Oscillator Basis and Scattering

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Oscillator Basis and Scattering

Oscillator basis is widely used is nuclear structure studies, in *ab initio* NCSM in particular.

Is there a way to relate directly results of shell model calculations with oscillator basis to scattering information?

I suggest to start from constructing oscillator basis. It can be generated using the Lanczos algorithm. As a result, it is possible to formulate a Lanczos scheme which combines naturally scattering and nuclear structure problems.

Oscillator Basis and Scattering

Plan:

Constructing infinite oscillator basis using Lanczos scheme. Free motion, Hamiltonian, boundary conditions for scattering and bound states.

How this scheme can be applied to *ab initio* studies of many-body systems.

Simple example: You obtained a state E_i in continuum in shell model (e.g., NCSM) calculation – how is it related to the experimental scattering information? Which E_i values are consistent with scattering phase shifts?

Important consequence: Sid Coon et al [PRC 86, 054002 (2012)] extrapolations for resonant states.

Lanczos algorithm

$\varphi_0 -$ arbitrary (random) pivot vector

$\varphi_{-1} = 0$

$\beta_0 = 0$

Iterations:

$\phi_{j+1} = H\varphi_j$

orthogonalizing ϕ_{j+1} to φ_j and φ_{j-1} and normalizing:

$\alpha_j = \langle \phi_{j+1} | \varphi_j \rangle$

$\tilde{\phi}_{j+1} = \phi_{j+1} - \alpha_j \varphi_j - \beta_j \varphi_{j-1}$

$\beta_{j+1} = ||\tilde{\phi}_{j+1}||$

$$\varphi_{j+1} = \frac{\tilde{\phi}_{j+1}}{\beta_{j+1}}$$

$$\langle \varphi_i | H | \varphi_j \rangle = \begin{pmatrix} \alpha_0 & \beta_1 & & & \\ \beta_1 & \alpha_1 & \beta_2 & & 0 \\ & \beta_2 & \alpha_2 & \ddots & \\ & & \ddots & \ddots & \beta_{N-1} \\ & 0 & & \beta_{N-1} & \alpha_{N-1} & \beta_N \\ & & & & \beta_N & \alpha_N \end{pmatrix}$$

Oscillator basis

* Matrix of the kinetic energy operator T is tridiagonal in oscillator basis: $T_{nm} = 0$ if $|n - m| > 1$.

$$T\varphi_n = T_{n,n-1}\varphi_{n-1} + T_{nn}\varphi_n + T_{n,n+1}\varphi_{n+1}$$

* Kinetic energy operator T generates oscillator basis
* either from below:

$$\varphi_0, \quad T\varphi_0 \Rightarrow \varphi_1, \quad T\varphi_1 \Rightarrow \varphi_2, \ \ldots$$

* or from above:

$$\ldots, \ \varphi_{M+1}, \ \varphi_M, \quad T\varphi_M \Rightarrow \varphi_{M-1}, \quad T\varphi_{M-1} \Rightarrow \varphi_{M-2}, \ \ldots, \ \varphi_0$$

Free Schrödinger equation

$$T\Psi = E\Psi$$

* Wave function expanded in oscillator basis:

$$\Psi = \sum_{n=0}^{\infty} a_n \varphi_n$$

* The kinetic energy matrix in oscillator basis is tridiagonal, hence a_n are solutions of a three-term recurrent relation (TRR):

$$T_{n,n-1}a_{n-1} + (T_{nn} - E)a_n + T_{n,n+1}a_{n+1} = 0$$

Free Schrödinger equation: TRR solutions

$$T_{n,n-1}a_{n-1} + (T_{nn} - E)a_n + T_{n,n+1}a_{n+1} = 0\ ; \qquad n > N$$

* Analytical expressions are known for linearly-independent solutions s_n and c_n of this TRR.

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

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

Free Schrödinger equation: TRR solutions

$$T_{n,n-1}a_{n-1} + (T_{nn} - E)a_n + T_{n,n+1}a_{n+1} = 0$$

* Properties of s_n and c_n for $E > 0$:

$$\sum_{n=0}^{\infty} s_n(E)\,\varphi_n = \Psi_E^0 = \sqrt{\frac{2}{\pi}}\,kr\,j_l(kr) \underset{r\to\infty}{\longrightarrow} \sqrt{\frac{2}{\pi}}\sin\left(kr - \frac{\pi l}{2}\right),$$

$$\sum_{n=0}^{\infty} c_n(E)\,\varphi_n \underset{r\to\infty}{\longrightarrow} \Psi_E^{0irreg} = \sqrt{\frac{2}{\pi}}\,kr\,n_l(kr) \underset{r\to\infty}{\longrightarrow} \sqrt{\frac{2}{\pi}}\,\cos\left(kr - \frac{\pi l}{2}\right).$$

* Any TRR solution a_n can be expressed as $a_n = \cos\delta\, s_n + \sin\delta\, c_n$ at $E > 0$, where δ is a scattering phase shift.

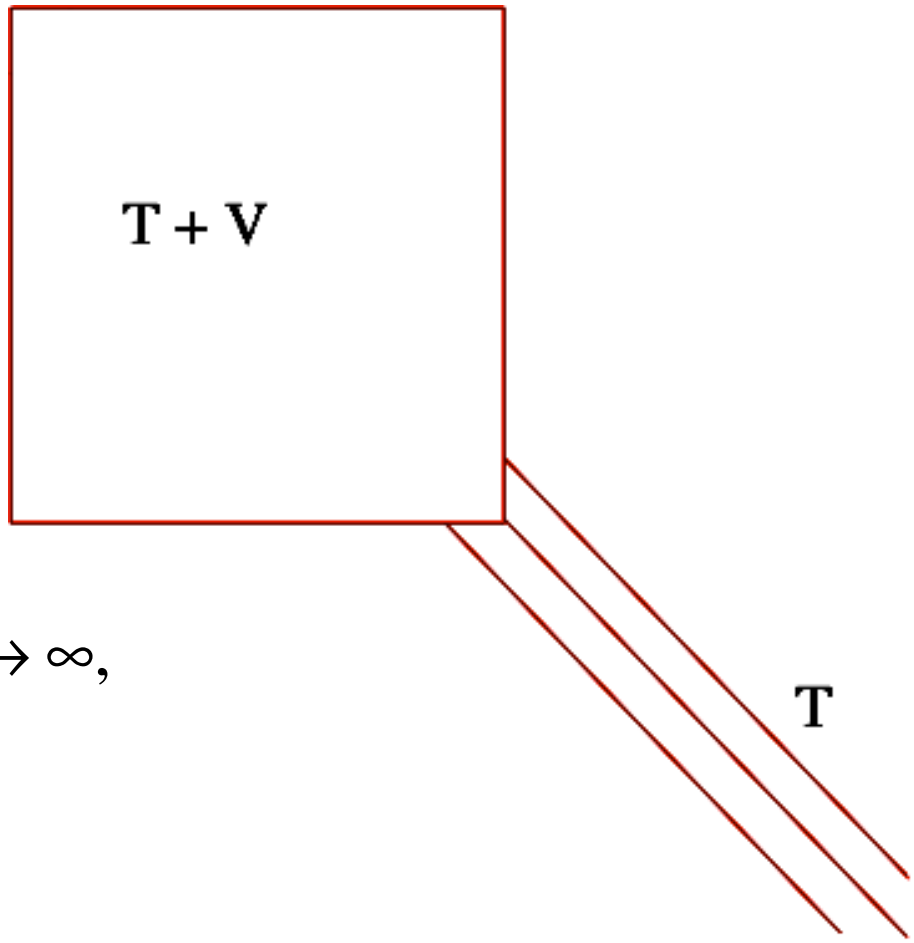
* For bound states ($E < 0$), a physically acceptable solution $c_n^+ = c_n + is_n$ rapidly decreases with n

Hamiltonian

$H = T + V$

A reasonable approximation is to truncate the potential energy matrix: $V_{nm} = 0$ for $n,m > N$, kinetic energy is not truncated.

Justification: kinetic energy m. e. increase with n linearly at large n: $T_{nn} \sim n,\ T_{n,n\pm1} \sim n,\ n \to \infty,$ while potential energy m. e. V_{nm} decrease with n and m.



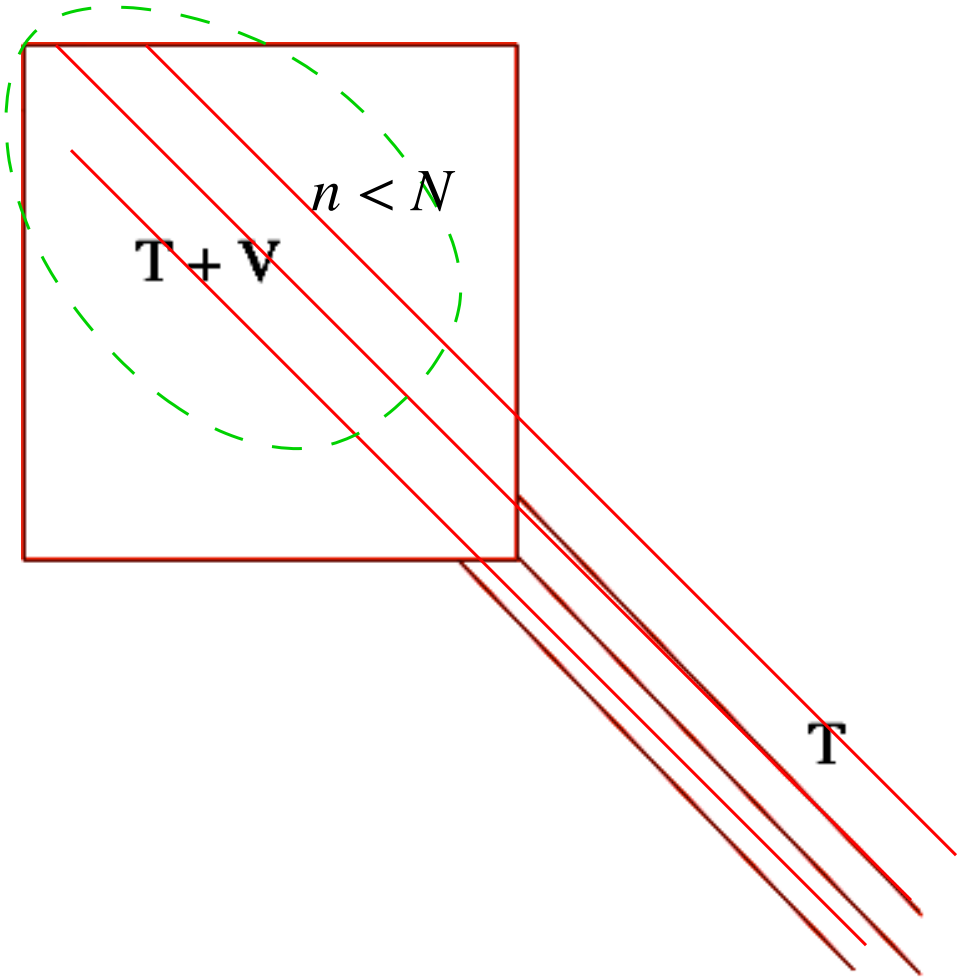
Lanczos algorithm

$H = T + V$

$V_{nm} = 0$ for $n,m > N$, kinetic energy matrix is infinite.

