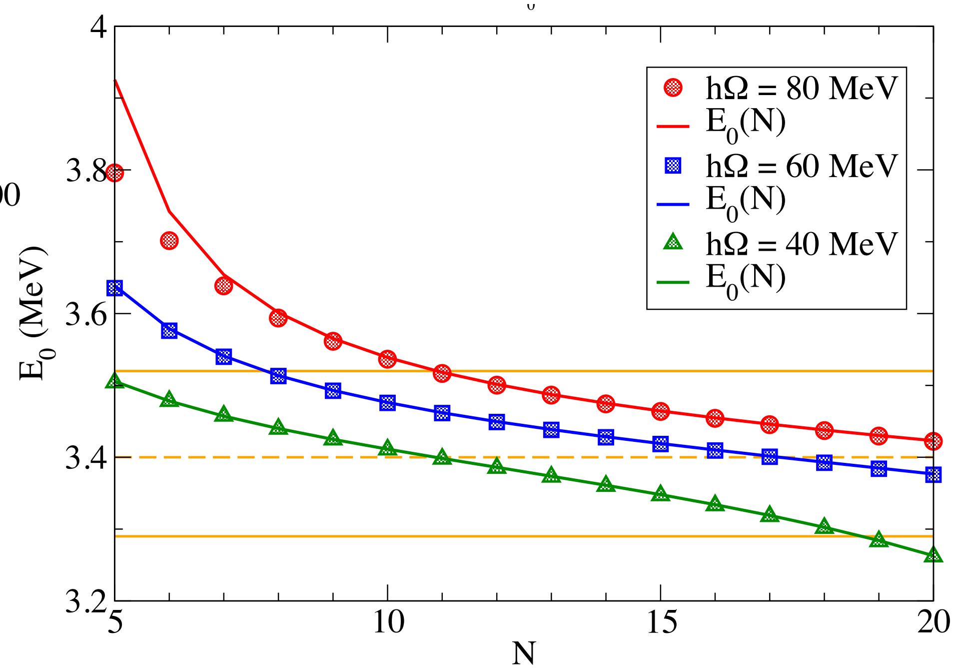
$$-\arctan\left(\frac{S_{N+1,l}(E_\nu)}{C_{N+1,l}E_\nu)}\right) = -\arctan\left(\frac{a\sqrt{E_\nu}}{E_\nu - b^2}\right) + c\sqrt{E_\nu}$$

$E_0(h\Omega)$



$dE_0/d(h\Omega) > 0$!

$E_0(N)$



Model 1: s-wave scattering

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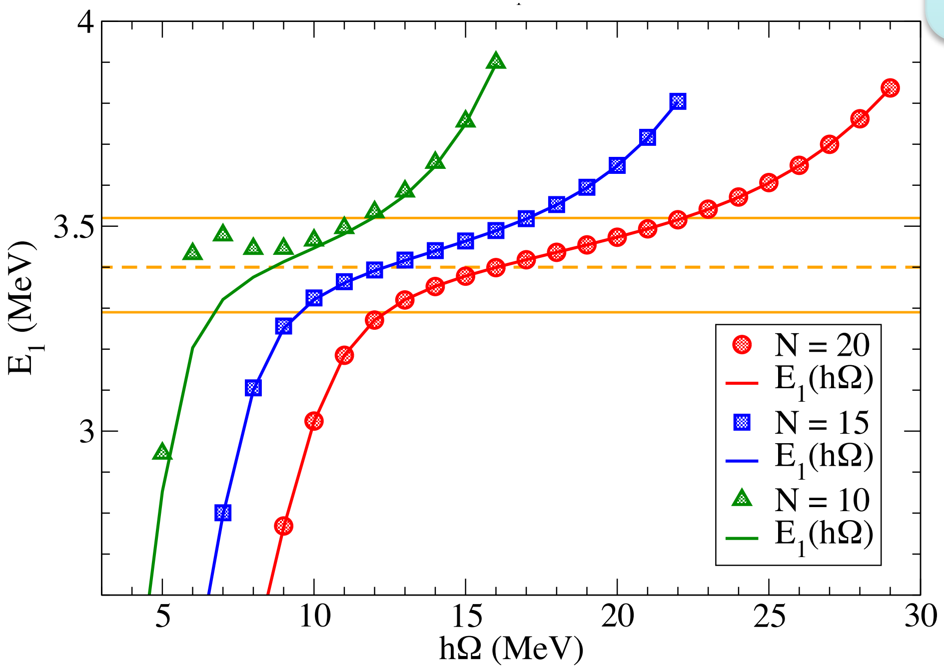
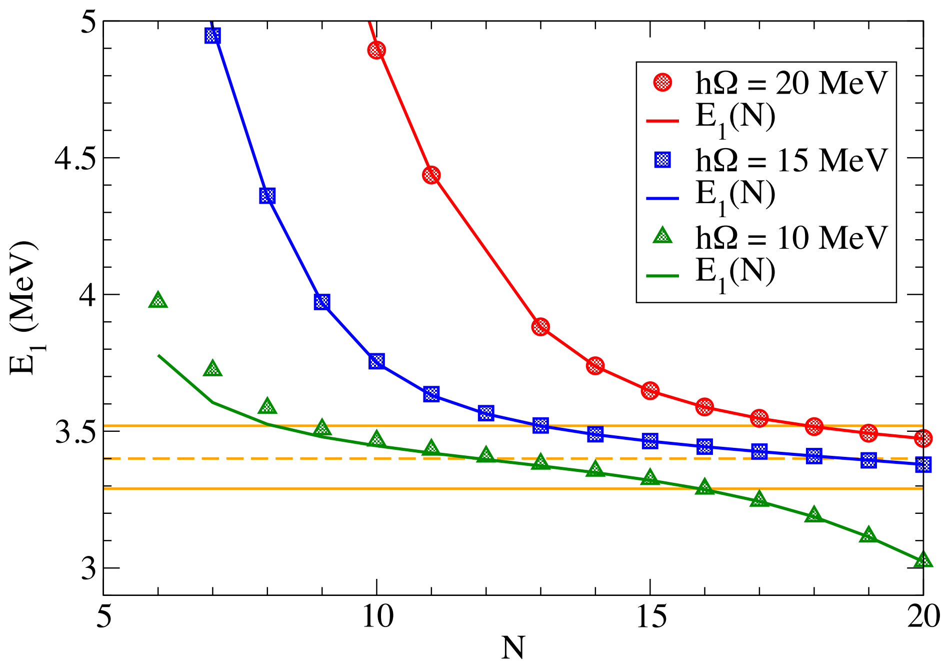
$E_1(\hbar\Omega)$



