

# Discretization of continuum for scattering problems



O.A. Rubtsova

in collaboration with

V.N. Pomerantsev, V.A. Kulikov

*Skobeltsyn Institute of Nuclear Physics,  
Moscow State University*



The IVth International School and Workshop  
on Few-Body Systems  
Khabarovsk  
1 October 2024

# Content:

1.  $L^2$  discretization.
2. Spectral shift function, spectral density and integrated density of states.
3. Finding scattering phase shifts from discretized spectra:
  - formalism,
  - numerical examples.
4. Union of spectra for solving multi-channel problems.
5. Multi-channel problems: examples.
6. Three-body problem.
7. Conclusion.

## Two-body problem

Consider at first two-body problem with the total Hamiltonian  $H$  and asymptotic Hamiltonian  $H_0$  (may include the Coulomb interaction).

The short-range interaction:

$$V = H - H_0$$

has a finite trace.

Resolvents of the Hamiltonians are taken in the following form:

$$R_0(E) = [H_0 - (E + i0)]^{-1}, \quad R(E) = [H - (E + i0)]^{-1}$$

## Different ways to solve the scattering problem

Schroedinger equation (differential):

$$H |\psi^{(+)}(E)\rangle = E |\psi^{(+)}(E)\rangle$$

Matching with asymptotical wf:

$$\psi^{(+)}(E, r) \xrightarrow{r \rightarrow \infty} h^{(-)}(E, r) + S(E) \cdot h^{(+)}(E, r)$$

$$S(E) = \exp(2i\delta(E)),$$

$S(E)$  – scattering matrix element which is related to observables.

Lippmann-Schwinger equation (integral):

$$|\psi^{(+)}(E)\rangle = |\phi_0(E)\rangle - R_0^{(+)}(E) V |\psi^{(+)}(E)\rangle$$

S-matrix is defined from the matrix element (integral) with exact scattering wave function:

$$S(E) = 1 + 2\pi iT(E)$$

$$T(E) = \langle \phi_0(E) | V | \psi^{(+)}(E) \rangle$$

One can also solve the equation for the T-matrix itself.

$S(E)$  is related to the scattering operator:  $S = \Omega^{(-)\dagger} \Omega^{(+)}$

Wave operators:  $|\psi^{(\pm)}(E)\rangle = \Omega^{(\pm)} |\phi_0(E)\rangle$

In the simplest case:

$$\phi_0(r) = \sqrt{\frac{2}{\pi}} \sin(kr), \quad \psi^{(+)}(r) \xrightarrow{r \rightarrow \infty} \sqrt{\frac{2}{\pi}} e^{i\delta} \sin(kr + \delta), \quad k = \sqrt{\frac{2mE}{\hbar^2}}$$

# L<sup>2</sup> discretization: expansion in some basis

Consider the Schroedinger equation for the wave function:  $H |\Psi\rangle = E |\Psi\rangle$

Let's expand the wave function over a finite set of L<sup>2</sup> functions  $\{|\phi_n\rangle\}_{n=1}^N$  ( $\langle\phi_n|\phi_n\rangle=1$ ) (forms a basis at  $N\rightarrow\infty$ ):

$$|\Psi\rangle = \sum_{n=1}^N C_n |\phi_n\rangle$$

This results in a generalized eigenvalue problem for the Hamiltonian matrix:

$$\det \| H_{nn'} - EI_{nn'} \| = 0 \quad H_{nn'} = \langle\phi_n|H|\phi_{n'}\rangle, \quad I_{nn'} = \langle\phi_n|\phi_{n'}\rangle$$

Discrete sets of energies:

$$\{E_j^0\}, j = 1, \dots, N \quad \text{for the asymptotic Hamiltonian } H_0$$

$$\{E_j\}, j = 1, \dots, N \quad \text{for the total Hamiltonian } H=H_0 + V$$

The positive eigenvalues ( $E_j > 0$ ) define the *discretized continuum*. The corresponding eigenfunctions have finite norms and usually are called as *pseudostates* of the continuum.

- Examples:**
- Harmonic oscillator representation,
  - bi-orthogonal Laguerre basis,
  - Gaussian basis and others.

## $L^2$ discretization: problem 'in a box' (finite volume)

A similar situation arises when solving scattering problem in a box (spherical cavity):

Conditions for the wave functions:

$$\psi_0(a) = 0$$

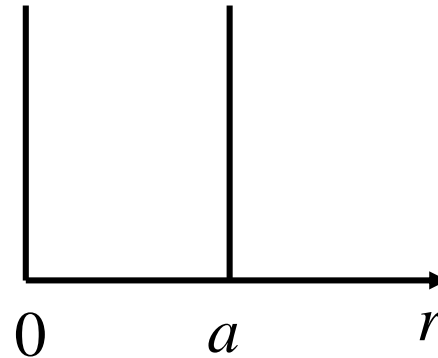
$$\psi(a) = 0$$

The asymptotic and total Hamiltonians have discrete but infinite spectra:

$$\{E_j^0\}, \{E_j\}, j = 1, \dots,$$

Wave-functions are  $L^2$  normalized as well.

- Examples:**
- Problems in finite volume,
  - QCD lattice calculations (Lüscher approach) and others.



# Spectral shift function

The **spectral shift function** corresponds to a pair of operators  $H_0$  and  $H=H_0+V$ :

$$\text{Tr} [f(H) - f(H_0)] = \int_{-\infty}^{\infty} dE f'(E) \xi(E) \quad \text{the trace formula (I.M. Lifshits 1952)}$$

The Birman-Krein equation (1962). Relation to the S-operator:

$$\det S(E) = \exp(-2\pi i \xi(E))$$

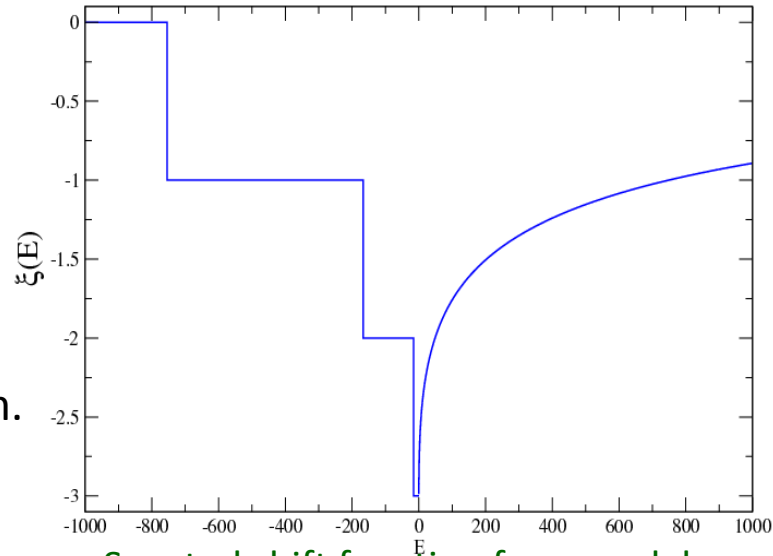
In one-channel case, SSF is proportional to the phase shift:

$$\xi(E) = -\frac{1}{\pi} \delta(E)$$

The SSF is also defined in the area of discrete spectrum. It takes integer values there:

$$\xi(E) = -\sum_{n=1}^{N_b} \theta(E - E_n), \quad E < 0$$

So that, the phase shift satisfies the Levinson theorem.



Spectral shift function for a model Hamiltonian with 3 bound states

M.Sh. Birman, A.B. Pushnitsky, **Spectral shift function, amazing and multifaceted**, Integr. equ. oper. theory **30**, 191 (1998).

# Continuum level density

Spectral density for a Hamiltonian with discrete spectrum:

$$\rho_b(E) = \text{Tr}[\delta(E - H_d)] = \sum_{n=1}^{N_b} \delta(E - E_n) \quad , \quad E_n - \text{eigen energies}$$

For continuous spectrum spectral density does not exist.

One can introduce the continuum level density:

$$\Delta(E) \equiv \frac{1}{\pi} \text{Tr} [\text{Im} R(E) - \text{Im} R_0(E)]$$

$$\tilde{\Delta}(E) = \sum_{n=1}^{N_b} \delta(E - E_n) + \Delta(E) = \text{Tr}[\delta(E - H) - \delta(E - H_0)] \Leftrightarrow \rho(E) - \rho(E_0)$$

Relation to the SSF (and phase shift  $\phi$ ):

$$\tilde{\Delta}(E) = -\frac{d\xi(E)}{dE} \quad \left( \Delta(E) = \frac{1}{\pi} \frac{d\phi(E)}{dE}, \quad E > 0 \right)$$

The SSF can be considered as integrated continuum level density:

$$\xi(E) = -\int_{-\infty}^E \tilde{\Delta}(E') dE' = -\sum_{n=1}^{N_b} \theta(E - E_n) - \int_{-\infty}^E \Delta(E) dE$$



# Continuum level density

The Krein-Fridel-Lloyd equation:

$$\Delta(E) = \frac{1}{2\pi i} \text{Tr} \left[ S^\dagger(E) \frac{d}{dE} S(E) \right] = \frac{1}{2\pi i} \frac{d}{dE} \ln \det S(E)$$

The trace equation:

$$\text{Tr} [f(H) - f(H_0)] = \sum_n^{N_b} f(E_n) + \int dE \Delta(E) f(E)$$

$\Delta(E)$  is widely used to find the resonance parameters:

$$\Delta(E) = \frac{1}{\pi} \frac{\Gamma/2}{(E - E_R)^2 + \Gamma^2/4} + \Delta_{bg}(E)$$

A. T. Kruppa and K. Arai, Phys. Rev. A **59**, 3556 (1999).

An interesting treatment of the spectral density and continuum level density can be found in the on-line book: [Chaos: classical and quantum \(chaosbook.org\)](http://chaosbook.org)

# Spectral density for the discretized continuum

For discretized spectrum, the separate spectral densities can be defined:

$$\rho_{0d}(E) = \sum_{j=1}^N \delta(E - E_j^0) \quad \text{for } H_0 \quad \text{and} \quad \rho_d(E) = \sum_{j=1}^N \delta(E - E_j) \quad \text{for } H$$

**Integrated densities of states (IDS):**

$$J_0(E) = \int_{-\infty}^E \rho_{0d}(E') dE' = \sum_{j=1}^N \theta(E - E_j^0), \quad J_0(E_j^0) = j \quad J(E) = \sum_{j=1}^N \theta(E - E_j), \quad J(E_j) = j$$

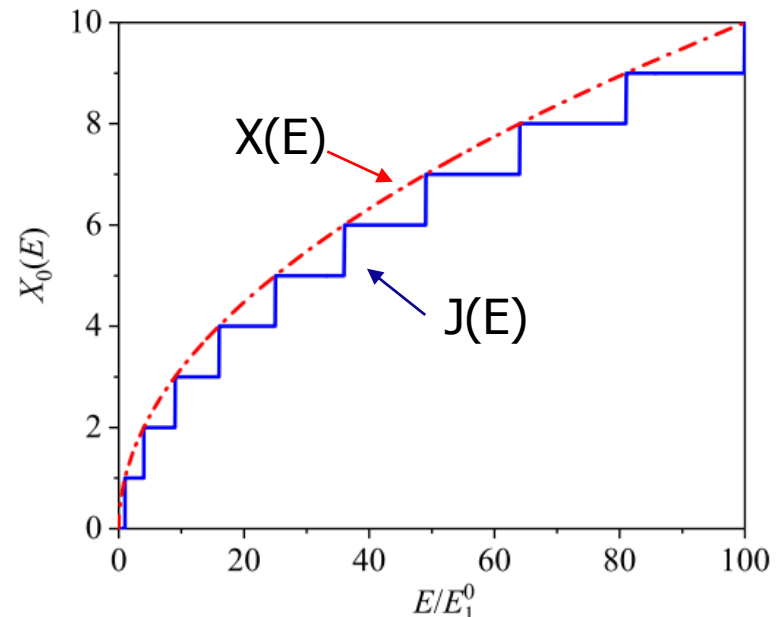
If we consider directly the differences:

$$\rho_d(E) - \rho_{0d}(E) \rightarrow \Delta(E)$$

$$-[J(E) - J_0(E)] \rightarrow \xi(E)$$

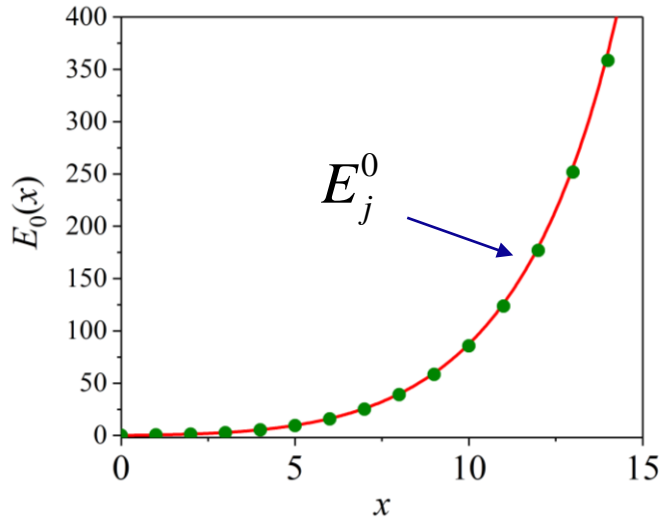
they do not contain any information about scattering.

One should construct smooth functions instead of the step-like ones:  $J(E) \rightarrow X(E)$ .

