Development of J-matrix approach for the analysis of resonant states obtained in no core shell model

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Highlights

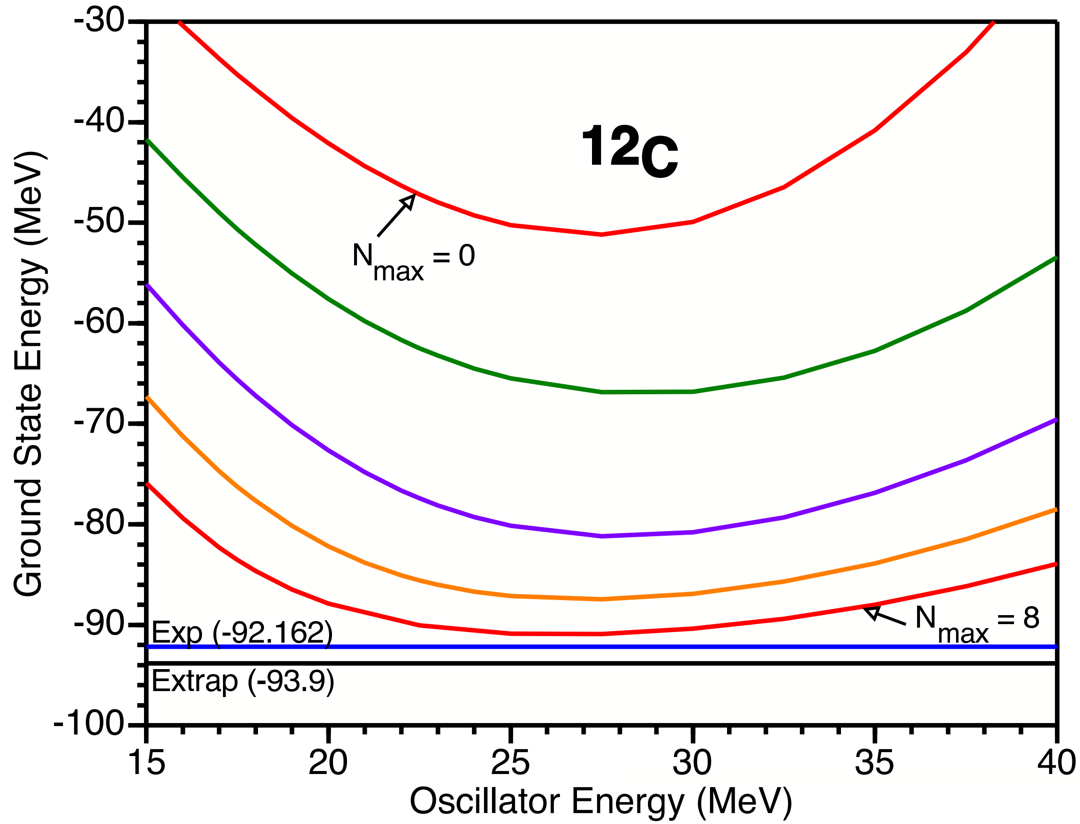
some general properties for oscillator basis calculations; this is the only relevance to NCSM

- ✓ Problem
- ✓ *J*-matrix formalism
- ✓ resonance information from E_λ

J-matrix ⟷ *NCSM: Nα scattering*

NB *this is still work in progress, some observations, examples*

Problem



Conventional:

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

Problem

Is it also true for resonant states?

Can we get resonance width from such calculations?

Opportunity:

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

$$H = H^0 + V$$

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

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

So, the phase shift at the eigenenergies E_j can be easily calculated!

Unfortunately, this does not work:

- *The dimensionality of the matrix is small, the average spacing between the levels is not well-defined.*
- *One needs sometimes D_j value below the lowest E_j^0*

J-matrix

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

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

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

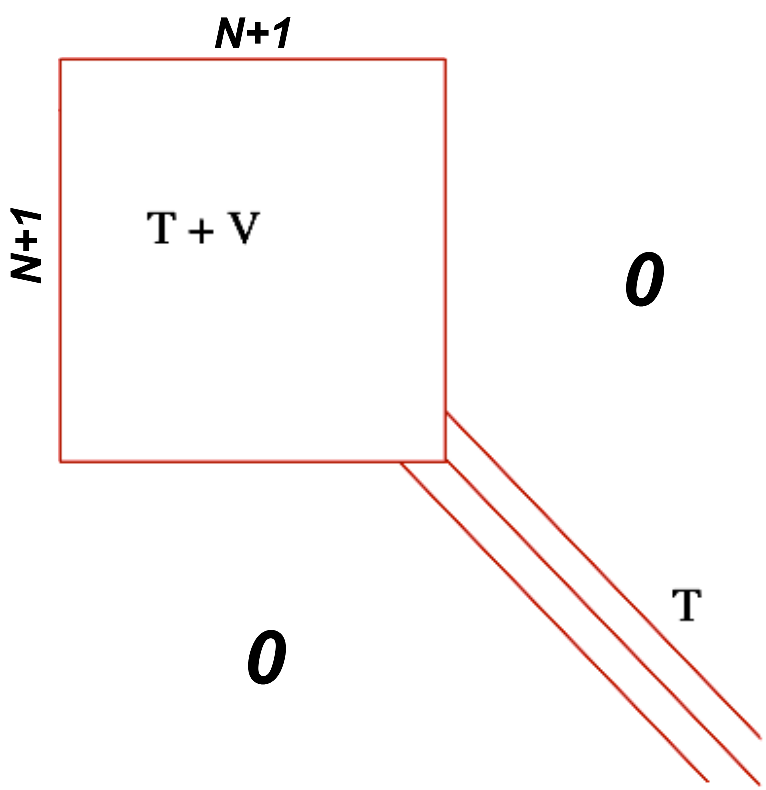
$r_0 = \sqrt{\hbar / m\omega}$, $\hbar\omega$ ***– oscillator parameters, m – reduced mass.***

$E = (q^2/2)\hbar\omega$ ***– c.m. energy,*** ***q = kr₀*** ***– dimensionless momentum.***