$dE_1/d(\hbar\Omega) > 0$!

$E_1(N)$



Model 1: s-wave scattering

Phase shift comparison

Resonance:

$E_r = 3.403 \ MeV$

$\Gamma \ = 0.225 \ MeV$

fit:

$E_r = 3.404 \ MeV$

$\Gamma \ = 0.223 \ MeV$

$a \ = 0.0605 \ MeV^{1/2}$

$b^2 = 3.4061 \ MeV$

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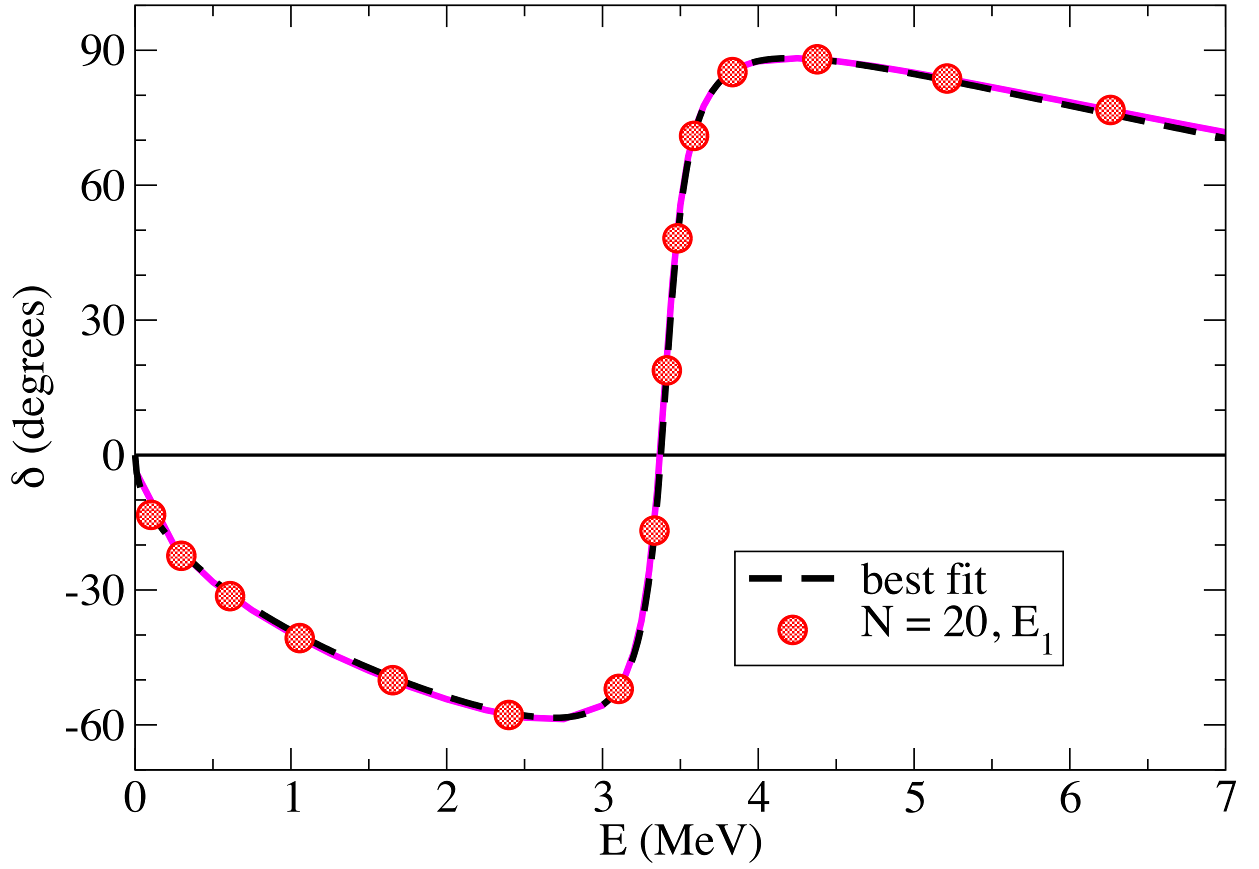


Model 2: d-wave scattering

Model potential

$$V(r)=V_0\frac{1}{1+\exp\left((r-R)/d_1\right)}+V_s\frac{d_2}{r}\frac{\exp\left((r-R)/d_1\right)}{\left[1+\exp\left((r-R)/d_1\right)\right]^2}$$