With H we first generate from above the oscillator basis functions φ_ν with $n \geq N$.

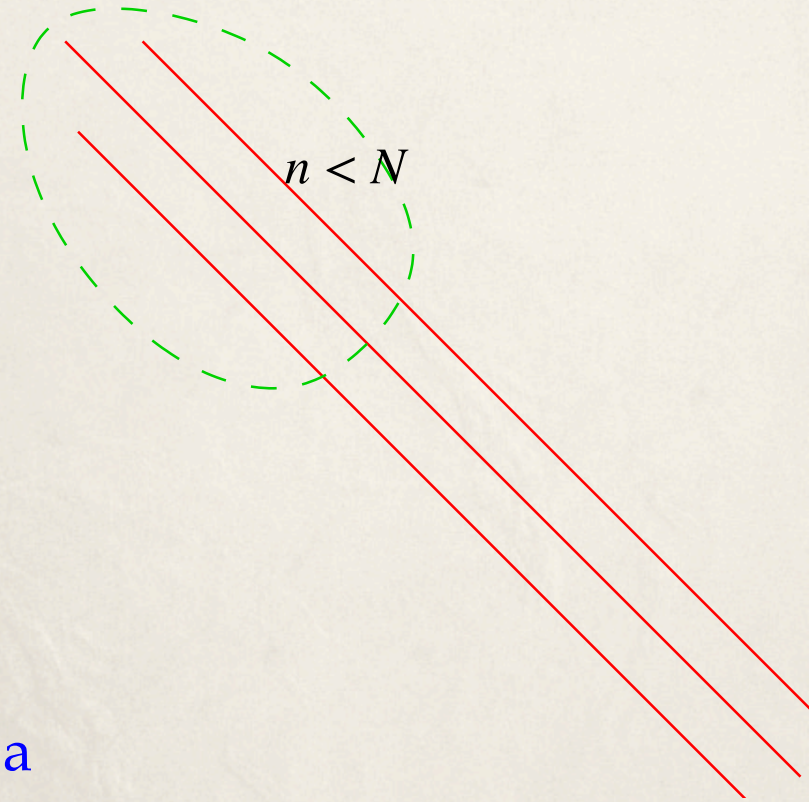
After that we construct Lanczos basis of states Φ_m which are superpositions of oscillator states φ_ν with $n \leq N$. H is tridiagonal in this basis.



Lanczos HORSE = *J*-matrix

HORSE = Harmonic Oscillator Representation of Scattering Equations

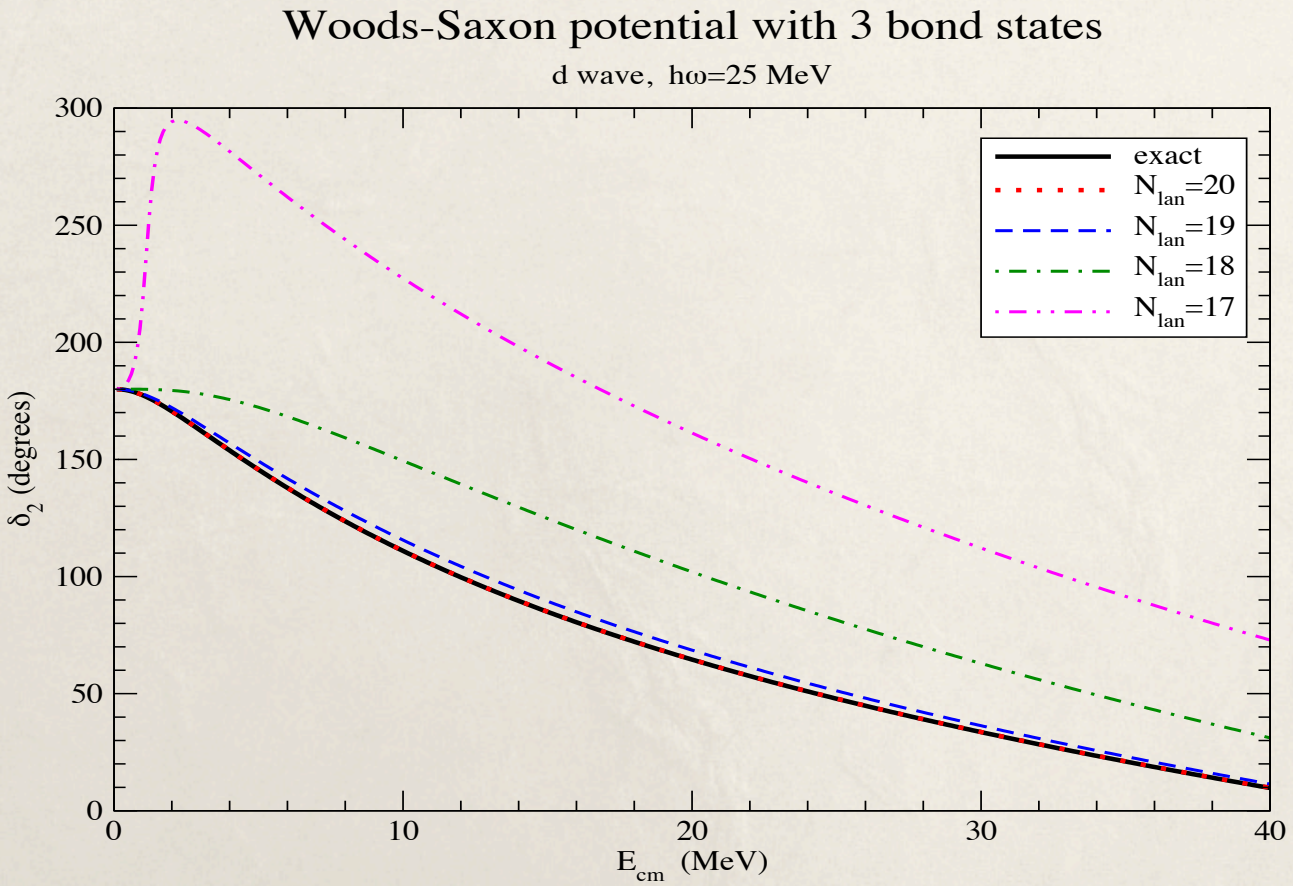
This is a reformulation of the *J*-matrix formalism known in scattering theory. Hopefully it is more convenient for realization of an *ab initio* no-core shell model approach to reactions.



We just extended a usual Lanczos procedure convenional for many-body applications which should be used with a different boundary condition: (i) scattering $a_n = \cos\delta\, s_n + \sin\delta\, c_n$ or (ii) decreasing a_n at large n.

How does it work and does it work at all?

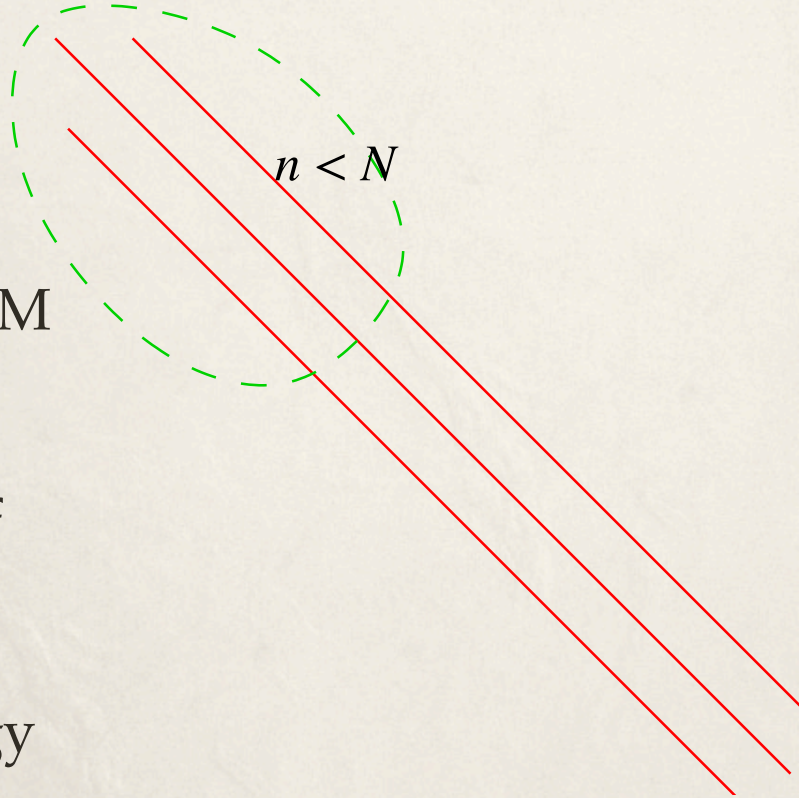
Scattering



Calculations are performed using the standard Lanczos algorithm with a specific pivot

Possible many-body *ab initio* applications

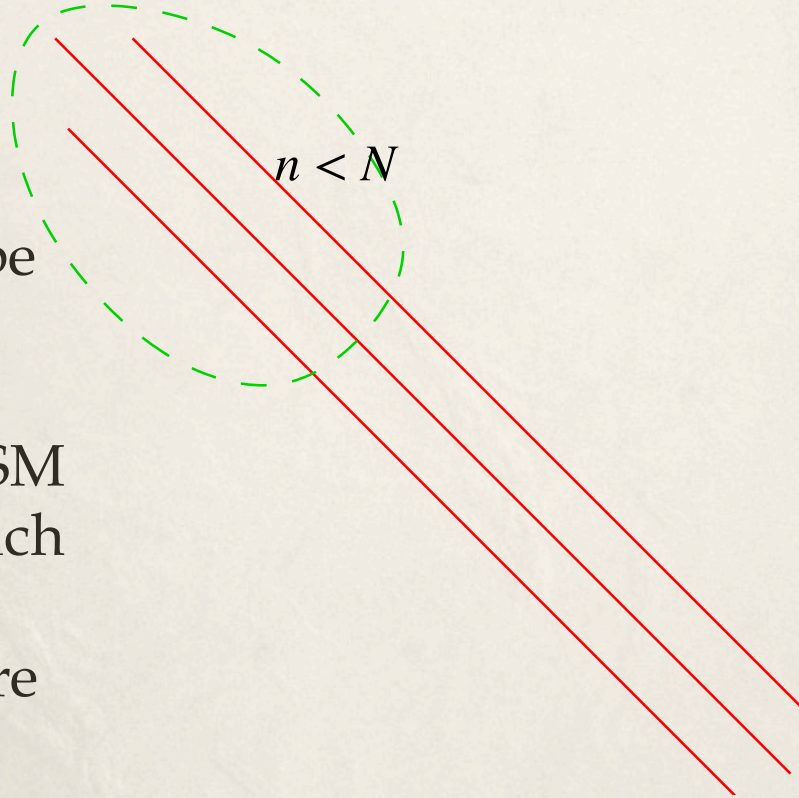
n-A scattering: if Ψ_A is obtained with N_{max}= 0, everything looks like a conventional Lanczos SM run in the A+1 system with a specific pivot vector. The SM Lanczos basis is extended analytically to involve states with large quanta. Interpretation of the results is different. If Ψ_A is obtained with N_{max}> 0, we need to add $N_{max}/2$ vectors to the conventional Lanczos scheme coupled by kinetic energy to the rest vectors.