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

J-matrix

Structure of Hamiltonian:



parameters: $N+1,\ \hbar\omega$

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:

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

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

$E_\lambda,\ \langle n|\lambda\rangle\ (\lambda = 0,1,\ldots,N)$ ***are obtained from*** $\sum_{n'=0}^{N} H^{l}_{nn'}\langle n'|\lambda\rangle = E_\lambda\langle n|\lambda\rangle,\ n \le N$

Regular and irregular oscillator solutions

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

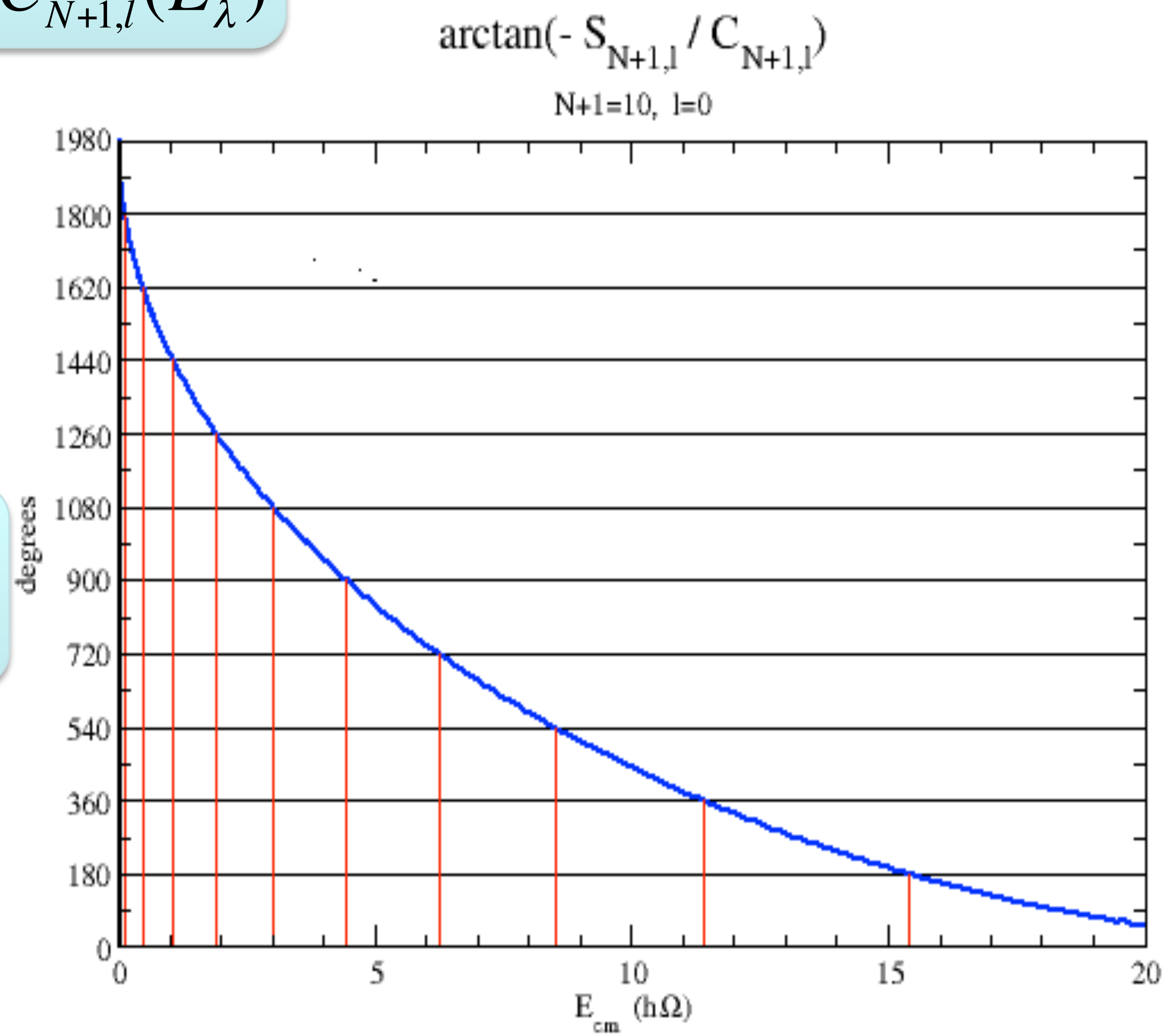
$$C_{nl}(q) = (-1)^l\sqrt{\frac{\pi r_0 n!}{\Gamma(n+l+3/2)}}\ \frac{q^{-l}}{\Gamma(-l+1/2)}\exp\left(-\frac{q^2}{2}\right)\Phi(-n-l-1/2,-l+1/2;q^2)\ .$$

J-matrix

$$E \to E_\lambda : \Rightarrow \tan\delta = -\frac{S_{N+1,l}(E_\lambda)}{C_{N+1,l}(E_\lambda)}$$

