Solving Few-Body Scattering Problems in a Discrete Representation by using GPU

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in collaboration with

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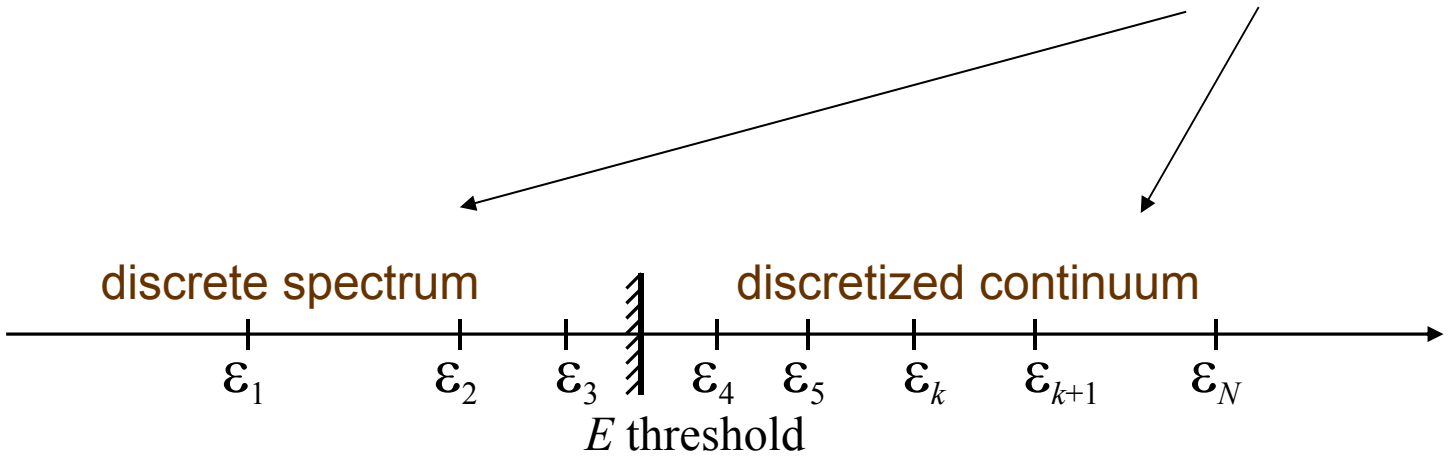
L2 discretization

$$H\,|\,\Psi\rangle = E\,|\,\Psi\rangle \longleftarrow |\,\Psi\rangle = \sum_{n=1}^{N} C_n\,|\,\phi_n\rangle,\ \langle\phi_n|\phi_k\rangle = \delta_{nk}$$

The eigenvalue problem: $\det\|\,H_{nn'} - E\delta_{nn'}\,\| = 0 \;\Rightarrow\; \{\varepsilon_n\}_{n=1}^{N},\ |\Psi_n\rangle$



The basic question: How to extract scattering information from pseudostates.

Weyl's eigendifferential formalism

Continuum wave functions don't have finite norms.

$$\langle \psi(E) | \psi(E') \rangle = \delta(E - E'), \quad |\Phi\rangle = \sum_{k=1}^{N_b} C_n |\psi_n\rangle + \int_0^\infty dE \; C(E) |\psi(E)\rangle.$$

When studying spectral theory for singular differential operators (in 1910), H. Weyl used the eigendifferential concept.

$$|\psi(E, \Delta E)\rangle = \int_E^{E+\Delta E} dE |\psi(E)\rangle$$

eigendifferential of the scattering wave function

An integration over some energy interval is just enough to make the w.f. to be normalizable:

$$\langle \psi(E, \Delta E) | \psi(E, \Delta E) \rangle = \Delta E$$

A complete system of wave functions for some Hamiltonian consists of bound states and eigendifferentials:

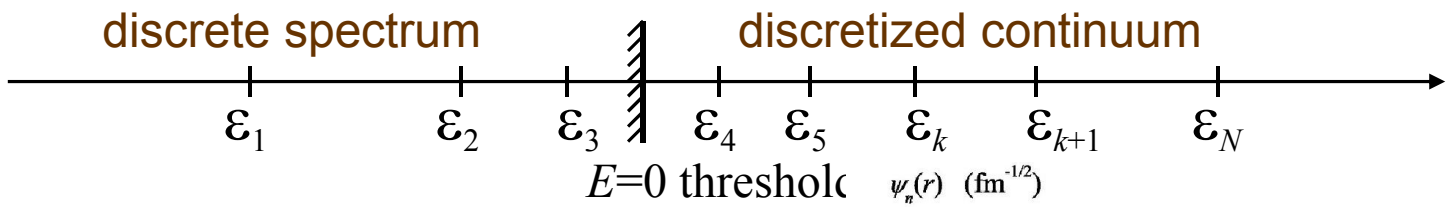
$$|\Phi\rangle \approx \sum_{k=1}^{N_b} C_n |\psi_n\rangle + \sum C(E) |\psi(E, \Delta E)\rangle.$$

The eigendifferential concept was used by pioneers of quantum physics H.Weyl, E. Wigner, H. Bethe and others to treat non-normalizable states (which do not belong to a Hilbert space) in a framework of the standard theory of Hermitian operators in a Hilbert space.

The details can be found in the textbook:
W. Greiner, Quantum Mechanics: An Introduction, Fourth. ed., Springer 2001.

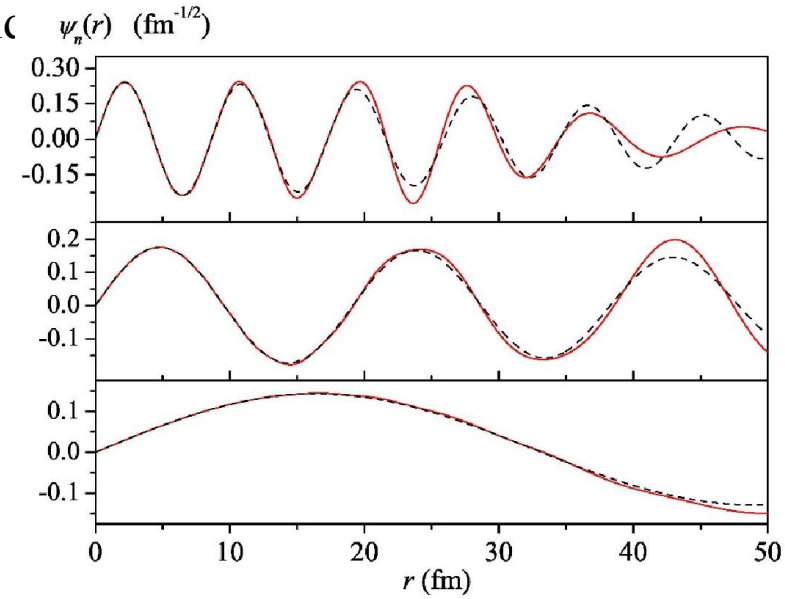
Pseudostates and eigendifferentials

$$|\Psi\rangle = \sum_{n=1}^{N} C_n |\phi_n\rangle \longrightarrow \quad H|\Psi\rangle = E|\Psi\rangle \quad \Rightarrow \{\varepsilon_n\}_{n=1}^{N}, \ |\Psi_n\rangle$$



Pseudostates have the same properties as eigendifferentials

$$\langle \psi_n | \psi_{n'} \rangle = \delta_{n,n'}, \quad \langle \psi_n | H | \psi_{n'} \rangle = \varepsilon_n \delta_{n,n'}$$



Comparison of pseudostates and eigendifferentials

Thus, one can treat pseudostates as approximations for eigendifferentials and construct the corresponding discretization bins.

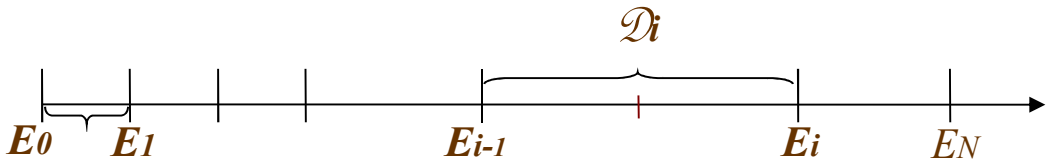
This statement has been used in the CDCC approach implicitly.

Stationary wave-packet formalism

Stationary wave packets and their properties

O.A. Rubtsova, V.I. Kukulin, V.N. Pomerantsev, Ann. Phys. 2015

Discretization of the continuum for some Hamiltonian *h*



$$[q_{i-1}, q_i], \quad q_i = \sqrt{2\mu E_i}$$ ← discretized momentum

Stationary wave packets are constructed as integrals of wave functions of h:

$$\langle \psi_q | \psi_{q'} \rangle = \delta(q - q')$$

$$|z_i\rangle = \frac{1}{\sqrt{B_i}} \int_{\mathcal{D}_i} f_i(q) |\psi_q\rangle dq, \; i = 1, \ldots, N$$

SWPs form an orthonormal set (jointly with possible bound states) :

$$\langle z_i | z_j \rangle = \delta_{ij} \qquad \langle z_i | z_0 \rangle = 0$$

bound state wf

The projector for SWP space of the Hamiltonian:

$$\mathfrak{p} = |z_0\rangle\langle z_0| + \sum_{i=1}^{N} |z_i\rangle\langle z_i|, \qquad \mathfrak{p}\, h\, \mathfrak{p} = \sum_{i=0}^{N} |z_i\rangle \varepsilon_i^* \langle z_i|$$

Spectral expansion of an operator $R(h)$ has a diagonal representation:

$$\mathfrak{p}R(h)\mathfrak{p} = \mathfrak{p}\int_{-\infty}^{+\infty} dE\,|\psi_E\rangle R(E)\langle\psi_E|\mathfrak{p} = \sum_{i=1}^{N}|z_i\rangle R_i\langle z_i|,$$

For continuous part of spectrum: $$R_i = \frac{1}{B_i}\int_{D_i} dE\; R(E)|f_i(E)|^2$$

Thus, one can get a diagonal finite-dimensional approximation for the resolvent of the Hamiltonian:

$$g^{(+)}(E) = [E + \mathrm{i}0 - h]^{-1} \quad \Rightarrow \quad \mathfrak{g}(E) = \sum_{n=1}^{N_b}\frac{|z_n\rangle\langle z_n|}{E - E_n} + \sum_{i=N_b+1}^{M}|z_i\rangle g_i(E)\langle z_i|$$

The eigenvalues:

$$g_i(E) = \frac{1}{D_i}\ln\left|\frac{E - \mathcal{E}_{i-1}}{E - \mathcal{E}_i}\right| - \frac{\mathrm{i}\pi}{D_k}\left[\theta(E - \mathcal{E}_{k-1}) - \theta(E - \mathcal{E}_k)\right], \quad E \in \mathfrak{D}_k,$$

Additional averaging on external energy:

$$g(E) \to \mathfrak{g}^k = \frac{1}{D_k}\int_{\mathcal{D}_k}\mathfrak{g}(E)dE, \quad E \in \mathcal{D}_k \longrightarrow g_i^k = \frac{1}{D_k D_i}W_{ki} - \frac{\mathrm{i}\pi}{D_k}\delta_{ik},$$

Stationary wave packets for different Hamiltonians

The free resolvent: $$g_0(E) = \left[E + i0 - h_0\right]^{-1} \Rightarrow \mathcal{g}_0(E) = \sum_{i=1}^{N} \left|x_i\right\rangle g_i(E) \left\langle x_i\right|$$

The total resolvent: $$g(E) = \left[E + i0 - h\right]^{-1} \Rightarrow \mathcal{g}(E) = \sum_{n=1}^{N_b} \frac{\left|z_n\right\rangle\left\langle z_n\right|}{E - E_n} + \sum_{i=N_b+1}^{M} \left|z_i\right\rangle g_i(E) \left\langle z_i\right|$$

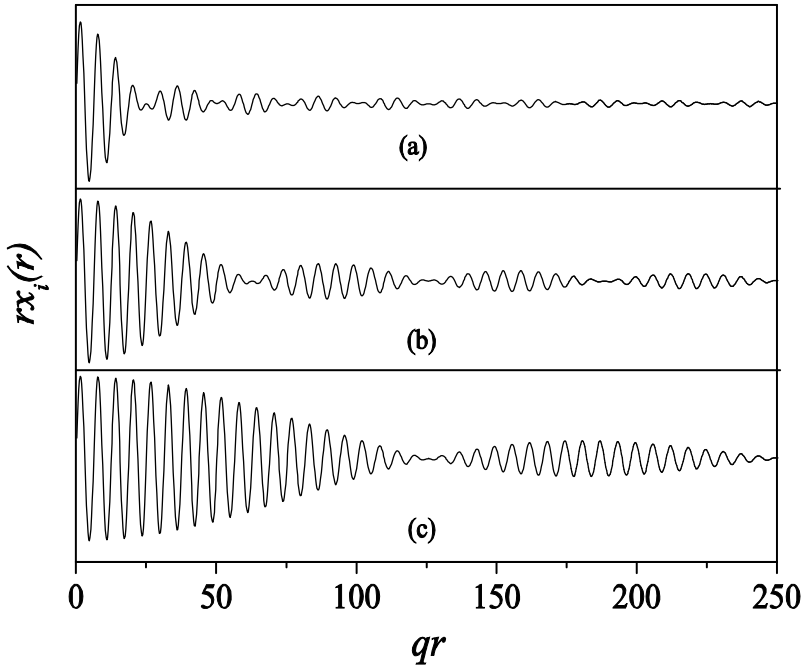
This property is also valid for Hamiltonians with long range interactions

The Coulomb resolvent: $$g_C(E) = \left[E + i0 - h_C\right]^{-1} \Rightarrow \mathcal{g}_C(E) = \sum_{i=1}^{N} \left|x_i^C\right\rangle g_i(E) \left\langle x_i^C\right|$$

