NOVEL TECHNIQUES FOR ULTRAFAST FEW-BODY SCATTERING CALCULATIONS

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Lecture 1

Part I:

Solving Quantum Scattering Problems on the Basis of Continuum Discretization

Contents

1. Discrete and continuous spectra of the Hamiltonian.

2. Weil's eigen-differentials method.

3. Stationary wave packets and their properties.

4. Description of the wave-packet formalism for solution of quantum scattering problems.

5. The case of a complex interaction potential.

6. Scattering of charged particles.

7. Relation between stationary wave packets and pseudo-states.

The eigenstates of the Hamiltonian

1. Discrete spectrum

$$H \mid \Psi_k \rangle = E_k \mid \Psi_k \rangle, \;\; k=1,..,M \quad (1)$$
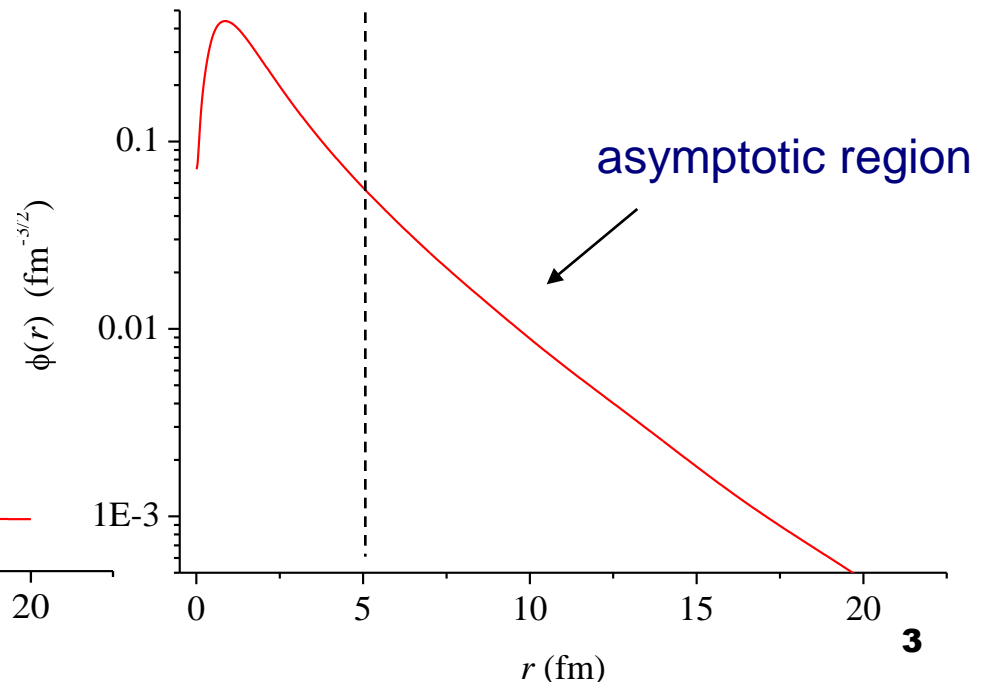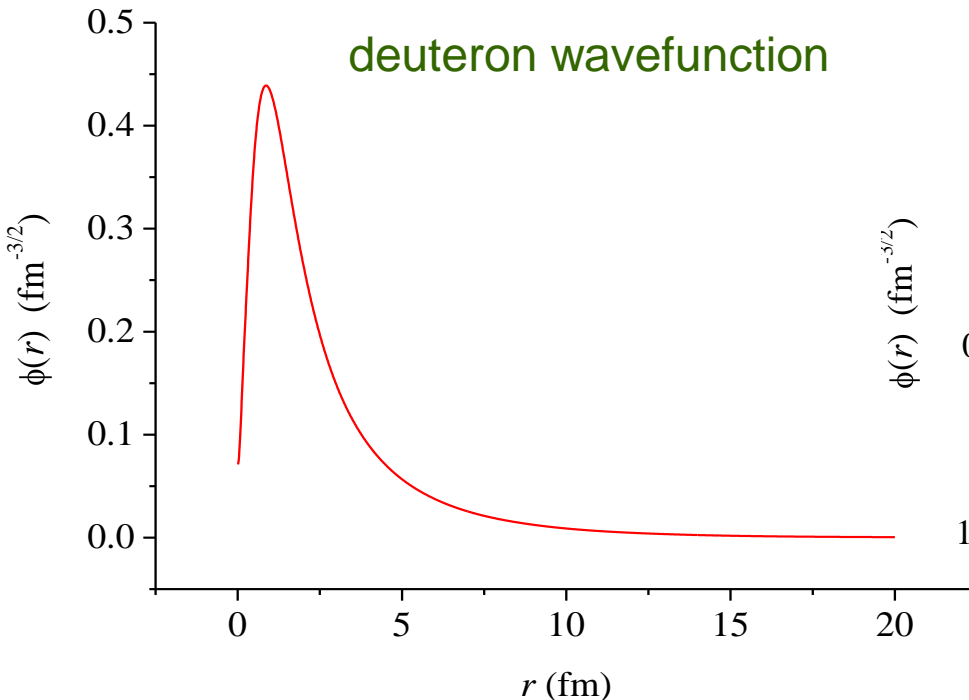
The solution of the Schrödinger equation exists at the discrete energy values E_k only.

$\langle r \mid \Psi_k \rangle = \Psi_k(r)$ — the wavefunction of the bound state.

The asymptotic boundary condition: $\quad \Psi_k(r) \underset{r \to \infty}{\sim} \exp(-\kappa r), \;\; \kappa = \sqrt{-2mE_k / \hbar^2}$

deuteron wavefunction

asymptotic region

2. Continuous spectrum

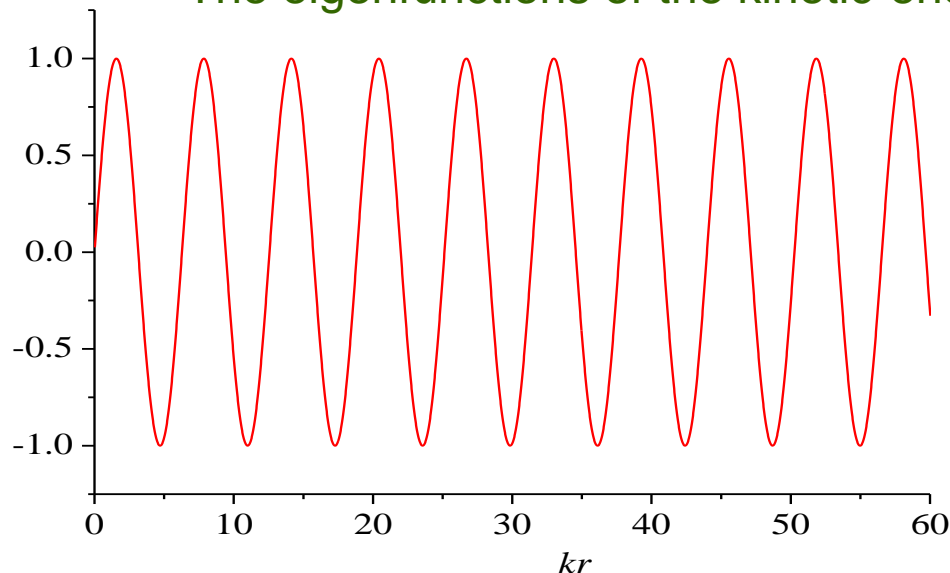$$H \mid \Psi(E) \rangle = E \mid \Psi(E) \rangle \qquad (3)$$

The solution of the Schrödinger equation (3) exists at arbitrary energy values $E \geq 0$.

The asymptotic boundary condition:

$$\Psi(E,r) \xrightarrow[r \to \infty]{} A(E) \sin (kr+\delta).$$

$A(E)$ — amplitude, δ — phase shift, $k=\sqrt{2E}$ — wave number.

The eigenfunctions of the kinetic-energy operator

$$\Psi(E;r) = A(E)\sin(kr)$$

States of continuous spectrum

For such states the wavefunctions do not descend in the coordinate space, i.e. they are unnormalized. Therefore, the description of continuous spectra of quantum-mechanical systems is not possible in a Hilbert space (in a strict sense).

For solution of this problem one may use
Weil's eigen-differentials method.

Let's define the eigen-differential of the continuous-spectrum wavefunction as an integral over a narrow energy bin:

$$\left|\Psi(E, E+\Delta)\right\rangle = \int\limits_{E}^{E+\Delta} \left|\Psi(E')\right\rangle dE'.$$

The so-defined states are normalized, i.e. belong to a Hilbert space.