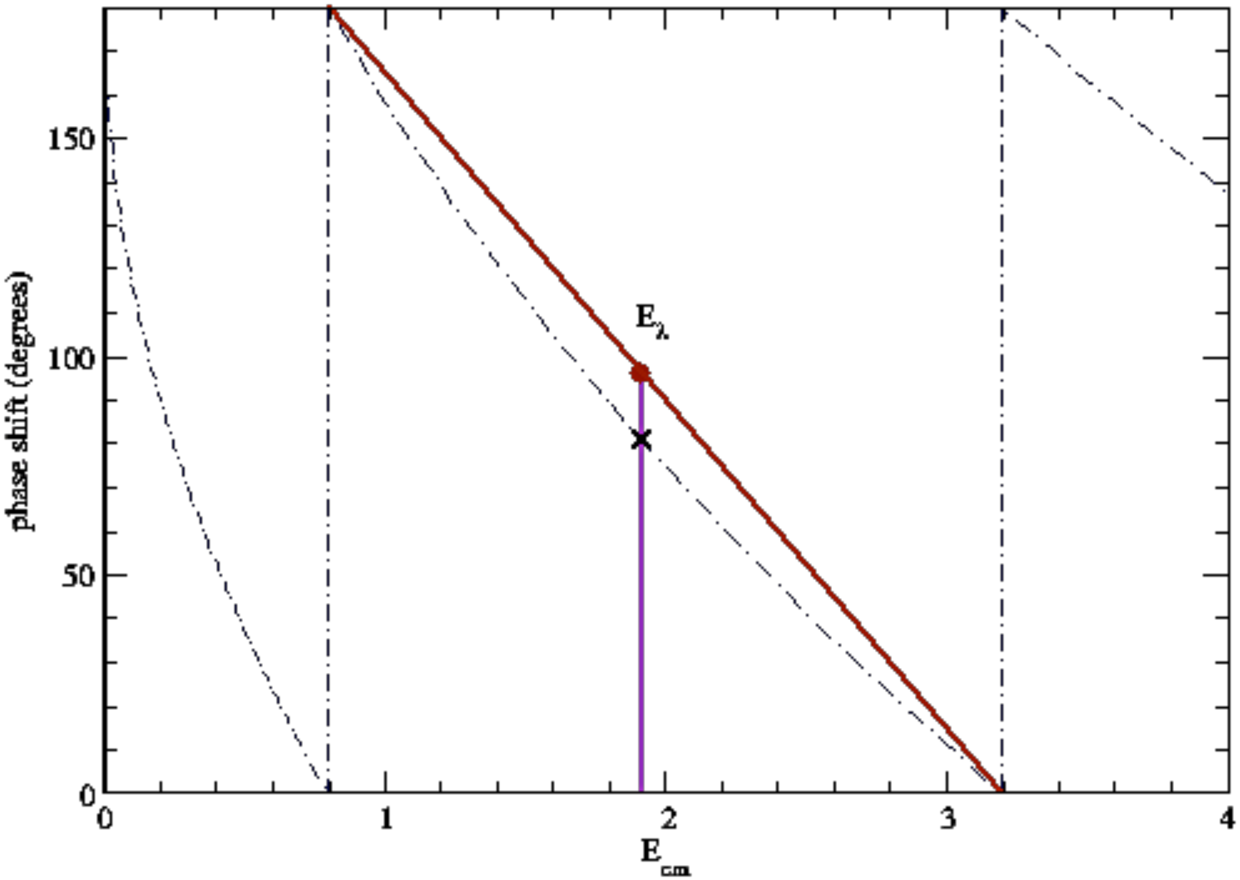
universal function

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



J-matrix

compare J-matrix with Lifshitz



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: ✖

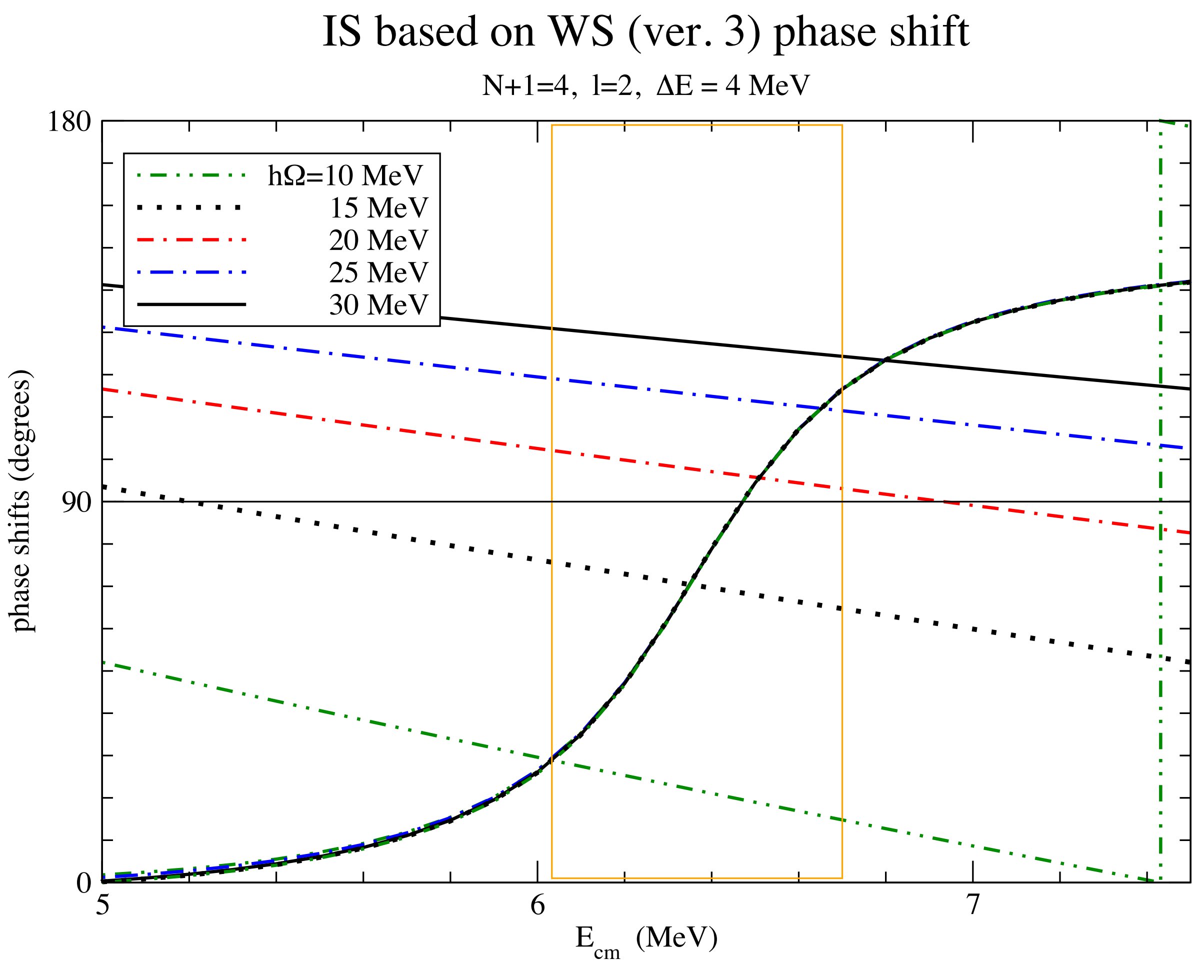
$$\delta(E_\lambda) = -\arctan\left(\frac{S_{N+1,l}(E_\lambda)}{C_{N+1,l}(E_\lambda)}\right)$$