$a_n = \cos\delta\, s_n + \sin\delta\, c_n,\ n \geq N.$

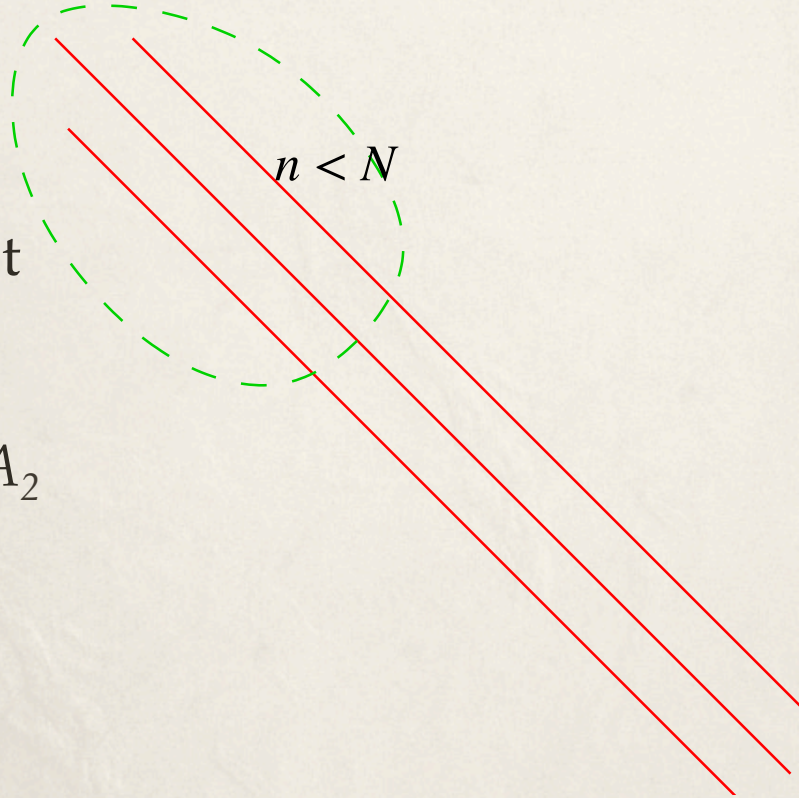
$$\Psi_{A+1} = \Psi_A \psi_{rel}$$

Possible many-body *ab initio* applications



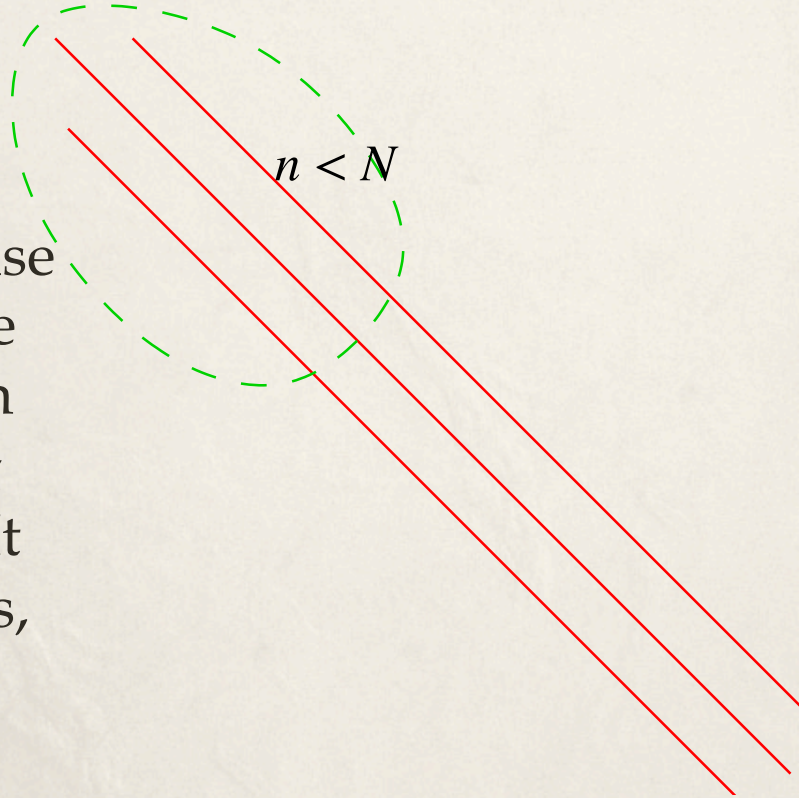
p-A scattering: Coulomb interaction can be included in the approach. One of the respective methods requires adding additional channel states in the Lanczos SM run in the A+1 system – the number of such states is about 50—80. Another method allowing for the Coulomb does not require adding additional channel states.

Possible many-body *ab initio* applications



$A_1 + A_2$ scattering: looks like that the most complicated problem now is transformation from the $A_1 + A_2$ cluster structure to the SM structure of the $A_1 + A_2$ system.

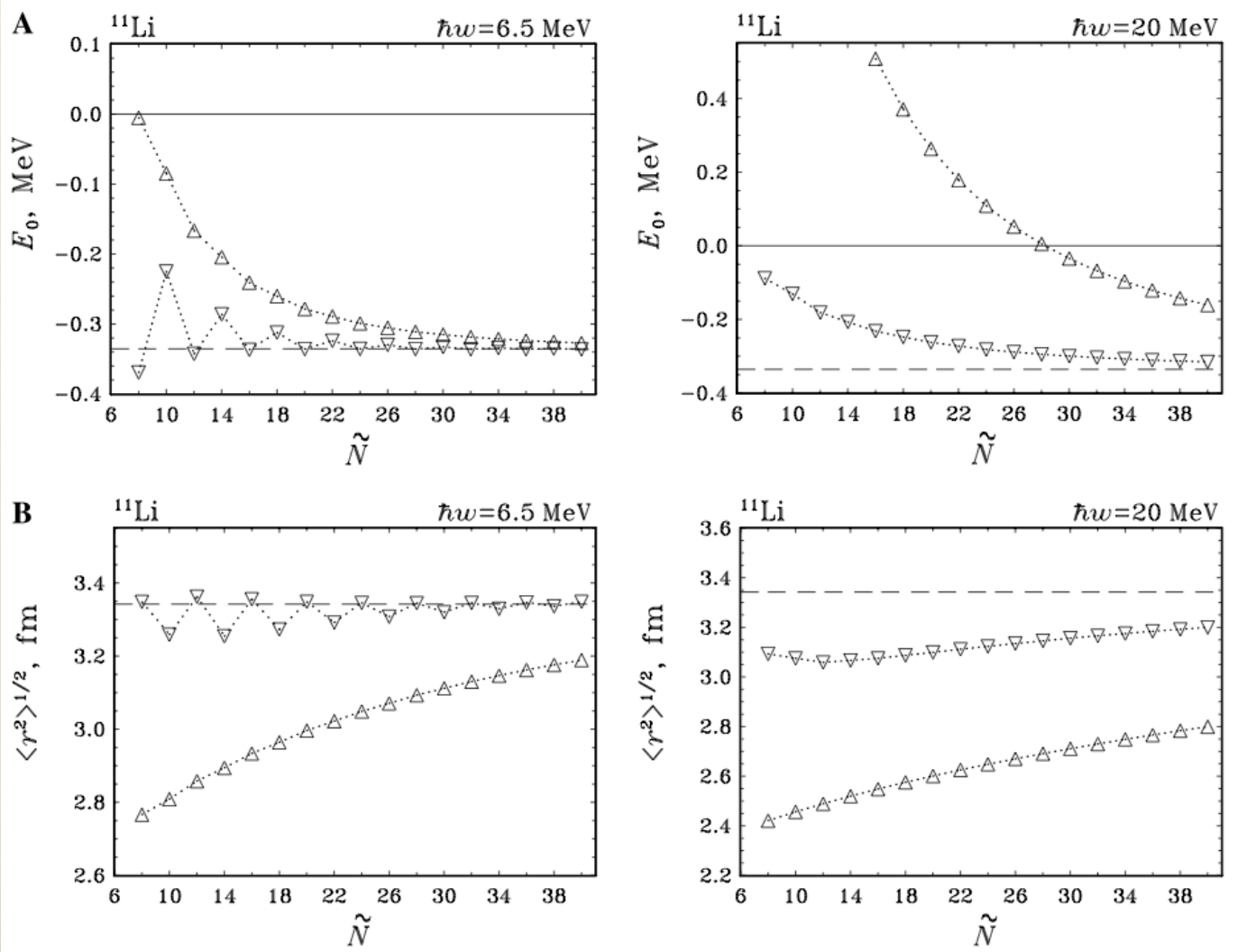
Possible many-body *ab initio* applications



Bound states: the TRR solutions a_n decrease with n when $n > N$ at $E < 0$. Extending the SM Lanczos basis by oscillator states with $n > N$ is equivalent to calculating binding energies as the respective S-matrix pole. It improves the variational binding energies, rms radii, EM transitions, etc.

How does it work and does it work at all?