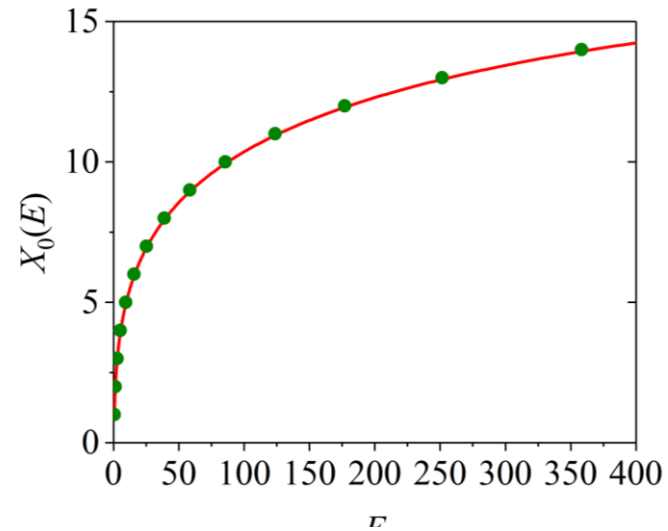


IDS for the problem  
in a finite volume

## Dependence of EVs on the index of state



## The inverse function

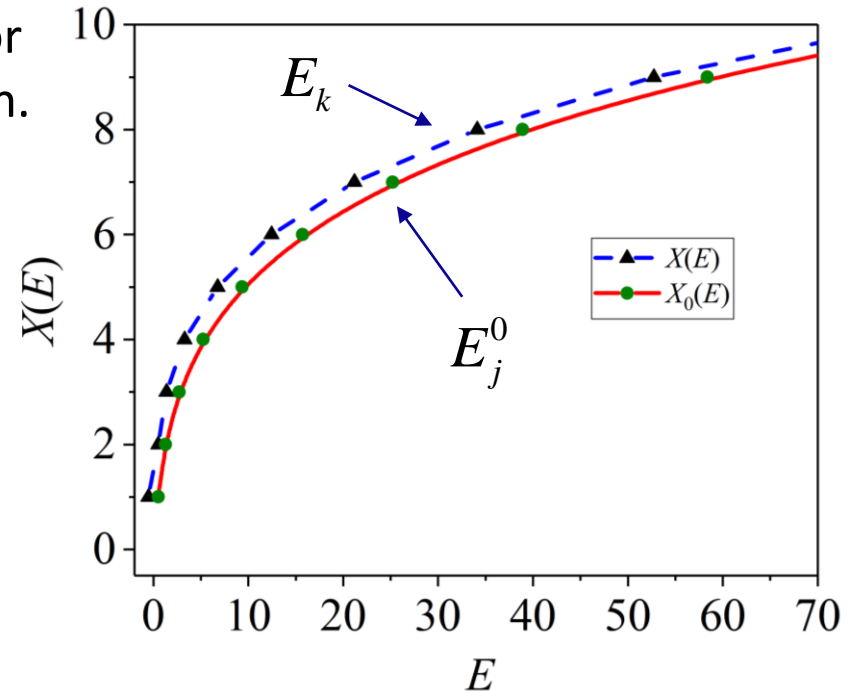


The similar function  $X(E)$  is defined for the spectrum of the total Hamiltonian.

Difference of  $X(E)$  and  $X_0(E)$  gives the SSF (and the phase shift) as continuous functions on energy:

$$\xi(E) = -[X(E) - X_0(E)]$$

$$\delta(E) = \pi[X(E) - X_0(E)]$$



# Quasi-continuous spectrum

(I.M. Lifshits, 1947)

For the initial Hamiltonian  $H_0$  with continuous spectrum, one considers a family of operators  $H_0(\alpha)$  with discrete spectra:

$$E_j^{0(\alpha)} = \lambda_0^{(\alpha)}(j\alpha) = \lambda_0(j\alpha) + O(\alpha),$$

$$D_j^{(\alpha)} \equiv E_{j+1}^{0(\alpha)} - E_j^{0(\alpha)} = \alpha \left[ \frac{d\lambda_0(u)}{du} \Big|_{u=j\alpha} + O(\alpha) \right]$$

( $\alpha$  is a small parameter)

- eigenvalues belong to some smooth monotonous function;
- one may consider a limit  $\alpha \rightarrow 0$ .

The respective family of total Hamiltonians  $H(\alpha) = H_0(\alpha) + V$  with EVs:  $E_j^{(\alpha)} = \lambda^{(\alpha)}(j\alpha)$

Relation for EVs of  $H(\alpha)$  and  $H_0(\alpha)$  (I.M. Lifshits):

$$E_j^{(\alpha)} = E_j^{0(\alpha)} + \alpha \frac{d\lambda_0(u)}{du} \Big|_{u=j\alpha} \xi_j^{(\alpha)}, \quad \xi_j^{(\alpha)} \rightarrow \xi(E_j) \quad \text{the spectral shift function}$$

If combine the r.h.s.:  $E_j^{(\alpha)} = \lambda^{(\alpha)}(\alpha j) \approx \lambda_0^{(\alpha)}(\alpha [j + \xi_j])$

An interaction causes a shift of EV along the same curve! Here  $\xi_j$  can be considered as **a non-integer shift of the index** of state.

One can define smooth integrated densities  $X_0$  and  $X$  as inverse functions:

$$\alpha X_0^{(\alpha)}(E) = [\lambda_0^{(\alpha)}]^{-1}(E), \quad \alpha X^{(\alpha)}(E) = [\lambda^{(\alpha)}]^{-1}(E)$$

$$\xi^{(\alpha)}(E) = -\left( X^{(\alpha)}(E) - X_0^{(\alpha)}(E) \right) \quad \xi(E) = \xi^{(\alpha)}(E) + O(\alpha)$$

# Spectral densities

The spectral shift function:

$$\xi(E) = -\left(X(E) - X_0(E)\right)$$

and the phase shift:

$$\delta(E) = \pi\left(X(E) - X_0(E)\right)$$

One can also define separate spectral densities:

$$\rho_0(E) \equiv \frac{dX_0(E)}{dE}, \quad \rho(E) \equiv \frac{dX(E)}{dE},$$

and the CLD as the difference: 
$$\Delta(E) = \frac{dX(E)}{dE} - \frac{dX_0(E)}{dE}$$

The functions  $X, X_0$  and  $\rho, \rho_0$  do not correspond to initial spectra and do not have finite limits when  $\alpha \rightarrow 0$ .

However, the limits for the differences, the functions  $\xi$  and  $\Delta$ , do exist.

## The properties of functions $X$ and $X_0$

$$\delta(E) = \pi \left( X(E) - X_0(E) \right)$$

$$X(E_j) = j \quad \longrightarrow \quad \delta(E_j) = \pi j - \pi X_0(E_j), \quad j = N_b + 1, \dots$$

At the points of the total Hamiltonian's spectrum, the phase shifts are defined by the function  $X_0$  only!

By using an expansion of  $X_0$  at the point  $E_k^0$  which is closest to  $E_j$  and

$$\frac{dX_0(E_k^0)}{dE} = \left[ \frac{dE_0(x=k)}{dx} \right]^{-1} \approx \frac{1}{D_k}$$

Approximation via the relative difference of EVs for the free and total Hamiltonian:

$$\delta(E_j) \approx \pi(j - k) + \pi \frac{E_k^0 - E_j}{D_k}$$

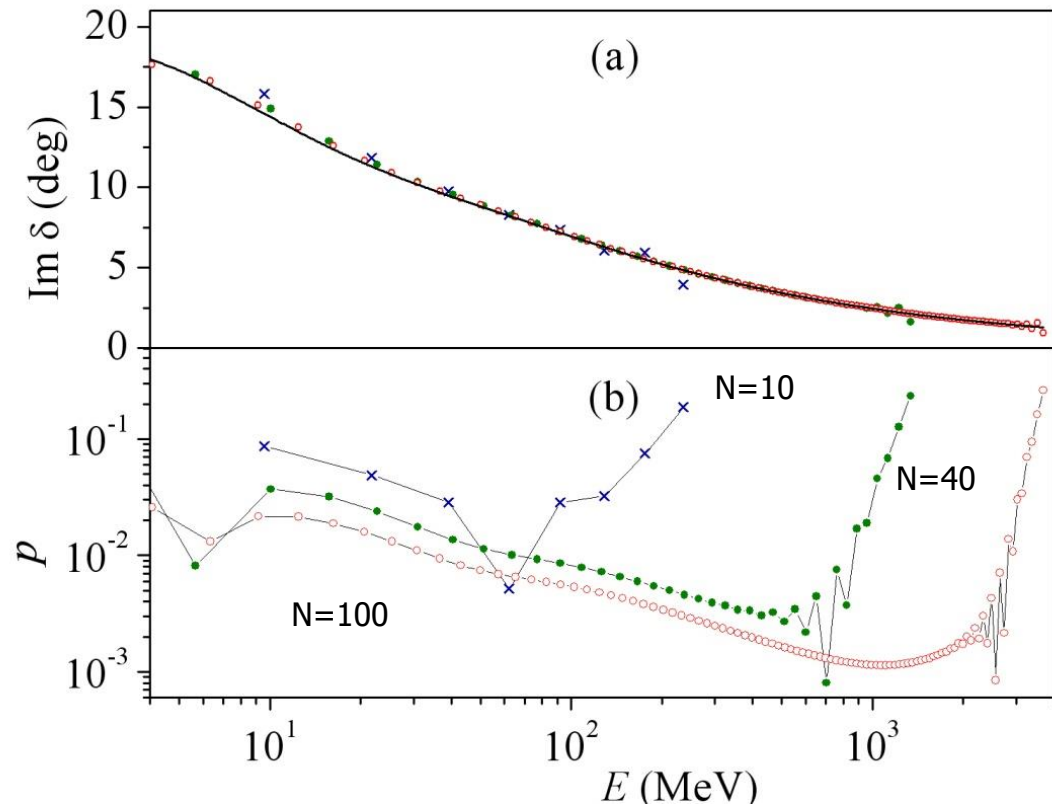
Numerical examples: O.A.R. et al., Phys. Rev. C **81**, 064003 (2010)

# Case of a complex-valued potential

$$V(r) = V_0 \exp(-\gamma r^2), \quad V_0 = -(40 + i10) \text{ MeV}, \quad \gamma = 0.25 \text{ fm}^{-2}$$

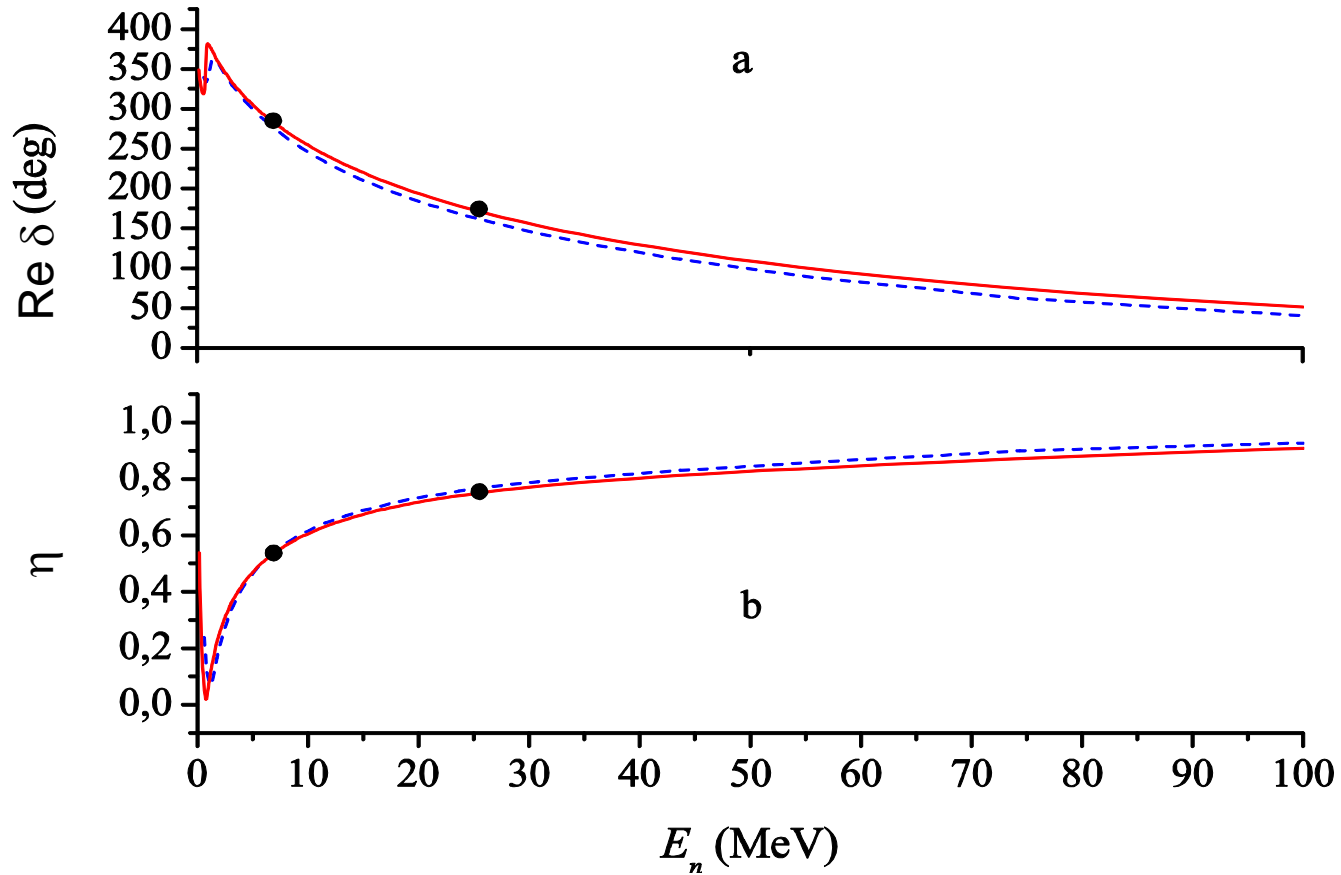
$$\delta(E_j^0) \approx -\pi \frac{E_j - E_j^0}{D_j} \Rightarrow \text{Im } \delta(E_j^0) \approx -\pi \frac{\text{Im } E_j}{D_j}$$