Behavior of free stationary wave packets

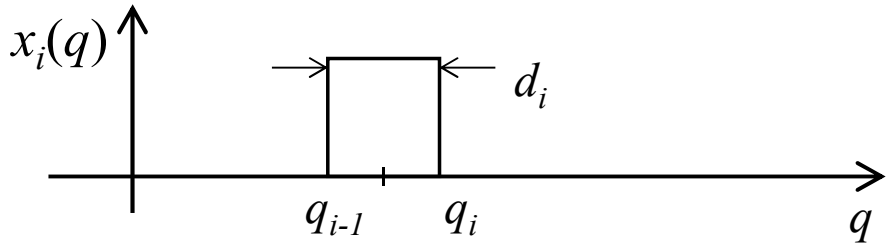
In configuration space

$$x_i(r) = \sqrt{d_i}\,\psi_{0q}(r)\,\frac{\sin(d_i r/2)}{d_i r/2}$$



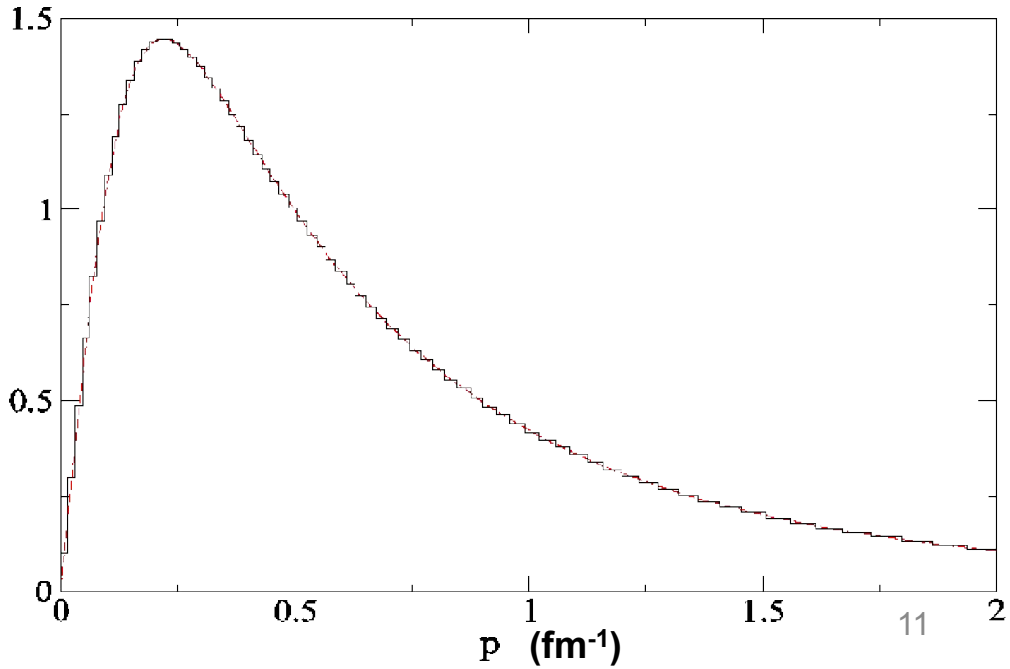
In momentum space

$$x_i(q) = \frac{f_i(q)\left[\theta(q-q_{i-1}) - \theta(q-q_i)\right]}{\sqrt{B_i}}$$



$f_i(q) = 1, \quad x_i(q)$ – is a step-like function

Deuteron wave function in the step-like WP basis



Example: the Lippmann-Schwinger equation for T-matrix:

$$t(E) = v + vg_0(E)t(E)$$

In momentum space:

$$t(E;q,q') = v(q,q') + \int dq'' \; \frac{v(q,q'')t(q'',q')}{E + i0 - (q'')^2/2m}$$

After a WP projection, one gets fully matrix equation:

$$\mathfrak{t}^k = \mathfrak{v} + \mathfrak{v}\mathfrak{g}_0^k \mathfrak{t}^k, \; E \in \mathcal{D}_k$$

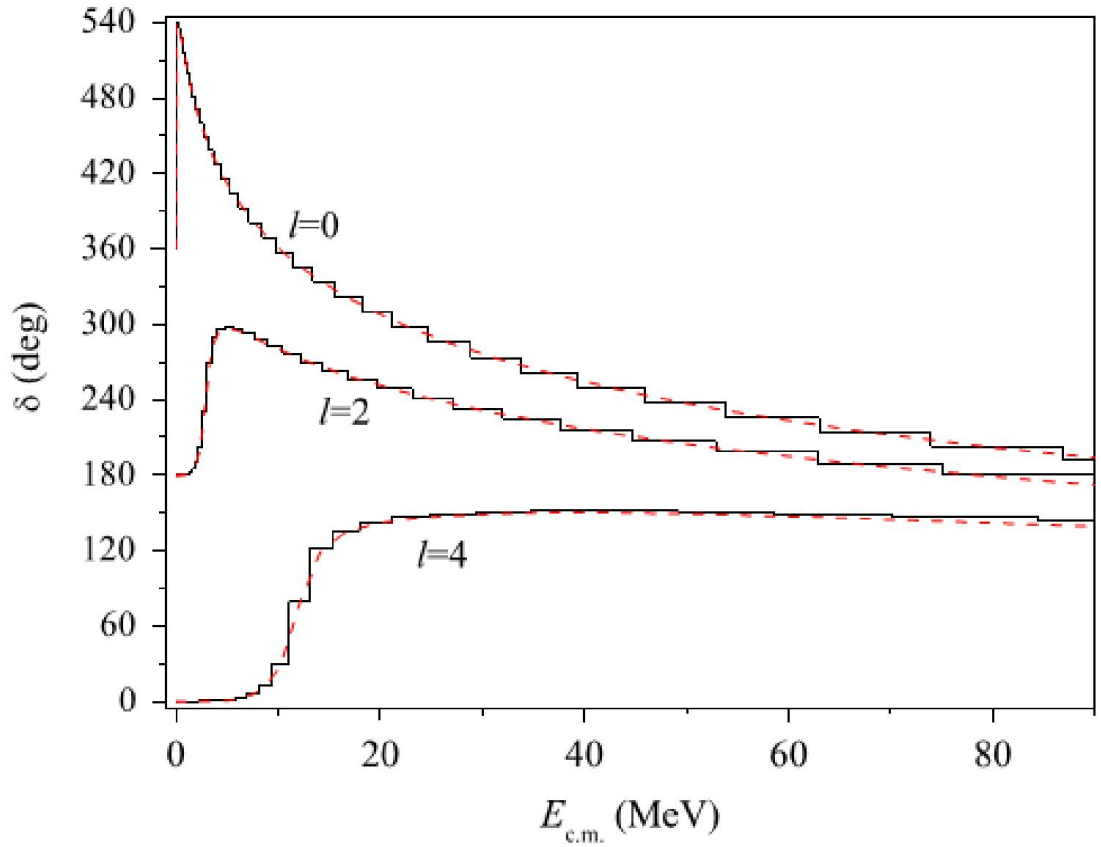
Off-shell t-matrix element: $$t(E;q,q') \approx \frac{t_{ij}^k}{\sqrt{D_i D_j}}, \quad \begin{matrix} E \in \mathcal{D}_k \\ q \in \mathcal{D}_i \\ q' \in \mathcal{D}_j \end{matrix}$$

The resulted T-matrix satisfies the unitarity condition.
This an exact T-matrix for the projected interaction operator $\mathfrak{v} = \mathfrak{p} V \mathfrak{p}$

Table 1
Comparison between the continuous representation for the scattering theory basic objects (in the momentum space) and their discrete analogs in the WP subspace for $E \in \mathfrak{D}_k$, $q \in \mathfrak{D}_i$ and $q' \in \mathfrak{D}_{i'}$.

	Continuous	Discrete WP
1. The free resolvent	$g_0(E; q, q')$	$[\mathfrak{g}_0]_i^k \delta_{i,i'}$.
2. The total resolvent	$g(E; q, q')$	$\mathfrak{g}_{i,i'}^k$.
3. The t-matrix	$t(E; q, q')$	$\mathfrak{t}_{i,i'}^k$.
4. The partial phase shift	$\delta(E)$	δ^k.

Partial phase shifts of α−α scattering



Solving via spectral methods

The spectral shift function formalism

I.M. Lifshits, Zh. Eks. Teor. Fiz. (JETP) **17**, 1017 (1947), *ibid* 1076 (1947)

The family of free operators $h_0^{(\alpha)}$ with quasi-continuous spectrum

$$E_j^0(\alpha) = f(j\alpha) + o(\alpha), \quad j = 1, \ldots$$

$$D_j^{(\alpha)} \equiv E_{j+1}^0(\alpha) - E_j^0(\alpha) = \alpha \left. \frac{df(u)}{du} \right|_{u=j\alpha} + o(\alpha), \quad j = 1, \ldots$$

The problem to solve:

How the spectrum of the initial Hamiltonian h_0 is changed by the inclusion of the perturbation (not small) v

The spectrum of the total Hamiltonian $h^{(\alpha)} = h_0^{(\alpha)} + v$

$$E_j(\alpha) = E_j^0(\alpha) + \xi\left(E_j^0\right) D_j^{(\alpha)} + O(\alpha), \quad j = 1, \ldots$$

the spectral shift function

The spectral shift function is defined for pair of operators h_0 and $h=h_0+v$

The trace formula (I.M. Lifshits, 1952.) for unperturbed and perturbed Hamiltonians

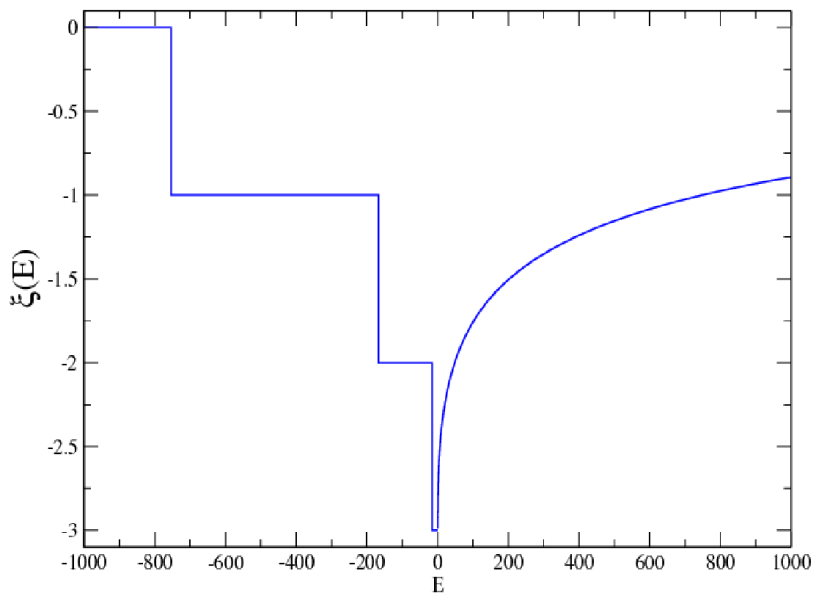
$$\mathrm{Tr}\left[f(h)-f(h_0)\right]=\int_{-\infty}^{\infty} f'(\lambda)\xi(\lambda)d\lambda$$

Birman-Krein formula (1962). Relation to the scattering operator.

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

In one-channel case this means $\delta(E)=-\pi\xi(E)$

SSF as function on the energy



M.Sh. Birman, A.B. Pushnitsky, *Spectral shift function, amazing and multifaceted*, Integr. Equ. Oper. Theory **30,** 191 (1998).

D. R. Yafaev, *Mathematical scattering theory. General theory*, Amer. Math. Soc., Providence, RI, 1992.

Moving back to the quasi continuous spectrum, one has the following formal expression for the SSF:

$$\xi\left(E_n^0\right) = \frac{E_n - E_n^0}{D_n} + O(\alpha)$$

Using further the Birman-Krein formula

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

we get the expression for the partial phase shifts in discrete points

$$\delta\left(E_n^0\right) = -\pi \frac{E_n - E_n^0}{D_n} + O(\alpha)$$

SSF and the spectral density

Spectral density for the discrete spectrum

$$\rho_b(E) = \sum_{n=1}^{N_b} \delta(E - E_n)$$

E_n – eigenvalues

It is related to the counting function

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

For the continuous spectrum, one should define the Continuum level density (CLD):

$$\Delta(E) \equiv -\frac{1}{\pi} \mathrm{Tr}\left[\mathrm{Im}\, G(E) - \mathrm{Im}\, G_0(E)\right]$$

It can be shown that CLD is directly related to the phase shift :

$$\Delta(E) = \frac{1}{\pi} \frac{d\delta(E)}{dE}$$

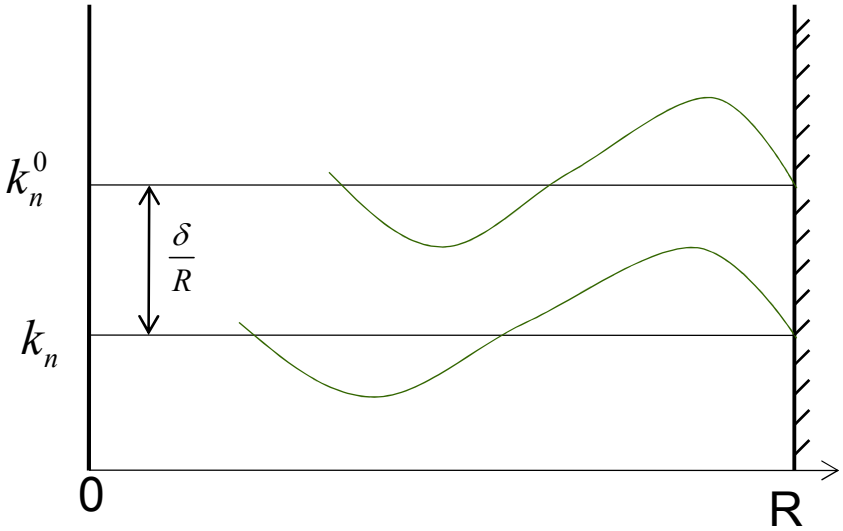
Thus, SSF can be treated as integrated density of states:

$$\xi(E) = -\int_{-\infty}^{E} dE' \left[\rho_B(E') + \Delta(E')\right]$$

Example: scattering inside a spherical box

Boundary condition for the free Hamiltonian:

$$\sin(k_n^0 R) = 0 \quad \Rightarrow \quad k_n^0 = \frac{\pi n}{R}, \; d_n = \frac{\pi}{R}$$



Boundary condition for total Hamiltonian:

$$\sin(k_n R + \delta_n^{(R)}) = 0 \quad \Rightarrow \quad k_n = \frac{\pi n - \delta_n^{(R)}}{R}$$

Thus, the phase shift satisfies the following relation:

$$\delta_n^{(R)} = -\pi \frac{k_n - k_n^0}{d_n}$$

Here the discrete SSF has a relation to the Lüscher approach.

Spectral shift function in the discrete representation

So, one can introduce the new approach to solve scattering problem by the continuum discretization on the base of this Birman-Krein formula and Lifshits discrte definition for the spectral shift function.