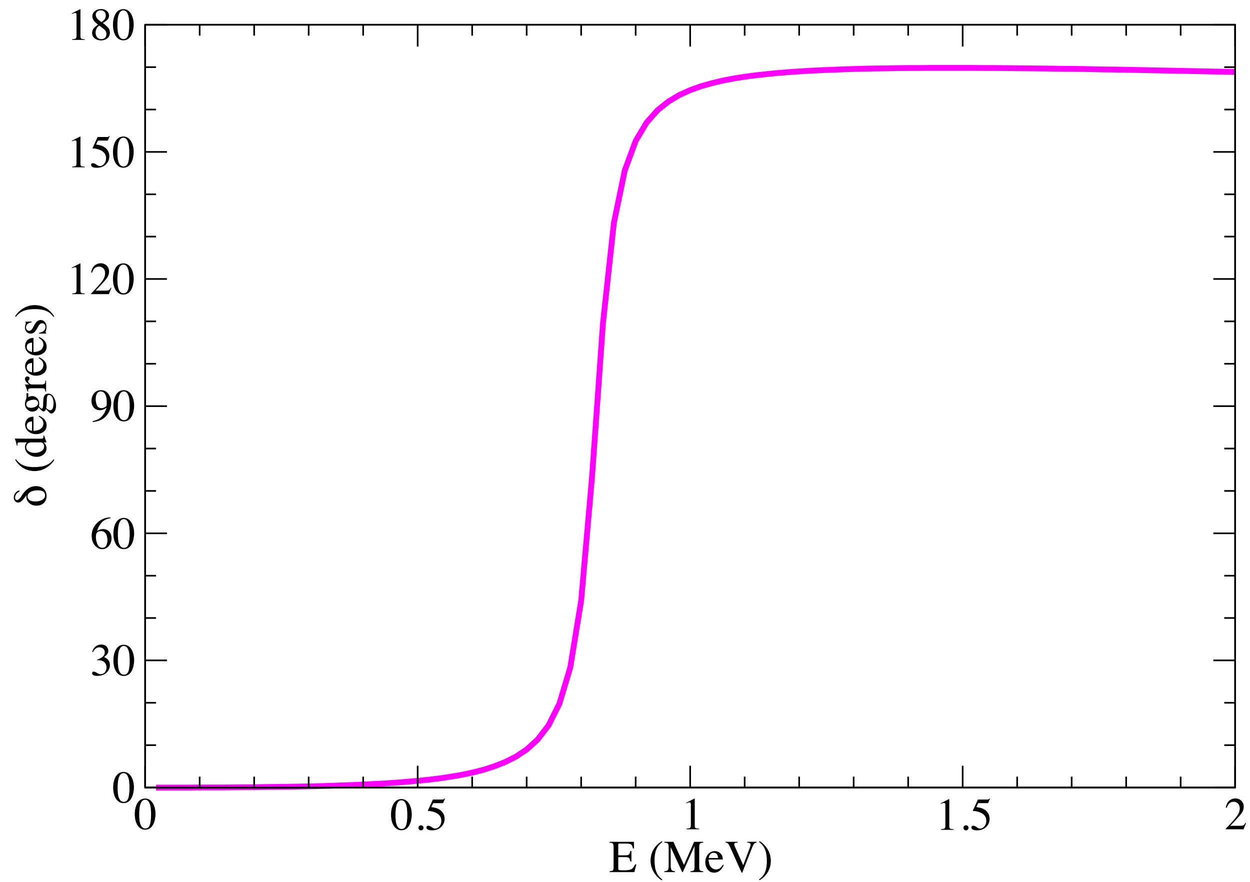
$$V_0=-48\ MeV,\ V_s=-20\ MeV,\ d_1=0.53\ fm,\ d_2=3.774\ fm,\ R=3.08\ fm$$

Resonance:

$$E_r=0.8319\ MeV$$
$$\Gamma=0.0612\ MeV$$

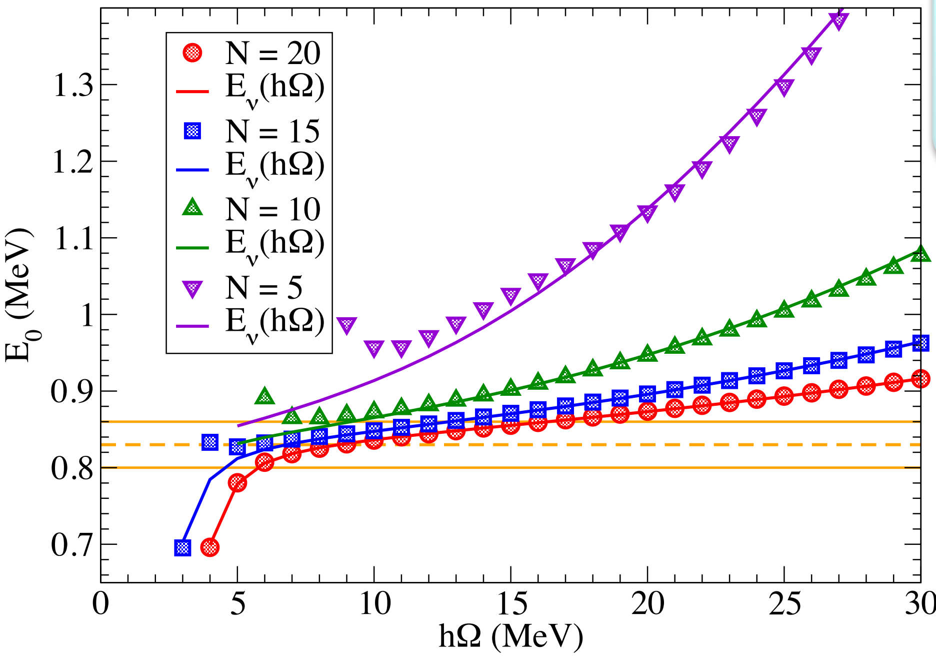
fit:

$$E_r=0.8319\ MeV$$
$$\Gamma=0.0589\ MeV$$
$$a=0.0317\ MeV^{1/2}$$
$$b^2=0.8324\ MeV$$
$$c=-0.0955\ MeV^{-1/2}$$