Then, according to the Weil's method, the complete set of orthogonal eigenstates of the Hamiltonian consists of the bound states and eigen differentials:

$$\left|\Psi_k\right\rangle_{k=1}^{N_b}, \left|\Psi(E, E+\Delta)\right\rangle\Big|_{E=0}^{\infty}$$

Eigen differentials

An arbitrary function from a Hilbert space can be expanded on this complete set of eigenstates:

$$\left|\Phi\right\rangle = \sum_{k=1}^{N_b} C_k \left|\Psi_k\right\rangle + \sum C(E,\Delta)\left|\Psi(E, E+\Delta)\right\rangle$$

The norm of the eigenfunction is defined as an integral

$$N = \int_{E}^{E+\Delta} \left\langle\Psi(E)\middle|\Psi(E')\right\rangle dE' = \left\langle\Psi(E)\middle|\Psi(E, E+\Delta)\right\rangle$$

In the limit of infinitesimal widths of the energy intervals the expansion for an arbitrary function turns to the "ordinary" form

$$\left|\Phi\right\rangle \xrightarrow[\Delta \to 0]{} \sum_{k=1}^{N_b} C_k \left|\Psi_k\right\rangle + \int_{0}^{\infty} C(E)\left|\Psi(E)\right\rangle dE$$

with the usual "norm"

$$\left\langle\Psi(E)\middle|\Psi(E')\right\rangle = \delta(E - E')$$
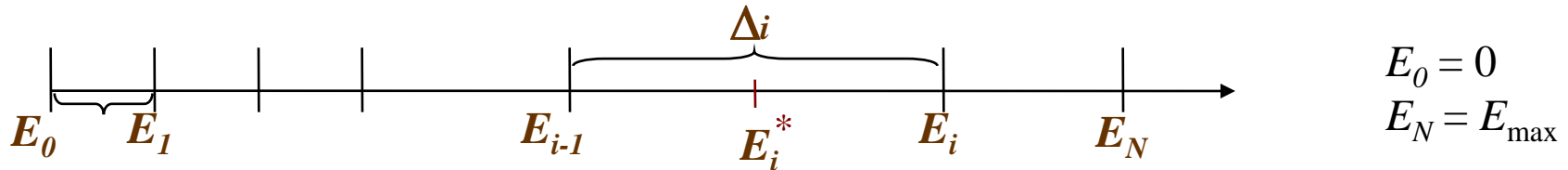
Stationary wave packets

Discretization of the continuous spectrum

Let's consider the free Hamiltonian H_0 (the kinetic-energy operator)

$$H_0 = -\frac{\hbar^2}{2m}\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2}\right], \quad \Psi_0(E,l;r) = \sqrt{\frac{2mk}{\pi\hbar^2}}rj_l(kr), \quad k = \frac{\sqrt{2mE}}{\hbar}$$

The "normalization" condition for the eigenfunctions: $\langle\Psi_0(E,l)|\Psi_0(E',l)\rangle = \delta(E-E')$

Let's divide the continuous spectrum of the H_0 into the energy bins $[E_{i-1},E_i]_{i=1}^N$:

$E_0 = 0$
$E_N = E_{\max}$

On each bin we can construct a stationary wave packet

$$|x_i\rangle = \frac{1}{\sqrt{\Delta_i}}\int_{E_{i-1}}^{E_i}|\Psi_0(E,l)\rangle dE \qquad i=1,..,N$$

Properties of the stationary wave packets

1. The set of SWP is orthonormalized:

$$\langle x_i | x_j \rangle = \frac{1}{\sqrt{\Delta_i \Delta_j}} \int_{E_{i-1}}^{E_i} \int_{E_{j-1}}^{E_j} \langle \Psi_0(E,l) | \Psi_0(E',l) \rangle dE dE' =$$

$$\frac{1}{\sqrt{\Delta_i \Delta_j}} \int_{E_{i-1}}^{E_i} \int_{E_{j-1}}^{E_j} \delta(E - E') dE dE' = \delta_{i,j} \frac{1}{\Delta_i} \int_{E_{i-1}}^{E_i} dE = \delta_{i,j}$$

After "packeting" the free-motion wavefunction becomes normalized!

2. Behavior of the "packet" function in the coordinate representation

$$\Psi_0(E,l;r) \approx \sqrt{\frac{2m}{\pi \hbar^2 k}} \sin\left(kr - \frac{l\pi}{2}\right), \quad kr \gg 1$$

$$x_i(r) \approx \sqrt{\frac{m}{\hbar^2}} \int_{k_{i-1}}^{k_i} \sqrt{\frac{2}{\pi k}} \sin\left(kr - \frac{l\pi}{2}\right) d\left(\frac{\hbar^2 k^2}{2m}\right) \approx \sqrt{\frac{2\hbar^2 k_i^*}{\pi m}} \int_{k_{i-1}}^{k_i} \sin\left(kr - \frac{l\pi}{2}\right) dk \approx$$
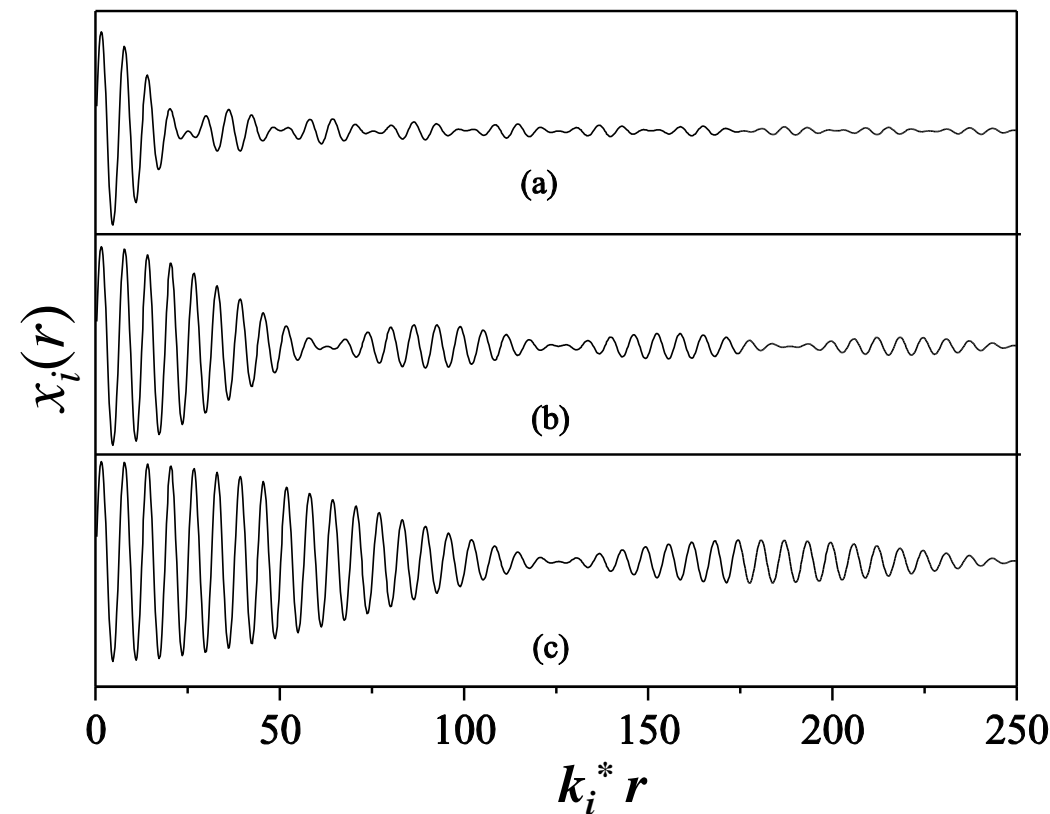
$$\approx \sqrt{\frac{2m\Delta_i}{\pi \hbar^2 k_i^*}} \sin\left(k_i^* r - \frac{l\pi}{2}\right) \frac{\sin(\frac{1}{2} d_i r)}{\frac{1}{2} d_i r}.$$

$$\boxed{\begin{array}{ll} \hbar k_{i-1} = \sqrt{2mE_{i-1}} & d_i = k_i - k_{i-1} \\ \hbar k_i = \sqrt{2mE_i} & E_i^* = \frac{1}{2}(E_{i-1} + E_i) \\ \hbar k_i^* = \sqrt{2mE_i^*} & \end{array}}$$

Behavior of the "packet" function in the coordinate representation

$$x_i(r) \approx \sqrt{\Delta_i}\ \Psi_0(E_i^*, l; r)\ \left[\frac{\sin(\frac{1}{2} d_i r)}{\frac{1}{2} d_i r} \right].$$

Coordinate dependencies of the wave packets for different ratios of their widths Δ_i to the energy eigenvalues E_i^*

$$\frac{\Delta_i}{E_i^*} = \begin{cases} 0.5 & (a); \\ 0.2 & (b); \\ 0.1 & (c). \end{cases}$$

The smaller the width of a wave-packet state the slower its decrease with distance.