Let's choose some finite L_2 basis and make subsequent diagonalization procedures for the free and the total Hamiltonians

$$\det\left\|\left[H_0\right]_{nn'} - E\delta_{nn'}\right\| = 0 \rightarrow \left\{E_j^0, D_j\right\} \qquad \det\left\|\left[H\right]_{nn'} - E\delta_{nn'}\right\| = 0 \rightarrow \left\{E_j\right\}$$

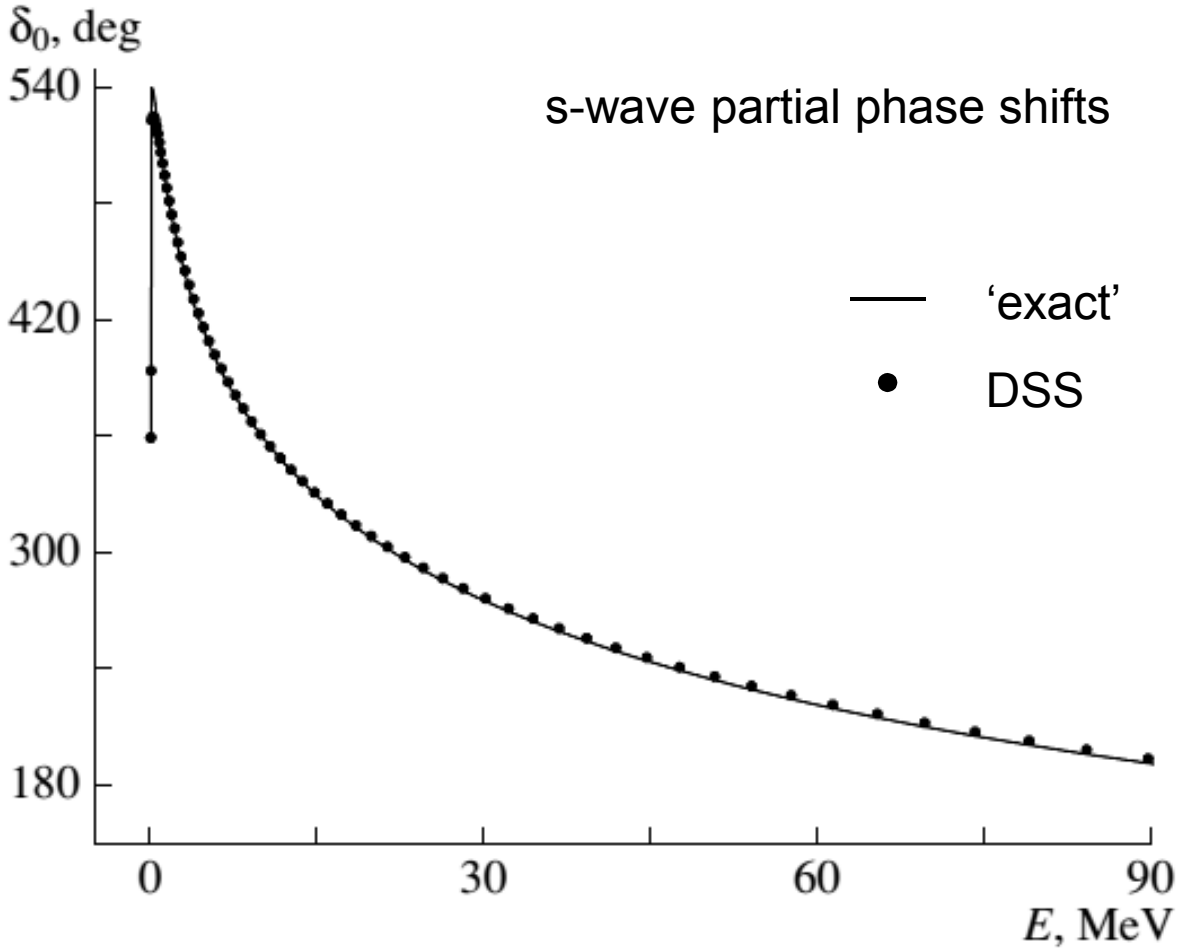
From the discrete definition of the SSF, one gets $\xi(E_j) \approx \xi_j = \dfrac{E_j - E_j^0}{D_j}$

Thus, partial phase shifts could be found from the explicit formula:

$$\delta(E_j) \approx -\pi \frac{E_j - E_j^0}{D_j}, \; j = 1, \ldots, N$$

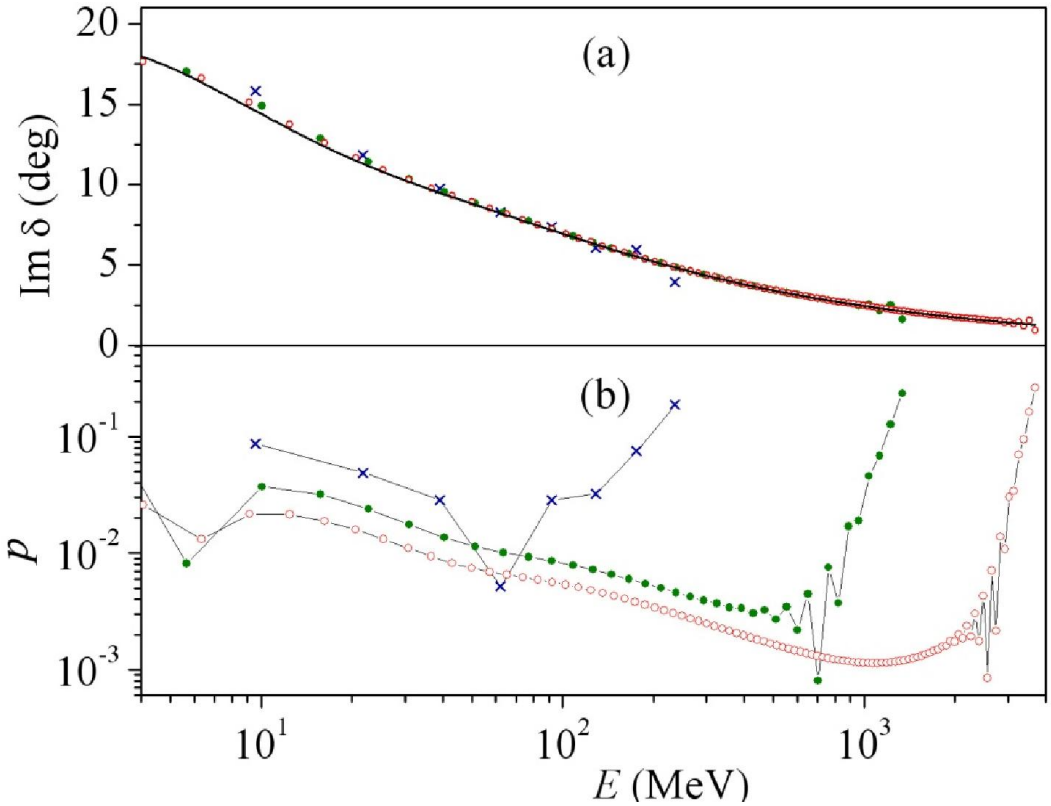
α–α scattering

$$h_C \to h = h_C + v_S$$

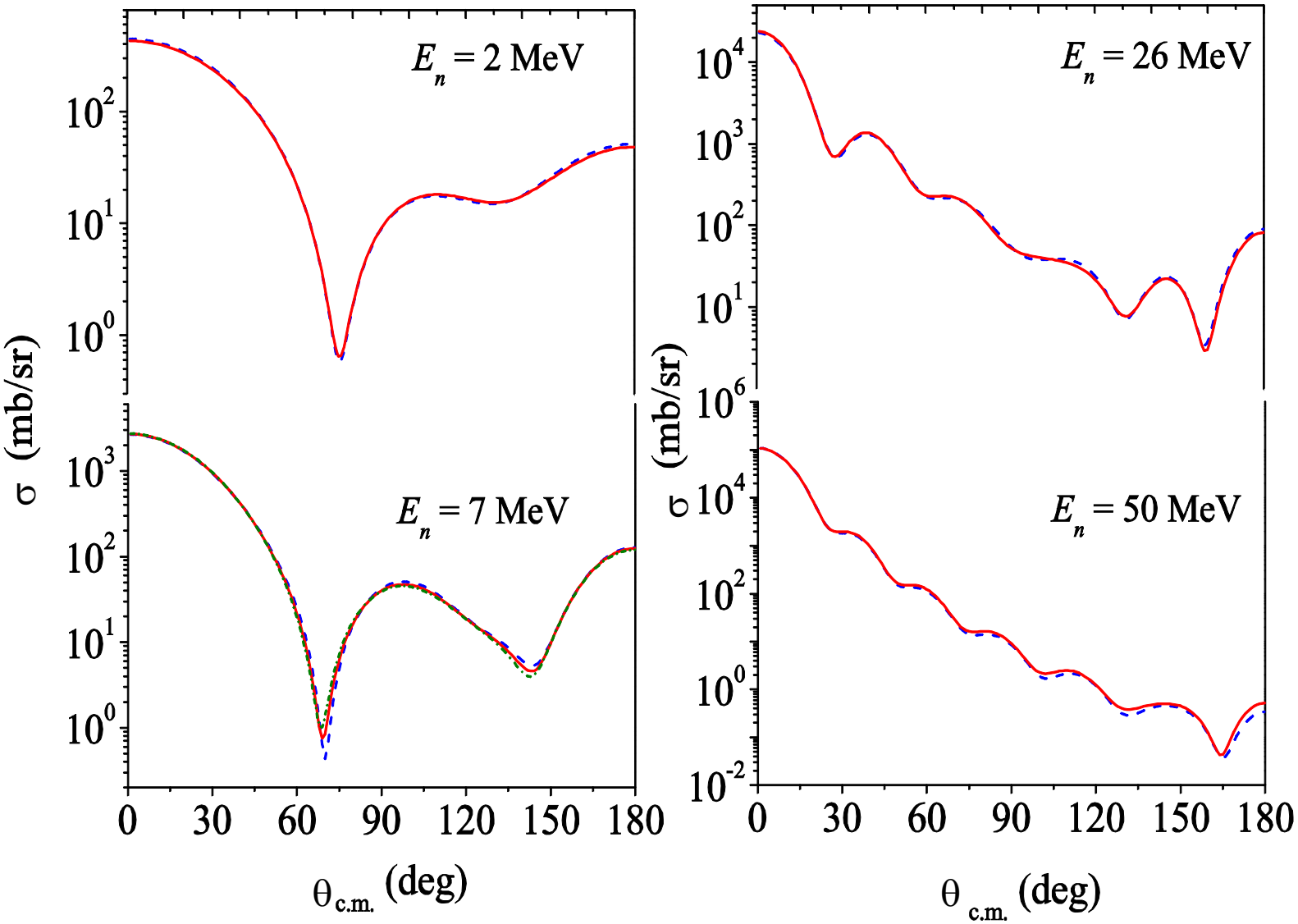


Case of complex potential

$$\delta(E_j^0) \approx -\pi \frac{E_j - E_j^0}{D_j} \quad \Rightarrow \quad \mathrm{Im}\ \delta\left(E_j^0\right) \approx -\pi \frac{\mathrm{Im}\ E_j}{D_j}$$



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



Multi-channel scattering problem

Multi-channel Hamiltonian:

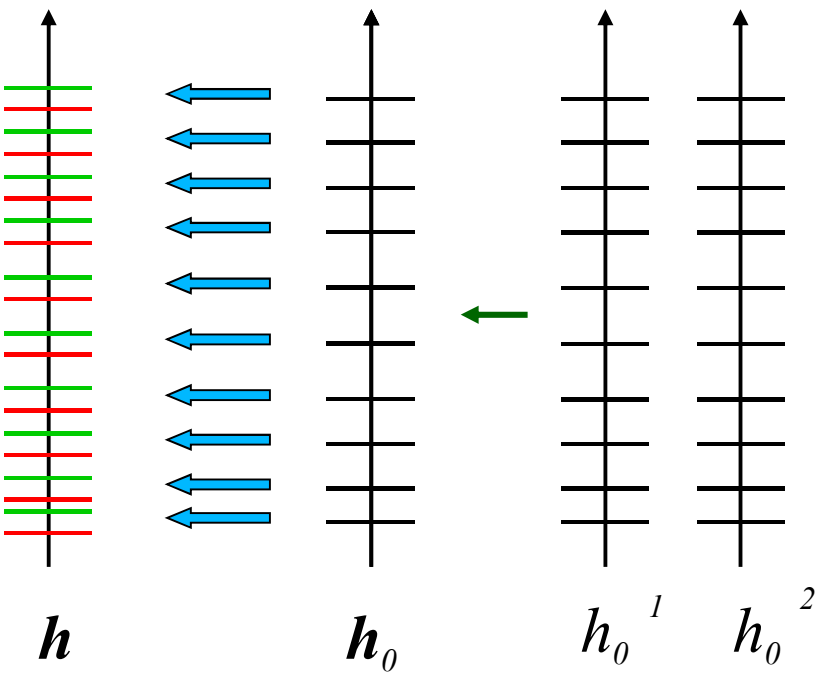
$$h_{\alpha\beta} = h_0^{\alpha}\delta_{\alpha\beta} + v_{\alpha\beta}, \quad \alpha, \beta = 1, \ldots, K$$

SSF theory does not allow to determine the separate phase shifts but the sum of eigenphases only:

$$\exp(-2\pi i \xi(E)) = \det S(E) \;\Rightarrow\; \xi(E) = -\frac{1}{\pi}\sum_{\kappa}\delta^{\kappa}(E)$$

Also, in the multi-channel case, the problem with L2 basis representation arises because the initial multichannel spectrum is degenerated, i.e. there are several solution at the one energy those correspond to different boundary conditions.

To treat correctly multi-channel pseudostates, one has to use the basis in which the dicretized free Hamitonian multichannel spectrum is **degenerate**.