Bound state:
^{11}Li in a cluster model
Note rms radius

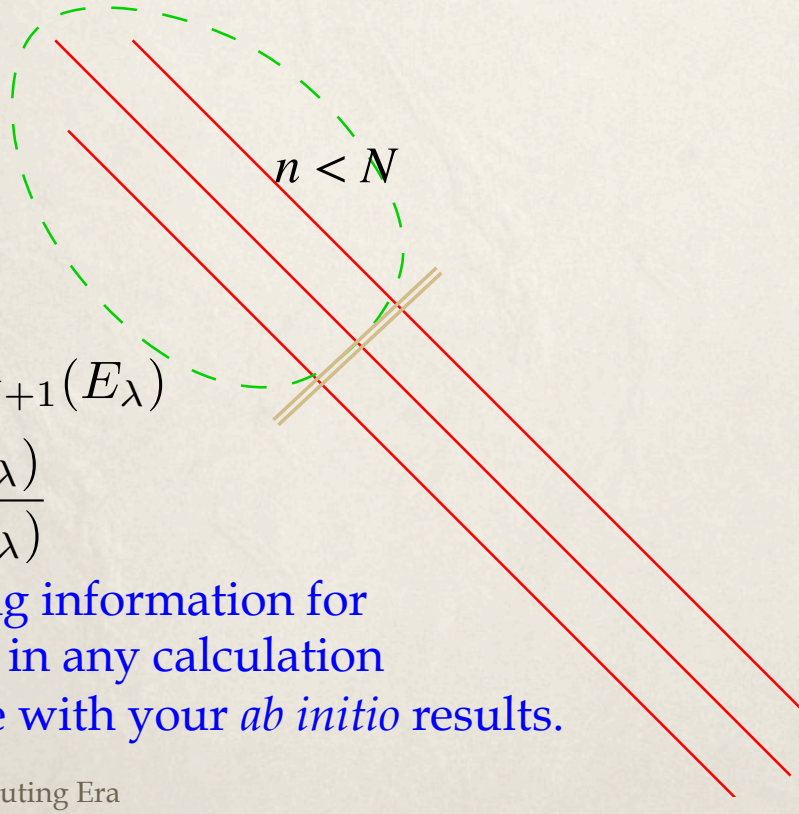


Relation to standard SM: Hamiltonian eigenstates

$$H_{n,n-1}a_{n-1} + (H_{nn} - E)a_n + H_{n,n+1}a_{n+1} = 0$$

Boundary condition: $H_{N,N-1}a_{N-1}(E_\lambda) + (H_{NN} - E)a_N(E_\lambda) = 0$

or $a_{N+1}(E_\lambda) = 0$



If the phase shifts are known experimentally, it is easy to solve numerically:

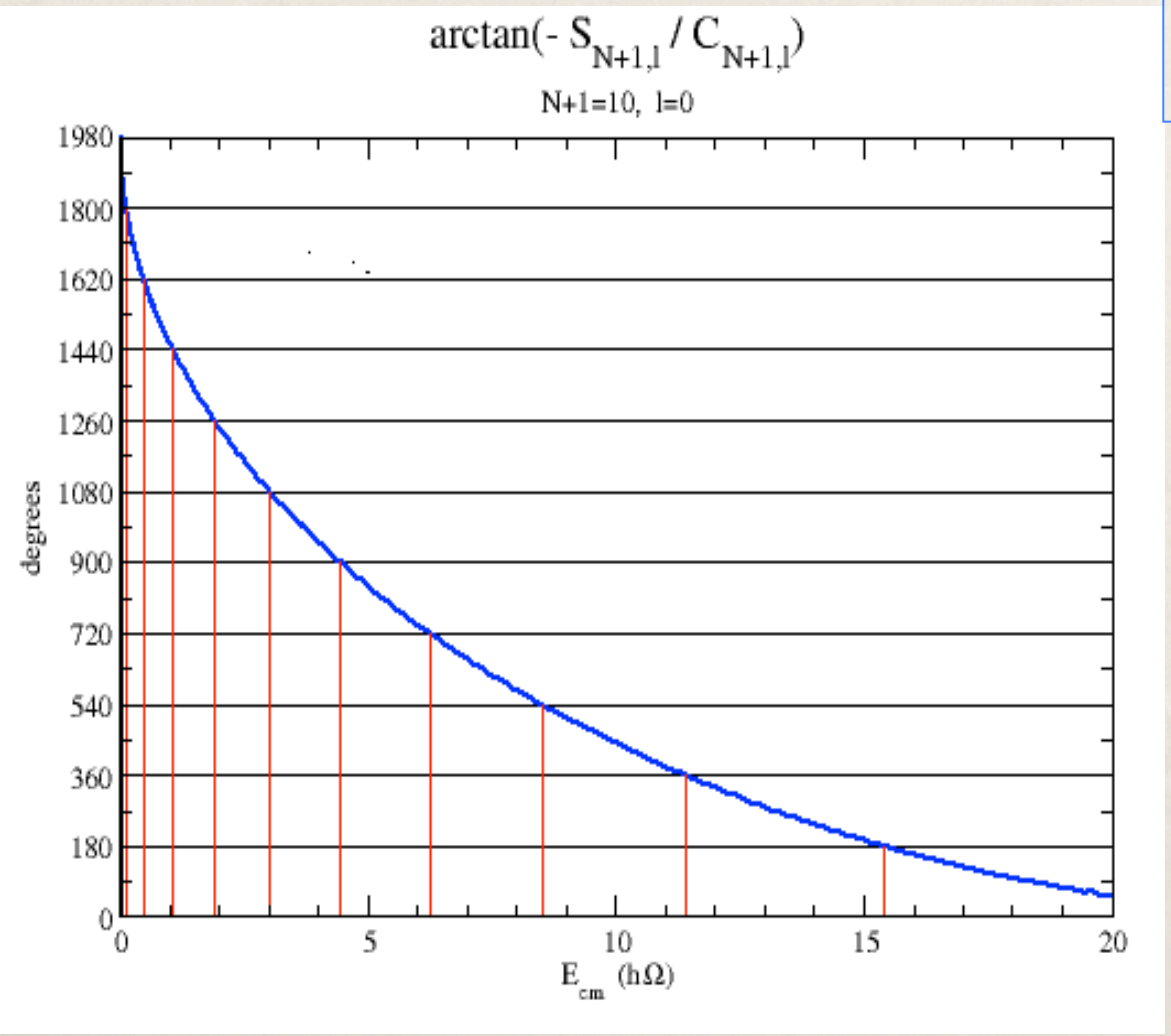
$$a_{N+1}(E_\lambda) = \cos\delta(E_\lambda)S_{N+1}(E_\lambda) + \sin\delta(E_\lambda)C_{N+1}(E_\lambda)$$

$$a_{N+1}(E_\lambda) = 0, \quad \text{hence} \quad \tan\delta(E_\lambda) = -\frac{S_{N+1}(E_\lambda)}{C_{N+1}(E_\lambda)}$$

E_λ are eigenstates that are consistent with scattering information for given $\hbar\Omega$ and N_{max}; this is what you should obtain in any calculation with oscillator basis and what you should compare with your *ab initio* results.

Universal function

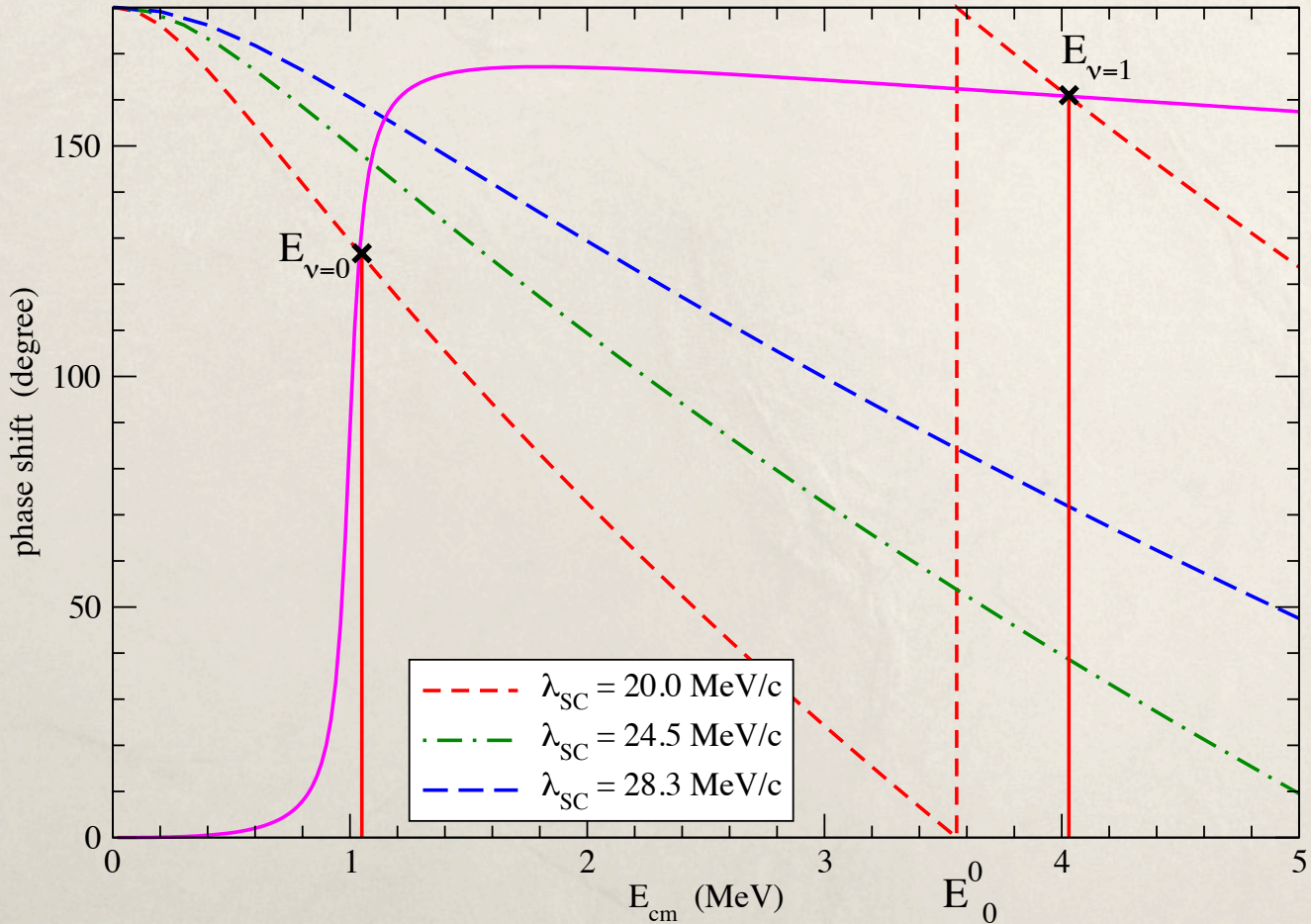
$$f_{nl}(E) = \arctan\left(-\frac{S_{nl}(E)}{C_{nl}(E)}\right)$$