The characteristic radius, for which the wave-packet function coincides with the exact state of continuous spectrum (up to the factor $\sqrt{\Delta_i}$), is

$$r_i = \frac{2}{d_i} = \frac{\hbar}{\sqrt{m}} \frac{2\sqrt{2E_i^*}}{\Delta_i}$$

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Thus the wave-packets can decay very slowly. Therefore, the basis constructed from such functions is very convenient for approximation of the continuous-spectrum eigenstates of some Hamiltonian H. This holds also for long-range interactions.

Because of infinitely large range of Coulomb forces, it is impossible to expand the exact Coulomb functions in the eigenfunctions of the kinetic-energy operator.

However, the Coulomb wave packets can be expanded on a finite set of free wave packets.

Thus, "packeting" the wavefunctions is an efficient tool for smoothing the singularities, appearing due to long-range interactions.
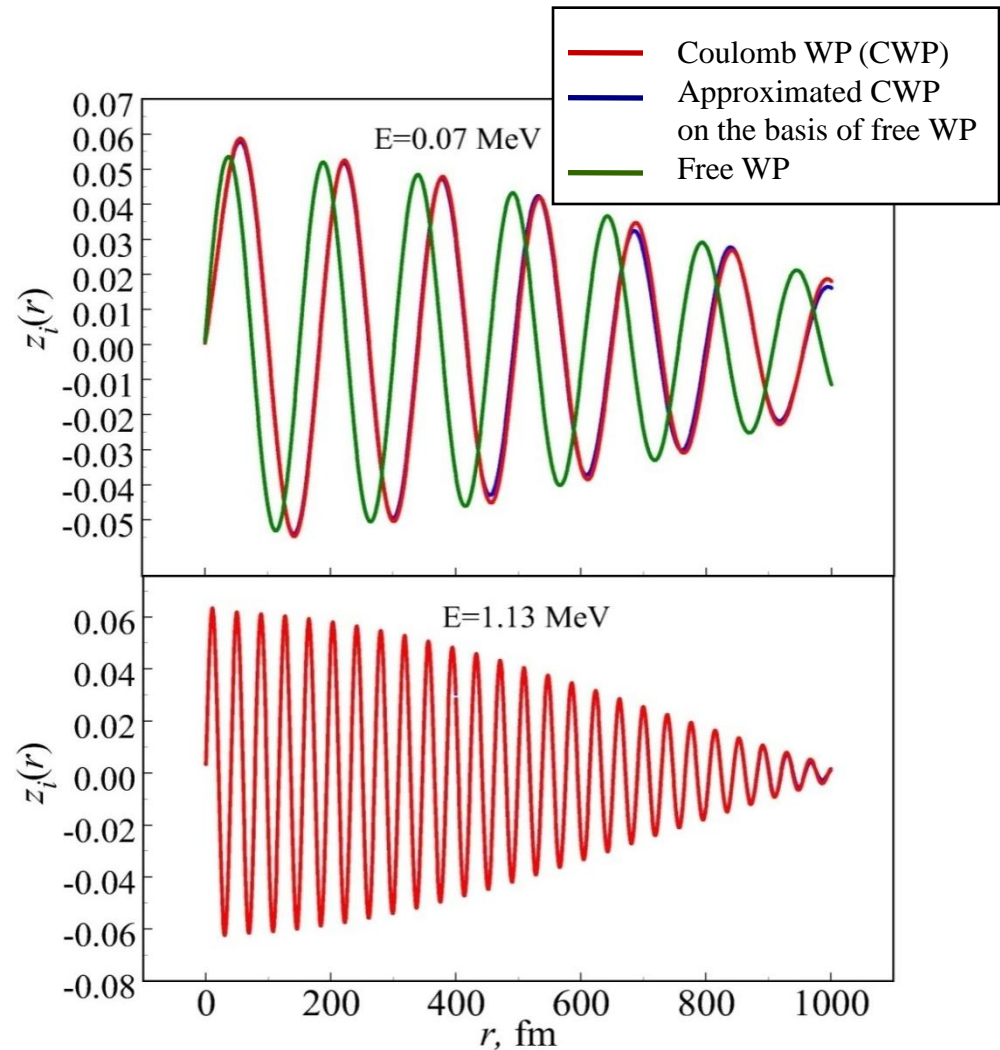
The formalism of stationary wave packets

With the use of the FWP basis, it is possible to construct the finite-dimensional analogs of the basic operators and equations of the quantum scattering theory.

Let's introduce the projector onto the wave-packet subspace (in each partial wave l):

$$\mathbb{P}^l = \sum_{i=1}^{N} |x_i^l\rangle\langle x_i^l|$$

The properties of projecting

1. Projection of an eigenfunction of the free-motion Hamiltonian H_0

Overlap integral of FWP and a plane wave:

$$\langle x_i|\Psi_0(E,l)\rangle = \frac{1}{\sqrt{\Delta_i}} \int_{E_{i-1}}^{E_i} \langle\Psi_0(E',l)|\Psi_0(E,l)\rangle dE' = \frac{1}{\sqrt{\Delta_i}} \int_{E_{i-1}}^{E_i} \delta(E-E') dE'$$

$$\langle x_i|\Psi_0(E,l)\rangle = \frac{1}{\sqrt{\Delta_i}} \left[\theta(E-E_{i-1}) - \theta(E-E_i)\right] = \begin{cases} \frac{1}{\sqrt{\Delta_i}}, & E \in [E_{i-1}, E_i], \\ 0, & E \notin [E_{i-1}, E_i]. \end{cases}$$

Thus, the result of projecting the eigenfunction of the Hamiltonian H_0 onto the wave-packet subspace is the wave-packet function on the interval, to which the energy E belongs:

$$\mathbb{P}^l |\Psi_0(E,l)\rangle = \left\{ \begin{array}{ll} \dfrac{|x_k^l\rangle}{\sqrt{\Delta_k}}, & E \in [E_{k-1}, E_k] \\ 0, & E > E_N \end{array} \right.$$

2. Projection of an operator, functionally depending on the Hamiltonian H_0

Let's consider an operator $R(H_0)$ depending upon H_0. Its spectral expansion in the complete basis of the H_0-eigenstates takes the form:

$$R(H_0) = \sum_l \int_0^\infty |\Psi_0(E,l)\rangle R(E) \langle \Psi_0(E,l)| dE.$$

Now let's apply the projectors from the left and from the right:

$$\mathbb{R}^l(H_0) \equiv \mathbb{P}^l R(H_0) \mathbb{P}^l = \sum_{i,j=1}^N |x_i^l\rangle \int_0^\infty \langle x_i^l|\Psi_0(E,l)\rangle R(E) \langle \Psi_0(E,l)|x_j^l\rangle \langle x_j^l|$$

$$\boxed{\mathbb{R}^l(H_0) = \sum_{i=1}^N |x_i^l\rangle \left[\frac{1}{\Delta_i} \int_{E_{i-1}}^{E_i} R(E) dE \right] \langle x_i^l|.}$$

General formula for wave-packet representation for an arbitrary function of H_0.

Finite-dimensional representation for the Hamiltonian itself looks as:

$$\mathbb{H}_0^l = \sum_{i=1}^{N} |x_i^l\rangle E_i^* \langle x_i|, \quad E_i^* = \frac{1}{\Delta_i} \int_{E_{i-1}}^{E_i} E \, dE = \frac{1}{2}(E_{i-1} + E_i).$$

So, the eigenvalues of the Hamiltonian matrix in the wave-packet basis coincide with the average points of energy intervals.

Finite-dimensional representation for the resolvent of the Hamiltonian H_0

The free resolvent is defined as

$$G_0(E) = [E + i0 - H_0]^{-1}$$

In the wave-packet representation we obtain the following expression:

$$\mathbb{G}_0^l(E) = \sum_{i=1}^{N} |x_i^l\rangle g_i(E)\langle x_i^l|, \quad g_i(E) = \frac{1}{\Delta_i} \int_{E_{i-1}}^{E_i} \frac{dE'}{E + i0 - E'},$$

$$g_i(E) = \frac{1}{\Delta_i} \ln \left| \frac{E - E_{i-1}}{E - E_i} \right| - \frac{i\pi}{\Delta_i} \left[\theta(E - E_{i-1}) - \theta(E - E_i) \right].$$

In the wave-packet representation the eigenvalues of the resolvent can be calculated in an explicit form.