Model 2: d-wave scattering

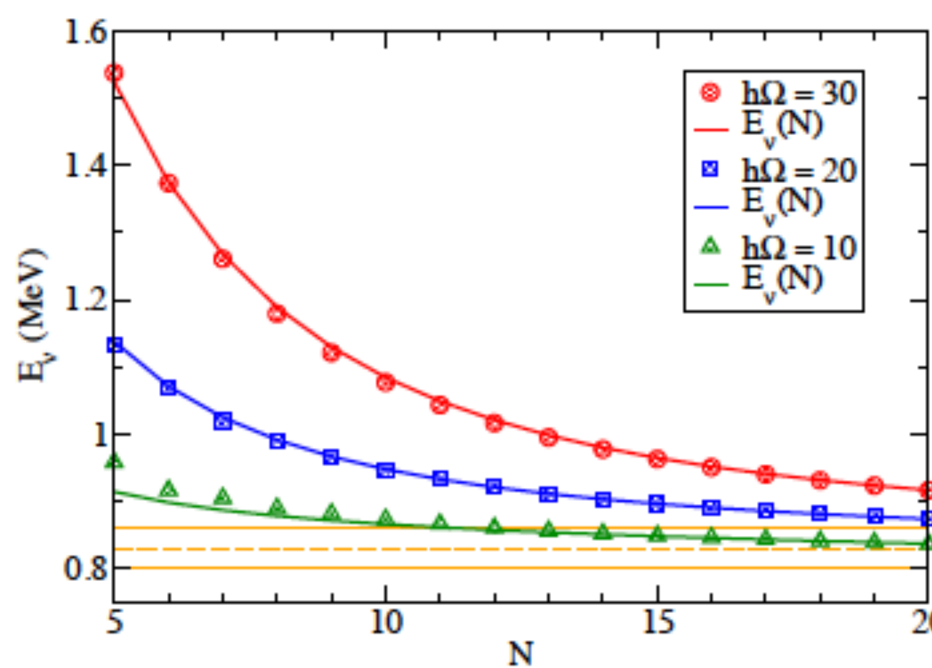
$E_0(h\Omega)$



$$-\arctan\left(\frac{S_{N+1,l}(E_\nu)}{C_{N+1,l}(E_\nu)}\right) = -\arctan\left(\frac{a\sqrt{E_\nu}}{E_\nu - b^2}\right) + c\sqrt{E_\nu}$$

$dE_0/d(h\Omega)$ should be >0 !

$E_0(N)$



Model 2: d-wave scattering

Phase shift comparison

Resonance:

$$E_r = 0.8319\ MeV$$

$$\Gamma = 0.0612\ MeV$$

fit:

$$E_r = 0.8319\ MeV$$

$$\Gamma = 0.0589\ MeV$$

$$a = 0.0317\ MeV^{1/2}$$

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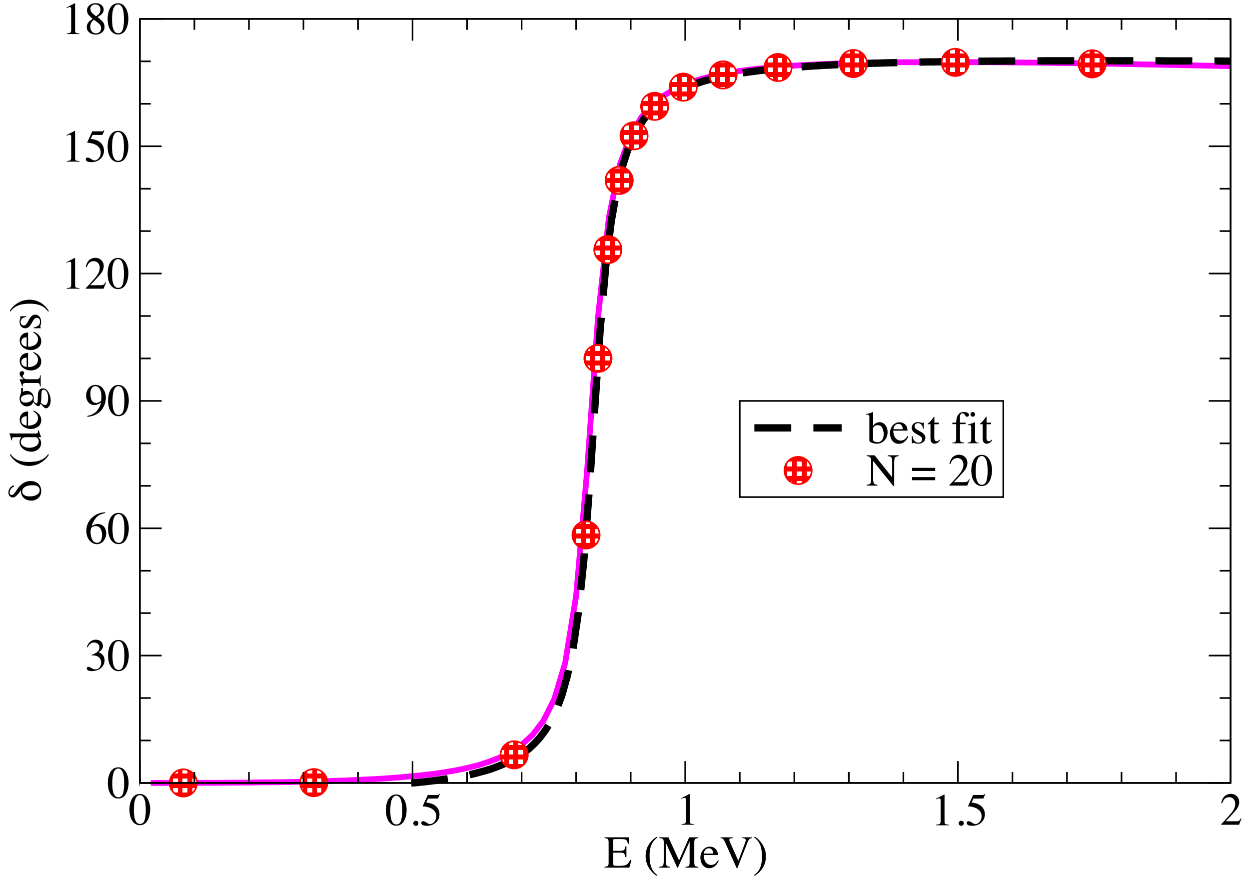
$$c = -0.0955\ MeV^{-1/2}$$