Calculation in the  
harmonic oscillator  
basis



# Complex non-local potential of Perey and Buck for neutron-nucleus scattering

$$V_{nA}(\mathbf{r}, \mathbf{r}') = -U(|\mathbf{r} + \mathbf{r}'|)W(|\mathbf{r} - \mathbf{r}'|)$$

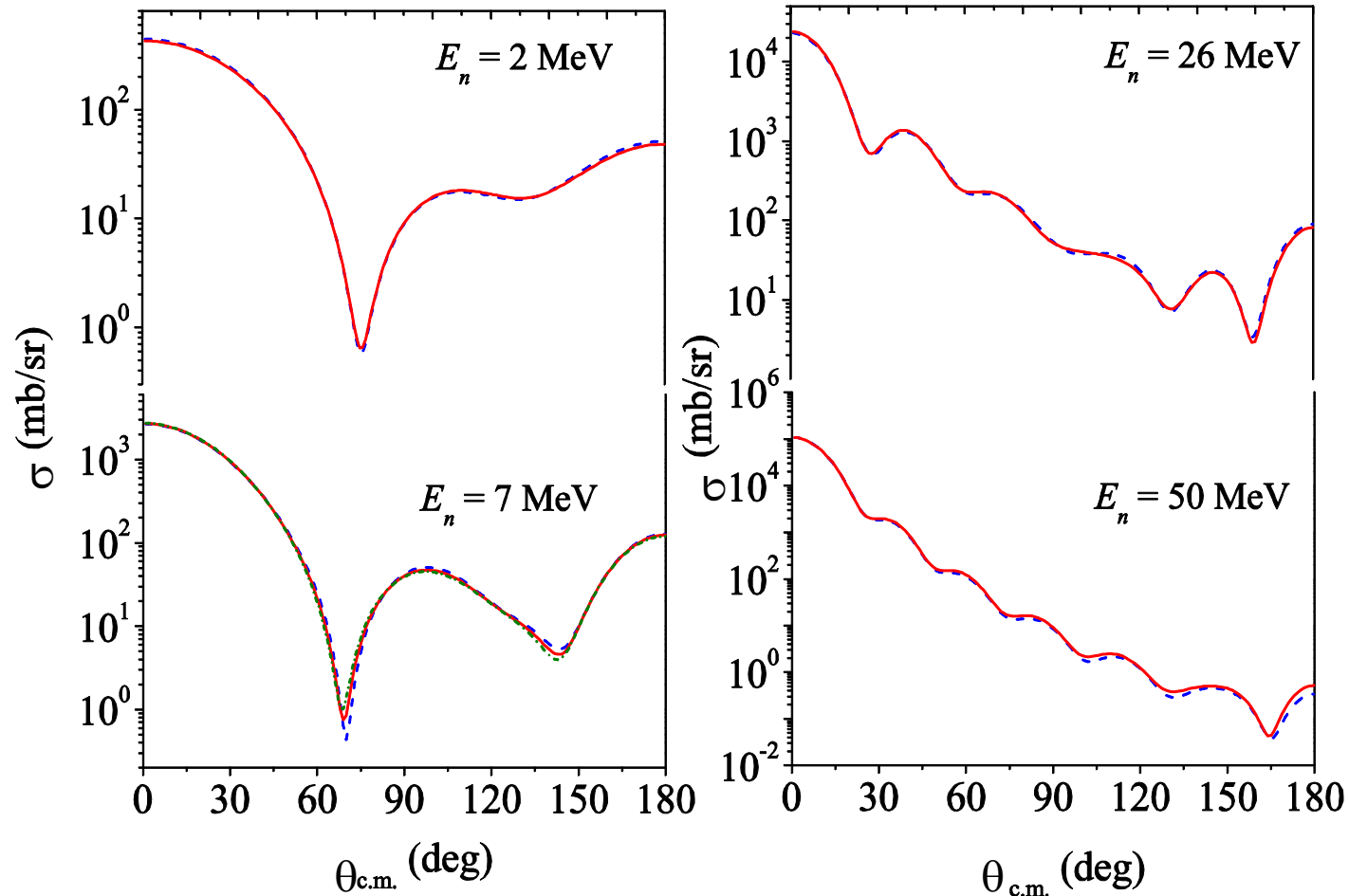


filled circles - results for local phase-equivalent potentials

Calculation in the stationary wave-packet basis.



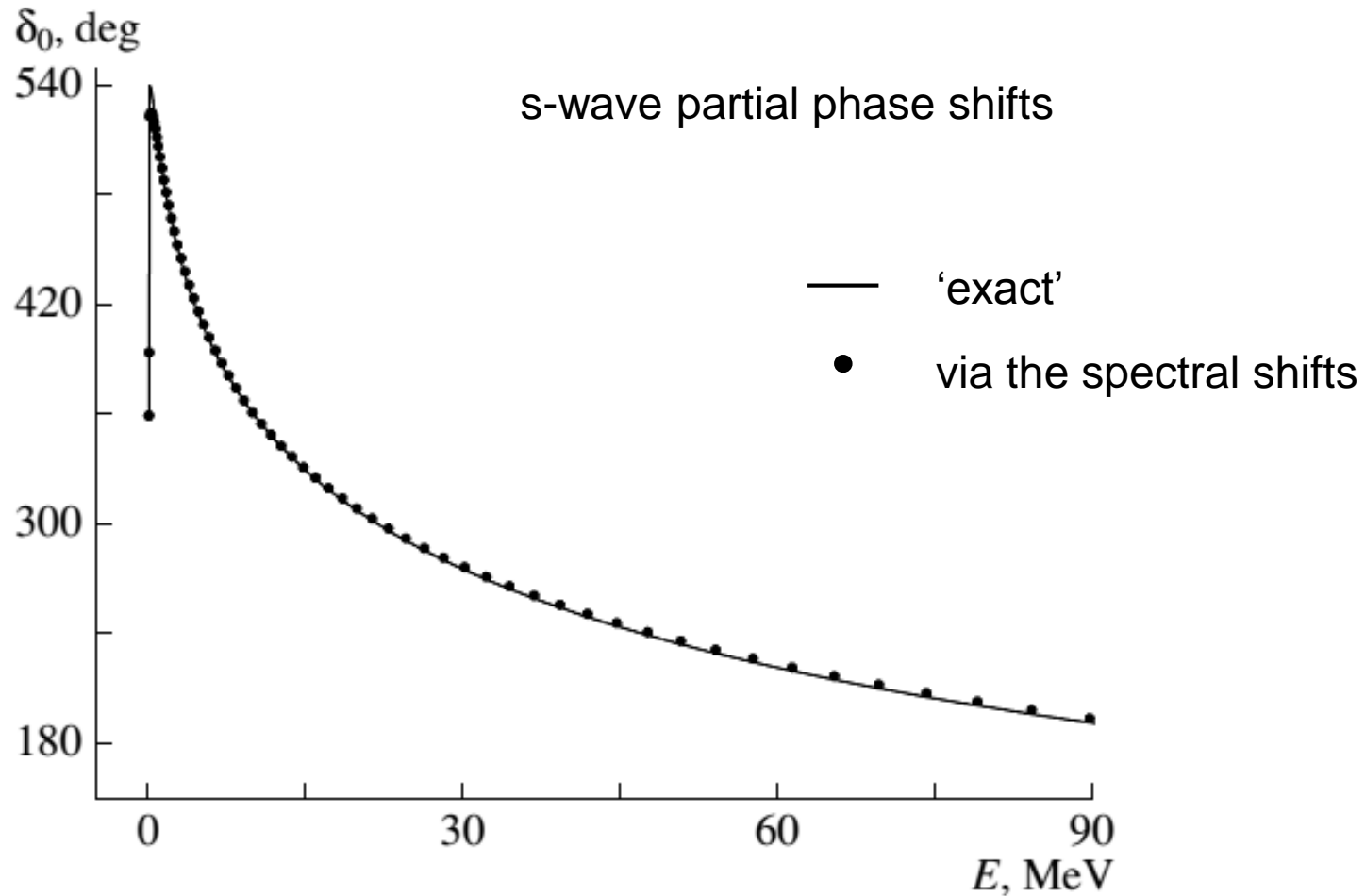
# Differential cross sections for neutron-nucleus scattering with non-local optical potential of Perey and Buck



Only a single diagonalisation procedure for each partial wave is required to get the cross sections in wide energy region.

# $\alpha$ - $\alpha$ scattering

$$H = H_0 + V_s, \quad H_0 = \frac{4e^2}{r}$$

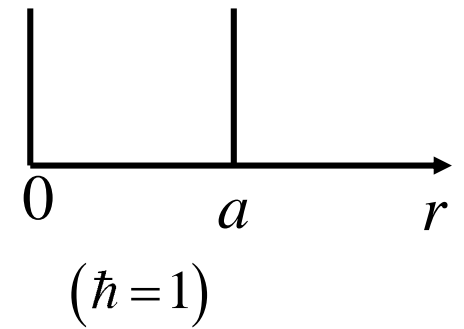


## Cases when $X_0$ is known explicitly

# Scattering problem in a finite volume

Discrete spectrum of the free Hamiltonian:

$$\sin(k_n^0 a) = 0 \Rightarrow k_n^0 = n \frac{\pi}{a}, \quad E_n^0 = \frac{1}{2m} \frac{\pi^2}{a^2} n^2, \quad n = 1, \dots$$



Integrated density of states (inverse):

$$X_0^{(a)}(E) = \frac{a}{\pi} \sqrt{2mE}$$

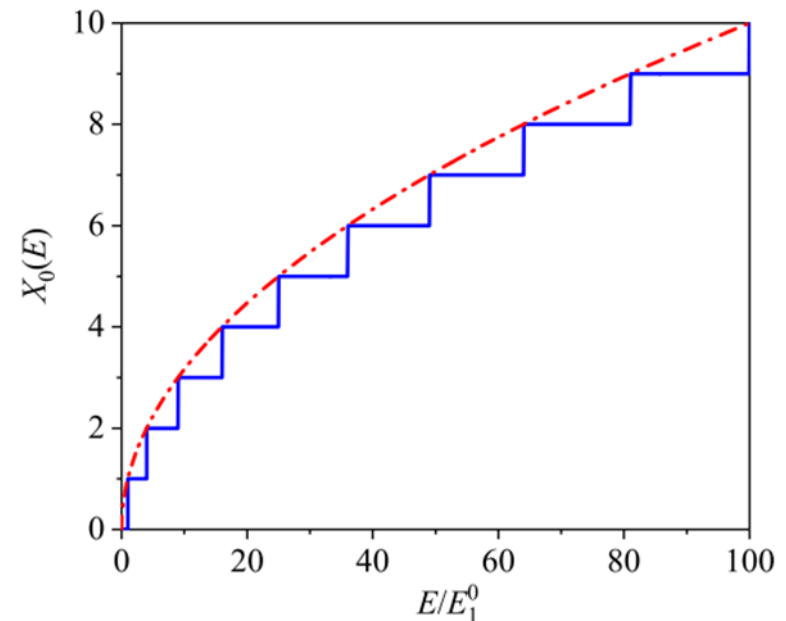
The small parameter:  $\alpha \sim \frac{1}{a}$

The phase shift at energies  $E_n$ :

$$\delta^{(a)}(E_n) = \pi n - a \sqrt{2mE_n}, \quad n = n_b + 1, \dots$$

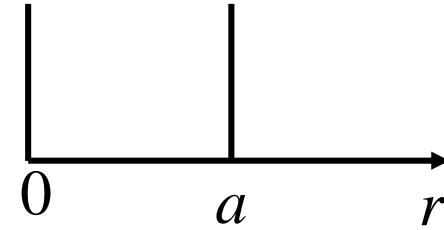
From the boundary condition:

$$\sin \left( a \sqrt{2mE_n} + \delta^{(a)}(E_n) \right) = 0$$



# Scattering problem in a finite volume

For  $l > 0$



$$\delta_l(E) = \eta_l(E) - \phi_l(E)$$

$$\phi_l(E) = \tan^{-1} \frac{j_l(ka)}{n_l(ka)}, \quad k = \sqrt{2mE}. \quad \text{hard sphere phase shift}$$

$\eta_l$  depends on interaction. It can be found by using the R-matrix method.

$$\delta^{(a)}(E_{nl}) = -\pi X_0^{(a)}(E_{nl}) = -\phi_l(E_{nl})$$

$E_{nl}$  - energies of states for which R-matrix is diagonal

The charged particle scattering can be considered similarly:

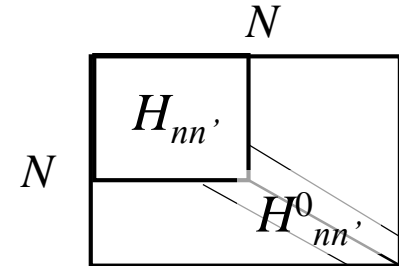
$$\phi_l(E) = \tan^{-1} \frac{F_l(ka)}{G_l(ka)}$$

## J-matrix approach

$$\delta(E) = \pi \left( X(E) - X_0(E) \right) \Rightarrow \delta(E_n) = \cancel{n\pi} - \pi X_0(E_n)$$

Matrix of the asymptotic Hamiltonian has a tri-diagonal (Jacobi) form.

Examples: the kinetic energy operator in the Harmonic Oscillator representation,  
the Coulomb Hamiltonian in bi-orthogonal Laguerre basis.



The SS-HORSE method (A.M. Shirokov et al., Phys. Rev. Lett. **117**, 182502 (2016)).  
At energies equal to EVs of the total Hamiltonian matrix, the phase shift has the simple expression:

$$\delta(E_{nl}) = f_{Nl}(E_{nl}), \quad f_{Nl}(E) \equiv -\tan^{-1} \frac{S_{N+1,l}(E)}{C_{N+1,l}(E)}$$

Function  $f_{Nl}$  does not depend on interaction.

$$\text{Integrated density: } X_0^{(N)}(E) = \frac{1}{\pi} \tan^{-1} \frac{S_{N+1,l}(E)}{C_{N+1,l}(E)}$$

The function  $X(E)$  can be also calculated in the HORSE method at any energy.