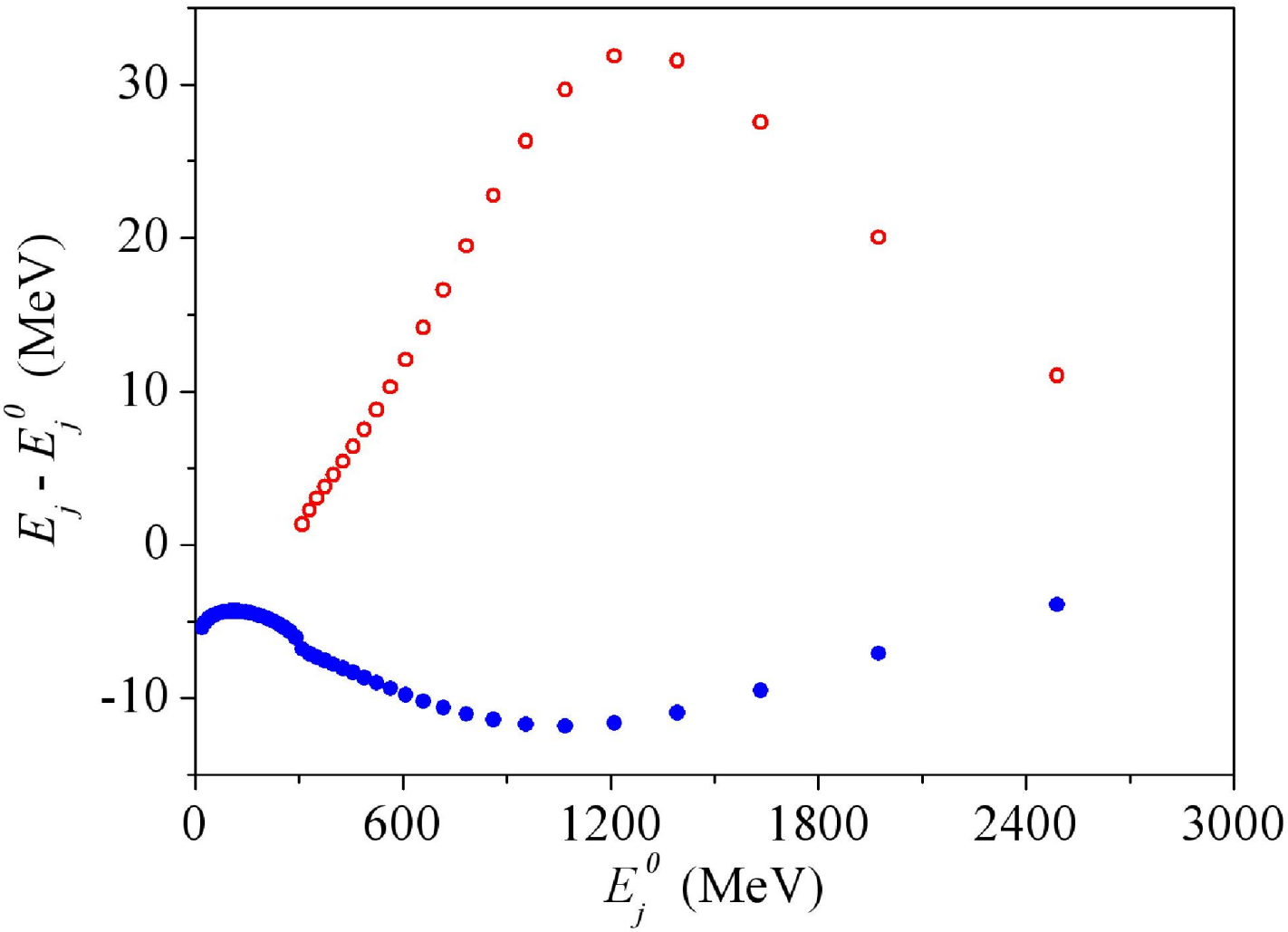
In a case of h_0 operator with degenerated eigenvalues, inclusion of interaction causes splitting of these multiple levels.

The important point here is that the alternation of the splitted levels doesn't change.

By this way, one can separate different branches in the total Hamiltonian spectrum.

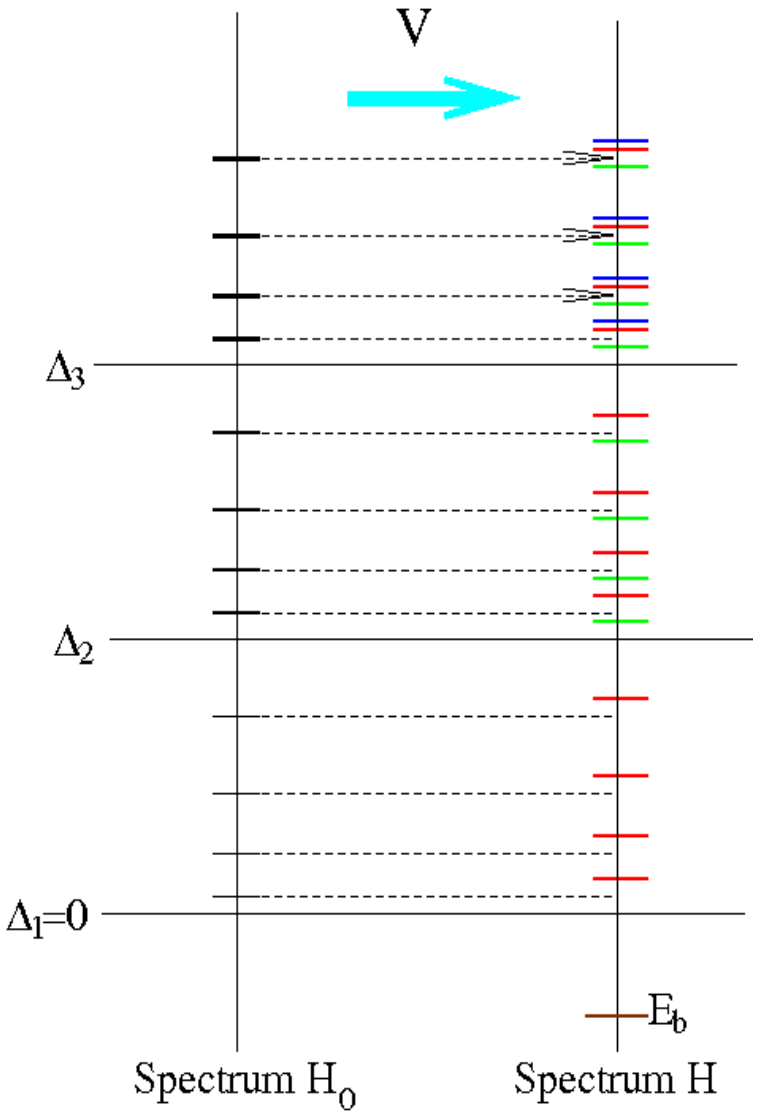
For a two-channel problem, one can separate two branches: 'even' and 'odd'.

Energy shifts for ‘even’ and ‘odd’ levels of two-channel problem



Generalization of the discrete SSF to the multi-channel case

PRC **81**, 064003 (2010); Phys. At. Nucl. **77**, 486 (2014)



In the multi-channel case, when one has discretized multiple free spectrum, it is rather simple to define spectral shifts for any branch of the discretize total Hamiltonian spectrum:

Thus, instead of the single SSF in the one-channel case, one has several spectral shift functions for each branch of the spectrum in the multi-channel case:

$$\xi_j^{(\kappa)} = \frac{E_j^{(\kappa)} - E_j^0}{D_j}, \quad \kappa = 1, \ldots, d$$

d – spectral multiplicity degree

Determination of the multi-channel S-matrix

The S-matix has a diagonal form in the eigenchannel representation.

$$S' = \begin{pmatrix} e^{2i\delta^{(1)}} & 0 & 0 \\ 0 & \dots & 0 \\ 0 & 0 & e^{2i\delta^{(d)}} \end{pmatrix}$$

$$\det S = \exp(2i\sum_{\kappa=1}^{d}\delta^{(\kappa)})$$

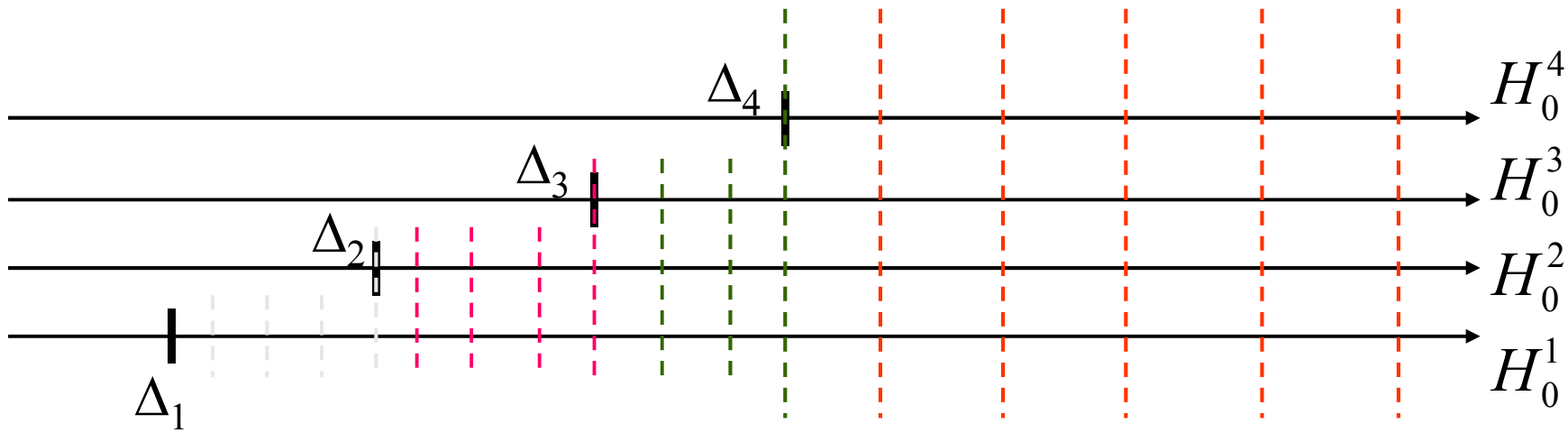
Generalization of the Birman-Krein formula:

$$\delta^{(\kappa)} = -\pi\xi^{(\kappa)} \;\Rightarrow\; \delta^{(\kappa)}(E_j^0) \approx -\pi\frac{E_j^{(\kappa)} - E_j^0}{D_j}$$

Thus, from the one-fold diagonalization of the total Hamiltonian matrix in the multi-channel wave-packet basis, one can evaluate partial phase shifts in the eigenchannel representation for a wide energy interval simultaneously.
This information is quite enough to find total cross section for example.

Construction of a multi-channel multiple spectrum

The free wave-packet basis is very convenient here, because one can construct the discretization bins ‘by hands’.



$$\left| x_i^{(\nu)} \right\rangle = \frac{1}{\sqrt{d_i}} \int_{q_{i-1}}^{q_i} \left| \psi_0^{(\nu)} \left(q - \sqrt{2\Delta_\nu} \right) \right\rangle dq$$

Matrix of the rotation form the eigenchannel representation to the initial ('experimental') channels.

At each energy, the initial S-matrix is related to the ER one by the rotation

$$S_{\mu\nu}(E) = \sum_{\kappa=1}^{d} U_{\kappa\mu}(E) S^{\kappa}(E) U^{*}_{\kappa\nu}(E), \;\; S^{\kappa} = \exp(2i\delta^{(\kappa)})$$

Matrix elements of the rotation matrix can be found just from the expansion coefficients for the pseudostates over free wave packets

$$\left| z_j^{(\kappa)} \right\rangle = \sum_{\nu=1}^{K} \sum_{i=1}^{N_\nu} C_{ji}^{(\kappa\nu)} \left| x_i^{(\nu)} \right\rangle$$

The total S-matrix can be found from the relation:

$$S_{\mu\nu}(E_i^0) \approx \sum_{\kappa=1}^{d} \mathrm{e}^{2i\delta_i^{(\kappa)}} \sum_{j=1}^{N_\kappa} C_{ji}^{(\kappa\mu)} C_{ji}^{*(\kappa\nu)}$$

For example, in two-channel case, one can use the Blatt-Biedenharn parametrization for the S-matrix

$$S(E)=\begin{pmatrix}\cos\varepsilon & \sin\varepsilon\\ -\sin\varepsilon & \cos\varepsilon\end{pmatrix}\begin{pmatrix}e^{2i\delta^{(1)}} & 0\\ 0 & e^{2i\delta^{(2)}}\end{pmatrix}\begin{pmatrix}\cos\varepsilon & -\sin\varepsilon\\ \sin\varepsilon & \cos\varepsilon\end{pmatrix}$$

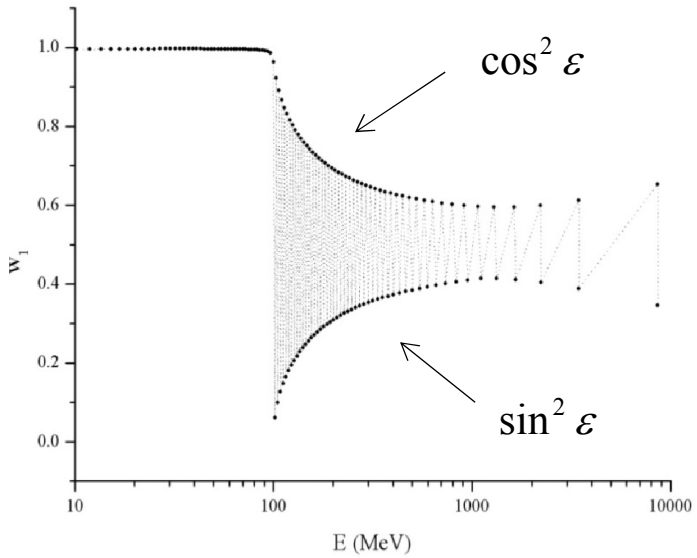
$$S_{11}(E)=e^{2i\delta^{(1)}}\cos^2\varepsilon+e^{2i\delta^{(2)}}\sin^2\varepsilon$$

The expansion of the pseudostate obtained via diagonalization in the two-channel WP basis

$$\left|z_i^{(\kappa)}\right\rangle=\sum_{j=1}^{N}C_{ij}^{(\kappa 1)}\left|x_j^{(1)}\right\rangle+\sum_{j=1}^{N}C_{ij}^{(\kappa 2)}\left|x_j^{(2)}\right\rangle,\ \kappa=1,2$$