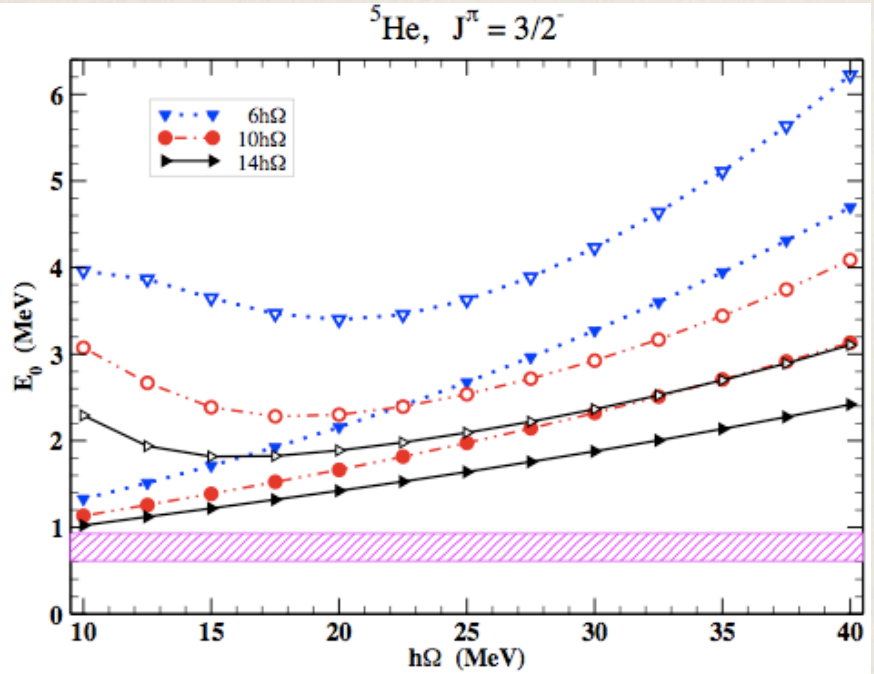
Phase shift and eigenvalue

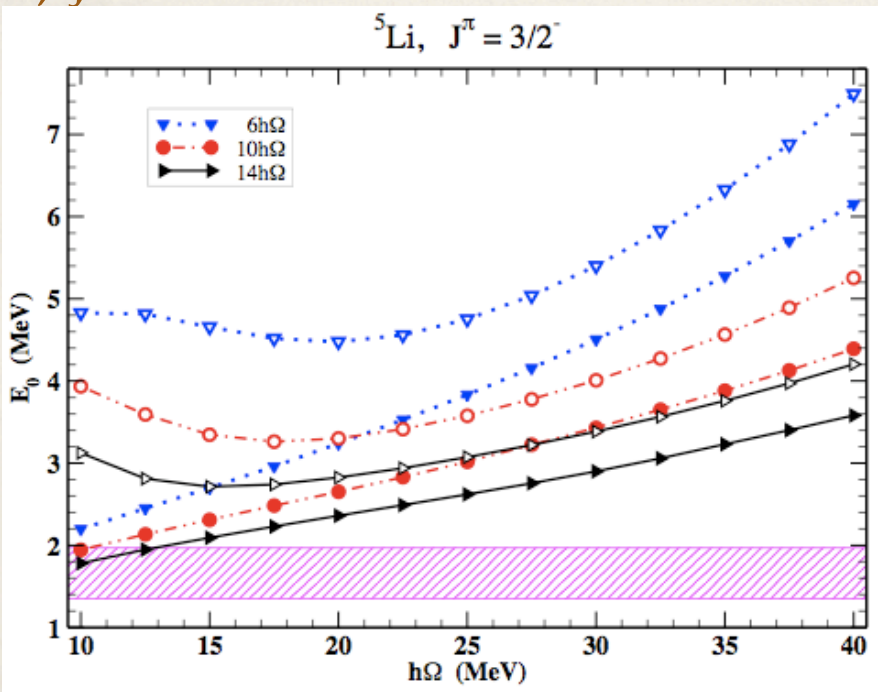
$$\tan\delta_l(E_\nu) = -\frac{S_{N+1,l}(E_\nu)}{C_{N+1,l}(E_\nu)}$$

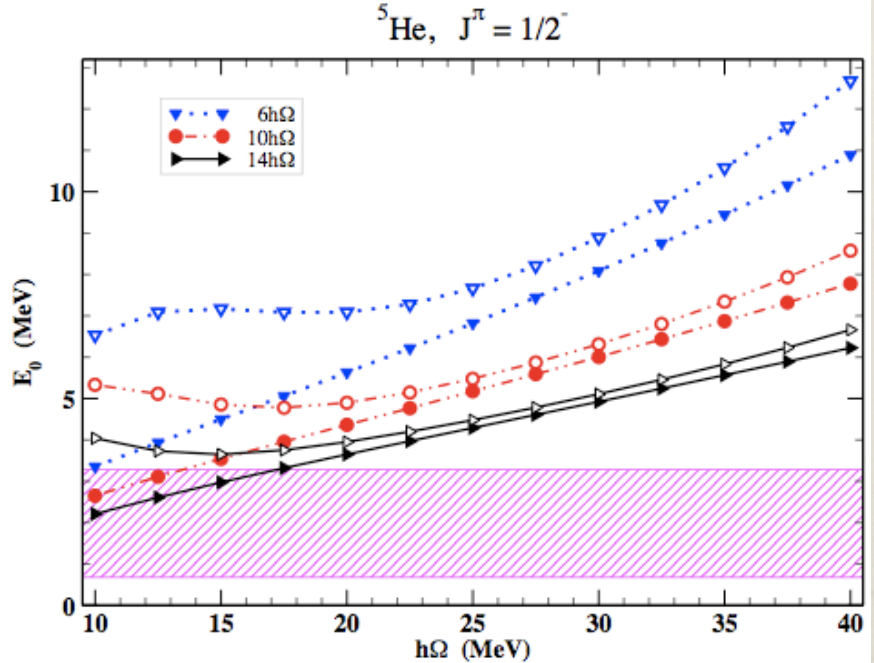
$$\lambda_{SC} = \sqrt{\left(m_N \hbar\Omega\right)/\left(N_{tot}+3/2\right)}$$