An additional averaging over energy

The finite-dimensional expression for the free resolvent may be used further on for calculation of scattering observables.

<u>The Lippmann-Schwinger integral equation for the T-matrix:</u>

$$T(E) = T(E) + V \, G_0(E) \, T(E)$$

V – interaction potential

$T(E)$ – scattering operator, related to the scattering amplitude at the real $E > 0$

The resolvent $\mathbb{G}_0(E)$ shows the singularities at the boundaries of the energy intervals at the real values of the energy E. To regularize these singularities, one can perform an additional averaging over energy:

$$\mathbb{G}_0(E) \mapsto \mathbb{G}_{0k} = \frac{1}{\Delta_k} \int_{E_{k-1}}^{E_k} \mathbb{G}_0(E) dE, \quad E \in [E_{k-1}, E_k].$$

averaged eigenvalues
of the free resolvent

$$\mathbb{G}_{0k} = \sum_{i=1}^N |x_i^l\rangle g_i^k \langle x_i^l|, \qquad g_i^k = -\frac{1}{\Delta_k \Delta_i} \sum_{s,t=0}^{1} (-1)^{s+t} (E_{k-s} - E_{i-t}) \ln |E_{k-s} - E_{i-t}| - \frac{i\pi}{\Delta_k} \delta_{i,k}.$$

Finite-dimensional (matrix) analog of the Lippmann-Schwinger equation

$$T(E) = T(E) + V\,G_0(E)\,T(E) - \text{integral LSE}$$

Let's replace the operators by their finite-dimensional analogs in the wave-packet basis, and also perform the additional averaging over energy. The result is the matrix equation

$$\mathbb{T}_k = \mathbb{V} + \mathbb{V}\mathbb{G}_{0k}\mathbb{T}_k, \quad E \in [E_{k-1}, E_k].$$

$$\mathbb{V} = \sum_{i,j=1}^{N} |x_i^l\rangle\langle x_i^l|V|x_j^l\rangle\langle x_j^l|, \quad \langle x_i^l|V|x_j^l\rangle \equiv \underbrace{\int_0^\infty x_i^l(r)V(r)x_j^l(r)r^2 dr.}$$

matrix element of an interaction potential

For a wide class of interactions the matrix elements of the potential operators can be calculated analytically in the wave-packet basis.

Finite-dimensional analog of the transition operator $T(E)$

$$\mathbb{T}_k \approx \sum_{i,j=1}^{N} |x_i^l\rangle\langle x_i^l|T(E_k^*)|x_j^l\rangle\langle x_j^l|$$

The matrix elements of the transition operator are defined as follows:

$$T_l(E_1, E_2; E) = \langle\Psi_0(E_1,l)|T(E)|\Psi_0(E_2,l)\rangle, \quad A_l(E) = T_l(E,E;E).$$

off-shell amplitude

on-shell scattering amplitude, related to observables

Wave-packet analogs:

$$T_l(E_1, E_2; E) \approx \frac{[\mathbb{T}_k]_{k_1,k_2}}{\sqrt{\Delta_{k_1}\Delta_{k_2}}}, \quad \begin{array}{l} E \in [E_{k-1}, E_k] \\ E_1 \in [E_{k_1-1}, E_{k_1}] \\ E_2 \in [E_{k_2-1}, E_{k_2}] \end{array},$$

$$A_l(E) \approx \frac{[\mathbb{T}_k]_{k,k}}{\Delta_k}$$

Thus, with the use of free-wave-packet basis, scattering observables can be found from the simple matrix equation. The only "input parameters" are the nodes of discretization and the matrix elements of the interaction potential in the wave-packet basis.

The unitarity condition for wave-packet analog of the transition operator

Let's rewrite the equation for wave-packet analog of the transition operator in the following form:

$$\mathbb{T}^{-1} = \mathbb{V}^{-1} - \mathbb{G}_0, \quad \mathbb{T}^{\dagger -1} = \mathbb{V}^{-1} - \mathbb{G}_0^{\dagger}$$

(here we omit the index k that defines the energy interval to which the wave-packet operators belong)

In the case of hermitian $\mathbb{V}$ we obtain:

$$\mathbb{T}^{\dagger} - \mathbb{T} = \mathbb{T}(\mathbb{T}^{-1} - \mathbb{T}^{\dagger -1})\mathbb{T}^{\dagger} = \mathbb{T}(\mathbb{G}_0^{\dagger} - \mathbb{G}_0)\mathbb{T}^{\dagger}.$$

It follows from this expression that the imaginary part of T-matrix is related to the imaginary parts of the resolvent eigenvalues g_i^k as

$$2\mathrm{Im}\mathbb{T}_{k,k} = \sum_{j=1}^{N} 2\mathrm{Im}g_j^k |\mathbb{T}_{j,k}|^2, \quad \Rightarrow \boxed{\mathrm{Im}\mathbb{T}_{k,k} = -\frac{\pi|\mathbb{T}_{k,k}|^2}{\Delta_k}.}$$

S-matrix elements:
$$S_k = 1 - 2\pi\mathrm{i}\frac{\mathbb{T}_{k,k}}{\Delta_k}$$

$$S_k S_k^* = 1 + \frac{2\pi\mathrm{i}}{\Delta_k}(\mathbb{T}_{k,k}^{\dagger} - \mathbb{T}_{k,k}) + \frac{4\pi^2}{\Delta_k^2}|\mathbb{T}_{k,k}|^2 = 1$$
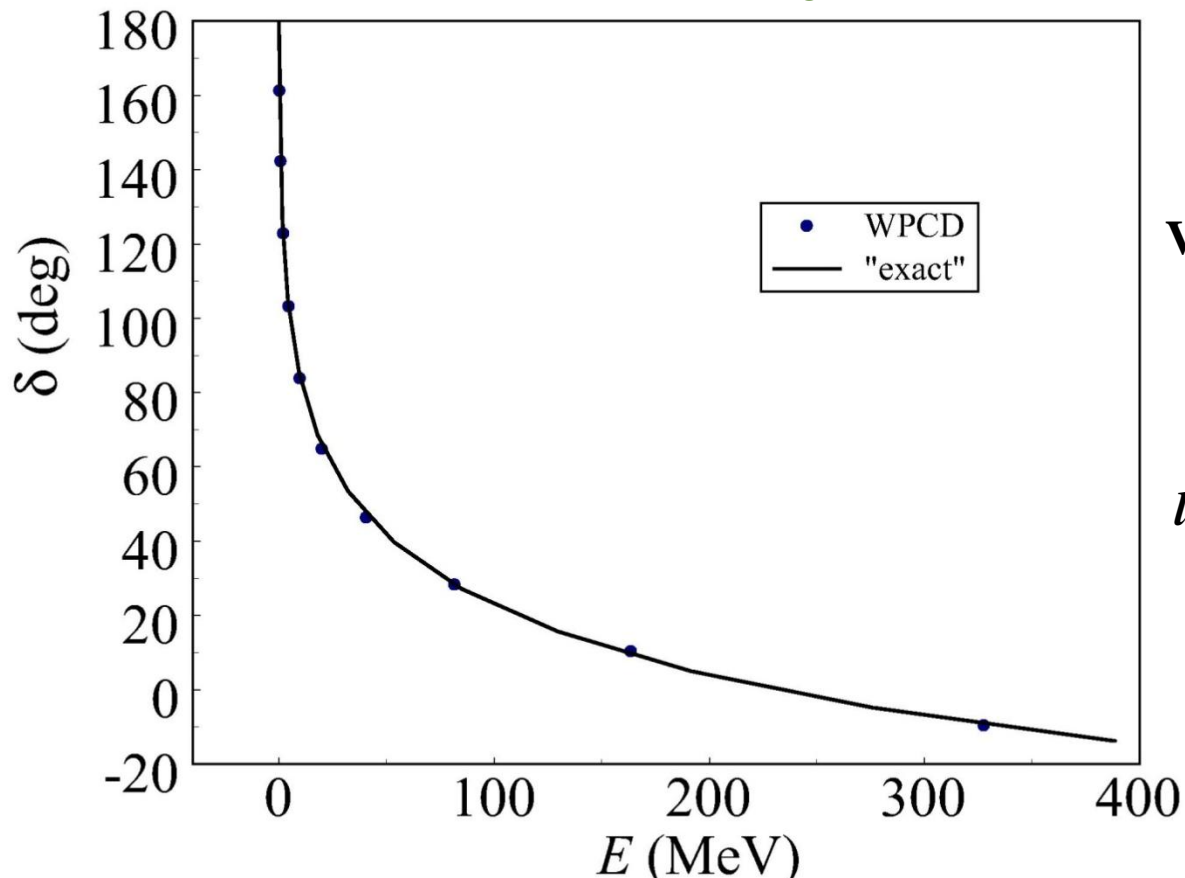
Thus, for hermitian potential operators S-matrix derived within the wave-packet approach is unitary: $|S_k| = 1.$