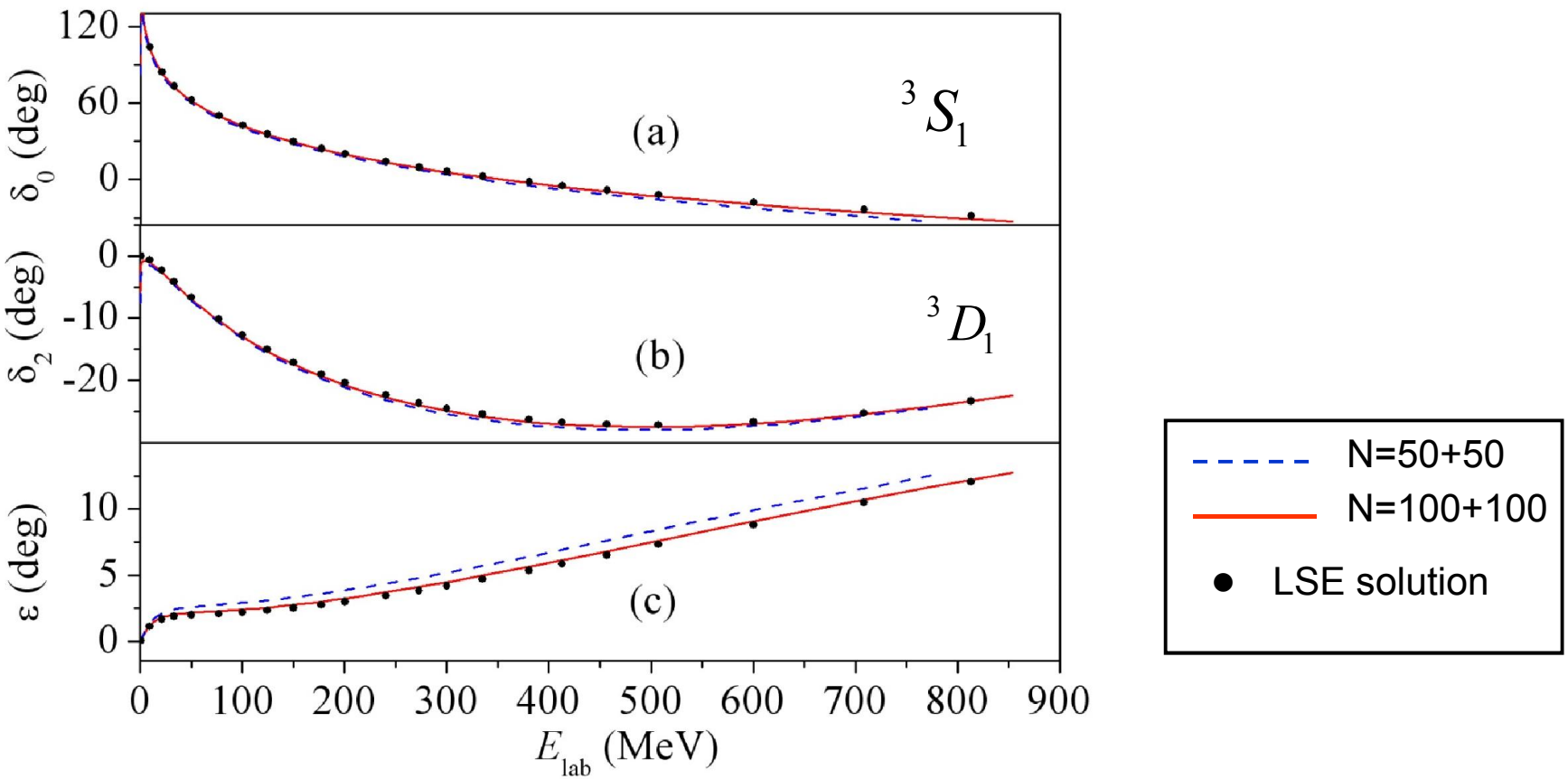
Then, the mixing angle can be defined from relations

$$\cos^2\varepsilon(E_j^0)\approx\sum_{j=1}^{N}\left|C_{ij}^{(11)}\right|^2,\ \sin^2\varepsilon(E_j^0)\approx\sum_{j=1}^{N}\left|C_{ij}^{(21)}\right|^2,$$



NN scattering via Moscow potential

The channel phase shifts and mixing angle in the Stapp parametrization

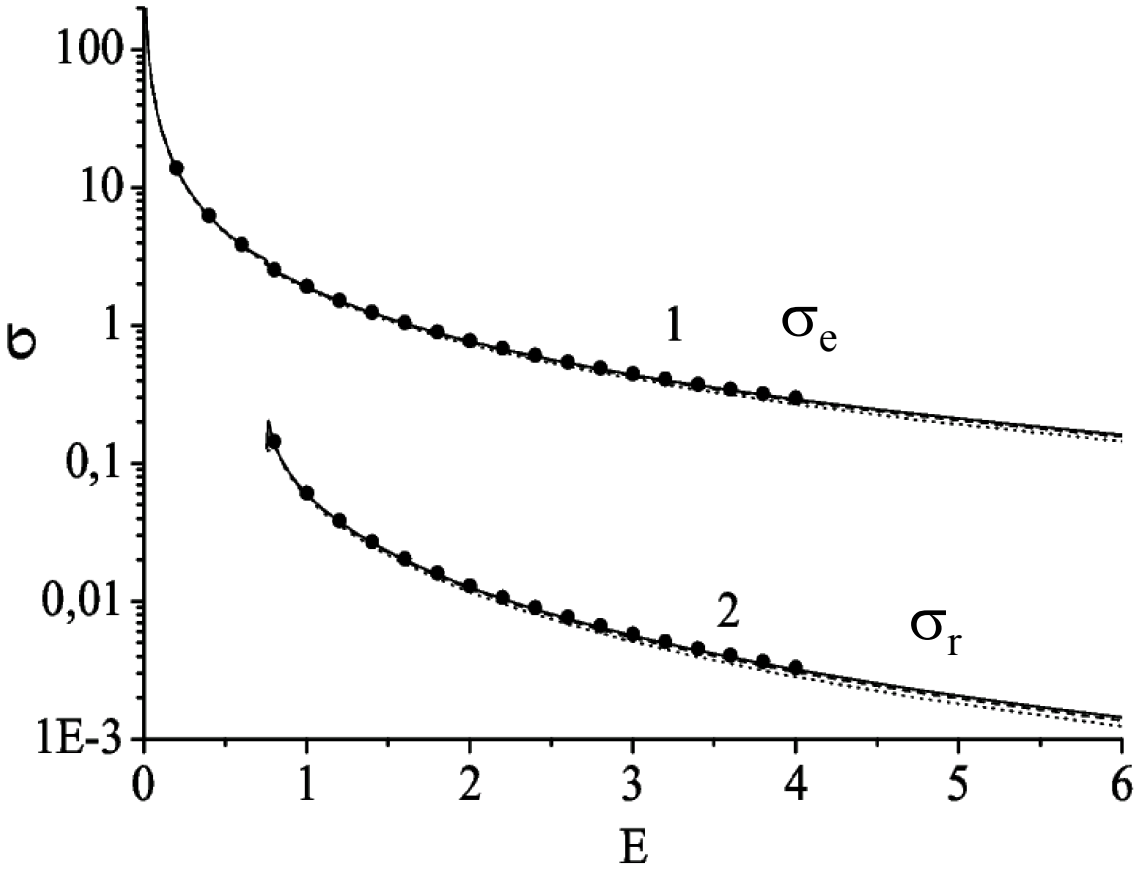


By one-fold diagonalization procedure, one gets multichannel S-matrix values at wide energy region.

Model e-H scattering

$V_{11}=V_{22}= -1.5\exp(-r)/r$
$V_{12}= -0.25\exp(-r)$,
$\Delta_2=0.75$

Elastic and reaction cross sections



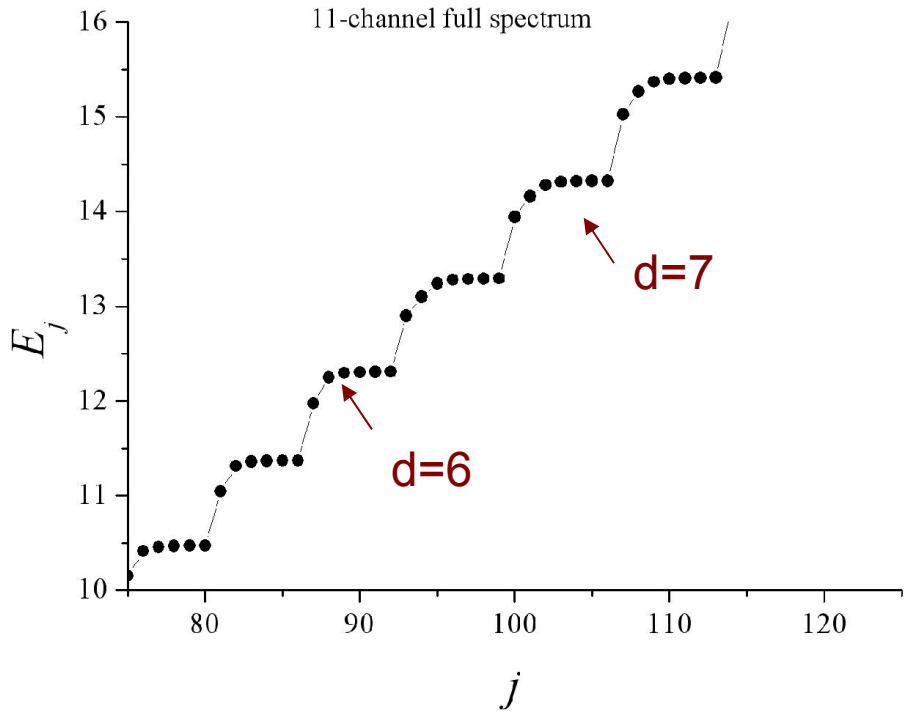
(points– B.H. Bransden and A.T. Stelbovics, J. Phys. B: At. Mol. Phys. **17**, 1877 (1984)).

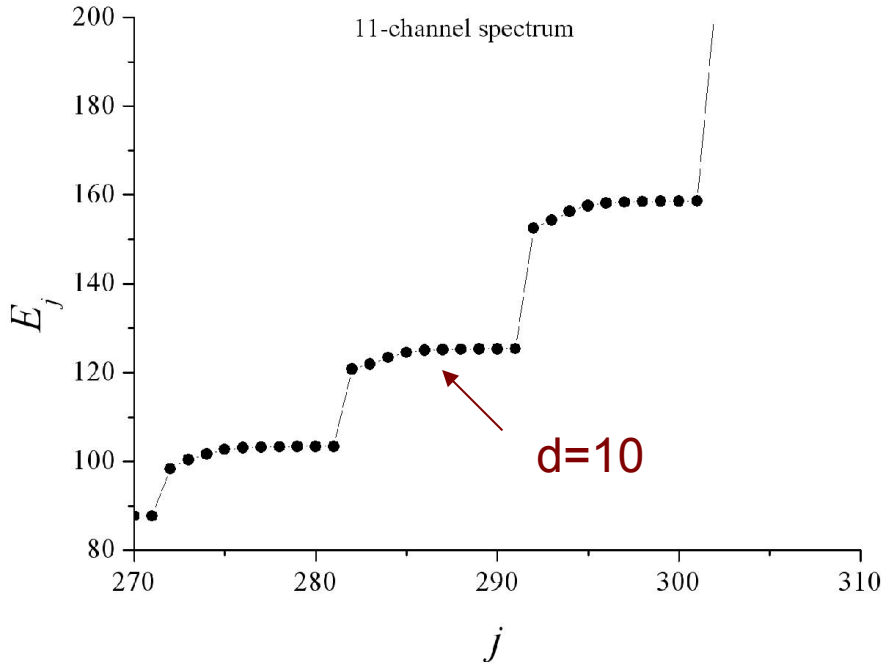
Model d+A problem

Two-body subHamiltonian h_{np} is discretized in Gaussian basis of dimension и K=11.

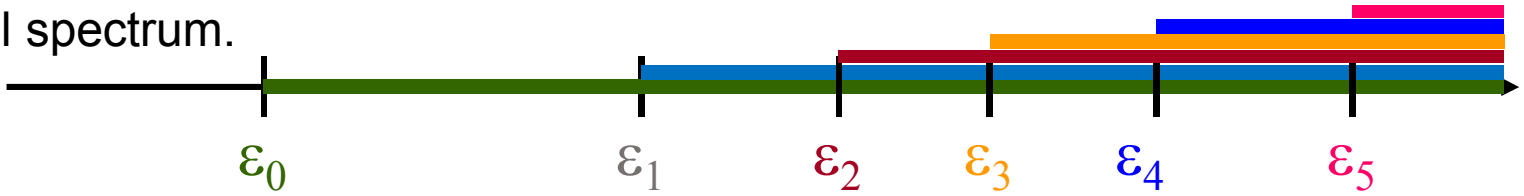
$$V_{nA}(r) = V_{pA}(r) = -V_0 \exp(-\gamma r^2),$$
$$V_0 = 15\ \mathrm{MeV},\ \gamma = 0.44\ \mathrm{fm}^{-2}$$

Total Hamiltonian discretized spectrum





One can see different series of pseudostates in different parts of the total multi-channel spectrum.



Off-shell T-matrix from the spectral expansion for the total resolvent

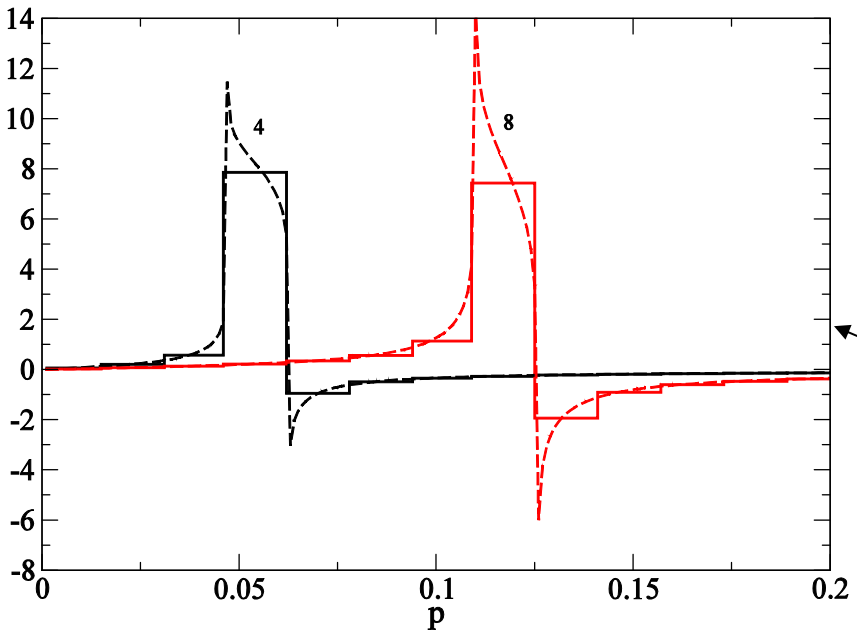
Scattering wave packets and pseudostates

Scattering wave packets (SWP) correspond to the total two-body Hamiltonian

$$h_1 = h_0 + v$$

are well approximated by pseudostates of the Hamiltonian matrix in the free WP basis:

$$\left| z_j \right\rangle \approx \sum_k C_{jk} \left| x_k \right\rangle$$



Exact scattering WPs for the Yamaguchi potential (dashed curves) and their approximations in the step-like WP basis (solid curves)

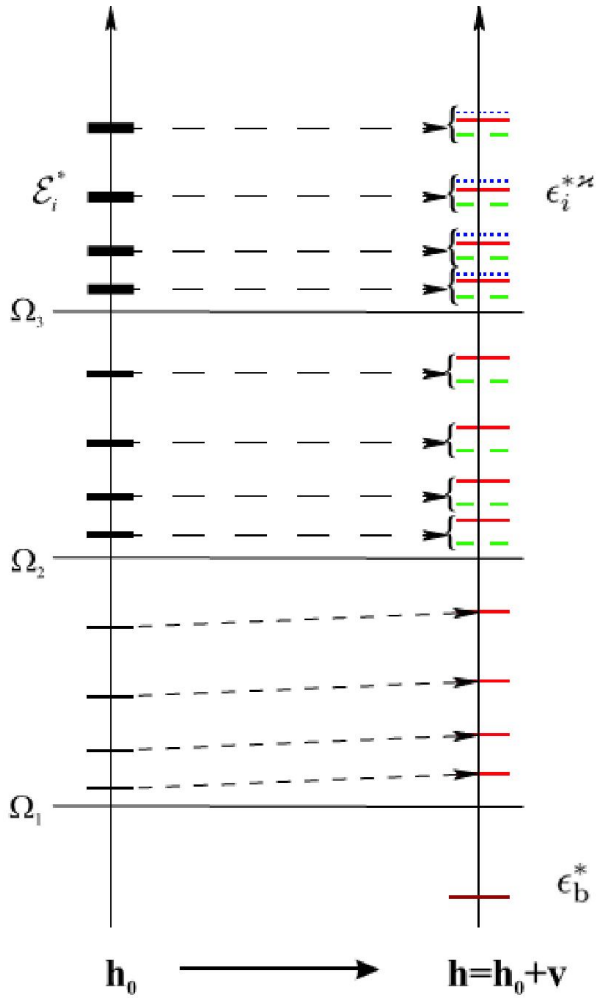
Thus, the free WP basis could be used to find two-body scattering WPs and bound states as well. The expansion over free WP states is valid even for the long-range Coulomb interaction!