Both functions, the continuum level density and the spectral shift function, can be used to find a resonance parameters.

At real energies near the resonance:

$$\Delta(E) = \frac{1}{\pi} \frac{\Gamma/2}{(E - E_R)^2 + \Gamma^2/4} + \Delta_{bg}(E)$$

$$\xi(E) = -\frac{1}{\pi} \arctan \frac{E - E_R}{\Gamma/2} + \xi_{bg}(E)$$

This leads to the following parametrization of the integrated spectral density:

$$X(E) = \frac{1}{\pi} \arctan \frac{E - E_R}{\Gamma/2} + X_{bg}(E) \quad (\xi(E) = X_0(E) - X(E))$$

# Calculations in the Gaussian basis



# Gaussian basis

Radial functions:  $\varphi_j(r) = A_{jl} r^l \exp(-\beta_j r^2)$ ,  $j = 1, \dots, N$

$$|\Psi\rangle = \sum_{n=1}^N C_n |\varphi_n\rangle, \quad \langle \varphi_n | \varphi_k \rangle = I_{nk}$$

Eigenvalue problems for  $H_0$  and  $H$ :

$$\det \| H_{nn'} - EI_{nn'} \| = 0 \rightarrow \{E_j^0\}_{j=1}^N \quad \{E_j\}_{j=1}^N$$

Scale parameters  $\beta_j$  can be chosen: the basis becomes complete at  $N \rightarrow \infty$

Below we use the Tchebyshev grid:

$$\beta_j = g_N(j), \quad \beta_j = \beta_0 \left( \tan \left[ \frac{j}{N+1} \frac{\pi}{2} \right] \right)^t, \quad j = 1, \dots, N$$

This basis is very convenient for approximation of bound states and few-body calculations.

Problems with approximation of continuum:

- sparse discretized spectrum;
- a non-orthogonal system – at rather moderate dimension it becomes numerically linear dependent.

# Union of discretized spectra

Let's construct discretized spectra corresponding to the same density of states  $X_0(E)$ .

Scale parameters:  $\beta_j = g_N(j), \beta_j = \beta_0 \left( \tan \left[ \frac{j}{N+1} \frac{\pi}{2} \right] \right)^t$

Consider a set of  $M$  bases with shifted scale parameters:

$$\left[ \beta_j^m = g_N(j + a_m - 1), j = 1, \dots, N \right]_{m=1}^M, \quad 0 < a_m < 1$$

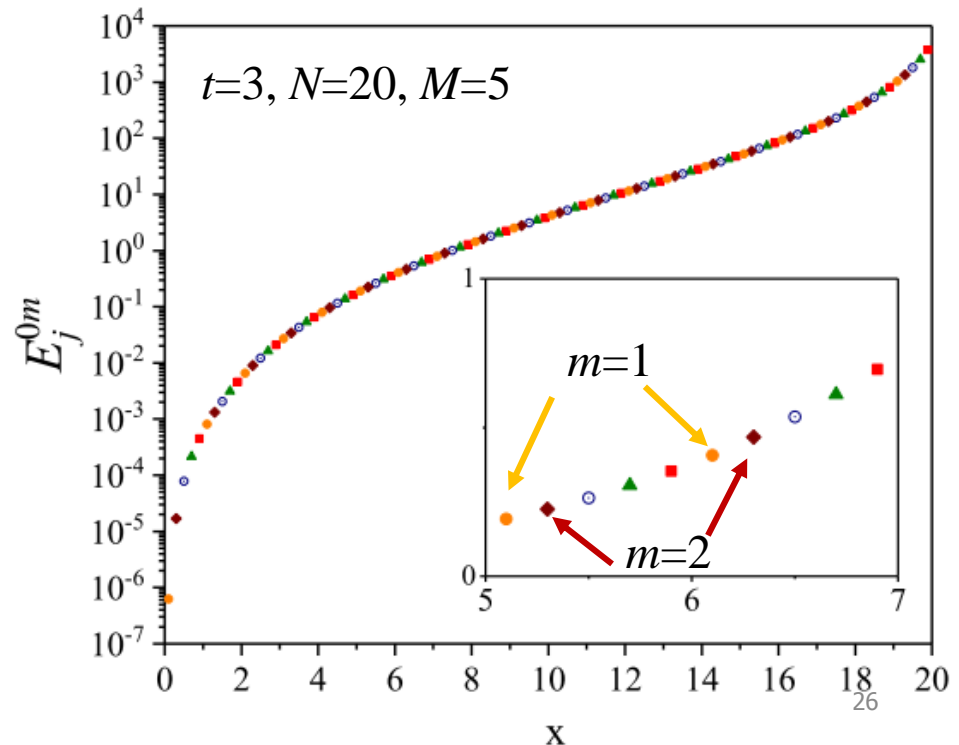
This imitates continuous dependence:

$$\beta(x) = g_N(x), \quad 0 < x \leq N$$

The eigenvalues (found from  $M$  eigenvalue problems) have the similar property - dependence on common index  $x$ :

$$E_j^{0m} = \lambda_0(x\alpha), \quad x = j + a_m - 1$$

$$\alpha \sim \frac{1}{N+1}$$



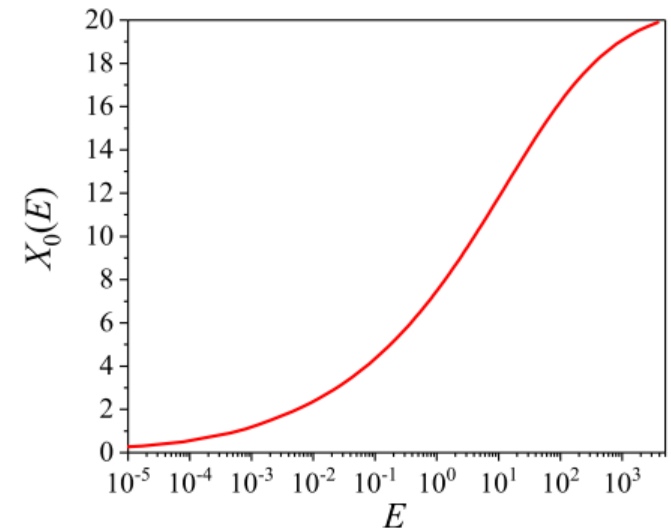
## Non-integer indices

Thus one can construct the ISD as follows:

$$X_0^{(N)}(E_j^{0m}) = j + a_m - 1, \quad \begin{matrix} j = 1, \dots, N \\ m = 1, \dots, M \end{matrix}$$

( to be compared with  $X_0^{(N)}(E_j^0) = j$  )

The integrated density of states reconstructed from 20 Gaussian bases



The same procedure for the spectrum of  $H$ :

$$X^{(N)}(E_k^m) = k + a_m - 1$$

The generalized relation for the phase shift:

$$\delta^{(N)}(E_k^m) = \pi \left[ k + a_m - 1 - X_0^{(N)}(E_k^m) \right], \quad 1 \leq k \leq N, \quad 1 \leq m \leq M$$

 non-integer value

## Numerical examples

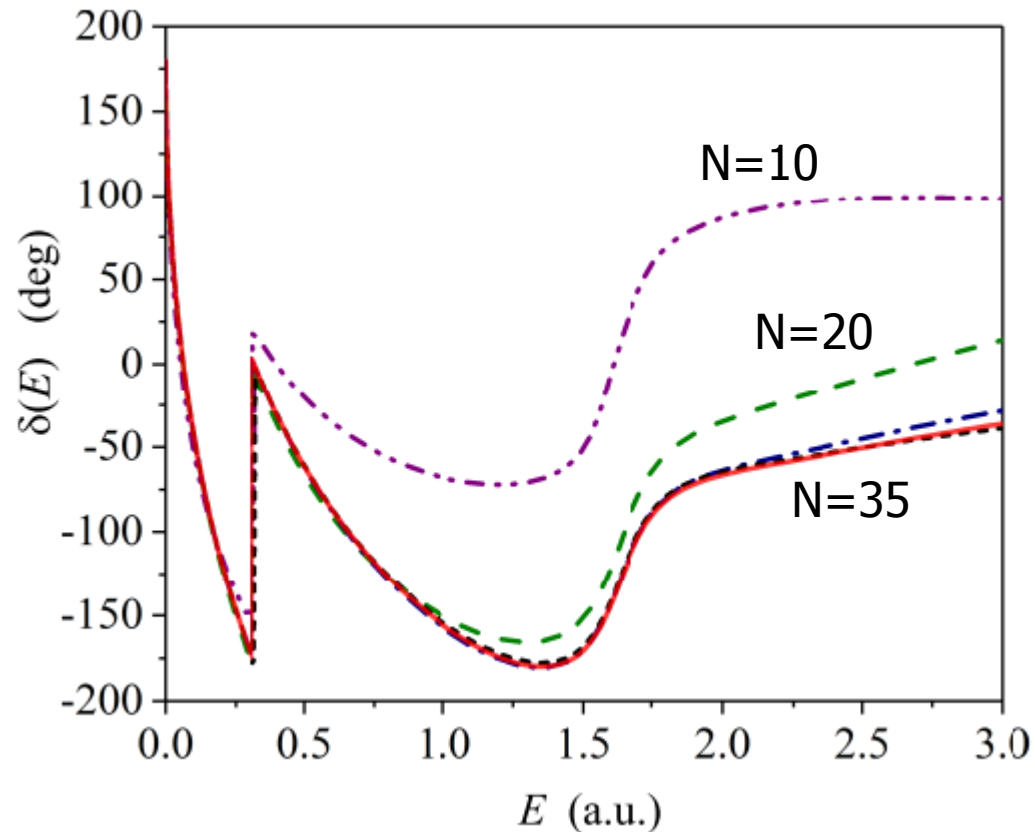
$$H_0 = T, \quad H = H_0 + V$$

$$V(r) = -8 \exp(-0.16r^2) + 4 \exp(-0.04r^2),$$

(Csoto et al., PRA 1990)

atomic units

orbital momentum  $L=0$



--- Direct solution  
of Schroedinger  
eq.

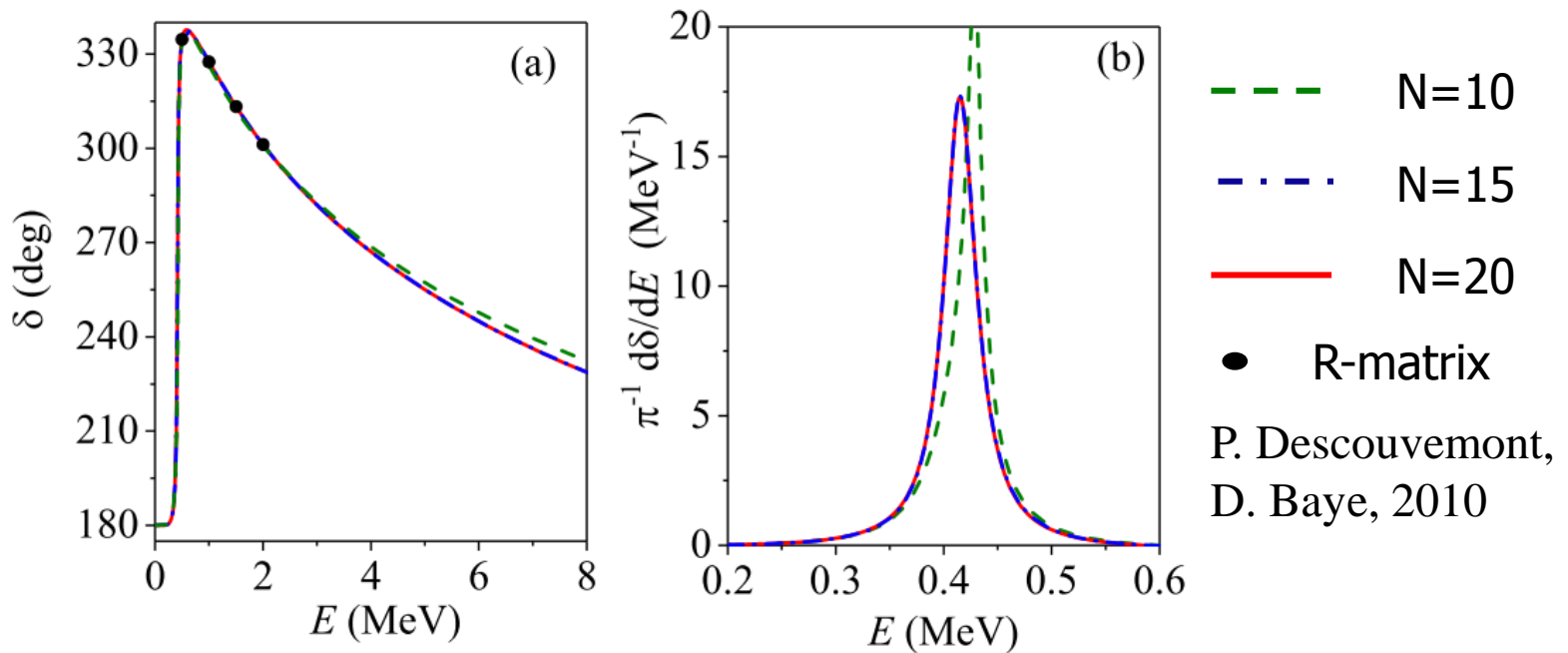
There is one bound state, and two resonances for this potential.