Illustrations for WP-technique: calculation of partial phase shifts

The partial phase shifts are easily found from the on-shell amplitude

$$A_l(E) = -\frac{e^{i\delta_l(E)} \sin \delta_l(E)}{\pi}$$

Phase shifts for n-p scattering

Malfliet-Tjon *NN* potential (MT III)

$$V(r) = V_R\, e^{-3.11r}/r - V_A\, e^{-1.55r}/r$$

V_R= 1438.7 MeV fm,
V_A= 626.9 MeV fm.

l=0

Finite-dimensional representations for operators

Along with finite-dimensional representations for transition operator, the wave-packet technique allows to build the FD-approximations for other operators of quantum scattering theory as well.

Resolvent of the total Hamiltonian

$$G(Z) = [Z - H]^{-1}$$

The resolvent identity (Lippmann-Schwinger equation for the resolvent):

$$\frac{1}{Z - H} - \frac{1}{Z - H_0} = \frac{1}{Z - H}[\cancel{Z} - H_0 - \cancel{Z} + H]\underbrace{}_{V}\frac{1}{Z - H_0}$$

$$\boxed{G(Z) = G_0(Z) + G(Z)VG_0(Z)}$$

in the wave-packet
$$\Rightarrow$$
representation

$$\boxed{\mathbb{G}(Z) = [\mathbb{G}_0^{-1}(Z) - \mathbb{V}^{-1}]^{-1}}$$

Note, that operators V^{-1} do not exist for local interaction potentials.

However, in the wave-packet representation the operator $\mathbb{V}^{-1}$ is defined simply as an inverse matrix for potential operator $\mathbb{V}$.

Resolvent of the total Hamiltonian

1) The finite-dimensional representation of the resolvent may be used for solving scattering problems at $Z = E + i0$. In doing this, it is convenient to apply an additional averaging over energy:

$$\mathbb{G}(E + i0) \longrightarrow \mathbb{G}_k = [\mathbb{G}_{0k}^{-1} - \mathbb{V}]^{-1}, \quad E \in [E_{k-1}, E_k].$$

The interrelation to the transition operator:

$$T(E) = V + V\, G(E{+}i0)\, V$$

2) For complex Z the finite-dimensional representation of the resolvent may be used for finding parameters of resonant states. The total resolvent has poles at the energies of bound and resonant states.

The transcendent equation

$$\boxed{\det \| [\mathbf{G}_0(Z)]^{-1} - \mathbf{V} \| = 0}$$

defines the bound-state and resonance poles. Here $\mathbf{G}_0$ and $\mathbf{V}$ are matrices of the operators in the wave-packet basis.

Equation for wavefunctions

The wavefunctions of the Hamiltonian, which describe scattering, satisfy the Lippmann-Schwinger equation:

$$|\Psi^{(+)}(E,l)\rangle = |\Psi_0(E,l)\rangle + VG_0(E+i0)|\Psi^{(+)}(E,l)\rangle$$

After replacing the exact scattering wavefunctions by their wave-packet analogs

$$|\Psi^{(+)}(E,l)\rangle \rightarrow |z_k^{(+)}\rangle, \qquad |\Psi_0(E,l)\rangle \rightarrow |x_k\rangle \qquad E \in [E_{k-1}, E_k]$$

the finite-dimensional analog of LSE takes the form

$$\boxed{|z_k^{(+)}\rangle = |x_k\rangle + \mathbb{V}\mathbb{G}_{0k}|z_k^{(+)}\rangle}$$

Solution of this equation may be written as

$$|z_k^{(+)}\rangle = \sum_{i=1}^{N}\Omega_{ik}|x_i\rangle \text{ , where } \Omega_{ik} \equiv \langle x_i | z_k^{(+)}\rangle = \overline{1 - \mathbb{G}_{0k}\mathbb{V}}^{-1}_{\ ik}$$

for the k-th interval, the expansion coefficients are defined by the k-th column of the matrix

Wave operator

Let's construct the total matrix of transformation from the free wave packets to the perturbed ones. For this purpose we gather the expansion coefficients for all Intervals $k=1,..,N$ in the matrix

$$
\Omega = \begin{pmatrix}
1-\mathbb{G}_{01}\mathbb{V}^{-1}{}_{11} & \cdots & 1-\mathbb{G}_{0N}\mathbb{V}^{-1}{}_{1N} \\
\vdots & \ddots & \vdots \\
1-\mathbb{G}_{01}\mathbb{V}^{-1}{}_{N1} & \cdots & 1-\mathbb{G}_{0N}\mathbb{V}^{-1}{}_{NN}
\end{pmatrix}
$$

It's easily seen that Ω is the matrix representation of the operator

Ω_{ik}

$$
\mathbb{O} = \sum_{k=1}^{N} |z_k^{(+)}\rangle\langle x_k| = \sum_{i,k=1}^{N} |x_i\rangle\langle x_i | z_k^{(+)}\rangle\langle x_k|,
$$

which is the finite-dimensional analog of Møller wave operator

$$
\Omega^{(+)} = \int_0^\infty |\Psi^{(+)}(E)\rangle\langle\Psi_0(E)| \, dE
$$

Complex interaction potential

The interaction between composite particles is usually defined by a non-local complex potential of the Perey-Buck form $V(\mathbf{r},\mathbf{r'}) = -U(/\mathbf{r}+\mathbf{r'}/)W(/\mathbf{r}-\mathbf{r'}/)$.

In the case of complex potential, the scattering phase is also complex. The decrease of elastic-scattering probability is characterized by a parameter which is called "inelasticity coefficient":
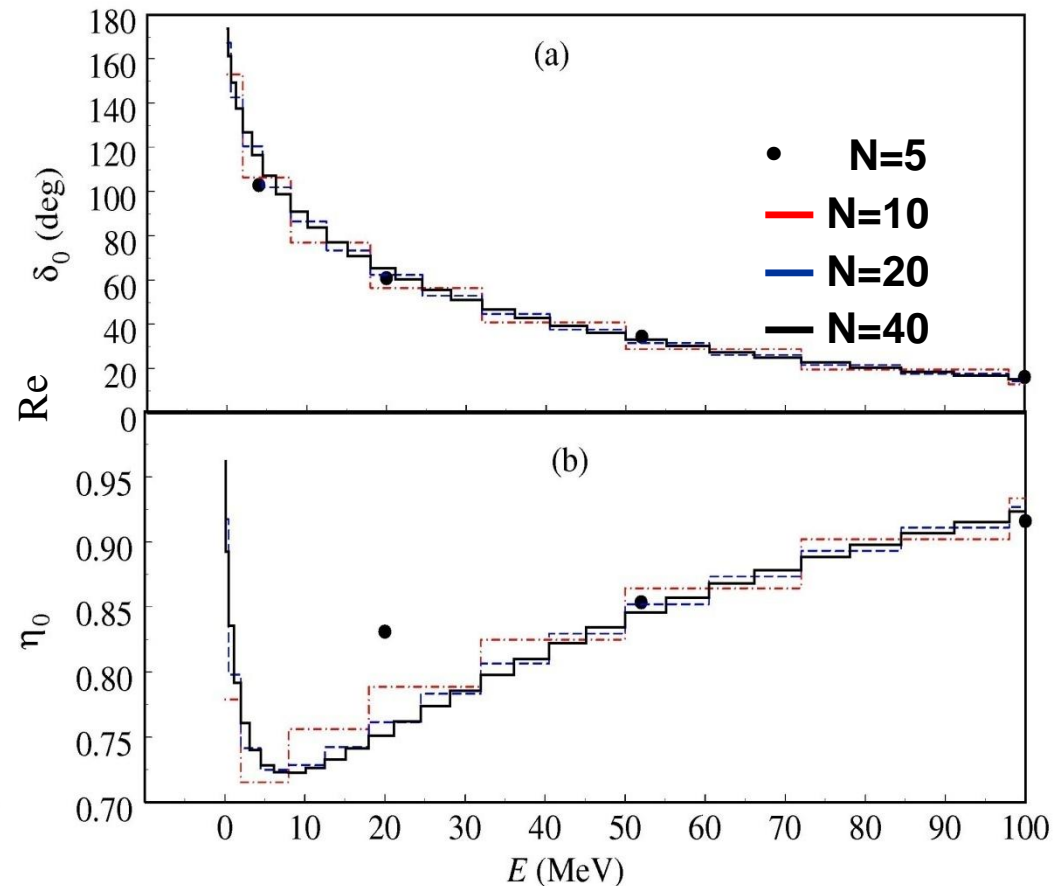
$$\eta_l = |S_l| = \exp[-2 \, \mathrm{Im} \, \delta_l(E)]$$