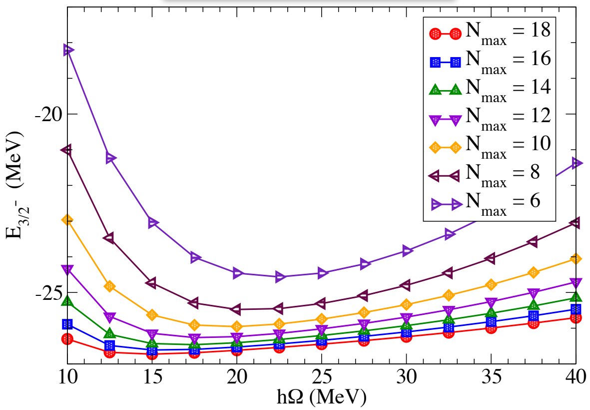


nα – scattering, resonance 3/2⁻

NCSM calculations for ^{5}He with JISP16

Redefined level energy from nα threshold: $E = E(^5\text{He}, 3/2^-) - E(^4\text{He}, gs)$

$E(^5\text{He}, 3/2^-)$



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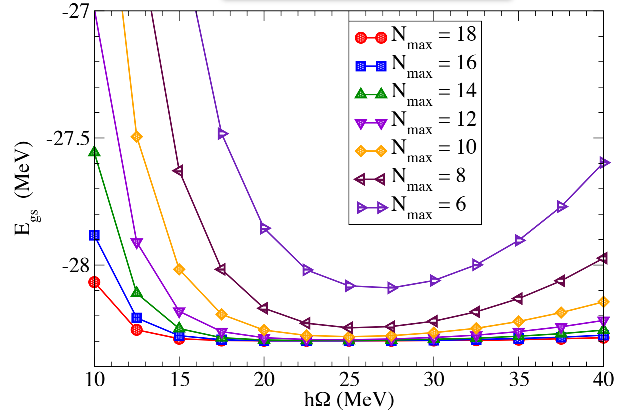
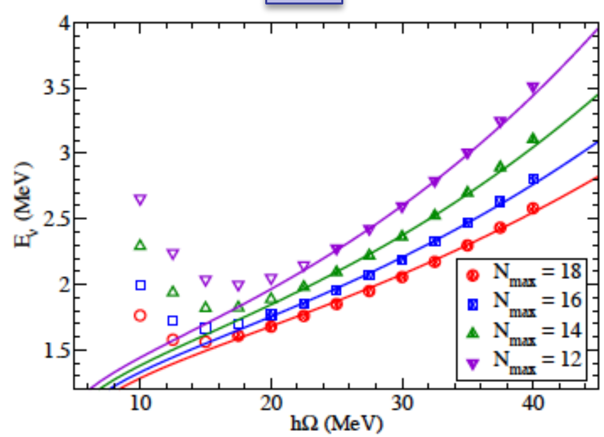
E(4He, gs)