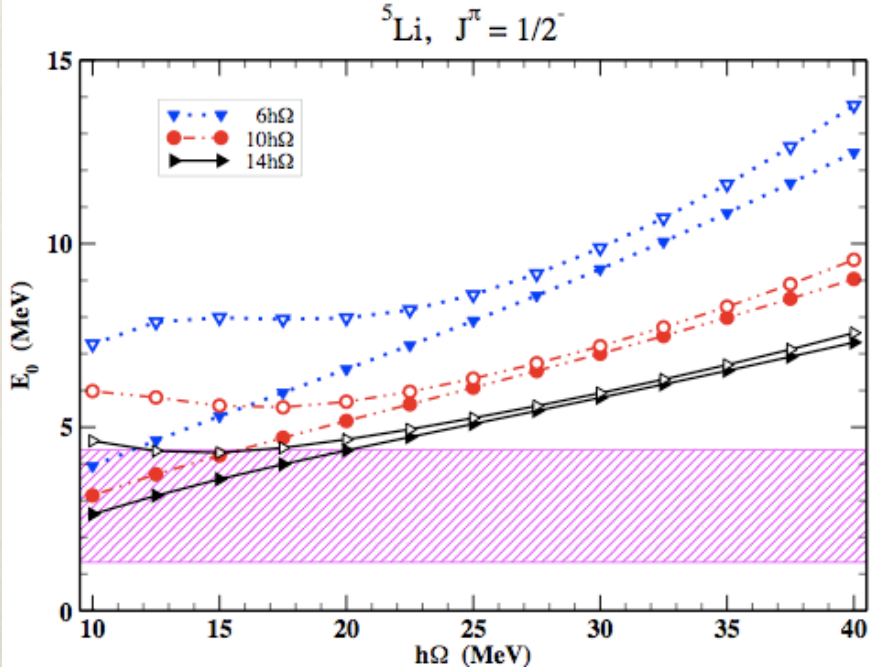


$N\alpha$ scattering and NCSM, JISP16

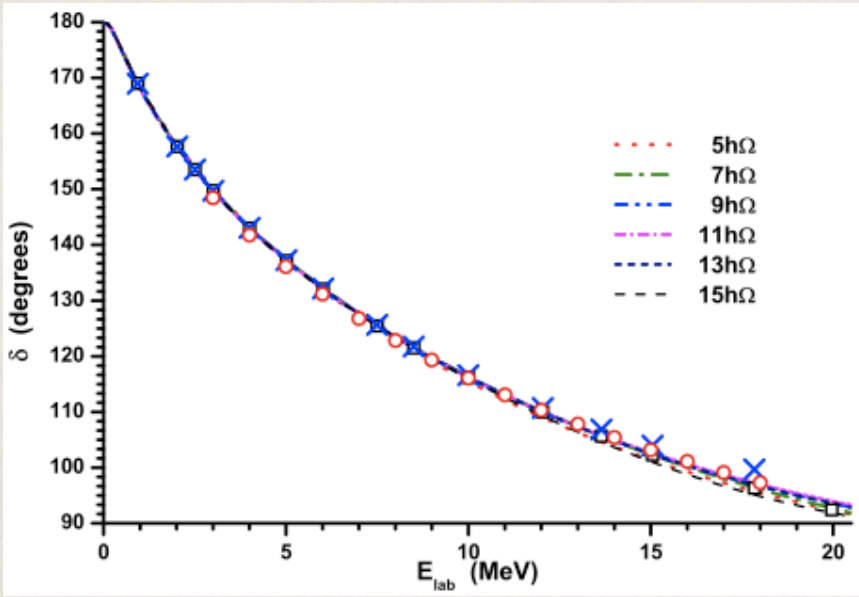


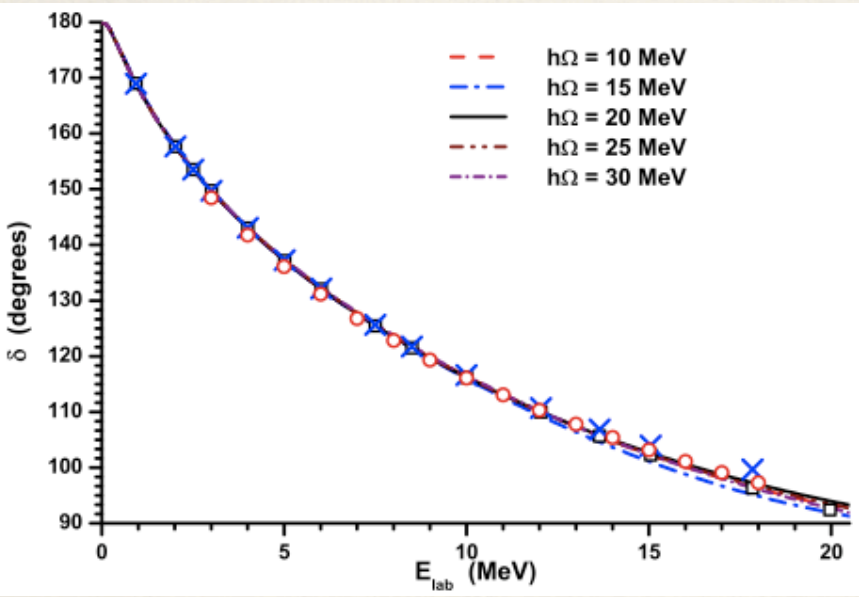


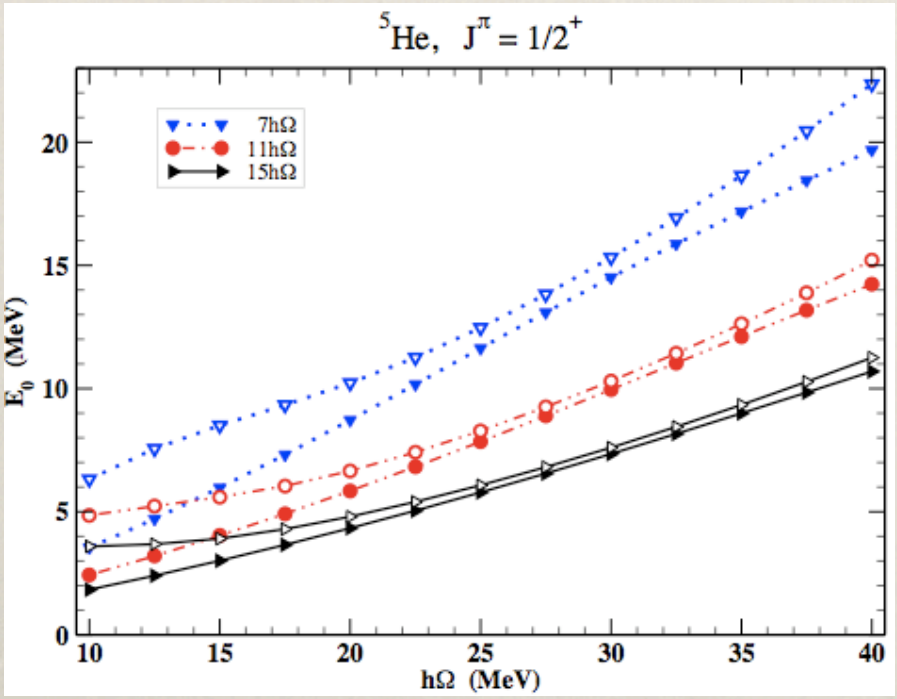


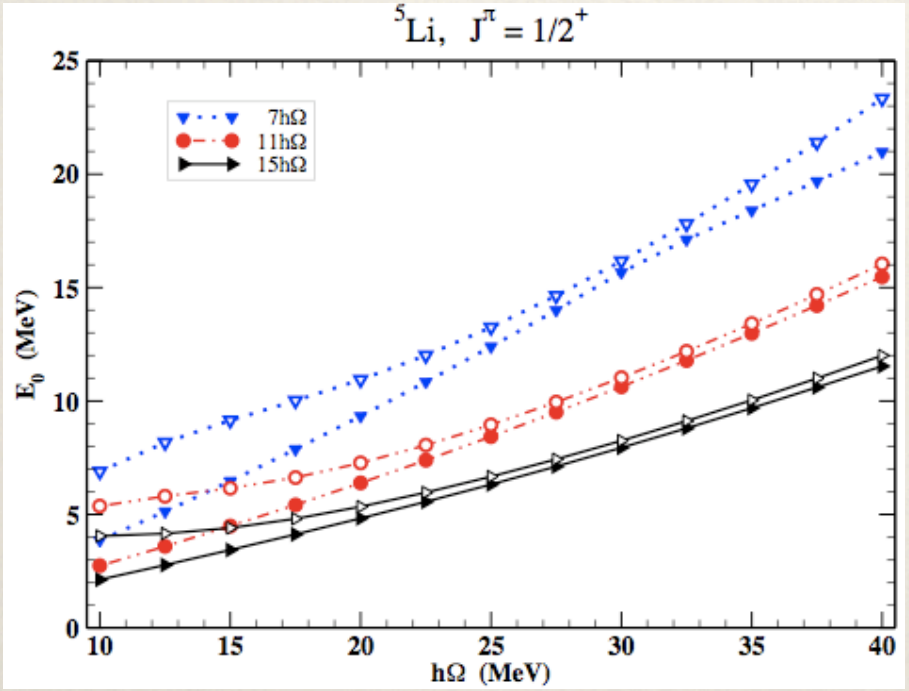


$N\alpha$ non-resonant scattering and NCSM, JISP16









S. Coon et al extrapolations

S. A. Coon, M. I. Avetian, M. K. G. Kruse, U. van Kolck, P. Maris, and J. P. Vary, PRC 86, 054002 (2012)

What is λ_{sc} dependence for resonances?

PHYSICAL REVIEW C **86**, 054002 (2012)

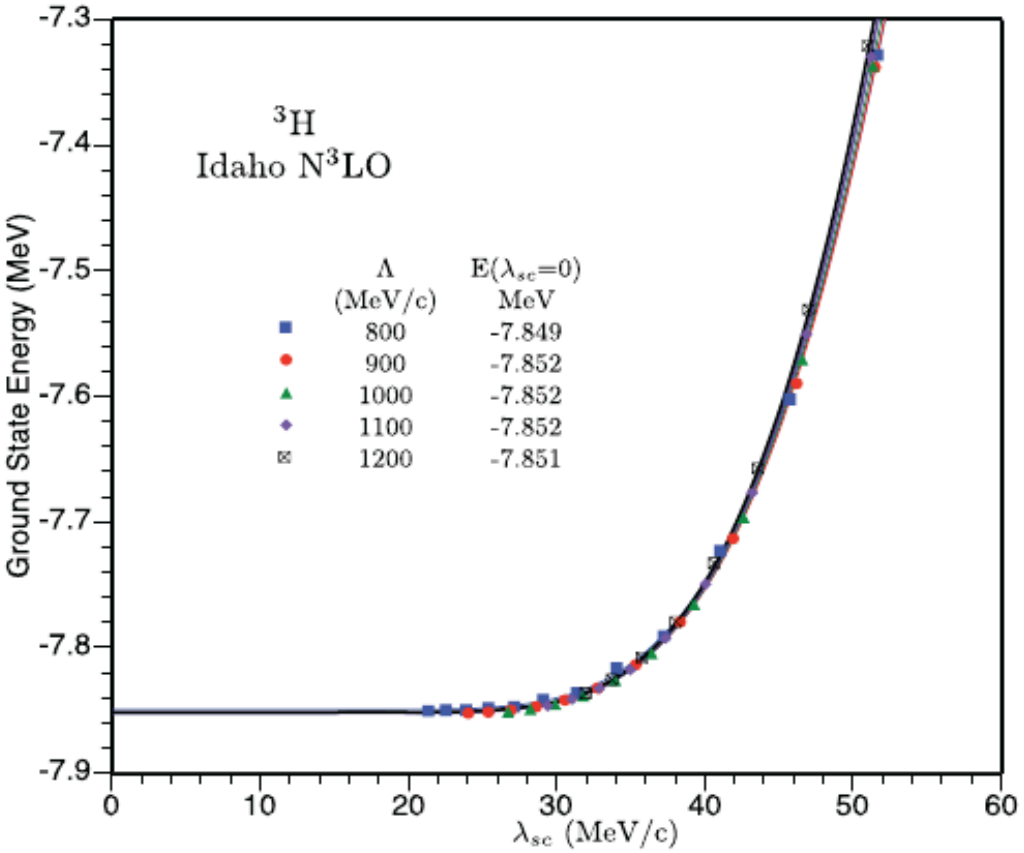


FIG. 7. (Color online) The ground-state energy of ^{3}H calculated at five fixed values of $\Lambda = \sqrt{m_N(N+3/2)\hbar\omega}$ and variable $\lambda_{sc} = \sqrt{(m_N\hbar\omega)/(N+3/2)}$. The curves are fits to the points and the functions fitted are used to extrapolate to the ir limit $\lambda_{sc} = 0$.

$$f_{nl}(E) = \arctan\left(-\frac{S_{nl}(E)}{C_{nl}(E)}\right)$$ scaling with $$\lambda_{SC} = \sqrt{\left(m_N \hbar\Omega\right)/\left(2n+l+3/2\right)}$$

Limit $n \to \infty$:

$$\begin{aligned} S_{nl}(q) \approx & q\sqrt{r_0}\,(n+l/2+3/4)^{\frac{1}{4}}\; j_l(2q\sqrt{n+l/2+3/4}) \\ \approx & \sqrt{r_0}\,(n+l/2+3/4)^{-\frac{1}{4}}\; \sin[2q\sqrt{n+l/2+3/4}-\pi l/2] \end{aligned}$$

$$\begin{aligned} C_{nl}(q) \approx & -q\sqrt{r_0}\,(n+l/2+3/4)^{\frac{1}{4}}\; n_l(2q\sqrt{n+l/2+3/4}) \\ \approx & \sqrt{r_0}\,(n+l/2+3/4)^{-\frac{1}{4}}\; \cos[2q\sqrt{n+l/2+3/4}-\pi l/2] \end{aligned}$$

$$q = \sqrt{\frac{2E}{\hbar\Omega}} \qquad q\sqrt{n+l/2+3/4} = \frac{\sqrt{m_N E}}{\lambda_{SC}}$$