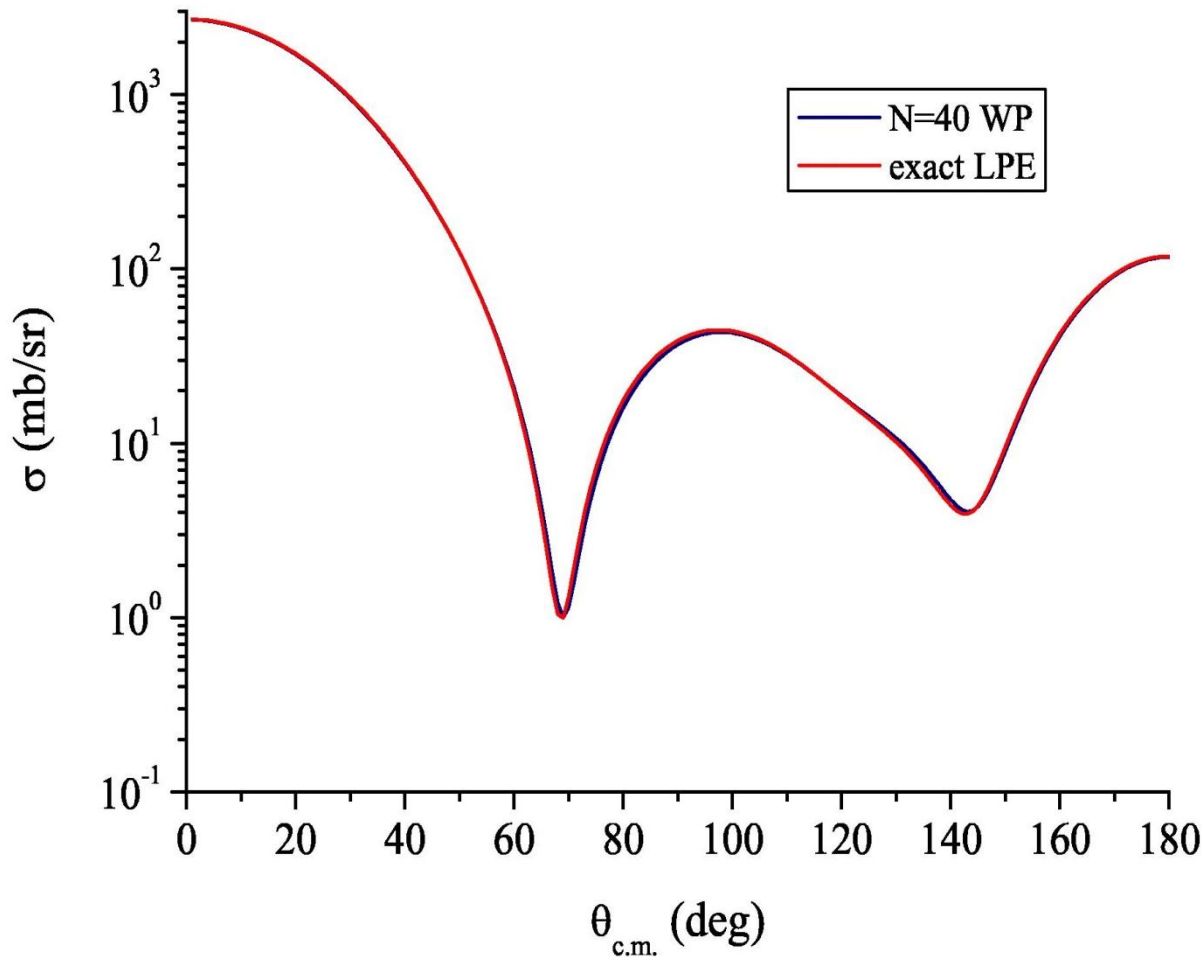Matrix elements for non-local interaction potential:

$$V_{ij}^l = \int_0^\infty \int_0^\infty x_i^l(r) V_l(r,r') x_j^l(r') r^2 r'^2 \, dr dr',$$

$$V_l(r,r') = \int \int Y_{lm}^*(\mathbf{n_r}) V(\mathbf{r},\mathbf{r'}) Y_{lm}(\mathbf{n_{r'}}) d\Omega_{\mathbf{r}} d\Omega_{\mathbf{r'}}.$$

Scattering of neutrons by the ^{56}Fe nucleus

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Differential cross section for n+^{56}Fe elastic scattering at the incident energy E_n=7 MeV

The differential cross section obtained within the wave-packet technique coincides with the cross section calculated for a local phase-equivalent potential.

Scattering of charged particles

The total Hamiltonian in the case of charged particles has the form

$$H = \underbrace{H_0 + V_C}_{H_C} + V_S \qquad V_C(r) = Z_1 Z_2 e^2/r, \;\; V_S(r) - \text{short-range potential}$$

The Hamiltonian H_C is used now as a "free" Hamiltonian. The basis functions are built from regular Coulomb functions (eigenfunctions of the Coulomb Hamiltonian H_C).

$$F_C(E, r) \approx \sqrt{\frac{2m}{\pi \hbar^2 k}} \sin\left[kr - \frac{1}{k}\ln(2kr) + \sigma\right], \quad \sigma = \arg\Gamma\left(1 + \frac{i}{k}\right), \quad kr \gg 1.$$

$$|x_i^C\rangle = \frac{1}{\Delta_i}\int_{E_{i-1}}^{E_i} |F_C(E)\rangle dE, \quad i = 1, \ldots, N.$$

$\longleftarrow$ Coulomb wave packets (CWP)

The equation for Coulomb-nuclear part of the transition operator:

$$\mathbb{T}_k^{\text{add}} = \mathbb{V}_S + \mathbb{V}_S \mathbb{G}_k^C \mathbb{T}_k^{\text{add}}, \qquad \mathbb{G}_k^C = \sum_{i=1}^{N} |x_i^C\rangle g_i^k \langle x_i^C|, \qquad \mathbb{V}_S = \sum_{i,j=1}^{N} |x_i^C\rangle\langle x_i^C|V_S|x_j^C\rangle\langle x_j^C|.$$