Mutlichannel stationary wave-packets

We can treat now multichannel pseudostates as approximations for scattering wave-packets defined in Eigenchannel representation:

$$|z_k^{\varkappa}\rangle = \frac{1}{\sqrt{C_k^{\varkappa}}} \int_{\Delta_k^{\varkappa}} w(E)|\tilde{\psi}^{\varkappa}(E)\rangle dE, \quad k = k_{\varkappa}, \ldots, N^{\varkappa},$$

$$\left| z_j^{(\kappa)} \right\rangle \approx \sum_{\nu=1}^{K} \sum_{i=1}^{N_\nu} C_{ji}^{(\kappa\nu)} \left| x_i^{(\nu)} \right\rangle$$



T-matrix from a Hamiltonian matrix diagonalization

Solution of the Lippmann-Schwinger eq.: $t(E) = V + Vg_0(E)t(E),$

can be represented in a form: $t(E) = V + Vg(E)V$

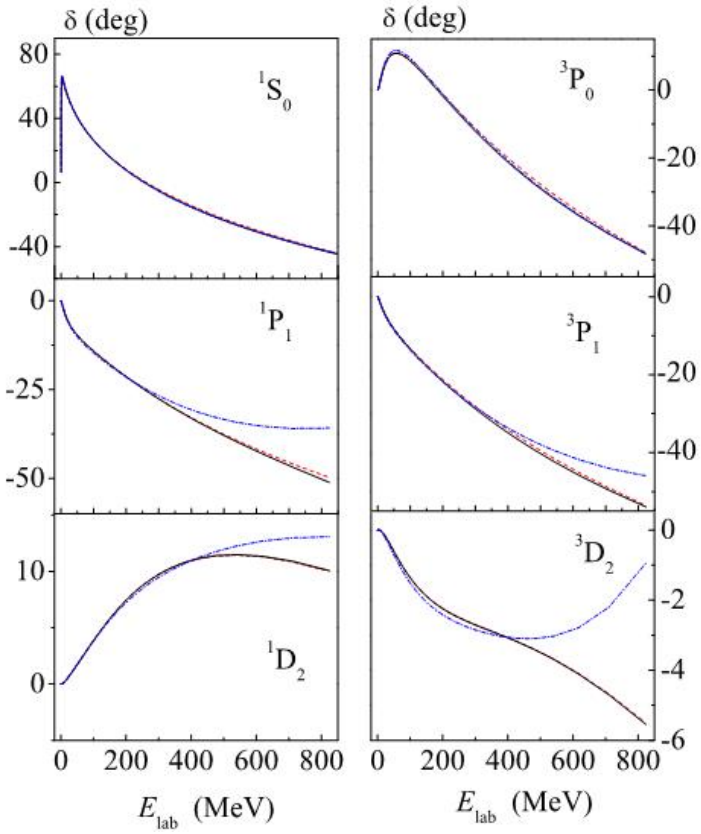
total resolvent

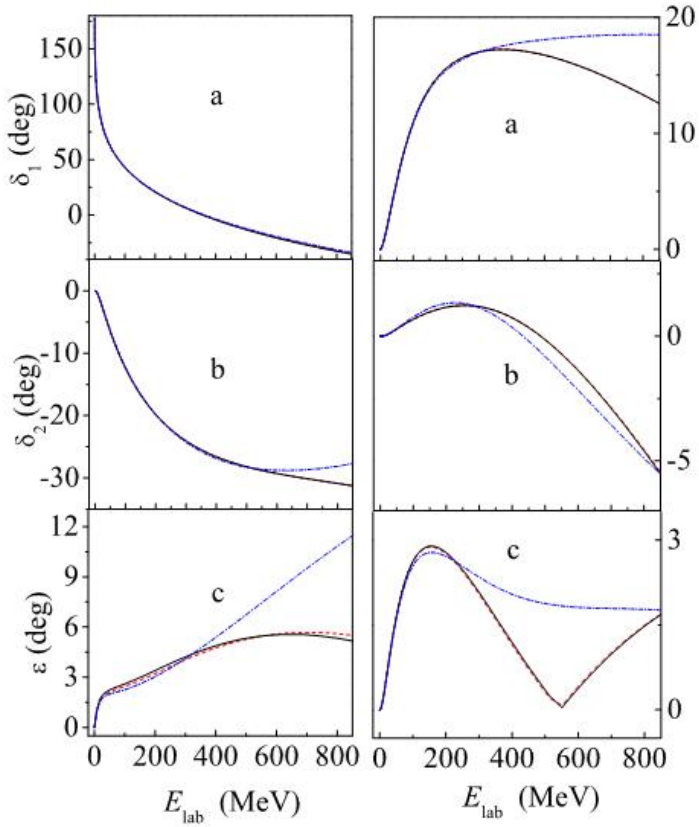
One can found a finite-dimensional approximation for g(E) in stationary wave-packet basis, employ multichannel pseudostate approximation and find the explicit relation for off-shell T-matrix

$$t_{\nu\nu'}(E) \approx \frac{\langle x_i^{\nu}|v|x_i^{\nu'}\rangle}{D_i} + \frac{\langle x_i^{\nu}|v|z_b\rangle\,\langle z_b|v|x_i^{\nu'}\rangle}{D_i(E-\epsilon_b^*)} + \sum_{\varkappa=1}^{K}\sum_{k=k_\varkappa}^{N^\varkappa}\frac{\langle x_i^{\nu}|v|z_k^{\varkappa}\rangle}{\sqrt{D_i}}g_k^{\varkappa}(E)\frac{\langle z_k^{\varkappa}|v|x_i^{\nu'}\rangle}{\sqrt{D_i}},$$

Off-shell T-matrix at many energies is found from a single diagonalization of the total Hamiltonian matrix.

Partial phase shifts for the NN scattering





CD Bonn

Nijmegen II

Partial phase shifts (a,b) and mixing angles (c) for the coupled channels $^3S_1$-$^3D_1$ (left) and $^3F_2$-$^3P_2$ (right) in the Stapp parametrisation.

The effective total Hamiltonian for the BGE

H. Muether et al., PRC 2016

An operator form of the Bethe-Goldstone equation:

$$T(K,W) = V + V\ Q(K)\ G_0(K,W)\ T(K,W),$$ where

$$G_0(K,W) = \left[W + i0 - H_0(K)\right]^{-1}, \quad \underbrace{H_0(K) = \int d\mathbf{k}\,|\mathbf{k}\rangle\left[e\left(|\mathbf{K}-\mathbf{k}|\right) + e\left(|\mathbf{K}+\mathbf{k}|\right)\right]\langle\mathbf{k}|}_{\text{the free Hamiltonian for two-nucleons in medium}}$$

The space of relative momentum is divided into two parts according to the action of the operator Q(K): its null subspace Γ and the 'Pauli-allowed' Q-subspace.

When the solution of the BGE can be formally written in a form:

$$T(W) = V + V\ Q^{\frac{1}{2}}\ G_Q(W)\ Q^{\frac{1}{2}}\ V$$

where G_Q is the resolvent of the effective Hamiltonian defined in Q-subspace:

$$H_Q = H_{0Q} + Q^{\frac{1}{2}}\ V\ Q^{\frac{1}{2}}, \quad G_Q(W) = \left[W + i0 - H_Q\right]_Q^{-1}$$

Now T-matrix at different W and *k* can be found by using the diagonalization technique.

To summarize:

There are three possibilities for solving two-body single- and multichannel problems:

1. Matrix analogs for integral equations:

$$t^k = v + v g_0^k t^k, \; E \in \mathcal{D}_k$$

2. On-shell observables for wide energy interval (simultaneously) can be found from the discrete spectral shift function formalism:

$$\delta(E_j) \approx -\pi \frac{E_j - E_j^0}{D_j}, \; j = 1, \ldots, N$$

3. Off-shell dependencies for wide energy interval (nearly simultaneously) can be found from the spectral expansion for the total resolvent

$$t_{\nu\nu'}(E) \approx \frac{\langle x_i^\nu | v | x_i^{\nu'} \rangle}{D_i} + \frac{\langle x_i^\nu | v | z_b \rangle \langle z_b | v | x_i^{\nu'} \rangle}{D_i (E - \epsilon_b^*)} + \sum_{\varkappa=1}^{K} \sum_{k=k_\varkappa}^{N^\varkappa} \frac{\langle x_i^\nu | v | z_k^\varkappa \rangle}{\sqrt{D_i}} g_k^\varkappa(E) \frac{\langle z_k^\varkappa | v | x_i^{\nu'} \rangle}{\sqrt{D_i}},$$

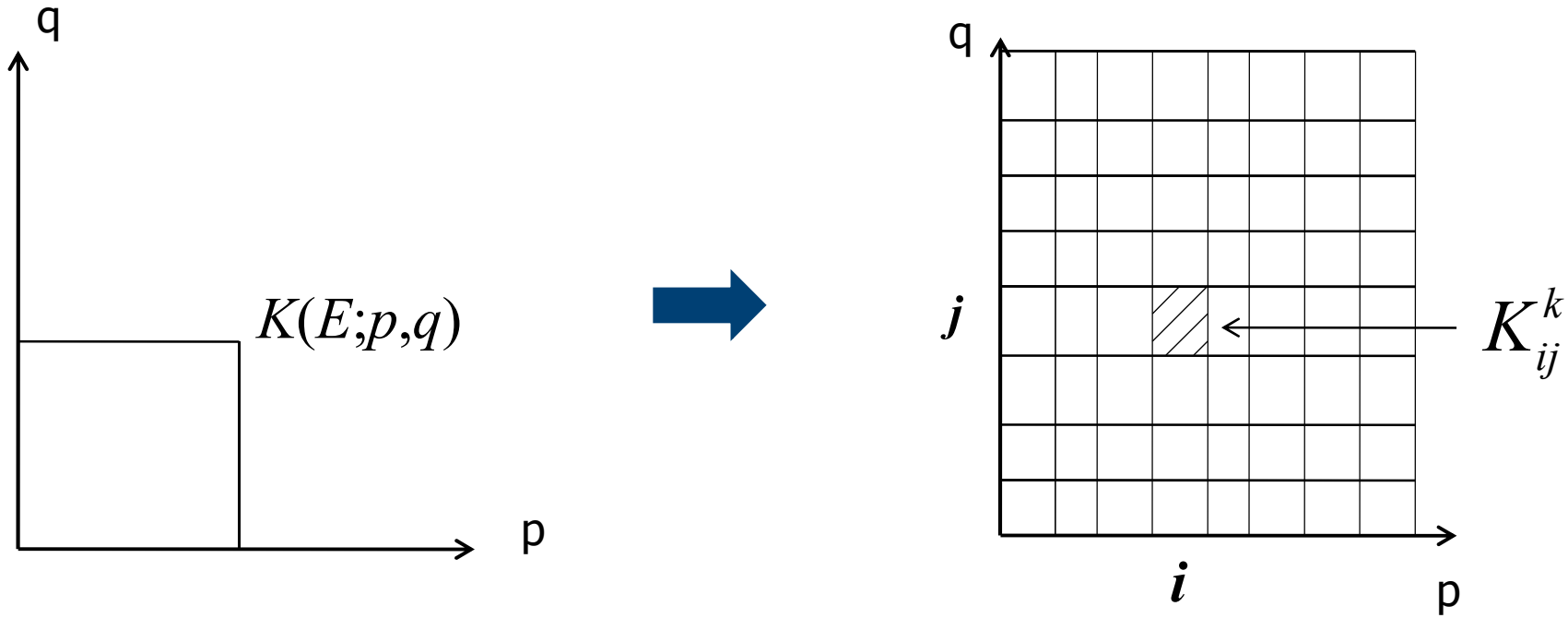
Few-Body Scattering Problem

Momentum lattice basis

The free motion three- (and few-body) Hamiltonian is a direct sum of the binary subHamiltonians, so the few-body basis functions can be constructed as direct products of the two-body ones.

$$H_0 = h_p^0 \oplus h_q^0 \;\Rightarrow\; \left|X_{ij}\right\rangle \equiv \left|x_i\right\rangle \otimes \left|y_j\right\rangle$$

Thus, in three- and few-body cases the WP basis space corresponds to a lattice in the momentum space. Thus we call the free WP basis as **the Lattice basis**.

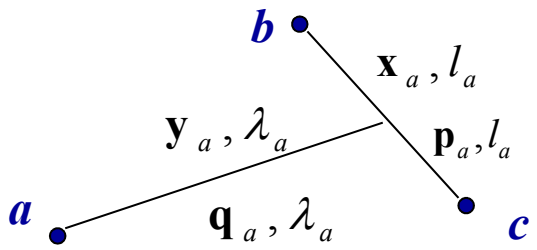


In the WP scheme, one has the discrete matrix function K^k_{ij} instead of continuous singular kernel of the integral equation $K(E;p,q)$. All the energy and momentum singularities are smoothed by the integration over the lattice cells.

Three-body channel resolvent

The total three-body Hamiltonian

$$H = H_0 + \sum_a v_a$$



One can define three channel Hamiltonians

$$H_a = H_0 + v_a = h_0^a \oplus h_a$$

Then, the channel WP basis states are direct products of two-body WPs for h_0^a and h_a subHamiltonians $\left| Z_{ij}^a \right\rangle \equiv \left| z_i \right\rangle \otimes \left| x_j \right\rangle$

In general few-body case, the WP basis should be constructed for each Jacobi coordinate. Such a basis corresponds to three-body scattering states of the channel Hamiltonian.