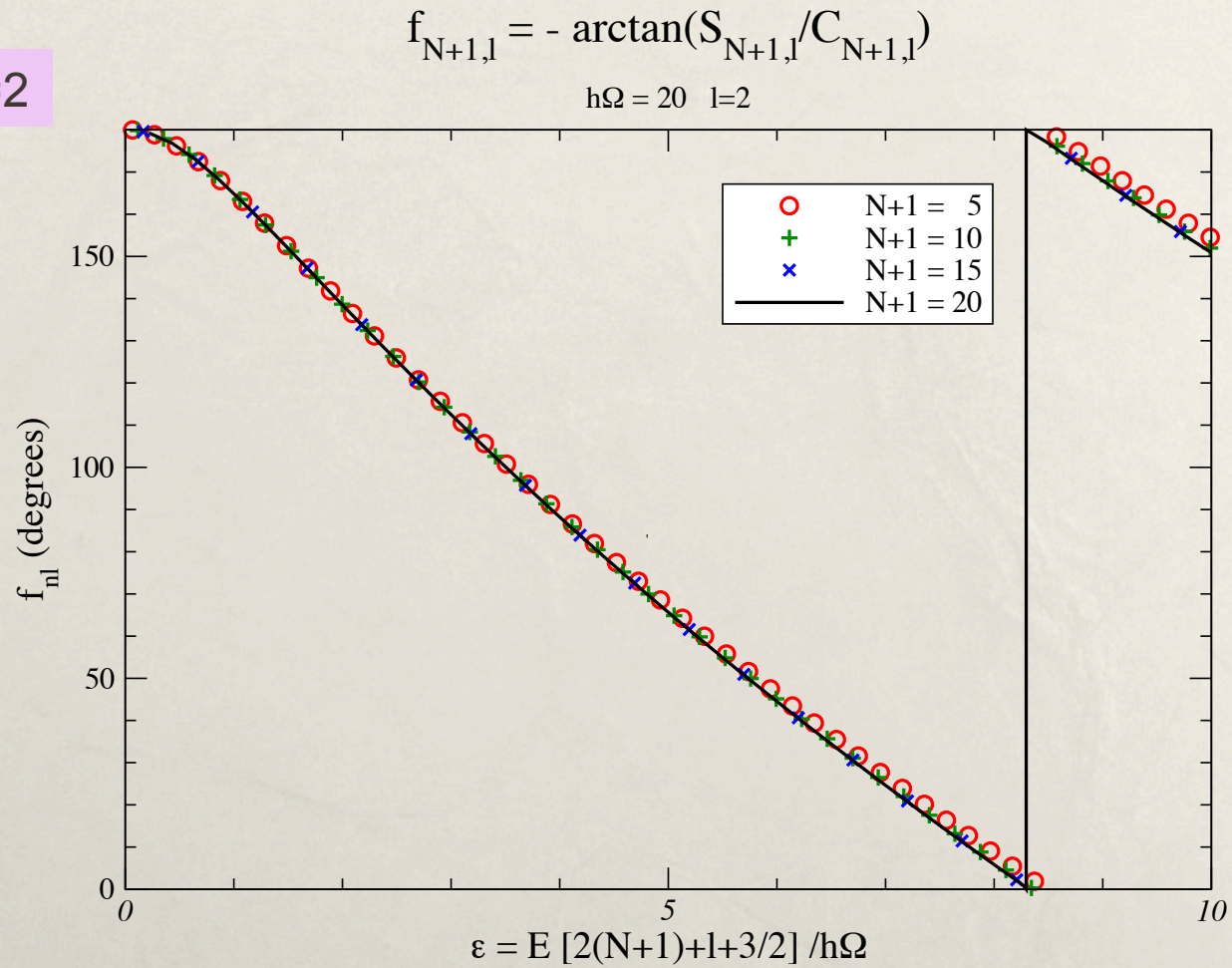
Universal function scaling

$$E_{cm}(\mathrm{MeV}) \Rightarrow \varepsilon = \frac{E_{cm}[2(N+1)+l+3/2]}{\hbar\Omega}$$

S.Coon et al (ir cutoff)

$$\lambda_{SC} = \sqrt{(m_N \hbar\Omega)/(N_{tot}+3/2)}$$

l=2

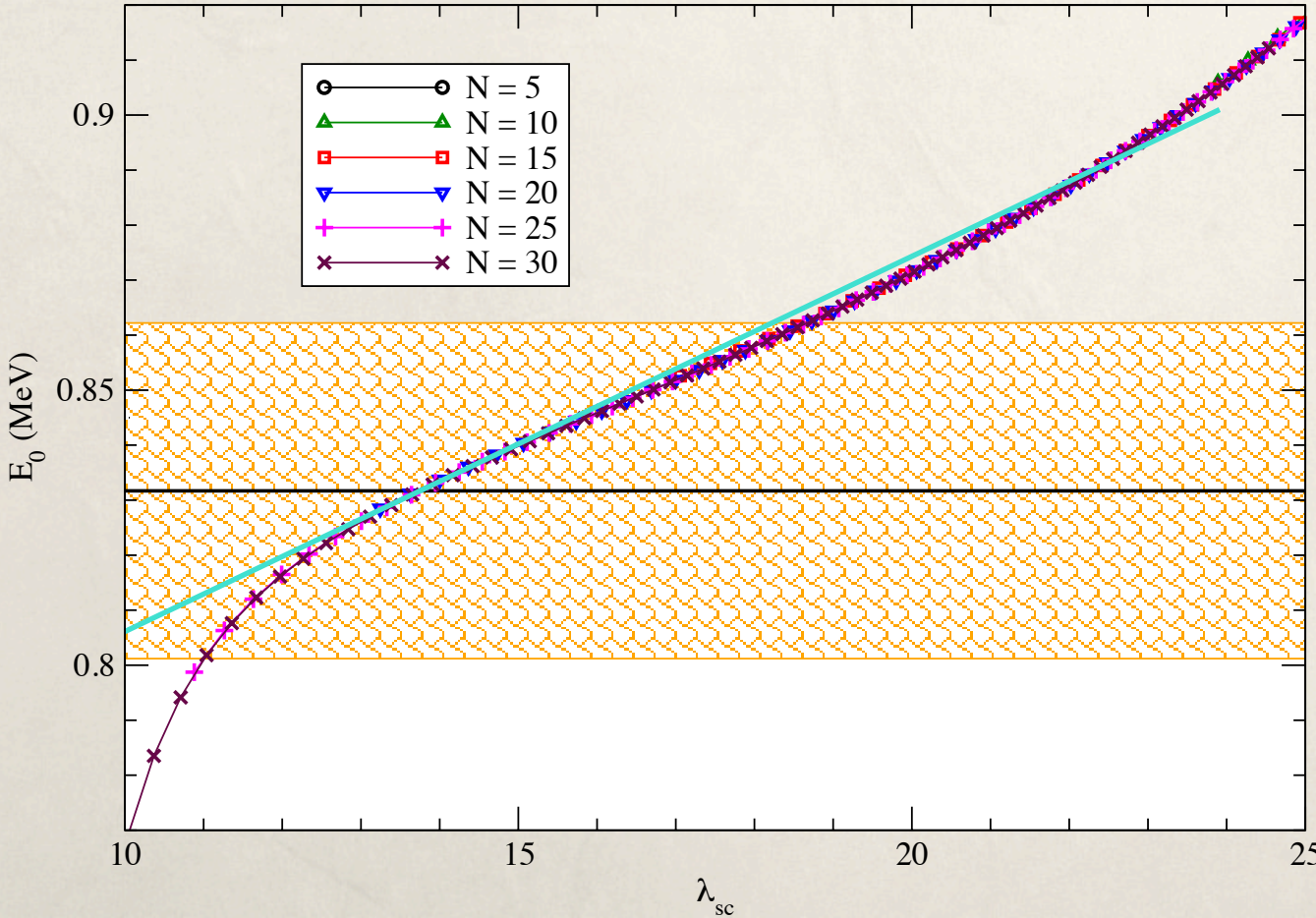


Breit–Wigner resonance

$$\left.\frac{dE_\nu}{d\lambda_{SC}}\right|_{E=E_r} = 2\left[\lambda_{SC}\left(\frac{Z}{\Gamma/2}+\frac{1}{E_r}\right)\right]^{-1}$$

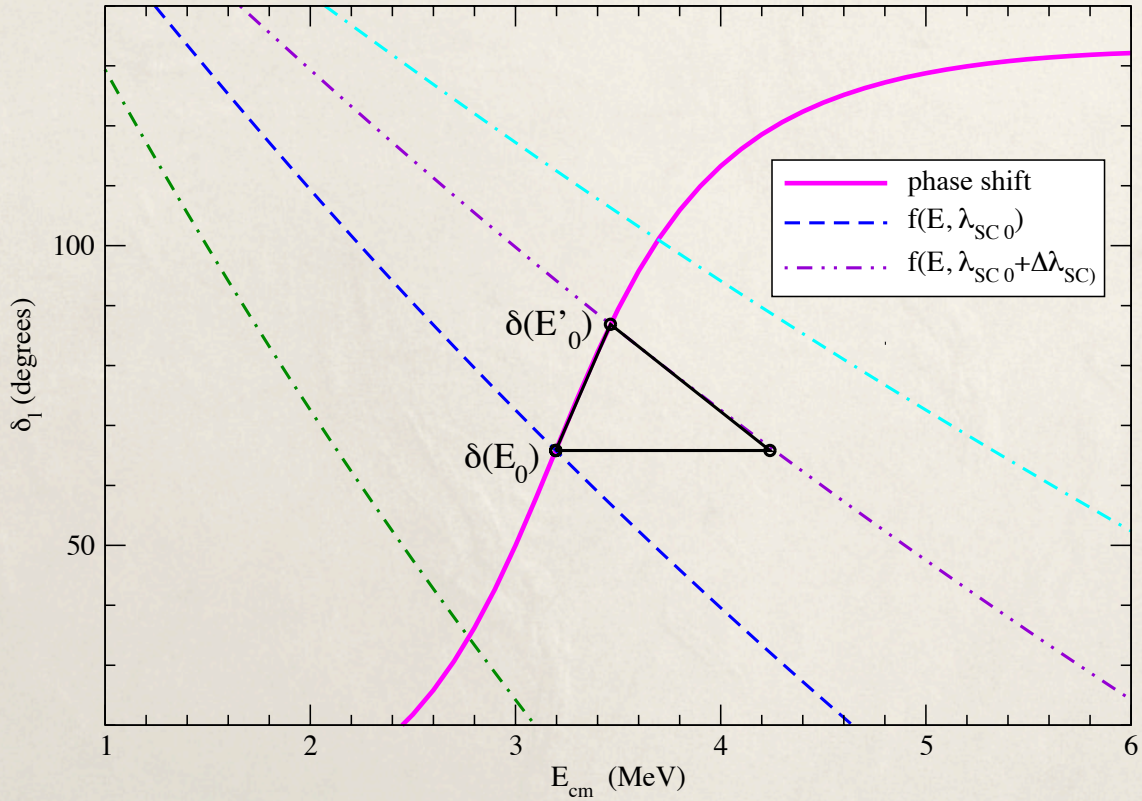
$$Z = \left(S^2_{N+1,l}(\varepsilon) + C^2_{N+1,l}(\varepsilon)\right)/q$$

$$\Lambda \geq 600 \ \text{MeV}/c$$



$$\left.\frac{d\delta_l}{dE}\right|_{E=E_v} = \frac{1}{\lambda_{SC}}\frac{1}{Z(q_v)}\left\{\frac{2}{dE_v/d\lambda_{SC}} - \frac{1}{E_v/\lambda_{SC}}\right\}$$