finite-dimensional representation of Coulomb resolvent

finite-dimensional representation of short-range potential operator

Illustration: the s- and d-wave Coulomb-nuclear partial phase shifts for α–α scattering
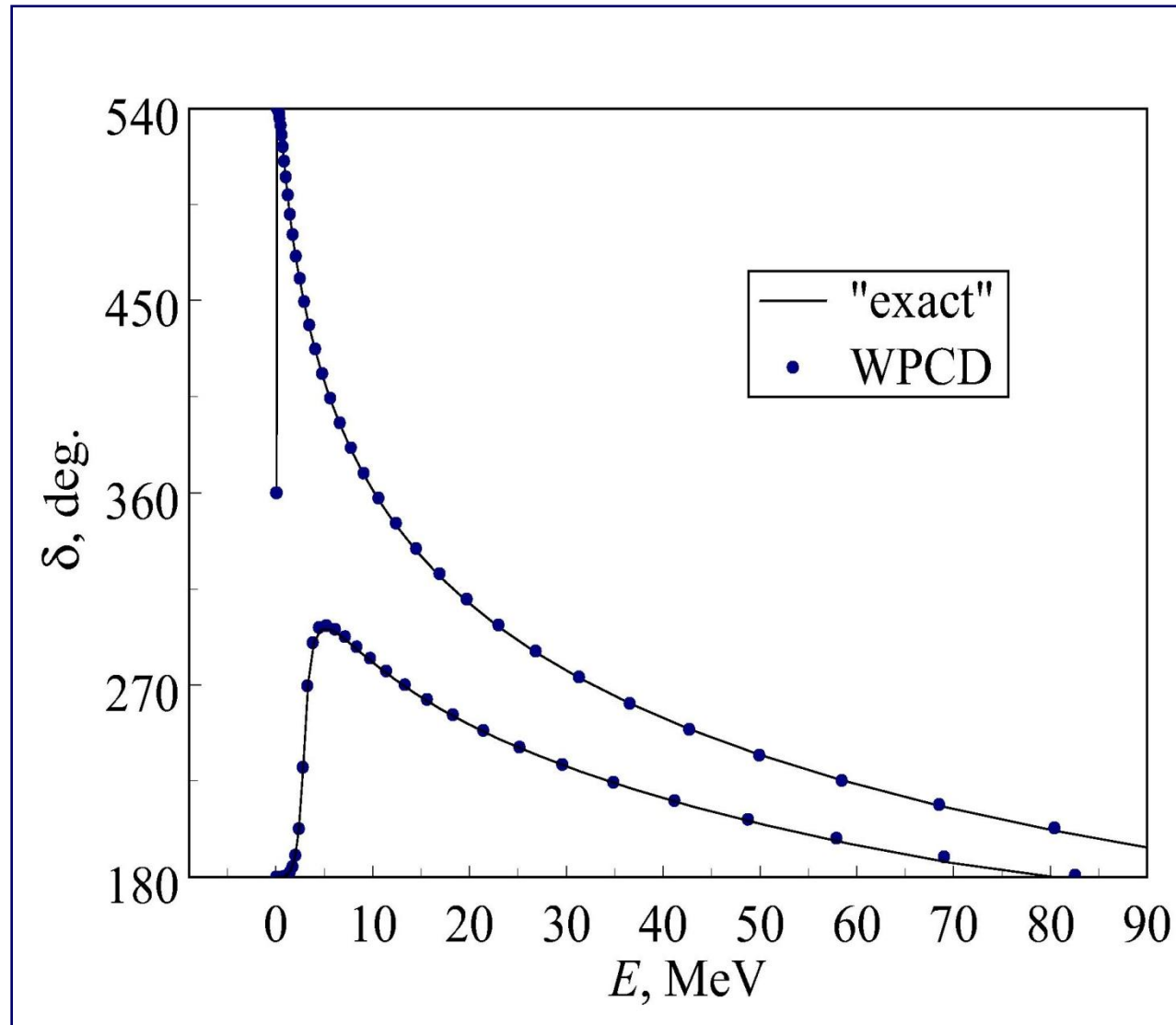
Interrelation between stationary wave packets and pseudo-states

Let's consider some basis of square-integrable functions

$$| \phi_n \rangle \, _{n=1}^{N}, \quad \langle \phi_{n'} | \phi_n \rangle = \delta_{n,n'}$$

The wavefunction of a quantum system satisfies the Schrödinger equation

$$H | \Psi \rangle = E | \Psi \rangle$$

Let's expand the wavefunction on our basis:
$$| \Psi \rangle = \sum_{n=1}^{N} C_n | \phi_n \rangle$$

The expansion coefficients C_n are found from the matrix equation

$$\sum_{n'=1}^{N} (H_{nn'} - E) C_{n'} = 0, \; n = 1, .., N, \quad H_{nn'} \equiv \langle \phi_n | H | \phi_{n'} \rangle$$

Non-trivial solution of this matrix equation is reduced to diagonalization of the Hamiltonian matrix, i.e. to finding the eigenvectors and eigenvalues of this matrix.

The eigenvalues are obtained from the equation:

$$\boxed{\det \| H_{nn'} - E \| = 0} \Rightarrow \quad \varepsilon_n \, _{n=1}^{N}$$
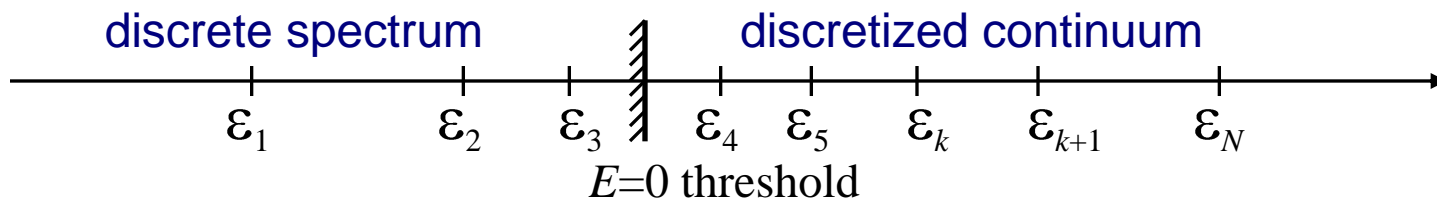
Eigenstates of the Hamiltonian matrix

As a result of diagonalization of the Hamiltonian matrix one obtains the complete set of eigen energies and eigenvectors

$$\varepsilon_n, \quad \left. C_i^n \right|_{i=1}^N \quad \rightarrow \quad |\bar{z}_n\rangle = \sum_{i=1}^N C_i^n |\phi_i\rangle, \quad n = 1,..,N$$

Eigenstates with energies $\varepsilon_n < 0$ ($n=1,..,N_b$) may be considered as approximations to bound states of initial Hamiltonian.

Eigenstates of the Hamiltonian matrix with positive energies $\varepsilon_n > 0$ ($n=N_{b+1},..,N$) correspond to the continuous spectrum of initial Hamiltonian.
As they are different from the exact scattering functions, such states are called as pseudo-states of the Hamiltonian.

discrete spectrum　　　　　　discretized continuum

ε_1　　　ε_2　ε_3　ε_4　ε_5　ε_k　ε_{k+1}　ε_N

$E=0$ threshold

Expansion of the Hamiltonian eigenfunctions on some basis of finite dimension leads to discretization of continuous spectrum of this Hamiltonian.

Properties of pseudo-states

1) Pseudo-states (together with bound states) form an orthonormalized set:

$$\left\langle \overline{z}_n \middle| \overline{z}_{n'} \right\rangle = \delta_{n,n'}, \quad n,n' = 1,..,N$$

2) The Hamiltonian matrix is diagonal in the pseudo-state representation

$$\left\langle \overline{z}_n \middle| H \middle| \overline{z}_{n'} \right\rangle = \varepsilon_n \delta_{n,n'}, \quad n,n' = 1,..,N$$

3) The wavefunctions of pseudo-states are proportional to exact continuous-spectrum functions in some restricted region of coordinate space and decrease outside of this region:

$$\overline{z}_n(r) \approx B_n \Psi(E;r), \quad r < r_0$$

Characteristic range r_0 depends on properties of the basis functions

If the range r_0 is greater than the range of interaction, then the pseudo-states can be used instead of exact wavefunctions for finding scattering observables.

The main problem here is the finding of the normalization coefficients B_n (normalization problem).

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The properties of pseudo-states are mainly the same as the properties of stationary wave packets.

Let's compare these states to each other. For this purpose, we shall use discretization parameters, for which the eigenstates of the Hamiltonian matrix coincide in the wave-packet and our L_2 bases.

As an example, we consider Gaussian basis $\phi_n(r) = D_n \exp(-\alpha_n r^2),$

D_n – normalization coefficients, α_n – basis parameters.