The main advantage of the discretization here is an explicit finite-dimensional representation for the few-body channel resolvent:

$$\boxed{G_a^{(+)}(E) = \sum \left[G_a \right]_{ij} \left| Z_{ij}^a \right\rangle \left\langle Z_{ij}^a \right|}$$

3N system (n-d scattering)

PRC 89, 064008 (2014)

The matrix analog of the AGS equation in the channel WP basis:

$$\mathbf{U} = \mathbf{P}\mathbf{V}_1 + \mathbf{P}\mathbf{V}_1\mathbf{G}_1\mathbf{U},$$

the channel resolvent

Elastic scattering amplitude can be found from a diagonal matrix element of **U**

$$e^{2i\delta(q_0)} - 1 \approx \frac{2m}{3q_0}\frac{U_{0j_0,0j_0}}{d_{j_0}}, \; q_0 \in (d_{j_0})$$

Breakup amplitude can be found from a non-diagonal elements of the same matrix **U**

$$T(p,q) \approx e^{i\delta_{NN}(p)} \frac{U_{0j_0,ij}}{\sqrt{d_{j_0} d_i d_j}}, \quad \begin{array}{l} p \in d_i \\ q \in d_j \\ q_0 \in d_{j_0} \end{array}$$

The free permutation matrix

The matrix of the particle permutation operator is just the matrix of the overlapping of the free WP bases defined in different Jacobi sets:

$$\left\langle X_{ij}{}^{a} \middle| P_{ab} \middle| X_{i'j'}{}^{a} \right\rangle = \left\langle X_{ij}{}^{a} \middle| X_{i'j'}{}^{b} \right\rangle$$

The permutation matrix for three identical particles can be found as follows:

$$P = P_{12}P_{23} + P_{13}P_{32}$$

$$\left\langle X_{ij} \middle| P \middle| X'_{i'j'} \right\rangle = \int\limits_{\mathcal{D}_{ij}} dpdq \int\limits_{\mathcal{D}_{i'j'}} dp'dq' \frac{P(p,q,p',q')}{\sqrt{d_i d_j d_{i'} d_{j'}}}$$

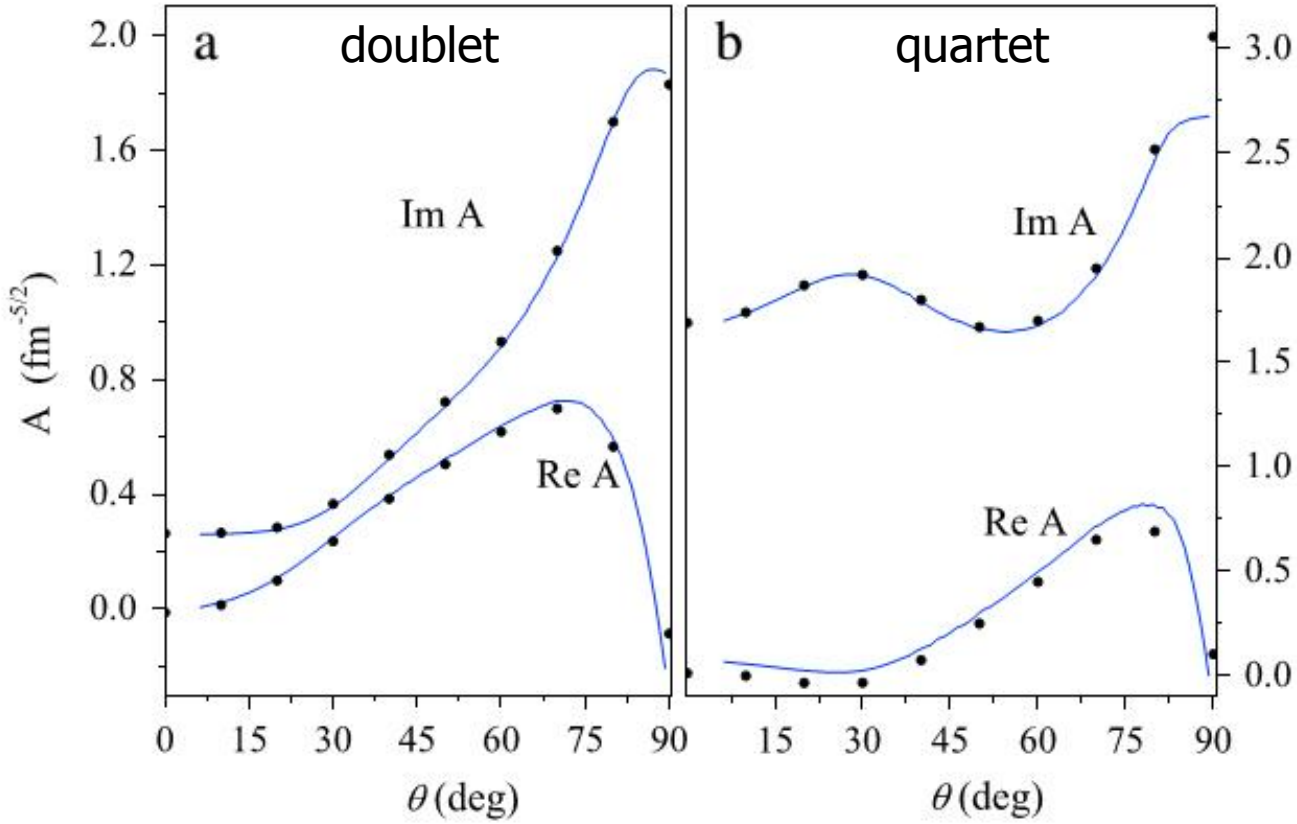
Here $P(p,q,p',q')$ is the kernel of the permutation operator in the momentum space.

The permutation operator matrix in the channel WP basis can be found using the expansion of the scattering WPs over the free ones

$$\left\langle Z_{ij}^{a} \middle| Z_{i'j'}^{b} \right\rangle = \sum_{ii'} O_{ik}^{*a} O_{i'k'}^{b} \left\langle X_{kj}^{a} \middle| X_{k'j'}^{b} \right\rangle = \sum_{ii'} O_{ik}^{*a} O_{i'k'}^{b} \left[P_0^{ab} \right]_{kj,k'j'}$$

n+d→n+n+p breakup amplitudes $^3S_1$

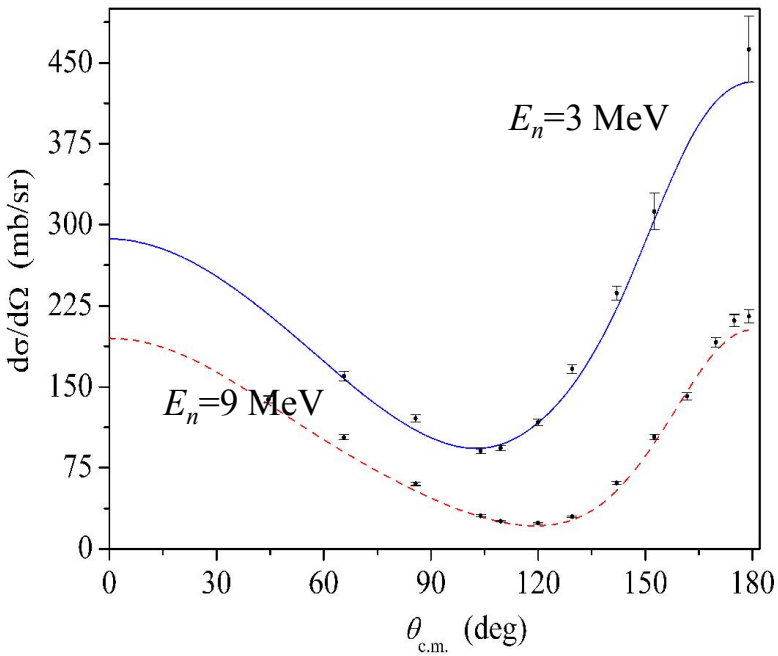
$$\psi(K,\rho) \xrightarrow[\rho\to\infty]{} \frac{A(\theta)}{(K\rho)^{5/2}} \qquad tg(\theta) = \frac{\sqrt{3}}{2}\frac{q}{p}$$

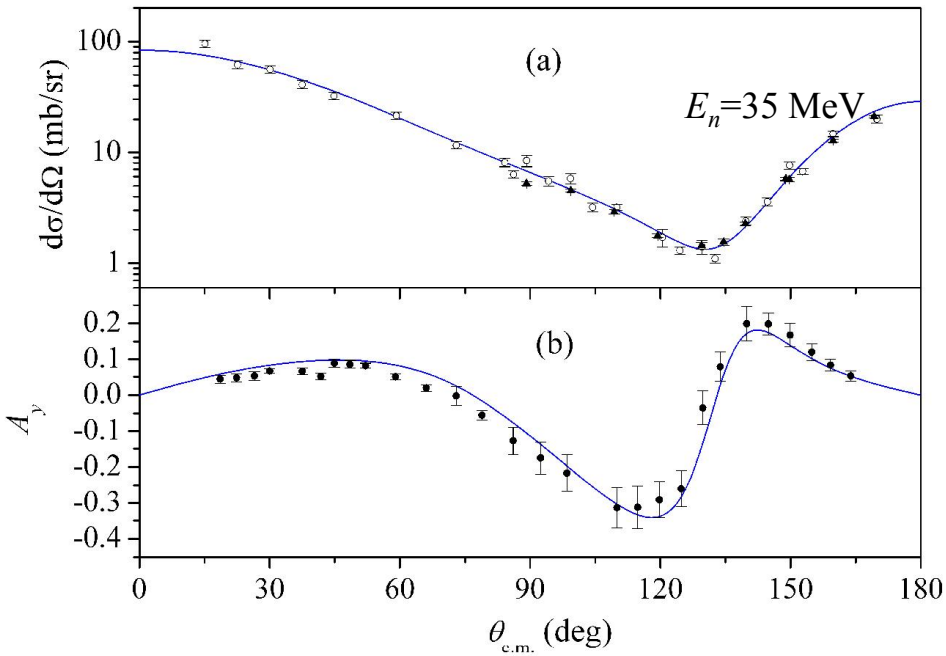


- Benchmark calculations (Friar et al., PRC 1995)
- Wave-packet

nd elastic differential cross sections for Nijmegen NN potential

Ann. Phys. 360, 613 (2015).
Com. Physics Commun. 204, 121 (2016)

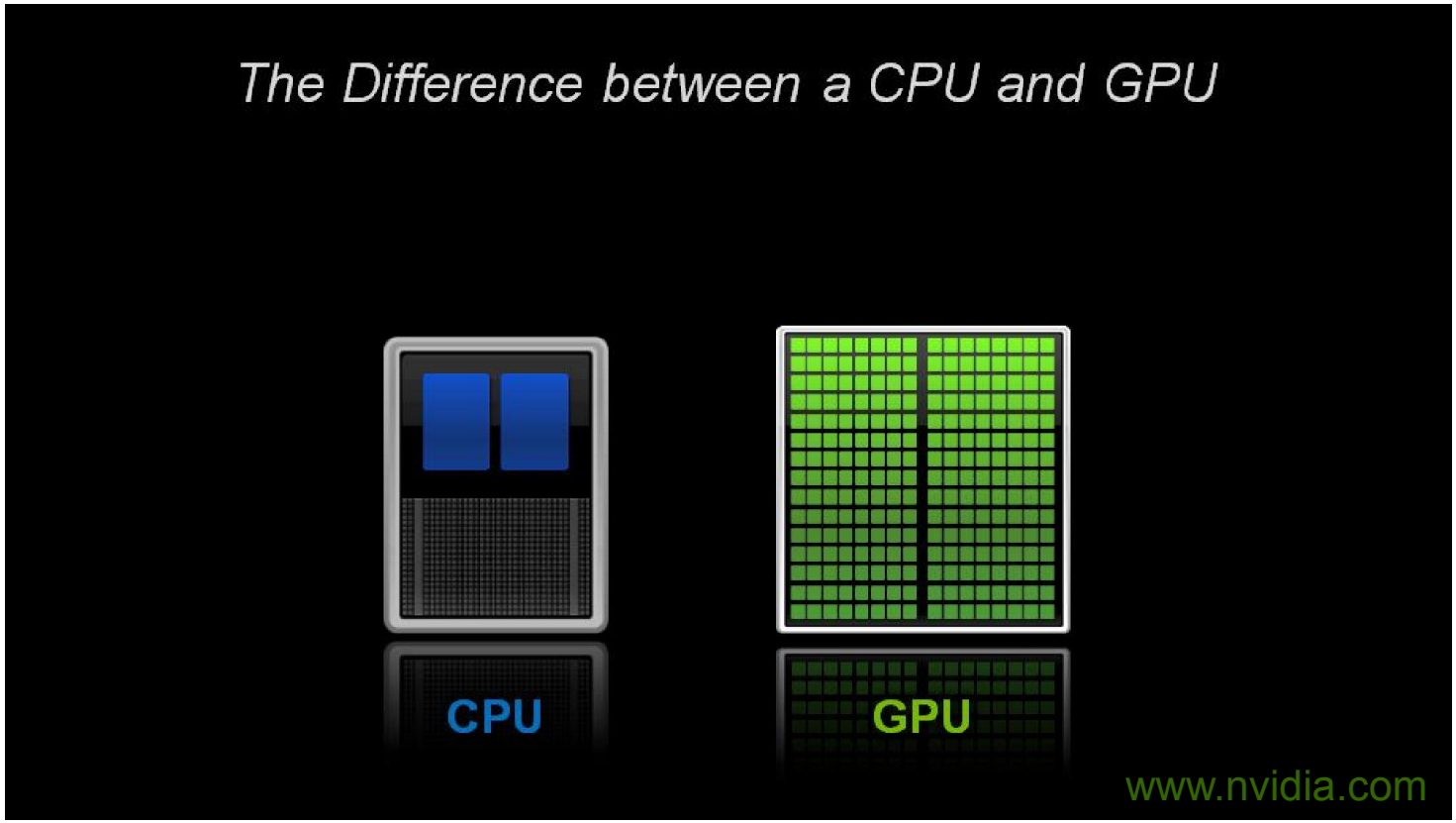




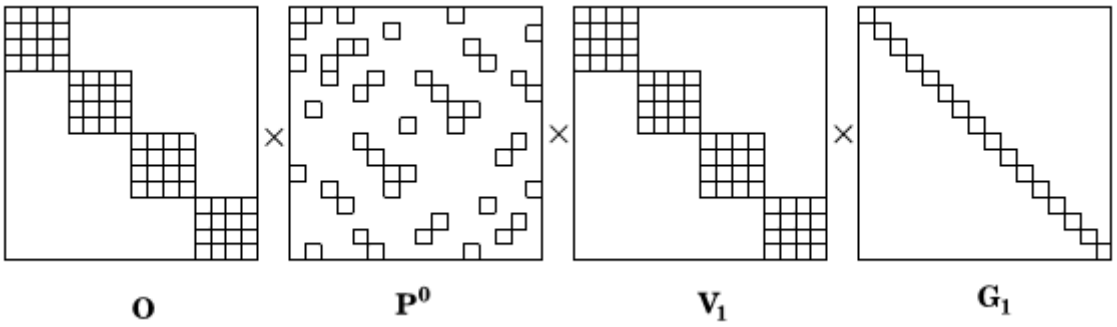
The calculations are prepared on an ordinary PC with a GPU.