J-matrix resonance information from E_λ

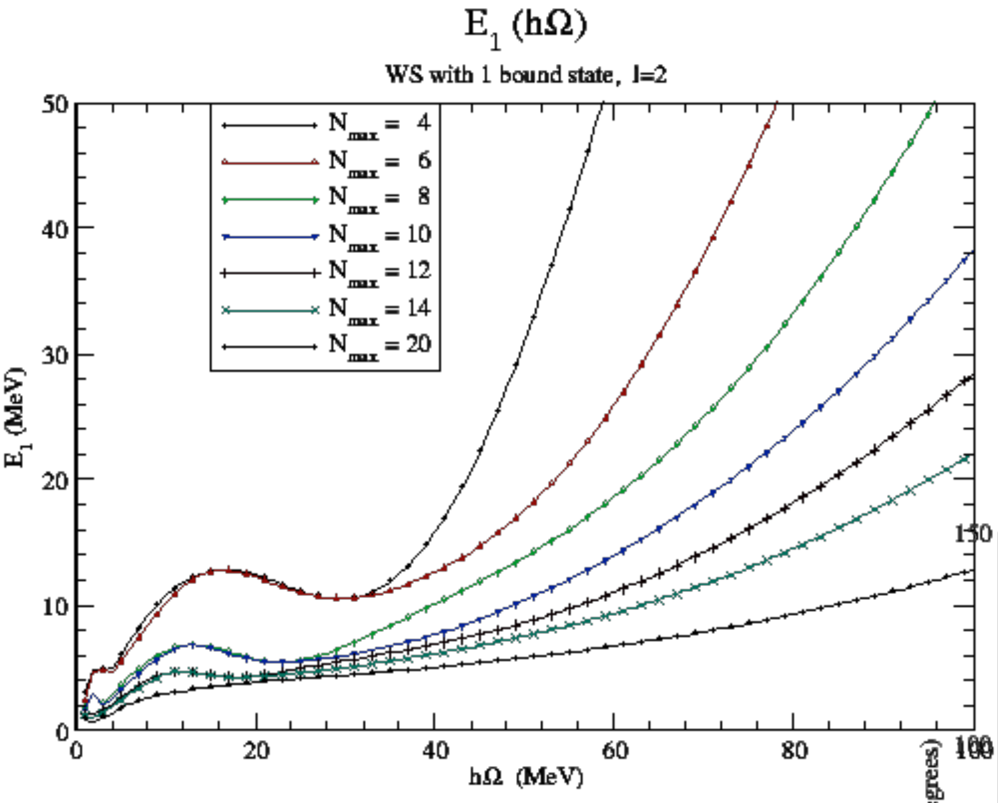
Let us try to extract resonance information from E_λ behavior only

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

- *E_λ should increase with $\hbar\omega$*
- *Within narrow resonance E_λ is nearly $\hbar\omega$-independent*
- *The slope of $E_\lambda(\hbar\omega)$ depends however on N_{max}, l, E_λ value*



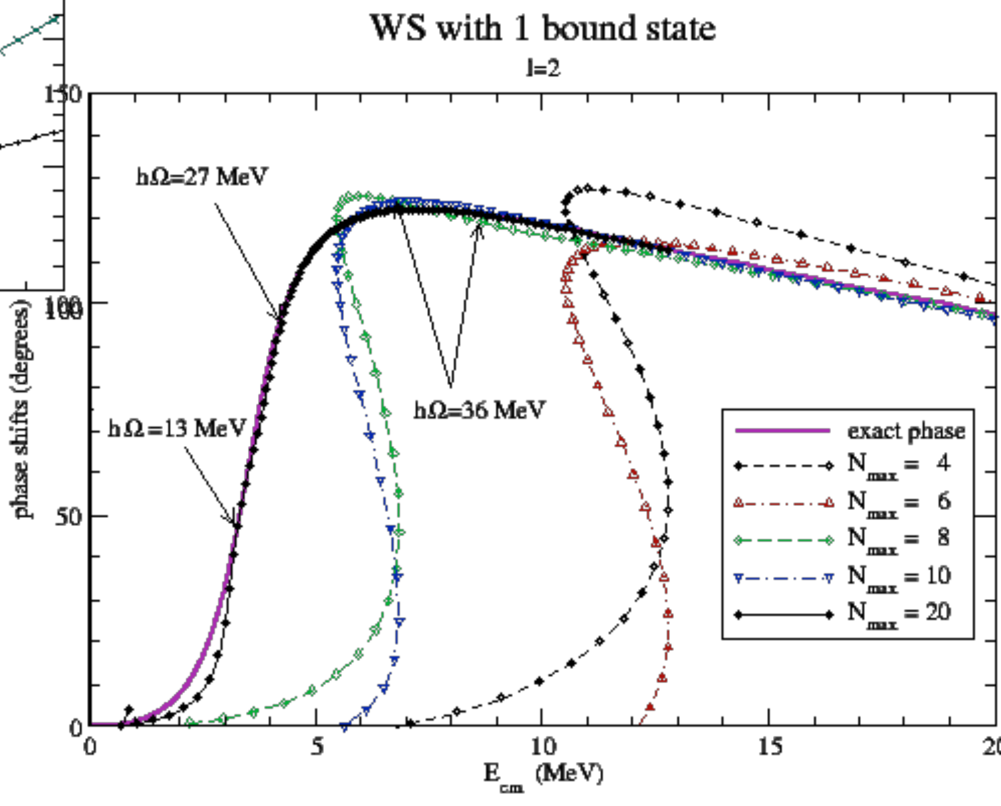
J-matrix



corresponding phase shift values

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

$E_\lambda(\hbar\omega)$ dependence



Resonance

- Breit-Wigner:

$$\delta^{BW} = \arctan \frac{\Gamma/2}{E_r - E} + \varphi$$

$$\tan \delta(E_\lambda) = -\frac{S_{N+1,l}(q_\lambda)}{C_{N+1,l}(q_\lambda)}$$

$$E_r = E_\lambda + \Delta_\lambda$$

- Simple approximation: φ=0

$$\tan \delta(E_\lambda) = -\frac{S_{N+1,l}(q_\lambda)}{C_{N+1,l}(q_\lambda)} = \frac{\Gamma/2}{\Delta}$$

$$\left. \frac{d \tan \delta(E)}{dE} \right|_{E=E_\lambda} = \frac{\Gamma/2}{\Delta^2}$$