# $p+^{12}\text{C}$ scattering

Unperturbed Hamiltonian includes Coulomb interaction:

$$H_0 = T + \frac{6e^2}{r}$$

Short-range nuclear potential:  $V(r) = V_0 \exp(-(r/r_0)^2)$ ,  $L=0$



There is a forbidden state.

$$E_R = 0.415 \text{ MeV and } \Gamma = 37 \text{ keV}$$

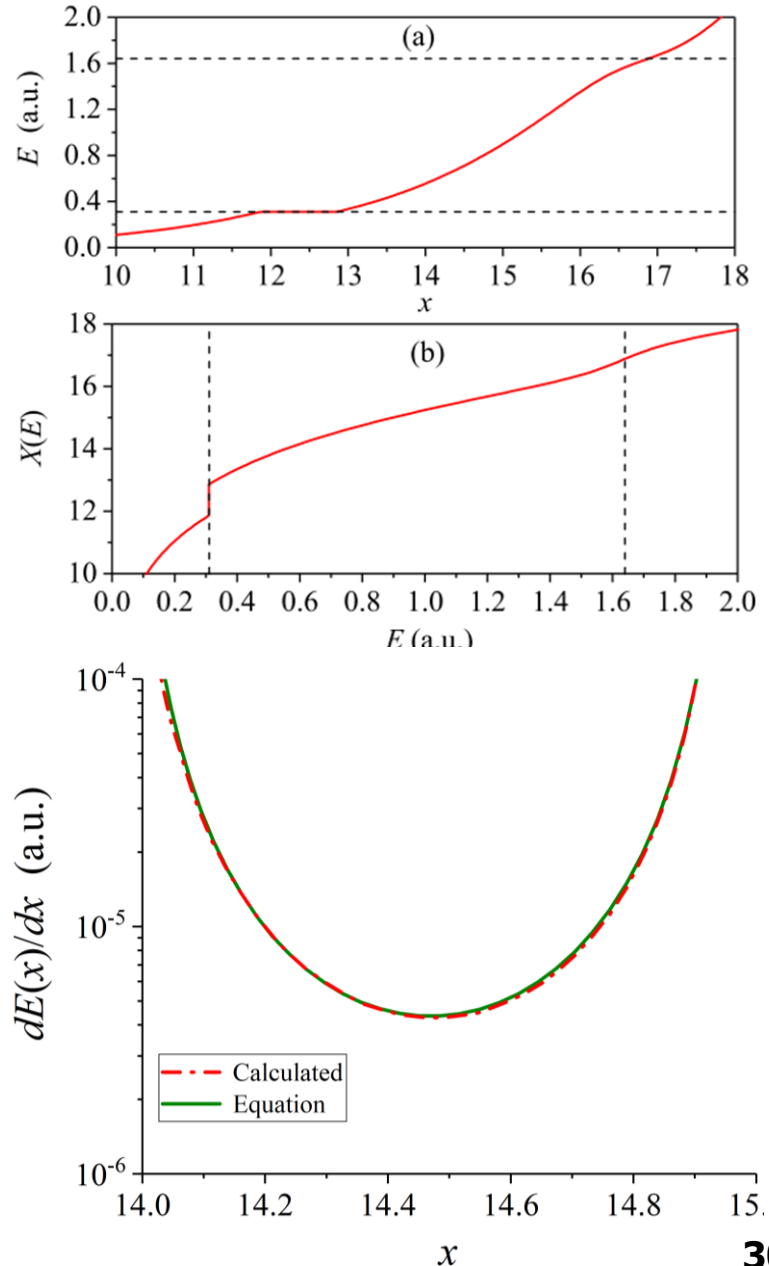
At real energies near the resonance position,  $E(x)$  has a 'plato' similarly to the stabilization approach of Hazi and Taylor.

One can find the parameters of the resonance from the integrated density  $X(E)$  for the total Hamiltonian:

$$X(E) = \frac{1}{\pi} \arctan \frac{E - E_R}{\Gamma/2} + X_{bg}(E)$$

For the narrow resonance  $\frac{dX(E)}{dE} \gg \frac{dX_0}{dE}$

$$\frac{dE(x)}{dx} \approx \pi \frac{\Gamma/2}{\cos^2 \pi(x - x_R)} \quad \Gamma \approx \frac{2}{\pi} \left. \frac{dE(x)}{dx} \right|_{x=x_R}$$



# Multi-channel problem

Total Hamiltonian:  $H_{\nu\nu'} = H_{0\nu} \delta_{\nu\nu'} + V_{\nu\nu'}, \quad \nu, \nu' = 1, \dots, K$

The spectrum is degenerated. At each energy  $E$ , there are  $K$  independent solutions.

The S-matrix elements: 
$$\mathbf{S}(E) = \mathbf{U} \begin{pmatrix} e^{2i\delta_1} & & 0 \\ & \ddots & \\ 0 & & e^{2i\delta_K} \end{pmatrix} \mathbf{U}^\dagger$$

In this case, still there is one spectral shift function:

$$\det \mathbf{S}(E) = \exp(-2\pi i \xi(E)), \quad \xi(E) = -\frac{1}{\pi} \sum_{k=1}^K \delta_k \quad \text{a sum of eigen phase shifts}$$

For this problem we employ the multichannel Gaussian set (forms a basis at  $N \rightarrow \infty$ ):

$$\{\varphi_{j l_\nu m_\nu}^\nu(\mathbf{r}) = A_{j l_\nu} r^{l_\nu} \exp(-\beta_j^\nu r^2) Y_{l_\nu m_\nu}(\hat{\mathbf{r}}), \quad j = 1, \dots, N^\nu\}_{\nu=1}^K$$

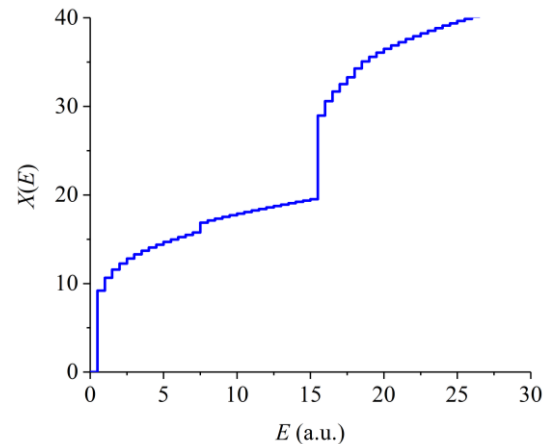
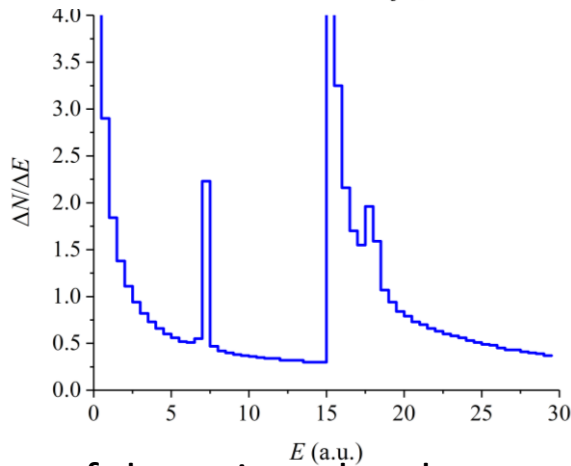
# 'Statistical' treatment of the united spectrum

Here we recover the integrated and spectral densities of states as numbers of the states below and near energy E correspondingly.

Let's divide the spectrum into intervals  $\Delta E_i$  and consider the values:

$$\rho_i = \frac{\Delta N_i}{\Delta E_i}, \quad X_i = \sum_{j \leq i} \rho_j \Delta E_j = \sum_{j \leq i} \Delta N_j$$

$\Delta N_i$  – number of states in an interval



In case of the union, the above values should be divided by the number of spectra M:

$$\rho_i^U = \frac{\Delta N_i}{M \Delta E_i}, \quad X_i^U = \frac{1}{M} \sum_{j \leq i} \Delta N_j$$

We have considered two types of such a treatment:

- intervals with a fixed number of states  $\Delta N$ ,
- intervals with a fixed energy  $\Delta E$ .

Both methods result in the same spectral and integrated densities.



## Two-channel model problem

$$H_0 = \begin{pmatrix} -\frac{1}{2} \frac{d^2}{dr^2} & 0 \\ 0 & -\frac{1}{2} \frac{d^2}{dr^2} + 15 \end{pmatrix}$$

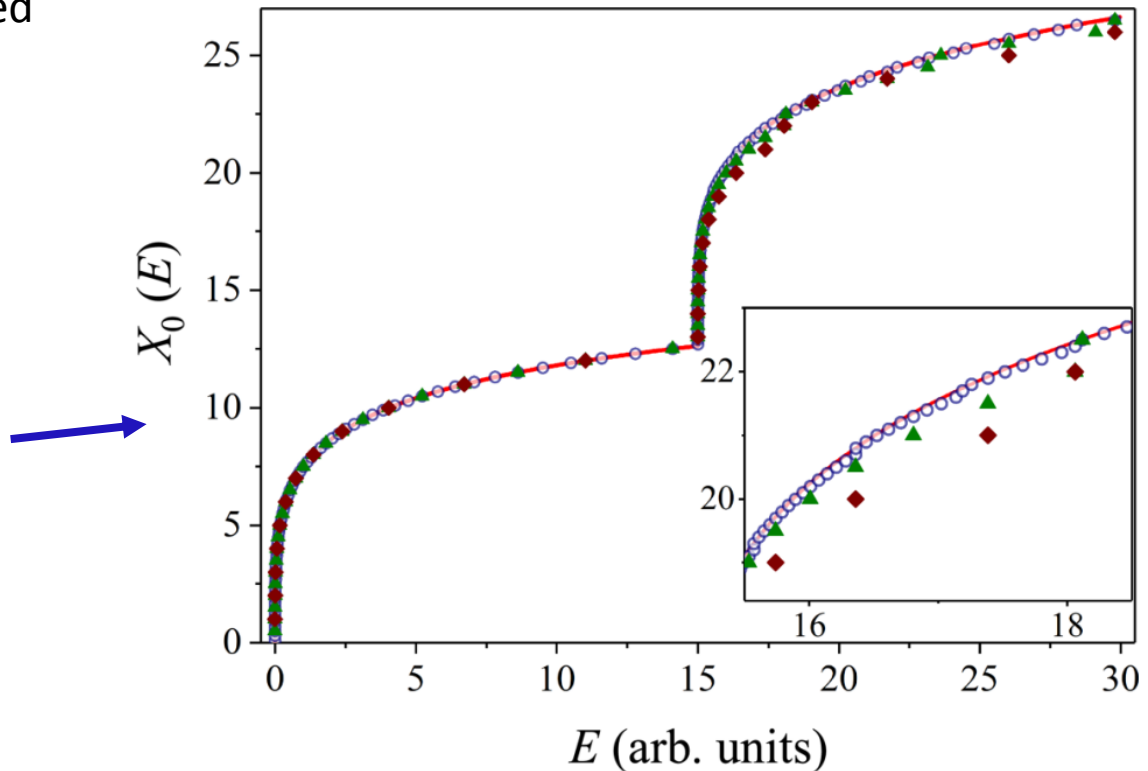
$$V(r) = \begin{pmatrix} 15e^{-0.5r^2} & 5re^{-r^2} \\ 5re^{-r^2} & 15(r^2 - r - 1)e^{-r^2} \end{pmatrix}$$

Integrated density for the asymptotic Hamiltonian is a sum of integrated densities for simple spectra:

$$X_0(E) = \sum_{v=1}^K X_{0v}(E)$$

The numerical reconstruction of  $X_0(E)$  with different multiplicity of union  $M$ .

- ◆  $M=1$
- ▲  $M=2$
- $M=10$
- exact sum  $X_0^1(E) + X_0^2(E)$



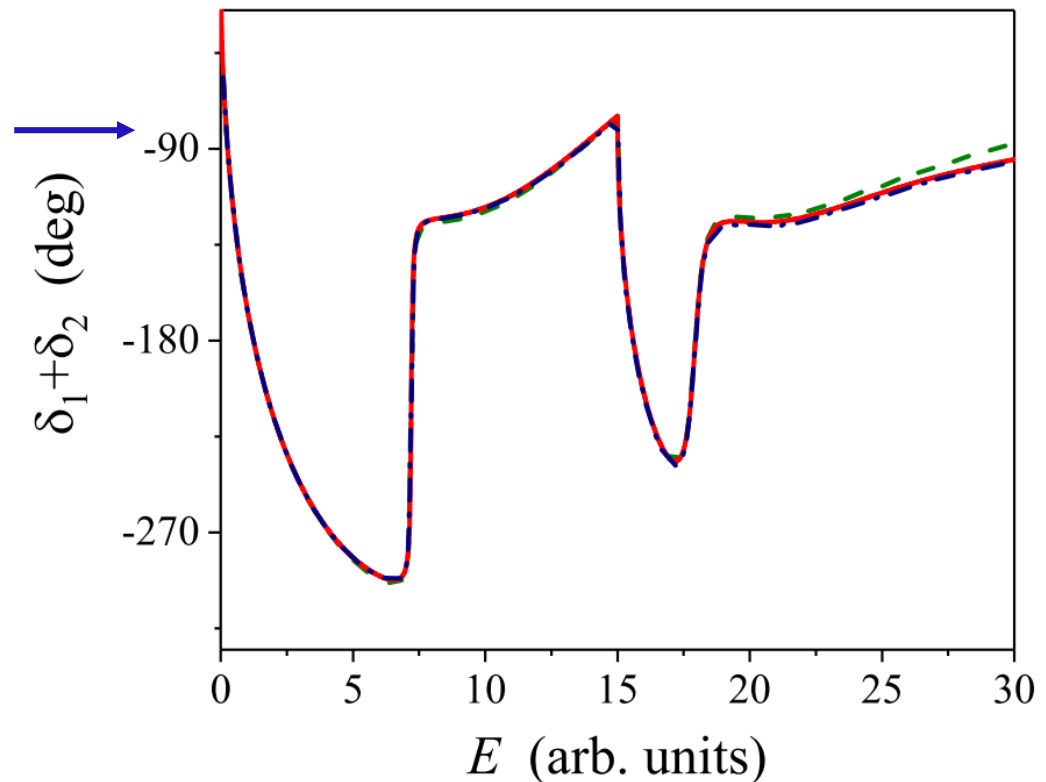
# Sum of the phase shifts

After calculation of the integrated densities for the total and asymptotic Hamiltonians  $X(E)$  and  $X_0(E)$ , one can find the sum of the phase shifts:

$$\sum_{i=1}^K \delta_i(E) \approx \pi [X(E) - X_0(E)]$$

Sum of the eigenphases for the model two-channel problem found from unions with  $M=160$  of Gaussian sets with dimensions:

- · —  $N_1=N_2=22$
- · —  $N_1=N_2=30$
- solution of Srchoed.eq.