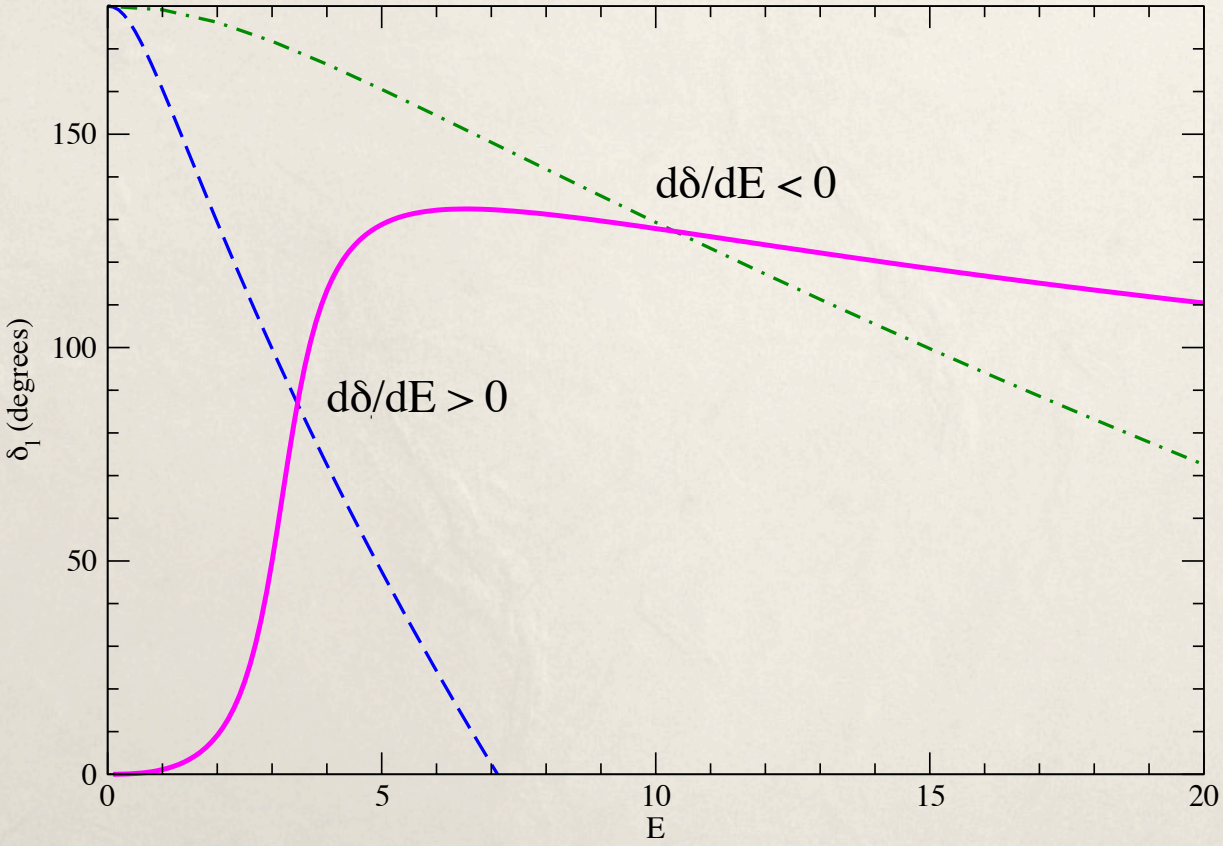
* Is it positive?



$$\left.\frac{d\delta_l}{dE}\right|_{E=E_\nu} = \frac{1}{\lambda_{SC}}\frac{1}{Z(q_\nu)}\left\{\frac{2}{dE_\nu/d\lambda_{SC}} - \frac{1}{E_\nu/\lambda_{SC}}\right\}$$

* Is it positive?

$$\frac{2E_\nu}{\lambda_{SC}} > \frac{dE_\nu}{d\lambda_{SC}}$$



$$\left.\frac{d\delta_l}{dE}\right|_{E=E_v} = \frac{1}{\lambda_{SC}}\frac{1}{Z(q_v)}\left\{\frac{2}{dE_v/d\lambda_{SC}} - \frac{1}{E_v/\lambda_{SC}}\right\}$$

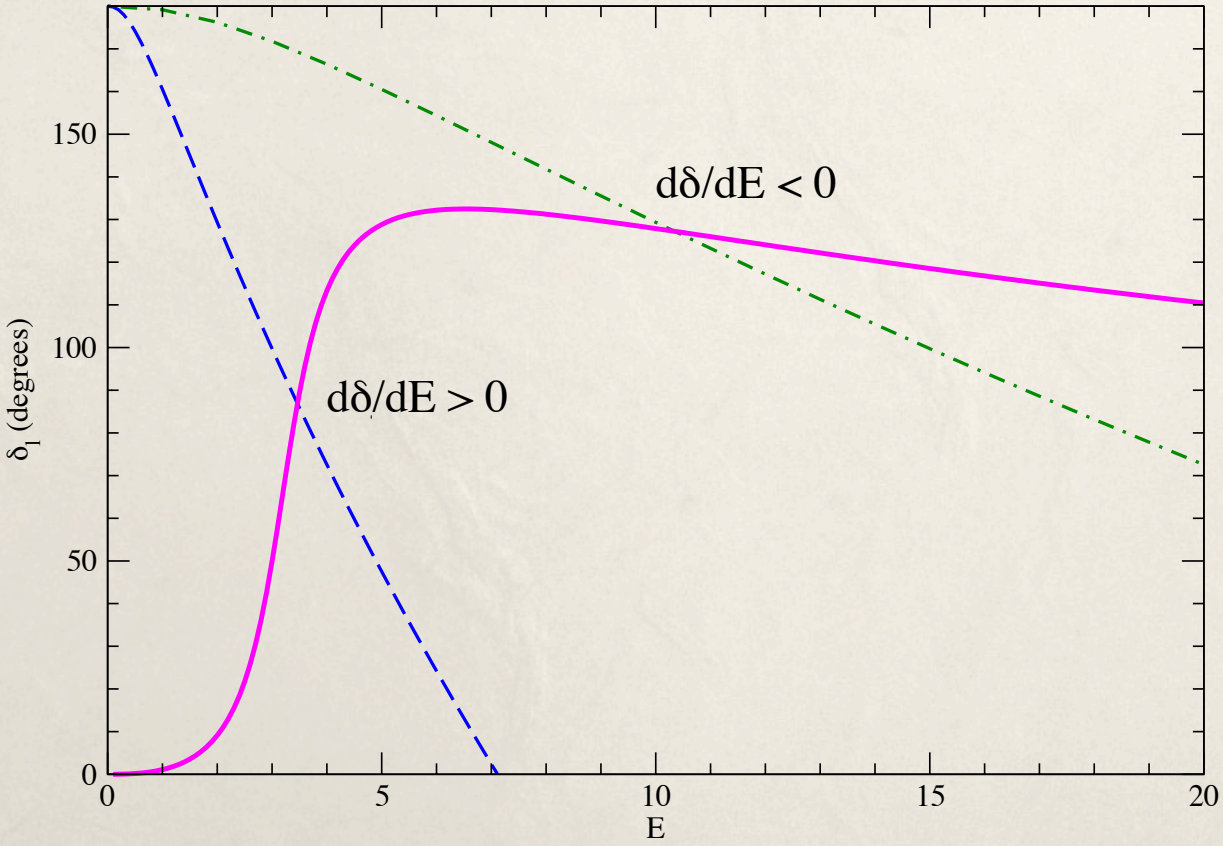
* Is it positive?

$\frac{d\delta}{dE} > 0$: ^{7}He $3/2^-$ $(14\hbar\Omega)$

($\Gamma \sim 150$ keV)

$\frac{d\delta}{dE} < 0$: ^{9}He $1/2^-$ $(12\hbar\Omega)$

($\Gamma \sim 100$ keV)

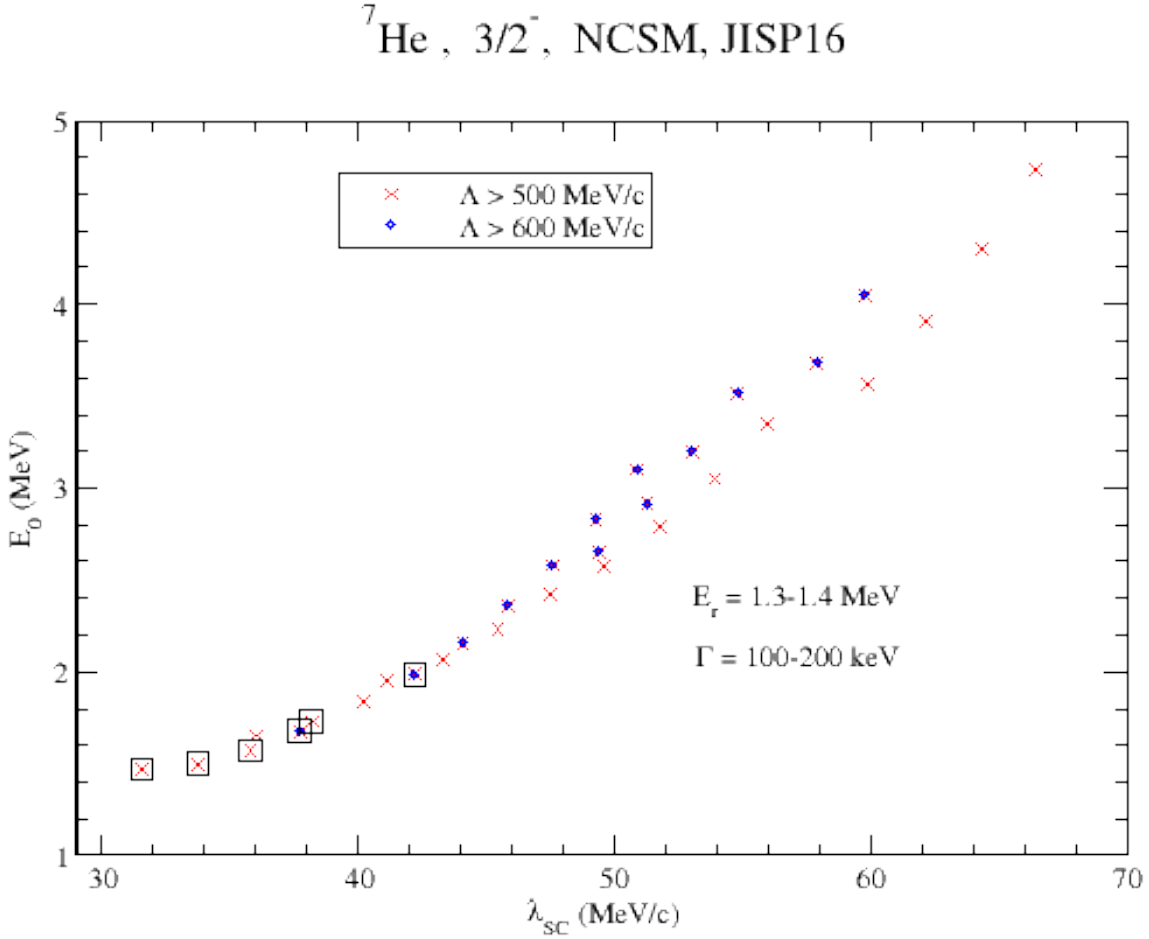


Example: ^{7}He, 3/2^{-}

Resonance:

E_r = 434 keV

Γ = 150 keV



Conclusions

* If the phase shifts are known experimentally, one can easily check whether states obtained in the shell model above the threshold are consistent with the phase shifts. These states should have sometimes energies far from the resonance and should be obtained in the case when there is no resonance with given J^{π}.
* If case when the eigenstate is found in the vicinity of the resonance, its width can be calculated.
* The Lanczos algorithm can be extended to calculate reactions within the shell model.

Main conclusion:

* Thank you!
* Happy birthday!