=

E

=

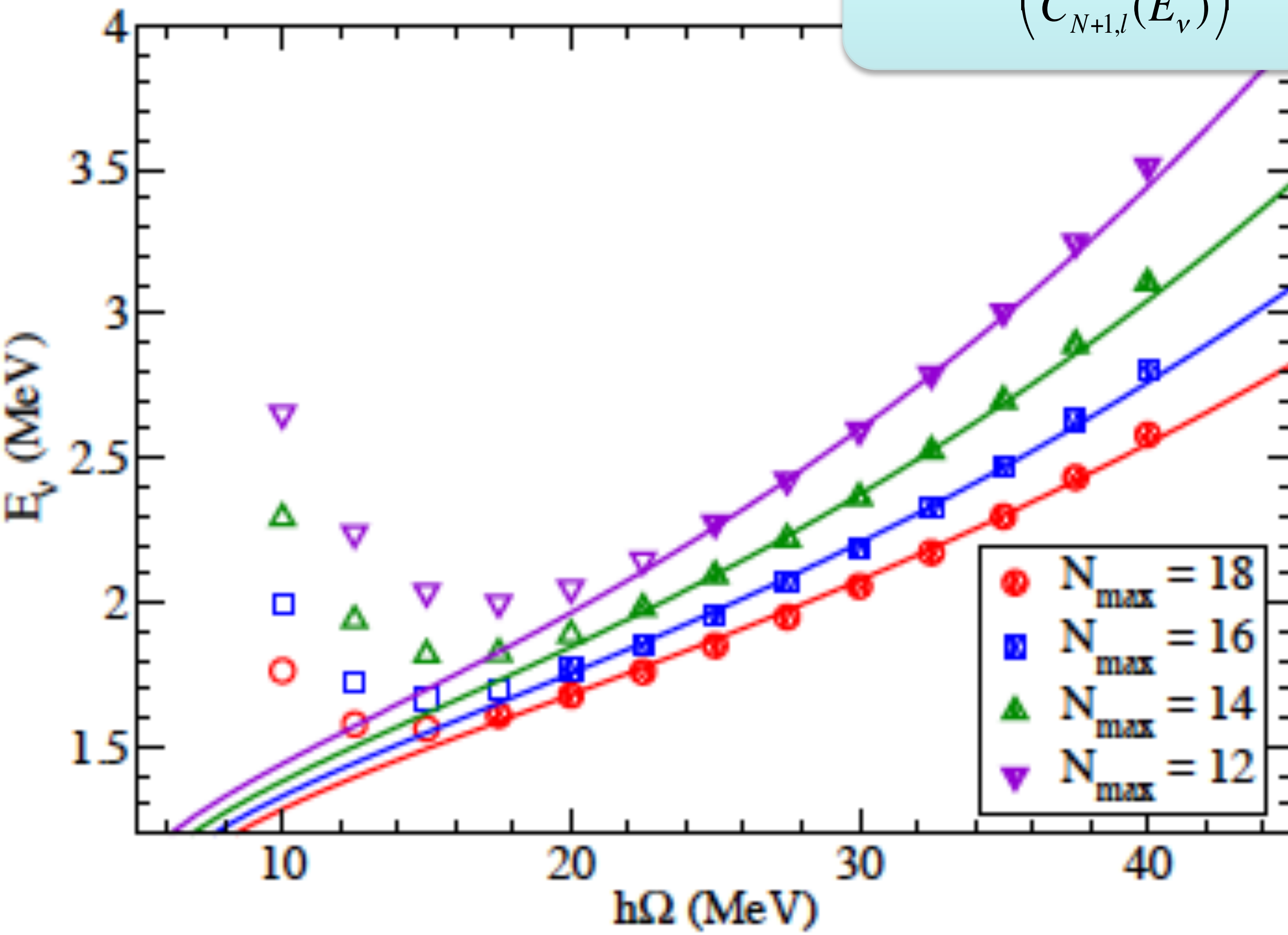


nα – scattering, resonance 3/2⁻

NCSM calculations for ^{5}He with JISP16

$$-\arctan\left(\frac{S_{N+1,l}(E_\nu)}{C_{N+1,l}(E_\nu)}\right) = -\arctan\left(\frac{a\sqrt{E_\nu}}{E_\nu - b^2}\right) + c\sqrt{E_\nu}$$

E(^{5}He, 3/2$^-$) – E(^{4}He, *gs*)



Best fit:

$a = 0.392\ MeV^{1/2}$

$b^2 = 1.286\ MeV$

$c = -0.475\ MeV^{-1/2}$

Resonance:

$E_r = 1.209\ MeV$

$\Gamma = 0.875\ MeV$

$\sqrt{\chi^2/datum} = 1.2^\circ$

nα – scattering, resonance 3/2⁻

Phase shift and resonances parameters

Resonance:

$E_r = 1.209\ MeV$

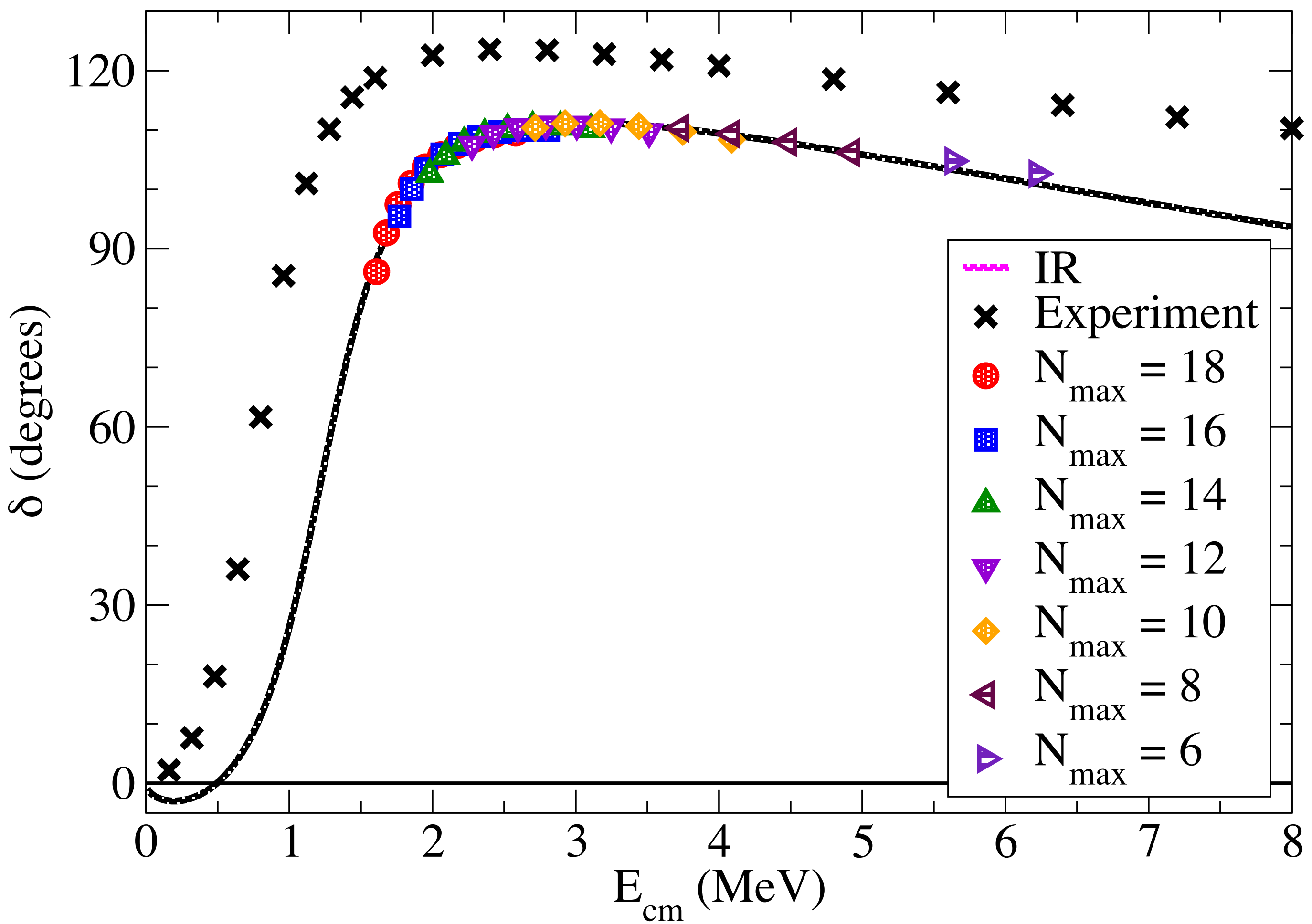
$\Gamma = 0.875\ MeV$

$\sqrt{\chi^2 / datum} = 1.2^\circ$

Experiment:

$E_r = 0.80\ MeV$

$\Gamma = 0.65\ MeV$

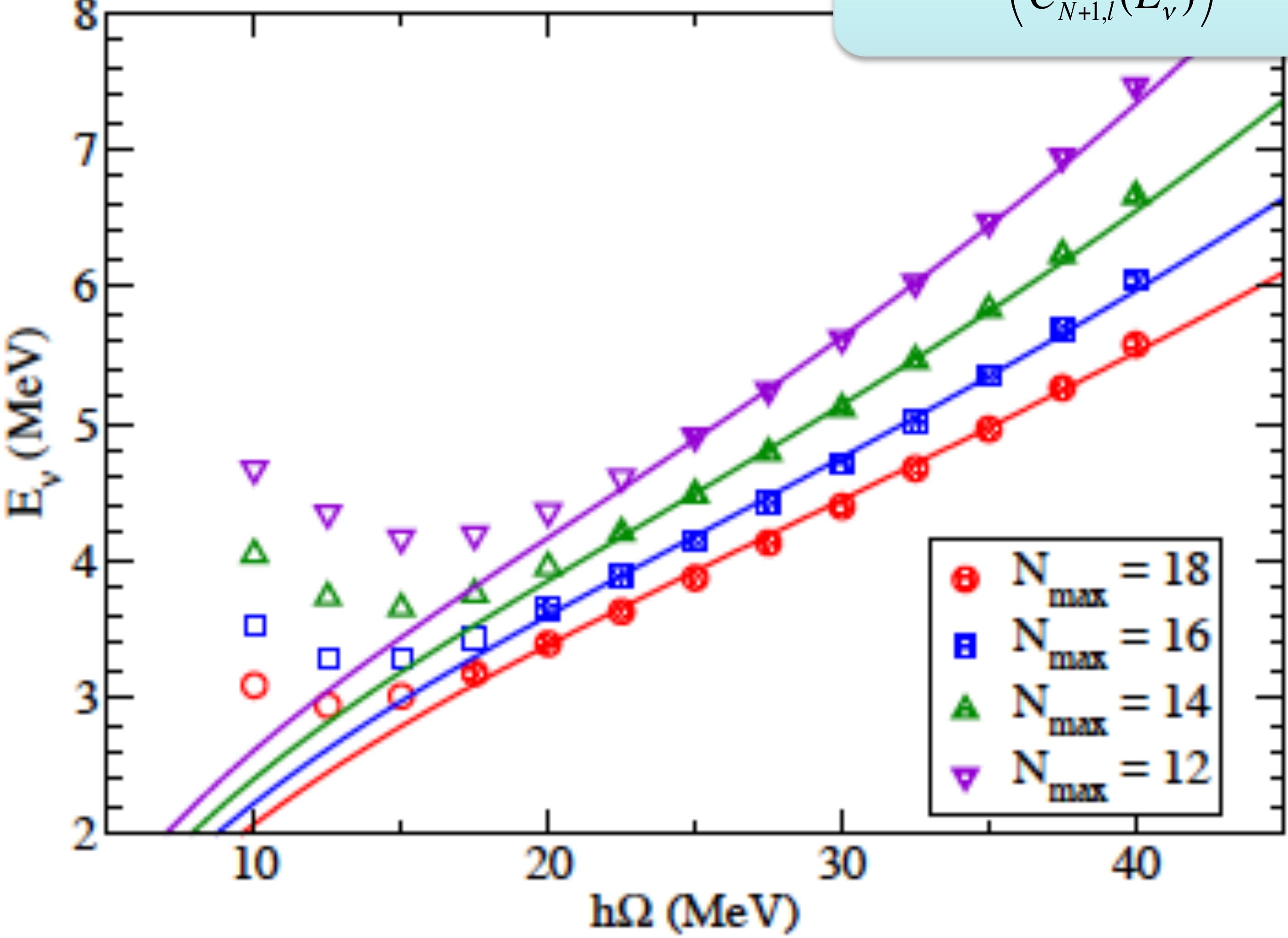


$n\alpha$ – scattering, resonance 1/2$^-$

NCSM calculations for ^{5}He with JISP16

$$-\arctan\left(\frac{S_{N+1,l}(E_\nu)}{C_{N+1,l}(E_\nu)}\right) = -\arctan\left(\frac{a\sqrt{E_\nu}}{E_\nu - b^2}\right) + c\sqrt{E_\nu}$$