Derivatives calculated through

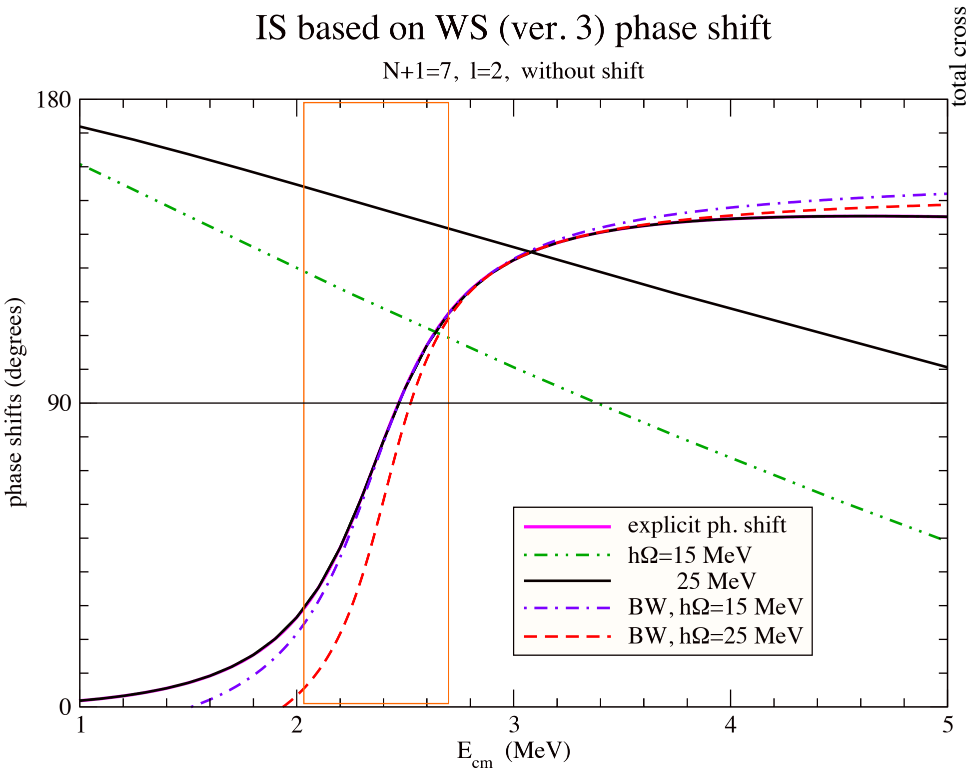
$$E_\lambda(\hbar\Omega), E_\lambda^{\pm}(\hbar\Omega \pm \Delta(\hbar\Omega))$$

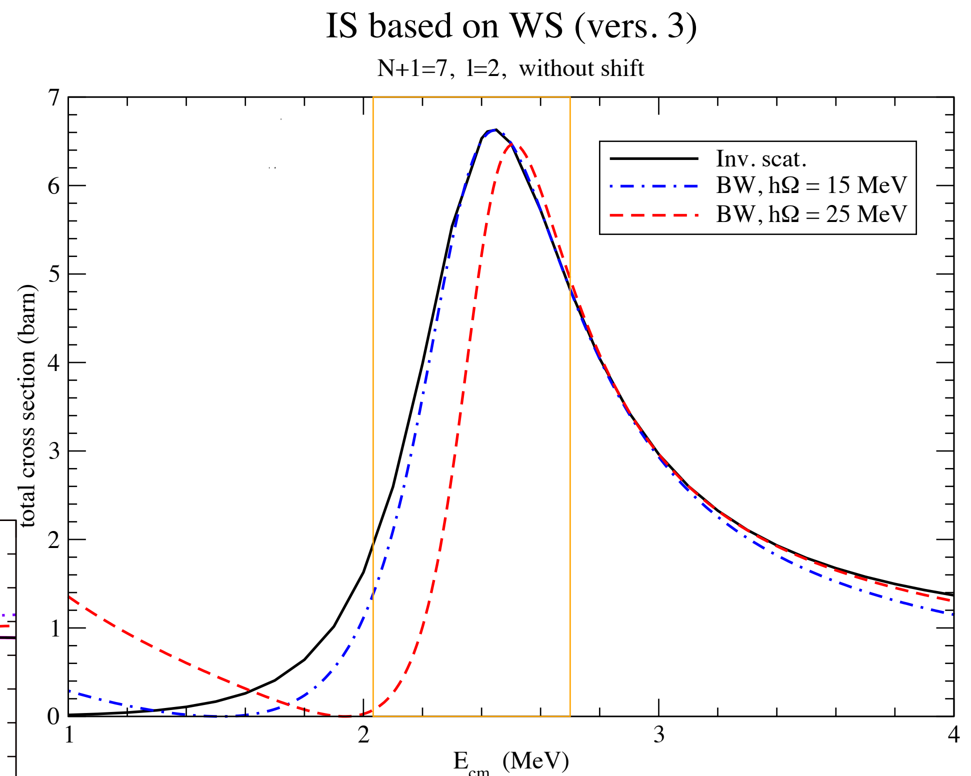
Do not expect to get a reasonable result for E_r or Γ if Γ/2Δ is small!