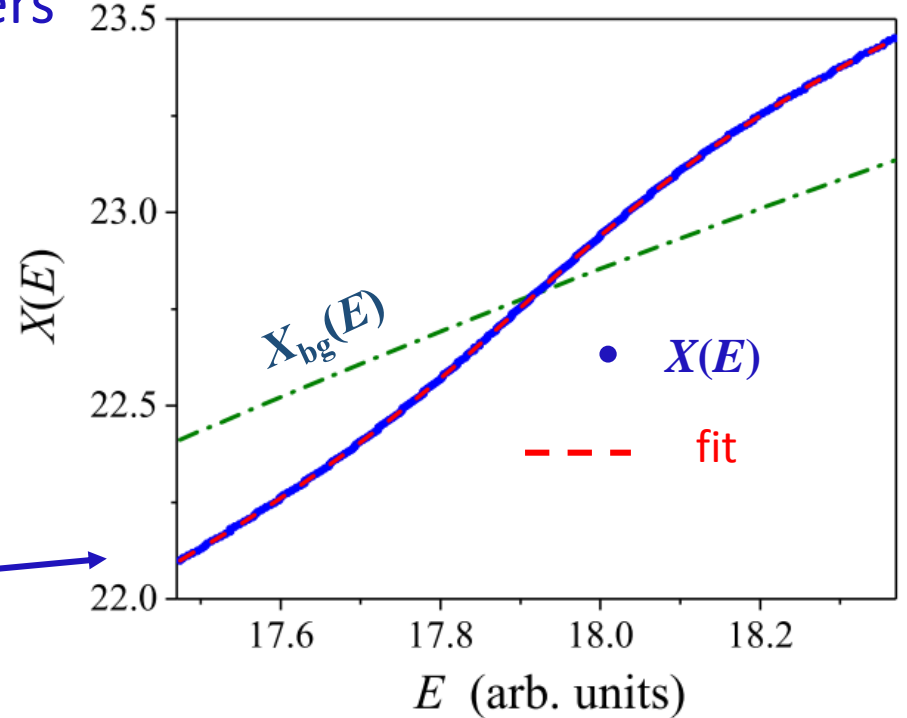
There two resonances for such a problem. The second resonance is above the threshold of the second channel.

## Finding the resonance parameters

The resonance term is present in the density of the total Hamiltonian. So that, one may try to fit only one integrated density:

$$X(E) = \frac{1}{\pi} \arctan \frac{E - E_R}{\Gamma/2} + X_{bg}(E)$$

Results of the fitting procedure



Parameters of the second resonance:

TABLE I. The parameters of the resonance  $E_R$  and  $\Gamma$  (in arb.units) found by fitting the functions  $X(E)$  and  $X(E) - X_0(E)$  for  $N_1 = N_2 = 22$  and different  $M$ .

$M$	$X(E)$		$X(E) - X_0(E)$	
	$E_R$	$\Gamma$	$E_R$	$\Gamma$
20	17.92(4)	0.59(5)	17.94(6)	0.58(7)
40	17.92(2)	0.60(2)	17.93(2)	0.58(2)
80	17.920(6)	0.596(6)	17.918(7)	0.591(8)
160	17.919(2)	0.594(2)	17.919(3)	0.589(3)

## A problem with tensor coupling in the interaction

The realistic model for NN interaction taking into account an additional non-nucleonic channel (with the dibaryon state).

$$\mathbf{H} = \mathbf{H}_0 + \mathbf{V}, \quad \mathbf{H}_0 = \text{diag}[T_S, T_D, E_0|\alpha\rangle\langle\alpha|],$$

$$\mathbf{V} = \begin{pmatrix} V_{SS}^{\text{ext}} & V_{SD}^{\text{ext}} & \mu_S|\varphi_S\rangle\langle\alpha| \\ V_{DS}^{\text{ext}} & V_{DD}^{\text{ext}} & \mu_D|\varphi_D\rangle\langle\alpha| \\ \mu_S|\alpha\rangle\langle\varphi_S| & \mu_D|\alpha\rangle\langle\varphi_D| & 0 \end{pmatrix}.$$

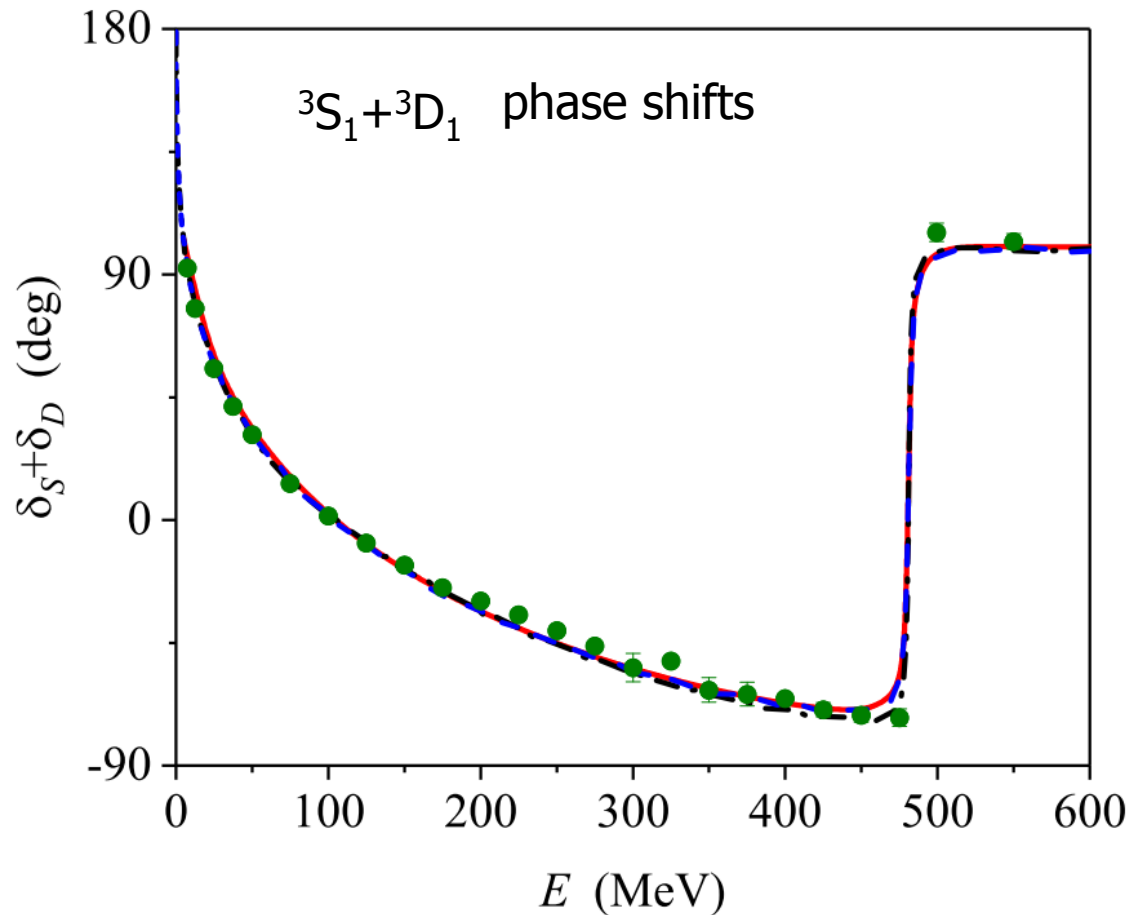
The sum of the eigen phase shifts for the coupled  ${}^3S_1 - {}^3D_1$  channels found using  $M=80$  Gaussian bases:

**black curve** -  $N_1 = N_2 = 10$

**blue curve**  $N_1 = N_2 = 30$

**red curve** - from a solution of the coupled Lippmann-Schwinger equations

**dots** - the SAID PWA data

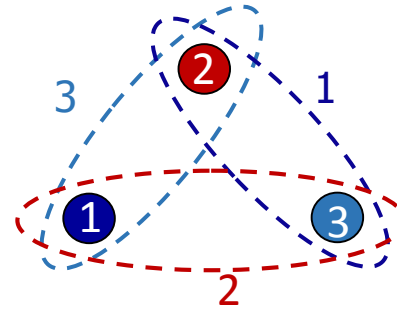


# Three-body problem

# Three-body problem

Total Hamiltonian:

$$H = H_0 + \sum_{i=1}^3 V_i$$



One has to consider **five** Hamiltonians in three-body case:

$H$  – the total Hamiltonian;

$H_0$  – the free Hamiltonian (kinetic energy operator);

$H_i = H_0 + V_i$  ( $i=1,2,3$ ) – three channel Hamiltonians

$$R_0(E) = [H_0 - (E + i0)]^{-1}, \quad R(E) = [H - (E + i0)]^{-1}$$

$$R_i(E) = [H_i - (E + i0)]^{-1}$$

# Three-body problem

The trace equation (Buslaev, Merkuriev 1970, the third virial coefficient):

$$\mathrm{Tr} \left[ f(H) - f(H_0) - \sum_{i=1}^3 (f(H_i) - f(H_0)) \right] = \sum_b f(E_b) + \frac{1}{\pi} \int_{E_{th}}^{\infty} dE \Omega(E) f(E)$$

Three-body spectral function:

$$\Omega(E) = \mathrm{Tr} \left[ \mathrm{Im} R(E) - \mathrm{Im} R_0(E) - \sum_{i=1}^3 (\mathrm{Im} R_i(E) - \mathrm{Im} R_0(E)) \right]$$

One may consider a three-body analog of the spectral shift function as an integral:

$$\xi_3(E) = - \int_{-\infty}^E dE' \left[ \sum_b \delta(E' - E_b) + \frac{1}{\pi} \Omega(E') \right]$$

One has to prove that this function exists.

## Three-body integrated spectral function

$$\xi_3(E) = - \int_{-\infty}^E dE' \left[ \sum_b \delta(E' - E_b) + \frac{1}{\pi} \text{Tr} \left( \text{Im} R(E') - \text{Im} R_0(E') - \sum_{i=1}^3 \{ \text{Im} R_i(E') - \text{Im} R_0(E') \} \right) \right]$$

In area of three-body discrete spectrum  $\xi_3(E)$  should be a step-like function similarly to SSF:

$$\xi_3(E) = - \sum_b \theta(E - E_b), \quad E < E_{th}$$

In a case, when there is two-body bound state in only one subsystem {23}, below the three-body breakup threshold ( $E=0$ ), only two terms contribute to the difference:

$$\xi_3(E) = - \sum_b \theta(E - E_b) - \frac{1}{\pi} \int_{E_{th}}^E dE' \text{Tr}[\text{Im} R(E') - \text{Im} R_1(E')], \quad E < 0$$

This should correspond to the sum of the eigen phase shifts of the total Hamiltonian similarly to the two-body case.

If the above three-body spectral function exists it should be represented as the difference of integrated densities for Hamiltonians in a case of continuum discretization:

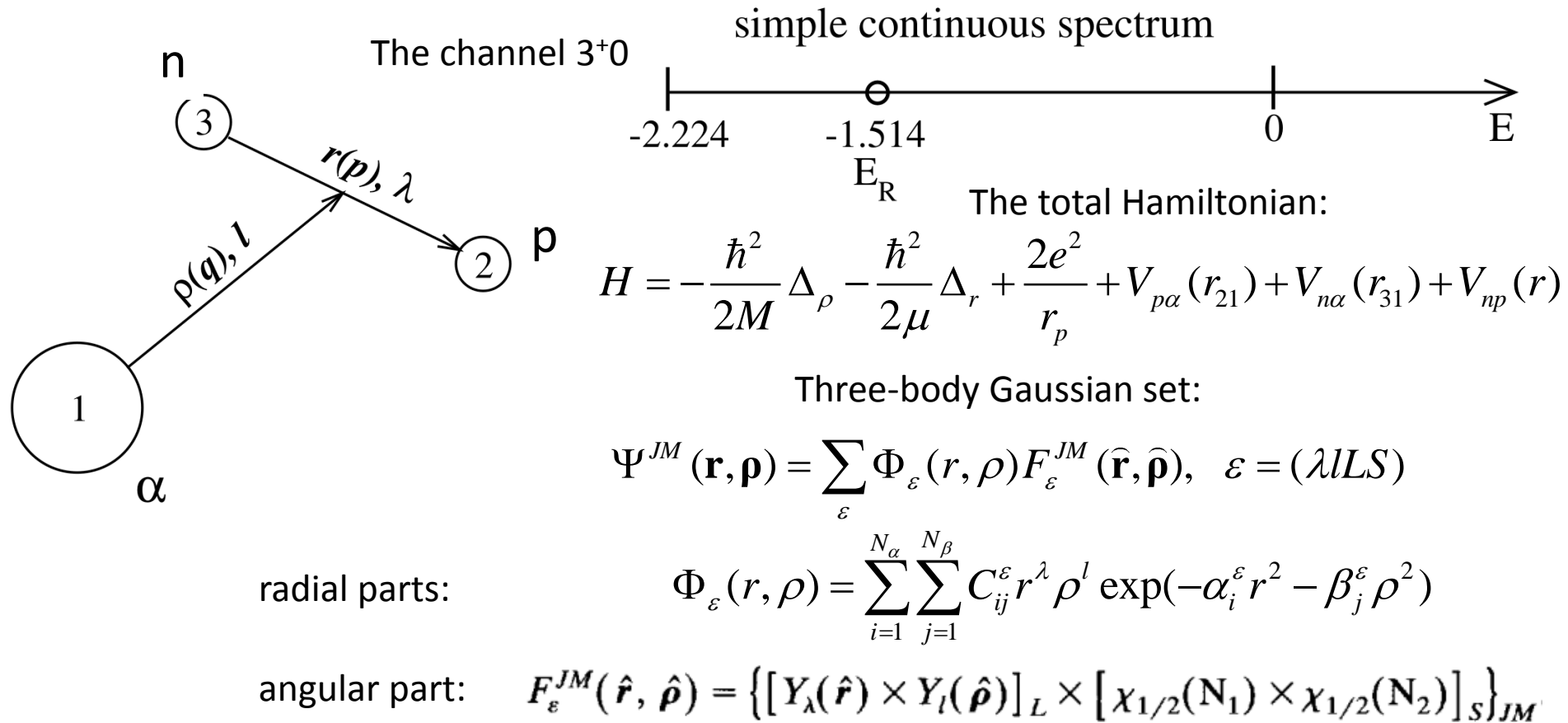
$$\xi_3(E) = - \left[ X(E) - X_0(E) - \sum_{i=1}^3 (X_i(E) - X_0(E)) \right]$$

This means that the corresponding difference should not depend on the basis dimension and should have a finite limit with increasing it to infinity.