$E(^5\text{He}, \tfrac{1}{2}^-) - E(^4\text{He}, gs)$



Best fit:

$a = 1.292\ MeV^{1/2}$

$b^2 = 3.432\ MeV$

$c = -0.535\ MeV^{-1/2}$

Resonance:

$E_r = 2.598\ MeV$

$\Gamma = 4.485\ MeV$

$\sqrt{\chi^2 / datum} = 0.8^\circ$

nα – scattering, resonance 3/2⁻

Phase shift and resonances parameters

Resonance:

$E_r = 2.598\ MeV$

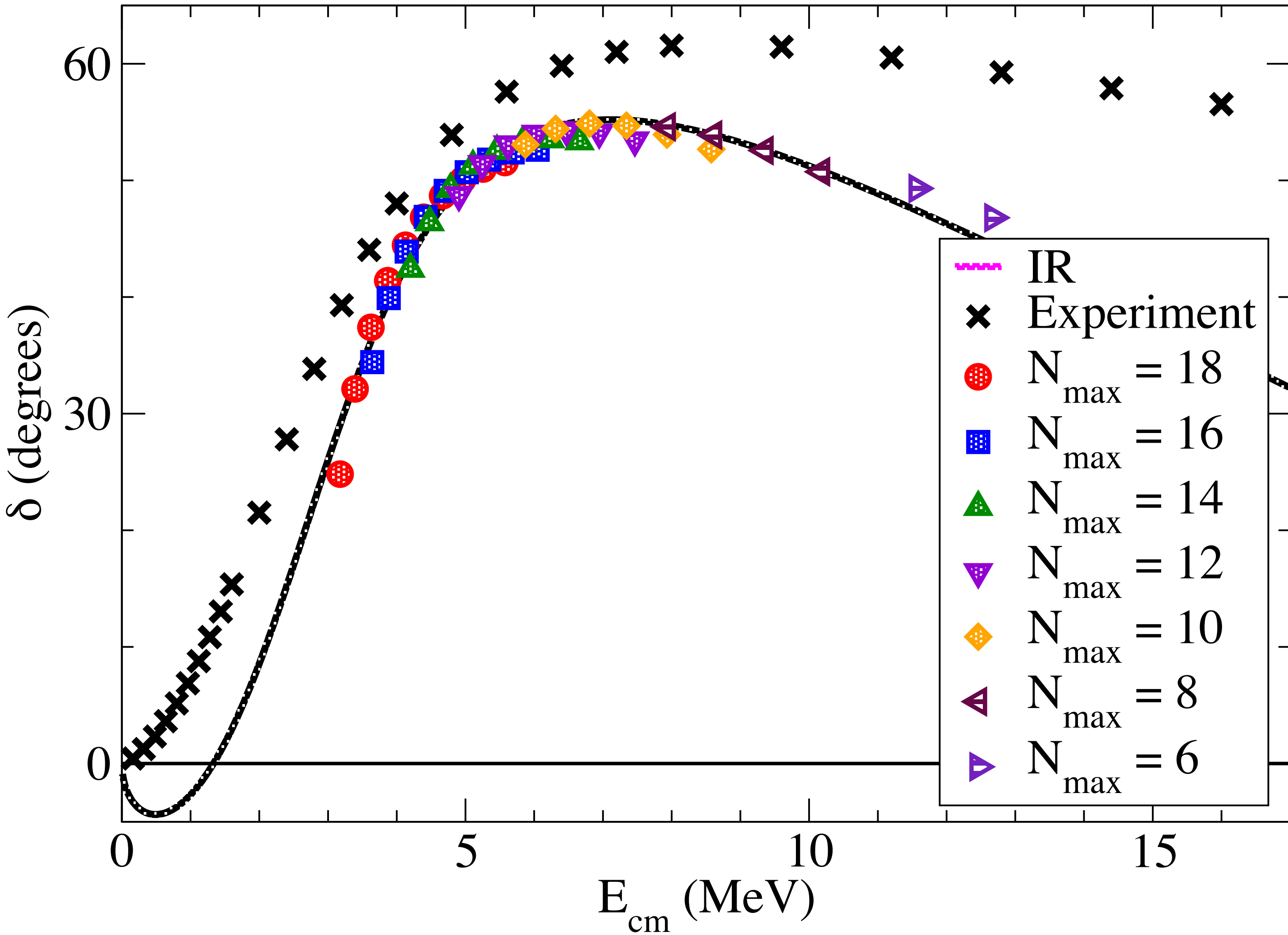
$\Gamma\ = 4.485\ MeV$

$\sqrt{\chi^2 / datum} = 0.8^\circ$

Experiment:

$E_r = 2.07\ MeV$

$\Gamma\ = 5.57\ MeV$



Conclusions

- *We suggest a new method to evaluate resonance energy and width. This method based on J-matrix is simple enough. But it works and provides a good estimate of resonance parameters.*

- *It seems that we achieved convergence of results for n*α *scattering extracted from NCSM calculations. It appears that disagreements between theory and experiment are due to JISP16, the NN interaction utilized in the study.*

Thank you!