If |Γ/2Δ| is large, we get good results for E_r, Γ and φ.

Resonance

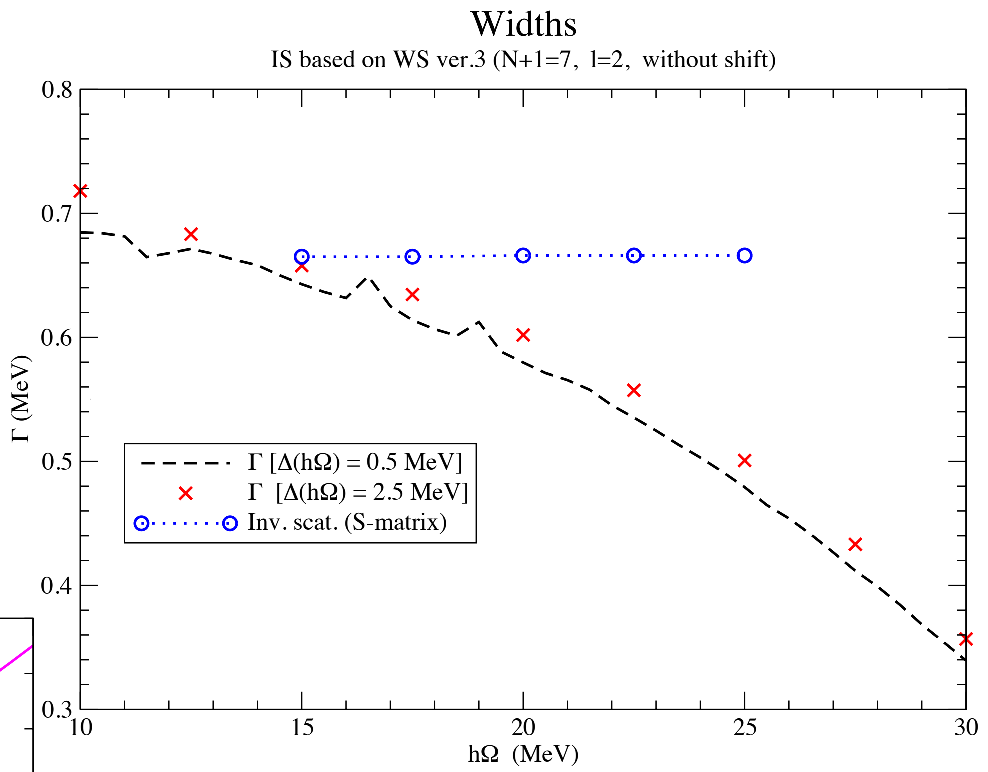
phase shift



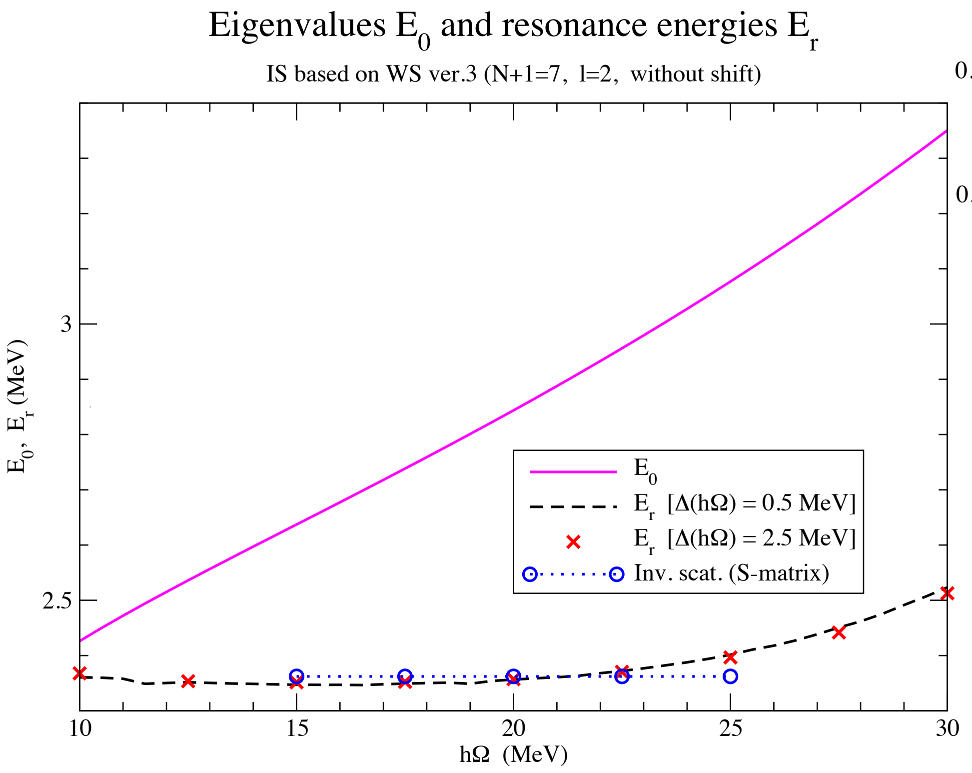


cross section

Resonance



Breit-Wigner: $E_r(\hbar\omega)$



Breit-Wigner: $\Gamma(\hbar\omega)$

Resonance

What can we do if we obtain E_λ
in a non-resonant region
above the resonance?