# $\alpha$ NN system in the three-cluster model

Consider a three-body model for  $\alpha$ -n-p system. **Below the three-body breakup threshold**, the spectrum of the total Hamiltonian is simple. Thus one can employ a similar treatment as in two-body case.



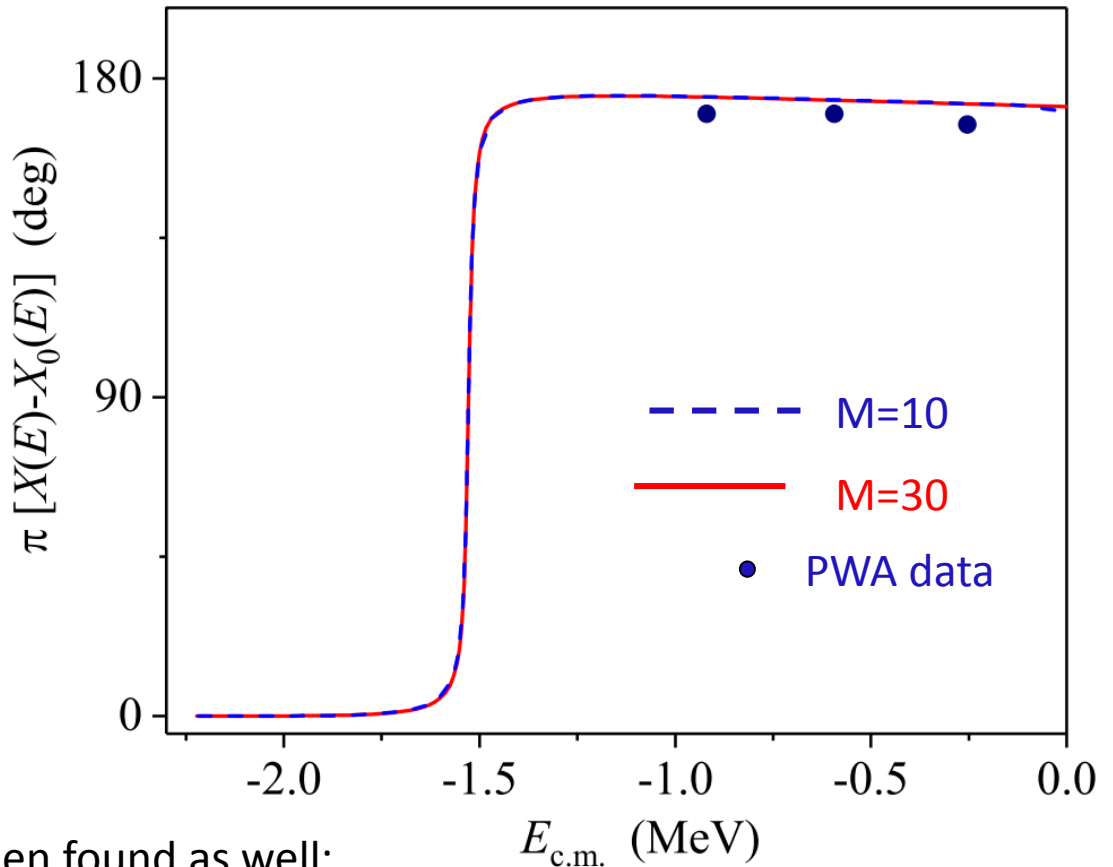
# $\alpha$ - d scattering below three-body breakup threshold

For the configuration  $3^+0$  one may calculate the partial  $\alpha$ -d phase shift  ${}^3D_3$  as the difference of spectral densities for the total and asymptotic Hamiltonians.

TABLE II. The quantum numbers and the dimensions of the basis components for a calculation of the  $3^+0$  state of  ${}^6\text{Li}$ .

$\gamma = \lambda L S$	$N_r \times N_p$
0221	$15 \times 20$
2021	$15 \times 20$
2221	$15 \times 20$
2231	$15 \times 20$
2241	$15 \times 20$
2421	$8 \times 8$
4221	$8 \times 8$
4041	$8 \times 8$

Here a variation of the basis parameters over relative np distance  $r$  has been employed to construct the union of  $M$  spectra.



The parameters for  ${}^6\text{Li}(3^+0)$  has been found as well:

$$E_R = -1.528 \text{ MeV}, \quad \Gamma = 22 \text{ keV},$$

The experimental values:  $E_R = -1.514 \text{ MeV}$ ,  $\Gamma = 24 \text{ keV}$ .

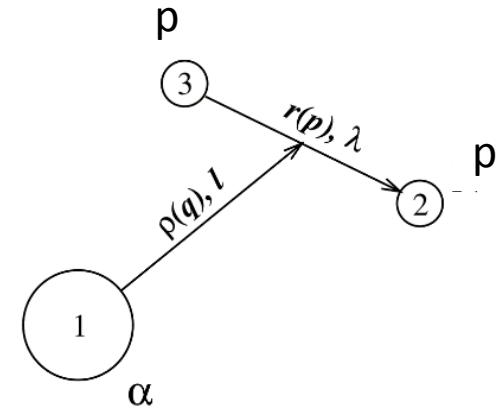
# Resonance above three-body breakup threshold

${}^6\text{Be}$  is considered as a three-body system  $\alpha+p+p$ :

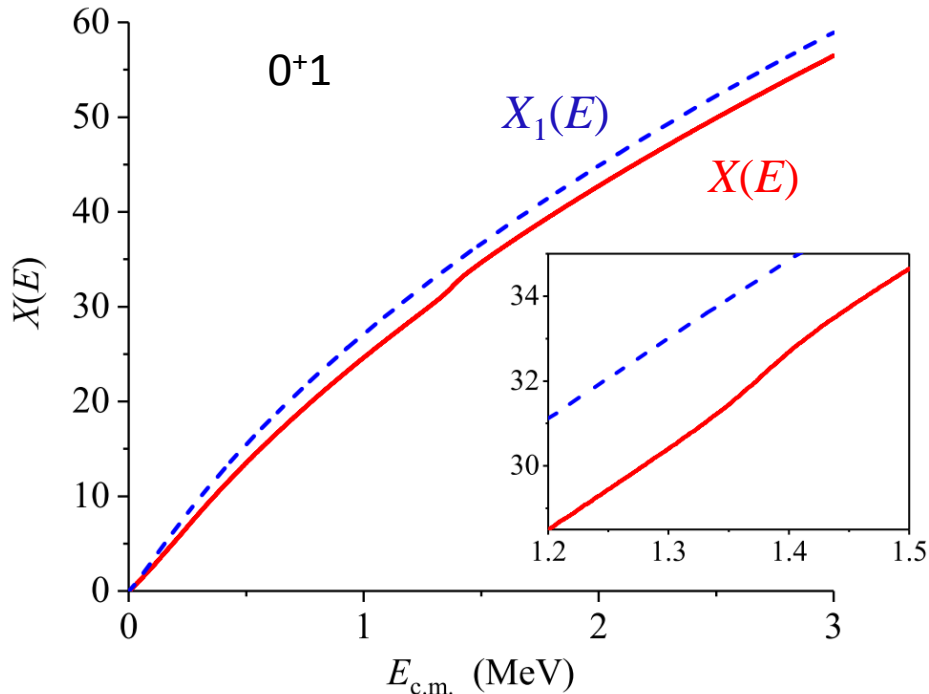
$$H = -\frac{\hbar^2}{2M} \Delta_\rho - \frac{\hbar^2}{2\mu} \Delta_r + \frac{2e^2}{r_{31}} + \frac{2e^2}{r_{21}} + \frac{e^2}{r} + V_{p\alpha}(r_{31}) + V_{p\alpha}(r_{21}) + V_{pp}(r)$$

One of asymptotic Hamiltonians:

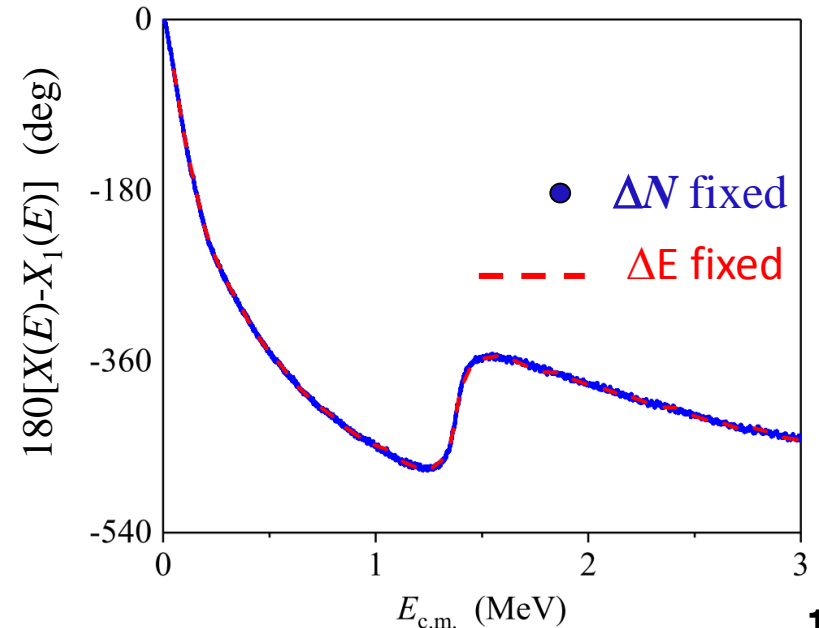
$$H_1 = -\frac{\hbar^2}{2M} \Delta_\rho - \frac{\hbar^2}{2\mu} \Delta_r + \frac{2e^2}{r_{31}} + \frac{2e^2}{r_{21}} + \frac{e^2}{r} + V_{pp}(r)$$



The united spectrum for each Hamiltonian is constructed by varying parameters over both Jacobi variables  $\mathbf{r}$  and  $\boldsymbol{\rho}$ .



The resonance is clearly seen in the difference of integrated densities



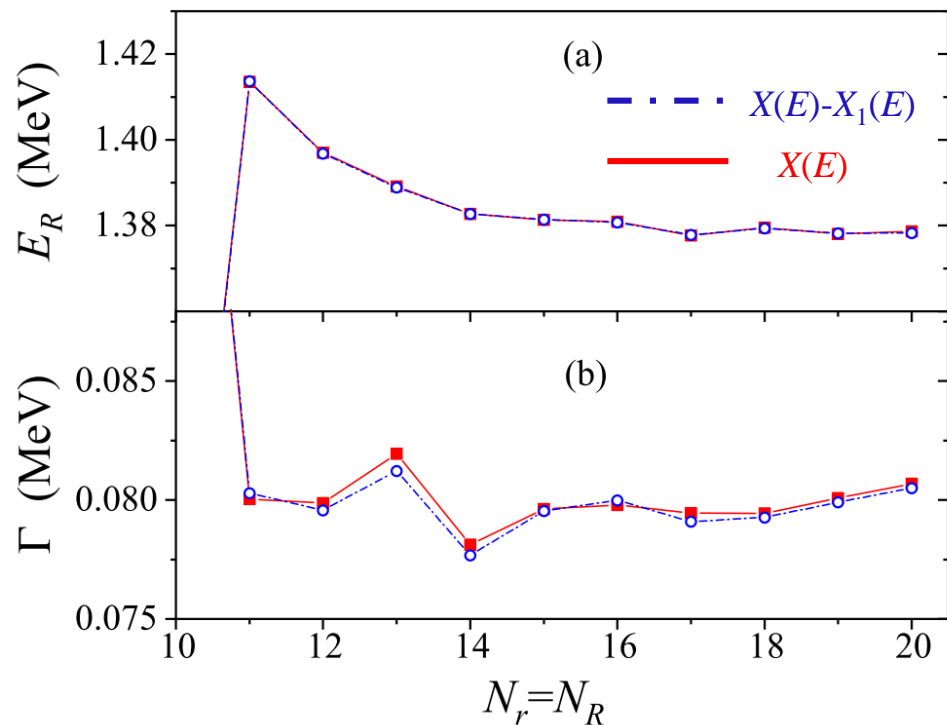
# Resonance 0<sup>+</sup>1

The taken partial configurations:

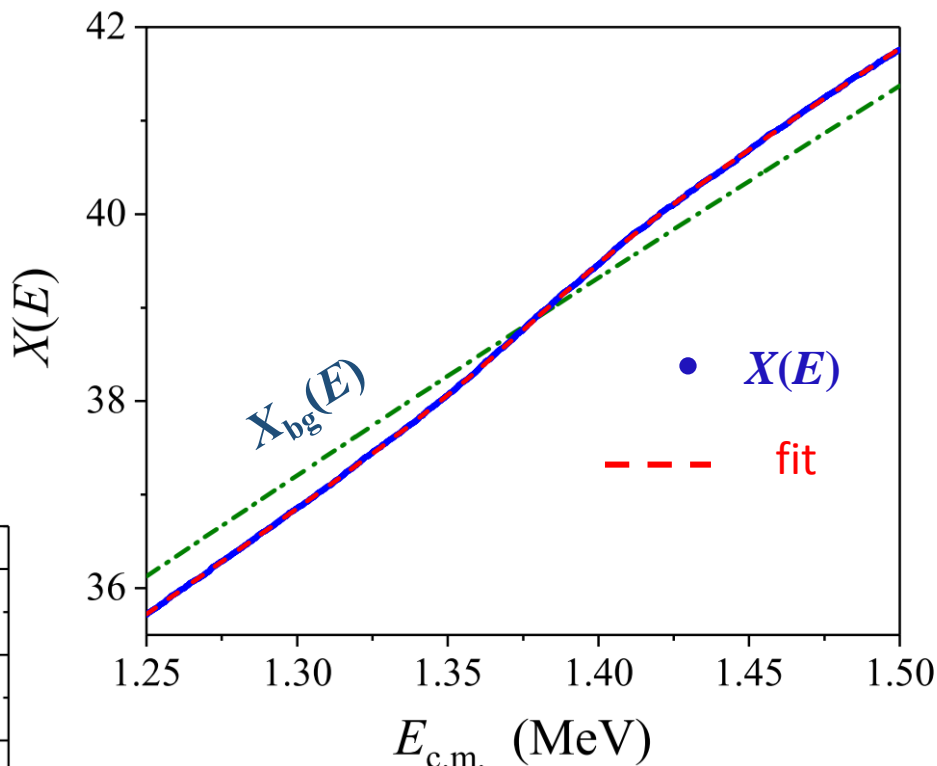
$$\gamma = \{\lambda, l, L, S\} = \{0000\}, \{1111\}, \{2200\}, \{3311\}$$

The resonance parameters has been found from the difference  $X(E)-X_0(E)$  and from a single density  $X(E)$ . Both results are very close.

Dependence on the basis dimension:



$$X(E) = \frac{1}{\pi} \arctan \frac{E - E_R}{\Gamma/2} + X_{bg}(E)$$



The found parameters for  ${}^6\text{Be}(1^+0)$  :

$$E_R = 1.379 \pm 0.001 \text{ MeV}, \Gamma = 79.8 \pm 0.5 \text{ keV}$$

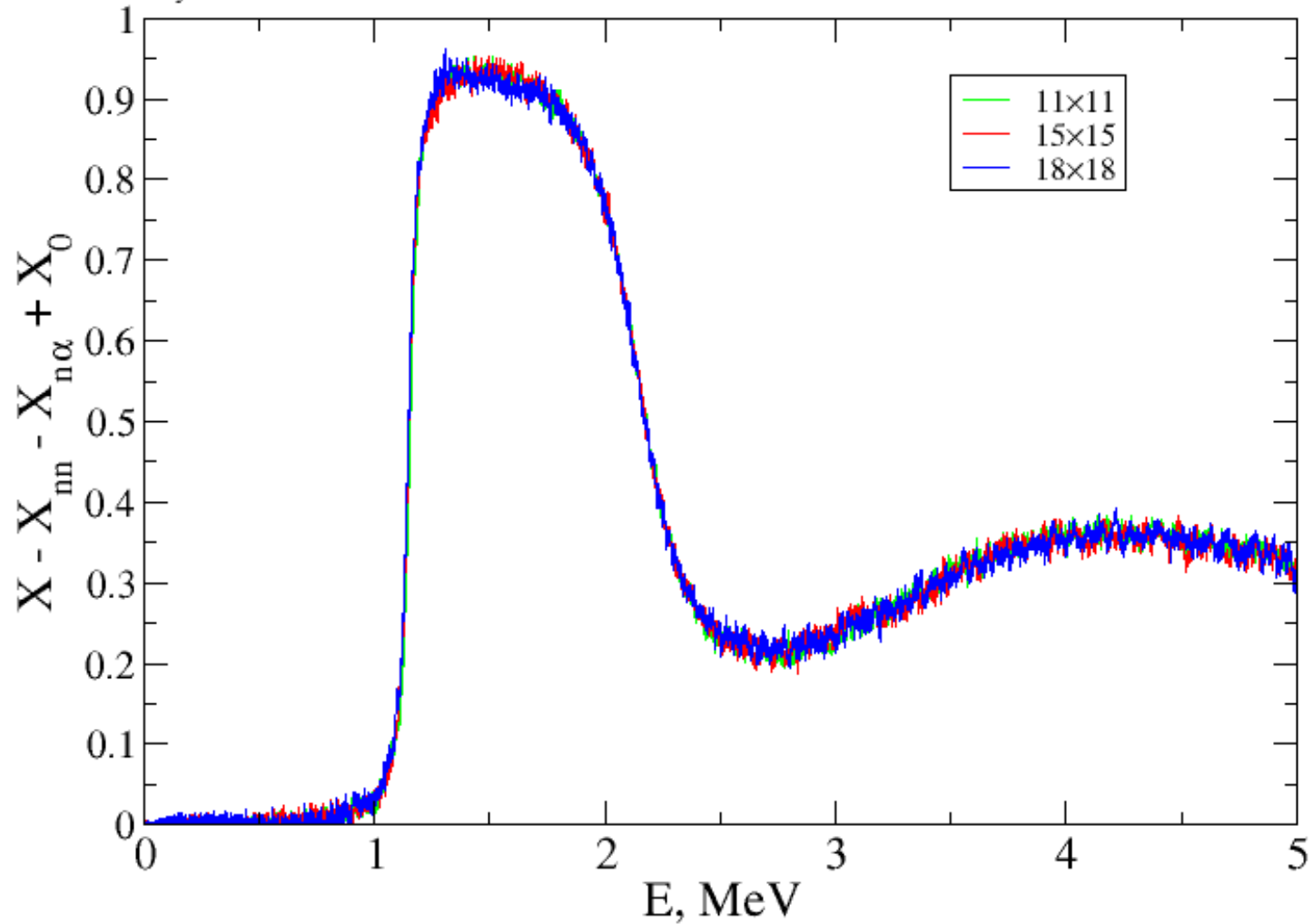
Experimental values:

$$E_R = 1.371 \text{ MeV}, \Gamma = 92 \text{ keV}$$

# Test of the integrated spectral function for $\alpha nn$ system

${}^6\text{He} (2^+ 1)$ , 7 channels

$(N_x \times N_y)$  are the basis dimensions for 3 main channels (>97% in wave function)



# Conclusions

We have discussed the formalism with continuous spectral densities and integrated densities for solving problems in continuum.

Integrated spectral densities are quite suitable for studying discretized spectrum within different  $L^2$  approaches.

We have demonstrated the efficiency of the method for finding the resonance parameters for the three-body problem with three charged particles as well.

The formalism with the three-body spectral function needs in further mathematical justification.

Important applications:

- study of two-proton radioactivity;
- study of existence of the three-neutron resonance for different modern models of NN interaction.

Three-body spectral function can be used for new treatment of the virial expansion.

The method with union of discretized spectra may be generalized for solving the scattering equations.

V.N.P., O.A.R., V.A.K., Phys. Rev. C **109**, 014002 (2024).

O.A. R., V.N.P., J.Phys. A **55**, 095301 (2022).

V.N.P., O.A.R., Phys. At. Nucl. **85**, 1087 (2022).

## Important references:

1. D. R. Yafaev, *Mathematical Scattering Theory: General Theory* (American Mathematical Society, Providence, RI, 1992).
2. M. S. Birman and A. V. Pushnitsky, *Integr. Equat. Oper. Th.* **30**, 191 (1998).
3. И.М. Лифшиц, *ЖЭТФ* **17**, 1017 (1947).
4. И.М. Лифшиц, *ЖЭТФ* **17**, 1076 (1947).
5. И.М. Лифшиц, *Успехи мат. наук* **7**, 171 (1952).
6. V. S. Buslaev and S. P. Merkuriev, *Theor. Math. Phys.* **5**, 1216 (1970).

**Thank you for your attention!**

# Спектральная плотность

Плотность состояний для дискретного спектра

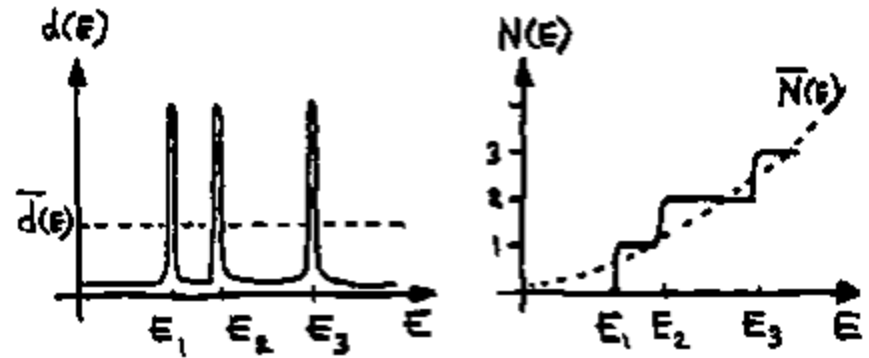
$$\rho(E) = \sum_n \delta(E - E_n)$$

Можно записать формальное равенство

$$\delta(E - E_n) = -\lim_{\varepsilon \rightarrow 0} \frac{1}{\pi} \operatorname{Im} \frac{1}{E - E_n + i\varepsilon} \Rightarrow \rho(E) = -\frac{1}{\pi} \lim_{\varepsilon \rightarrow 0} \operatorname{Im} \operatorname{Tr} \left( [E + i\varepsilon - H]^{-1} \right)$$

Спектральная плотность может быть представлена как производная от счетной функции

$$\rho(E) = \frac{dN}{dE}, \quad N(E) = \sum_n \theta(E - E_n)$$



Chaos: classical and quantum ([chaosbook.org](http://chaosbook.org))



# Union of the discretized spectra

Radial functions of the Gaussian set depend on set of parameters  $\beta$ :

$$\varphi_j(r) = A_{jl} r^l \exp(-\beta_j r^2), \quad j = 1, \dots, N$$

The parameters  $\beta_j$  are given on some mesh (the set is complete (forms a basis)

in a limit  $N \rightarrow \infty$ ):

$$\beta_j = \beta_0 g\left(\frac{j}{N+1}\right), \quad j = 1, \dots, N$$

Additional sets of the parameters are introduced by shifting the index ( $0 \leq a < 1$ ):

$$\beta_j(a) = \beta_{j-a} = \beta_0 g\left(\frac{j-a}{N+1}\right), \quad j = 1, \dots, N$$

It has been shown that the corresponding eigenvalues are shifted along the same curve:

$$\{\beta_{j-a}\}_{j=1}^N \Rightarrow \{E_j(a)\}_{j=1}^N$$

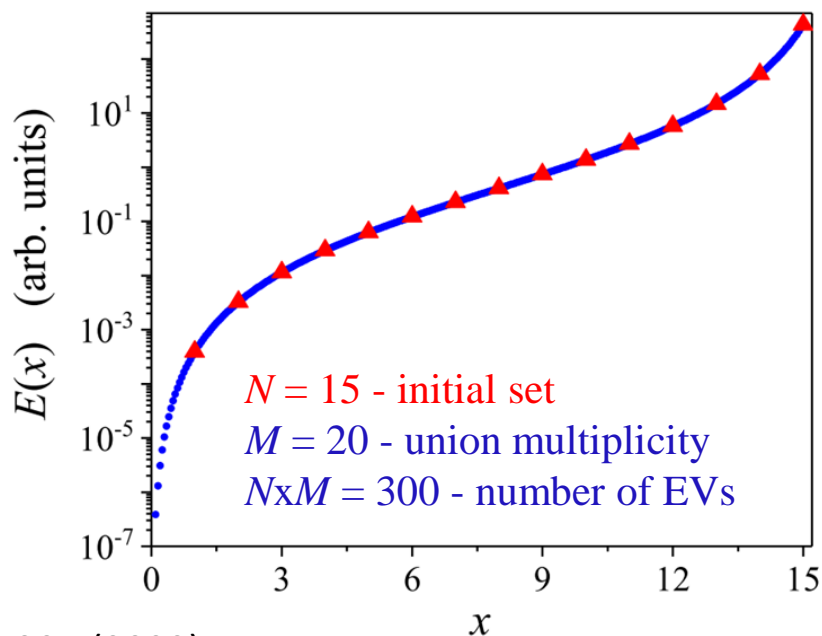
$$E_j = E(j), \quad E_j(a) = E(j-a).$$

Thus, the set of indices

$0 \leq a_1 \leq \dots \leq a_m \leq \dots \leq a_M < 1$   
generates a union of eigenvalues

$E(j-a_m)$  (see the Fig.)

This property allows to reconstruct a continuous dependence  $E(x)$  and integrated density  $\chi(E)$  for a simple spectrum.



# Narrow two-channel resonance

$$H = -\frac{1}{2} \frac{d^2}{dr^2} + H_0(x) + V(x, r) \quad (\text{Noro, Taylor, 1980})$$

$$V = \begin{pmatrix} -1.0 & -7.5 \\ -7.5 & 7.5 \end{pmatrix} r^2 e^{-r}$$

$$\frac{dE(x)}{dx} \approx \pi \frac{\Gamma / 2}{\cos^2 \pi(x - x_R)}$$

$$E_R = 4.768 \text{ a.u.}$$

$$\Gamma = 0.0014 \text{ a.u.}$$

(V.A. Mandelshtam et al.:  $E_R = 4.768 \text{ a.u.}$   
 $\Gamma = 0.00142 \text{ a.u.}$  )

Thresholds  $E_1 = 0, E_2 = 0.1 \text{ a.u.}$