Practical solution on a GPU

GPU – graphics processing unit



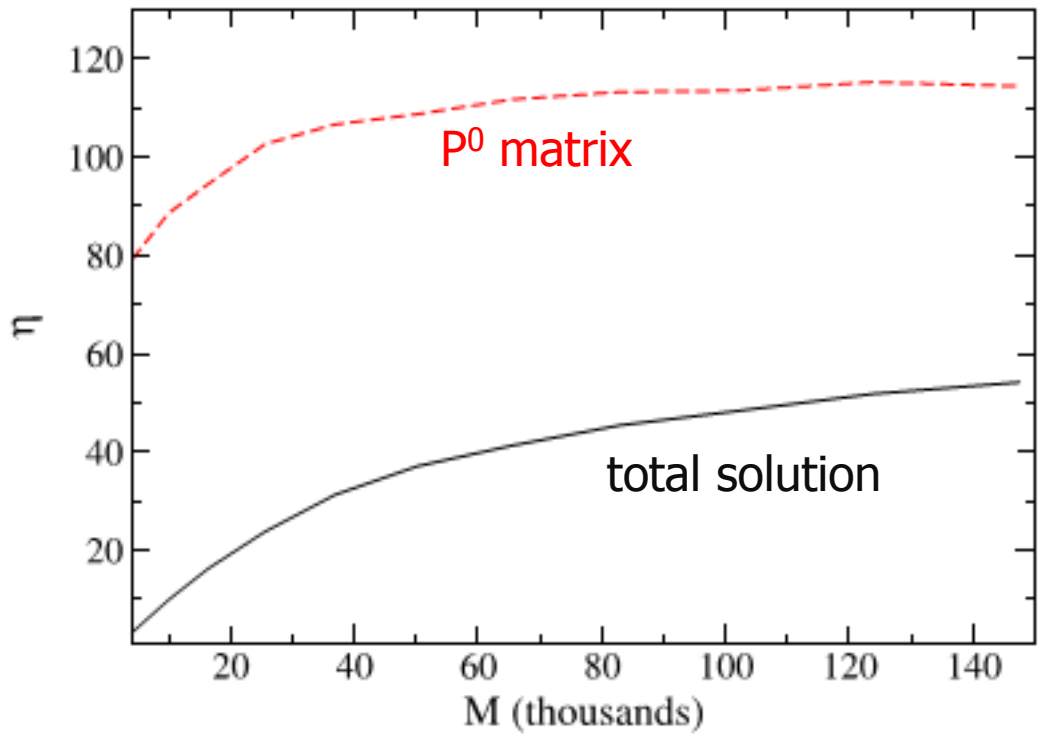
Practical solution on a GPU



The optimized algorithm for the solution of the realistic nd scattering problem consists of the following main steps:

1. Construction of three-body WP basis including preparation of two- body bases (via diagonalization of the pairwise NN subHamiltonian matrix in the free WP basis). Calculation of channel resolvent G_1.
2. Selection of nonzero elements of the overlap matrix.
3. Calculation of nonzero elements of the overlap matrix.
4. Solution of the resulted matrix equation by iterations using the Pade-approximant technique.

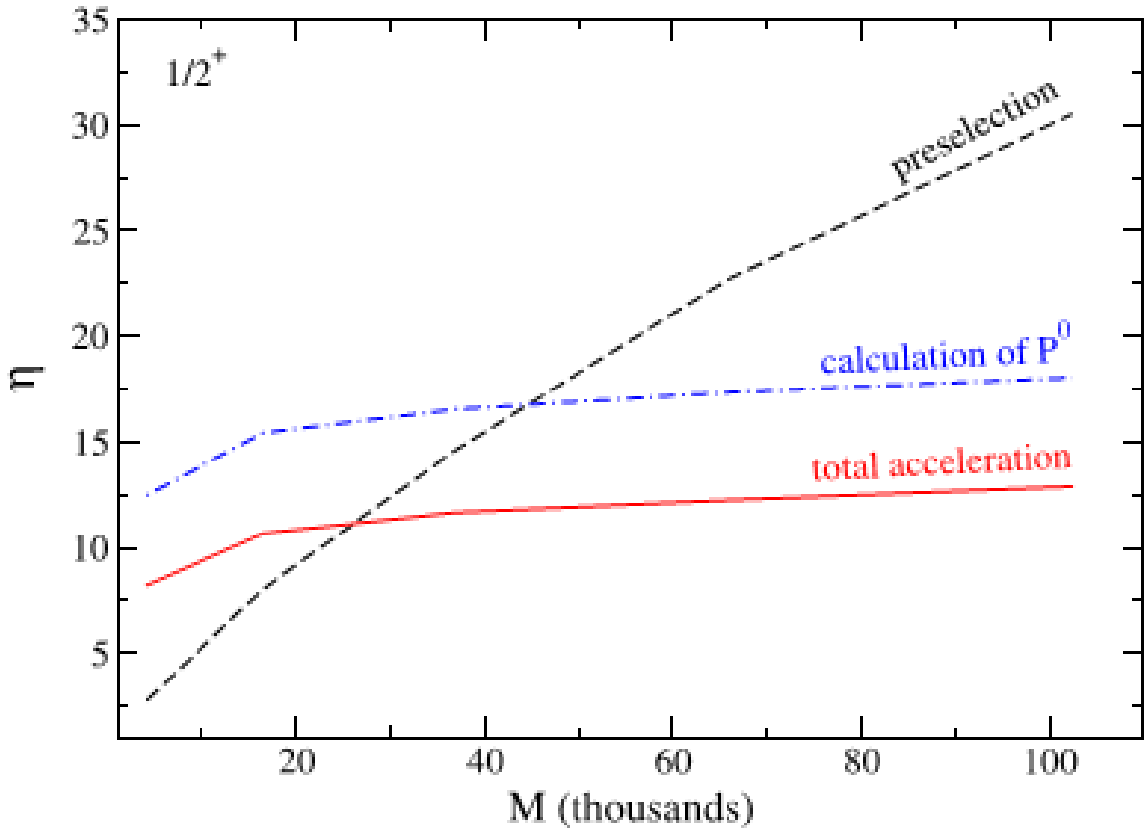
Acceleration for a solution of nd scattering problem with MT III potential



As a result, we found the acceleration for the overlap matrix calculation in 90-110 times, and the total acceleration in 10-50 times according to different basis dimension. The total acceleration keep growing with the dimension increasing.

Solution of the nd elastic scattering problem with fully realistic NN interaction

The GPU acceleration ratio η = t(CPU)/t(GPU) for the complete solution (solid line) and the overlap matrix calculation (dashed) versus the matrix dimension M in solution of 18-channel Faddeev equations for partial nd elastic amplitude.



Conclusions

Continuum discretization and stationary wave-packet formalism are shown to be convenient and effective tools for solving few-body scattering problems.

The approach can be applied to few-body problems in different other branches of quantum physics, e.g. in the quantum chemistry, solid state theory etc.

Some developments such as discrete spectral shift function formalism is suitable just for the discrete representation.

Other applications: Ann. Phys. **360**, 613 (2015).

Thank you for your attention!

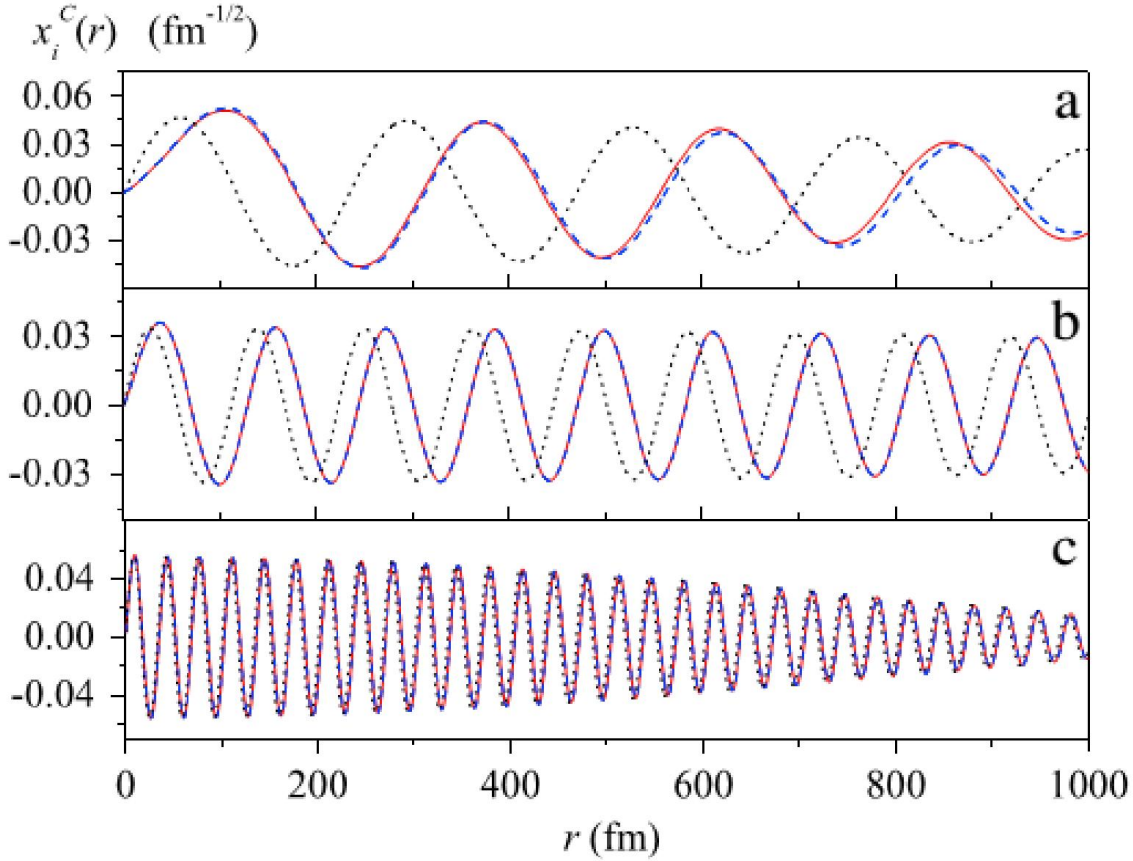


Fig. 5. The exact s-wave Coulomb WPs (dashed curves), the pseudostates found via the free WP basis (solid curves) and the free WPs at the same energy (dotted curves) for pp system at three center of mass energies: $E_{\text{c.m.}} = 0.03$ MeV (a), $E_{\text{c.m.}} = 0.133$ MeV (b) and $E_{\text{c.m.}} = 1.474$ MeV (c). In the case (c) the Coulomb phase shift is rather small, so that three curves are very close to each other.

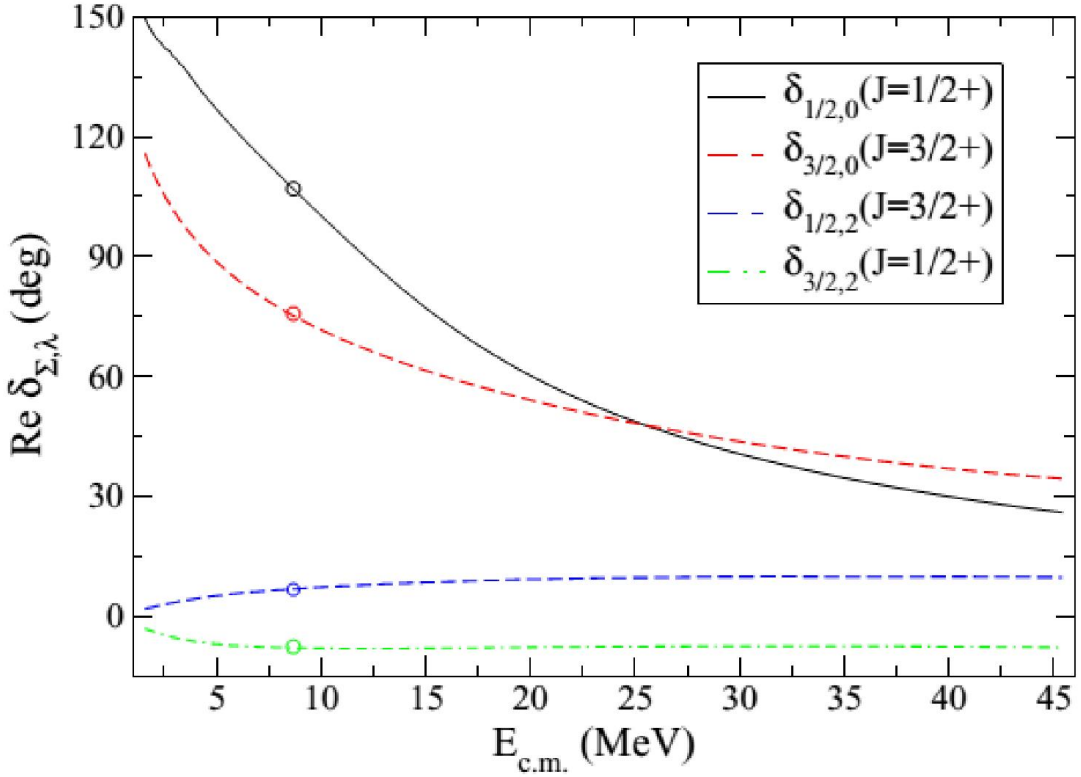
Advantages

• The multi-dimensional integral equation with singular kernel is replaced by simple matrix form with regular (averaged and smoothed) matrix elements.

• Due to matrix form for the permutation operator P, there is no need in time consuming multi-dimensional interpolations of a current solution when one iterates the equation kernel.

•The energy dependence remains in the resolvent matrix only (which is diagonal). So that, calculations at many energies can be done with the same permutation matrix P.

Partial phase shifts of the elastic nd scattering obtained within the WP approach (solid lines) and within the standard Faddeev calculations (circles).



• The scheme is suitable for a parallelization and realization on GPU.

Table 1
Runtime (in s) for separate steps of complete solutions of realistic *nd* scattering problem.

	Step	CPU time	GPU time
1.	Processing input data	30	30
2a.	Pre-selection for $\mathbb{P}^0$	12	1.9
2b.	Calculation of nonzero elements of $\mathbb{P}^0$	4558	524
4.	Iterations and Pade summation	1253	1250
	Total time	5852	1803