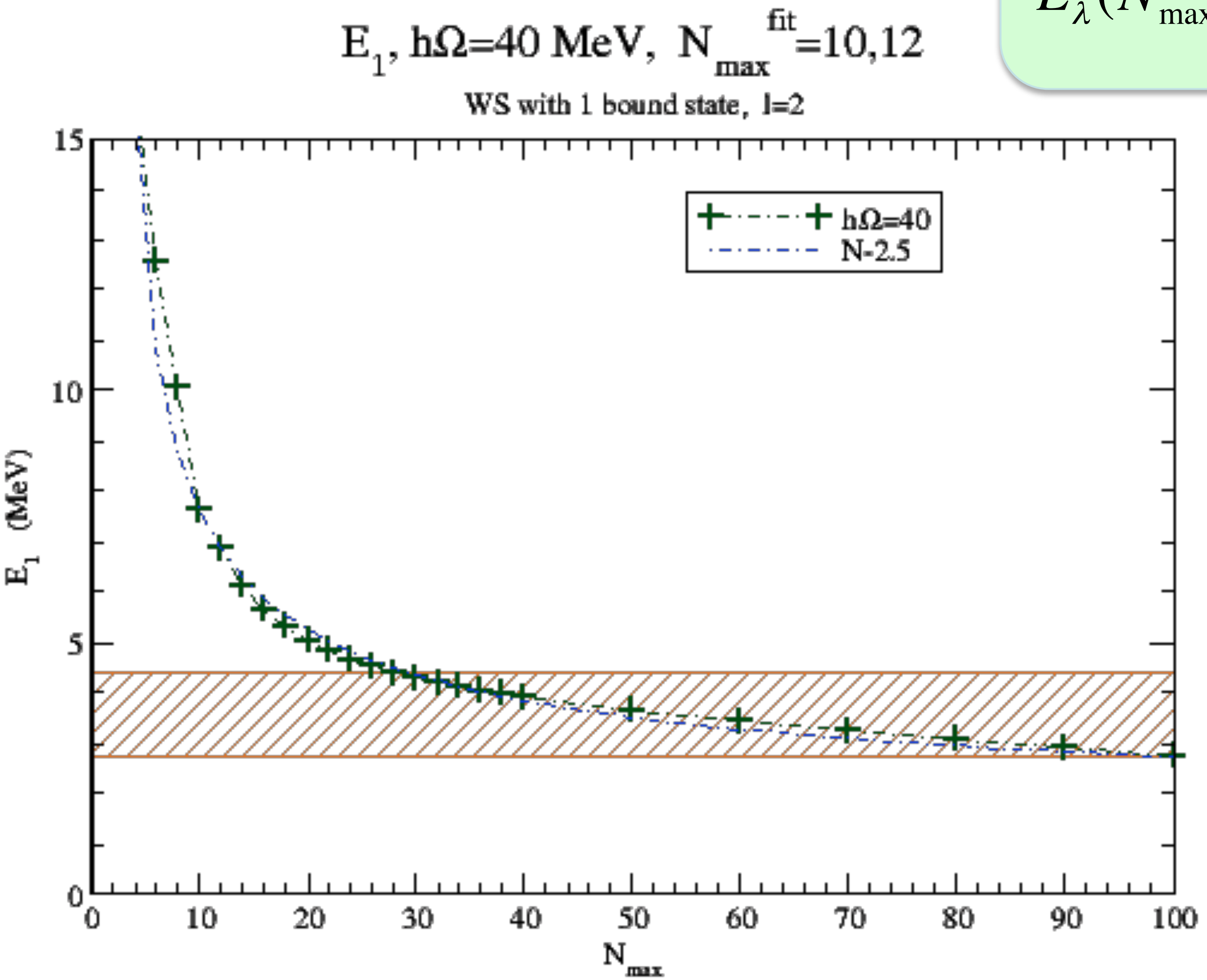
- We can extrapolate energies to larger (but finite) N_{max} value when E_λ is in the resonant region.

Expected dependence is $E_\lambda(N_{\mathrm{max}}) \approx A \frac{\exp(-a\sqrt{N_{\mathrm{max}}+b})}{\sqrt{N_{\mathrm{max}}+b}}$

Resonance

extrapolation

$$E_\lambda(N_{\max}) \approx A\frac{\exp(-a\sqrt{N_{\max}+b})}{\sqrt{N_{\max}+b}}$$

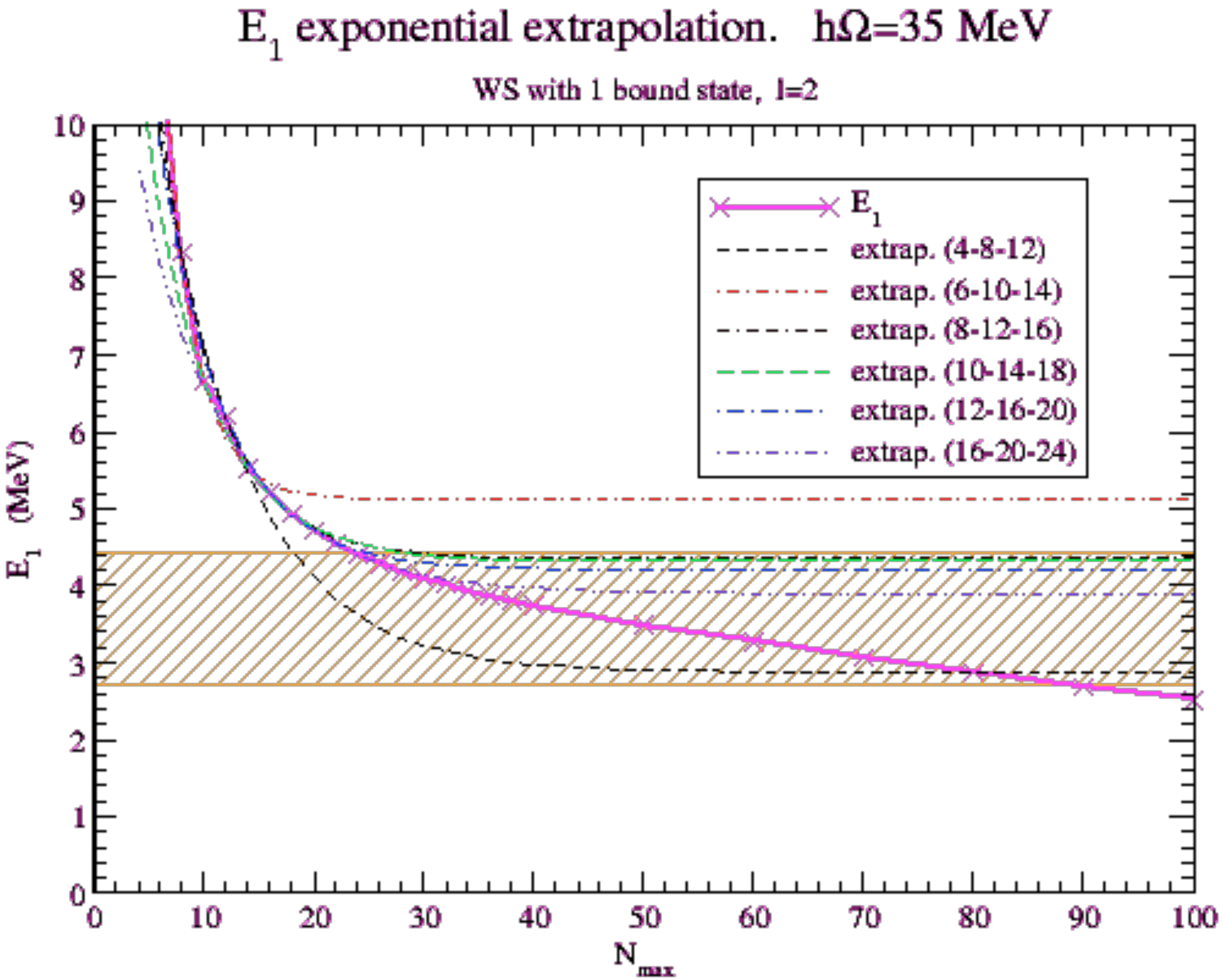


This works. However this extrapolation seems to be unstable and inconvenient

Resonance

More convenient is
an exponential xtrapolation

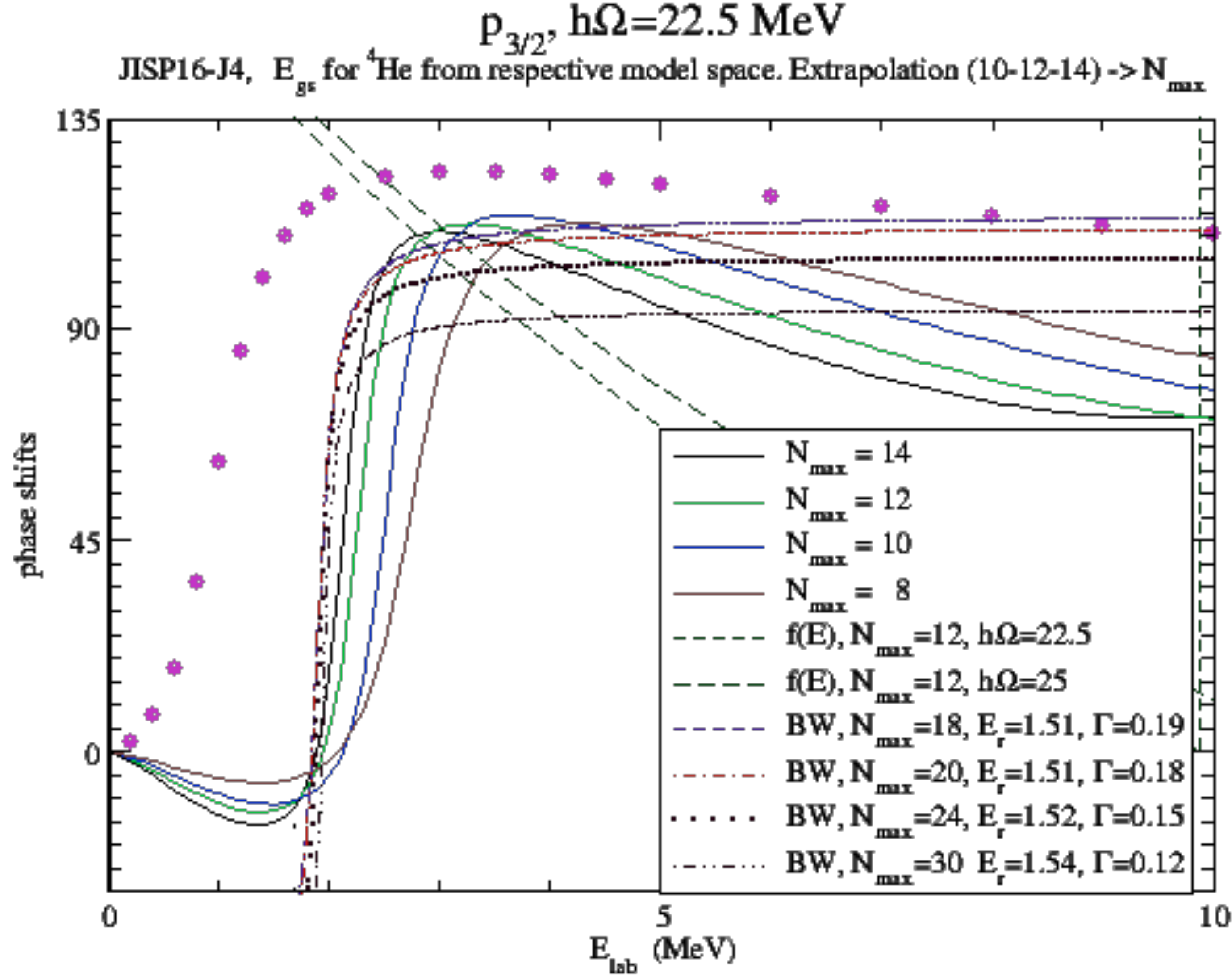
$$E_\lambda(N_{max}) = a\exp(-cN_{max}) + E_\lambda(\infty)$$



nα scattering

Resonance parameters obtained from NCSM calculations for ^{5}**He**

- We get stable E_r and Γ;
- Γ is too small as compared with experiment.



Conclusions

- *The best way to compare the calculated results with experiment is to use "experimental" phase shifts and get E_λ consistent with scattering data using simple inverse scattering technique.*

- *Studying $\hbar\omega$ dependence of E_λ obtained in NCSM, one can get resonance energy and width. However, usually an extrapolation to a reasonable N_{max} value is required.*

Спасибо за внимание!