Example: distribution on the basis of geometric progression

$$\alpha_n = \alpha_0 a^n$$


n, **pseudo-state number**
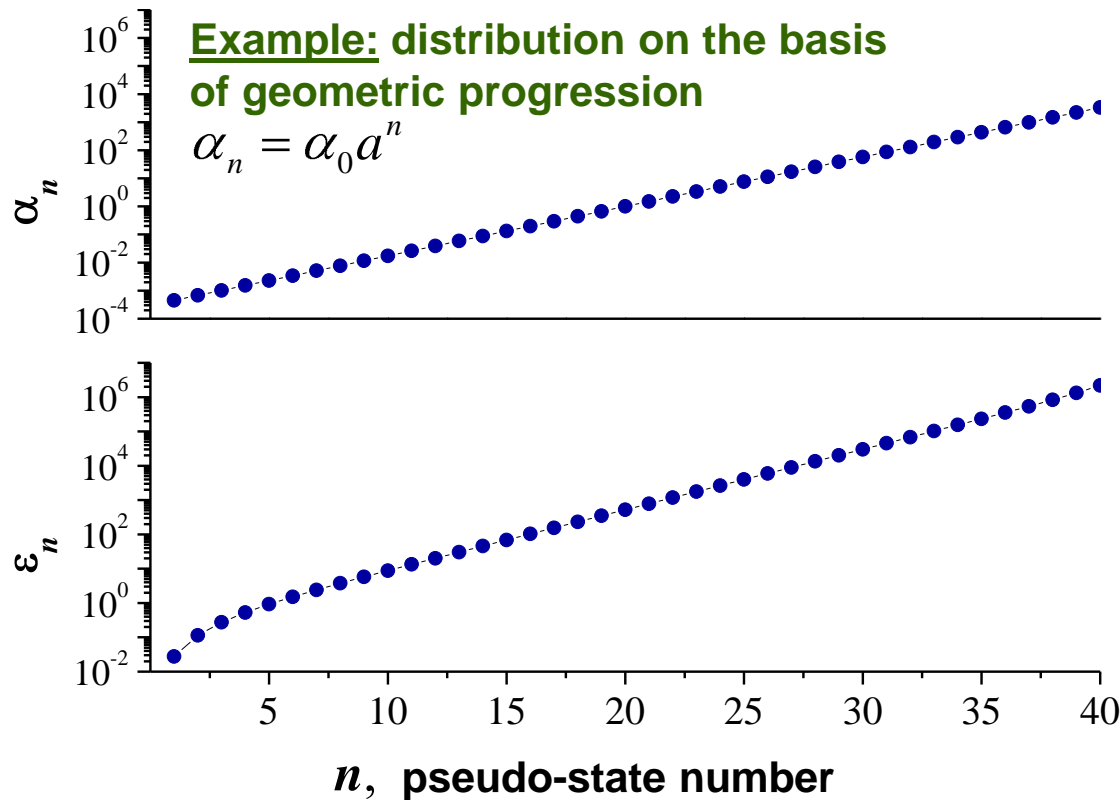
Let's construct the pseudo-state spectrum for the kinetic-energy operator H_0 on this basis.

As a result of diagonalization, we obtain the set of eigenvalues ε_n and respective pseudo-state functions $\overline{x}_n(r).$

Let's now divide the continuous spectrum of the Hamiltonian H_0 into bins, so that the average points E_i^* of the bins to coincide with the eigenvalues ε_i of the Hamiltonian matrix in the chosen Gaussian basis.

We may then construct the stationary wave packets $x_i(r)$ using this decomposition of the H_0 continuous spectrum.

Let's compare directly the coordinate dependencies for two different types of functions (wave-packet states and pseudo-states), corresponding to the same eigenvalues of the discretized Hamiltonian spectrum.
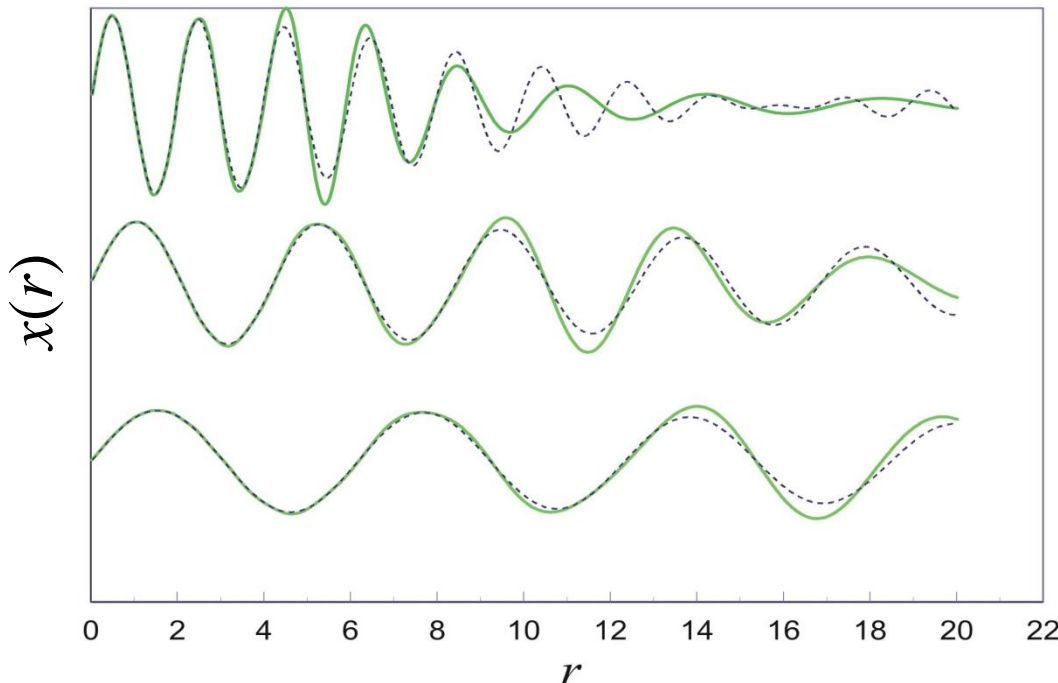
The both types of wavefunctions almost coincide in a restricted region $r<R$ and fall in different ways outside this region.
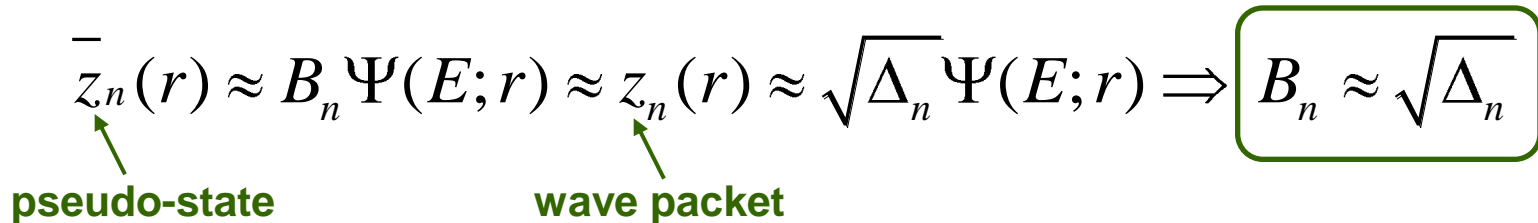
Thus, the amplitudes of wavefunctions agree within some restricted region R.

A new treatment of pseudo-states

So, the above direct comparison between pseudo-states and stationary wave packets allows to draw the following conclusions:

1. The Hamiltonian pseudo-states, obtained by diagonalization of its matrix built on some L_2-basis, should be considered as approximations to stationary wave packets rather that for exact scattering functions.

2. The normalization coefficients B_n when passing from pseudo-states to exact continuous-spectrum functions depend on the distribution of discrete energies of pseudo-states and are equal to the square roots of the widths of discretization intervals which these pseudo-states are associated with.

$$\bar{z}_n(r) \approx B_n \Psi(E;r) \approx z_n(r) \approx \sqrt{\Delta_n}\,\Psi(E;r) \Rightarrow \boxed{B_n \approx \sqrt{\Delta_n}}$$

pseudo-state   **wave packet**

3. The wave-packet formalism may be used for solution of scattering problems on an arbitrary L_2-basis. So, in practical calculations, the wave-packet states can be replaced by the respective pseudo-states of the free Hamiltonian on the chosen basis.

Reconstruction of discretization widths from eigen energies

As a result of Hamiltonian diagonalization a discrete set of eigen energies is obtained. For using pseudo-states in the calculations the end points of discretization intervals and bin widths should be found from this energy distribution.
A few possible ways of doing this exist.

1. Recursive procedure

$$E_0 = 0,\ E_1 = 2E_1^*;\ \boxed{E_i = 2E_i^* - E_{i-1}, i = 1,..,N,}\ \Delta_i = E_i - E_{i-1}$$

After performing this procedure the eigenvalues turn out to be located precisely in the average points of the bins. However, the entire energy distribution is used for determination of local widths. If this distribution is defined by inhomogeneous function, then the local concentration in one part of the spectrum will influence all bins. This may lead to some distortions, for example, to non-physical negative widths.

2. "Local" formula

$$\boxed{\varepsilon_k = f(k),\ \Delta_n = \left.\frac{df(k)}{dk}\right|_{k=n}}$$

Simplified version:

$$\Delta_n = \frac{1}{2}\left(\varepsilon_{n+1} - \varepsilon_{n-1}\right),\ n = 2,..,N-1,$$

$$\Delta_1 = \varepsilon_2 - \frac{\Delta_2}{2},\ \Delta_N = \varepsilon_N + \frac{\Delta_{N-1}}{2}.$$

To illustrate this procedure we show here the phase-shift calculations on the harmonic-oscillator basis.

We found the phase shifts for the Austern potential (model complex interaction of the deuteron with heavy nuclei):

$$V(r) = (V_0 + iU_0)\exp(-\gamma r^2)$$

$V_0 = -100$ MeV
$U_0 = -10$ MeV, $\gamma = 0.0625$ fm^{-2}

discretized spectrum of the kinetic-energy operator

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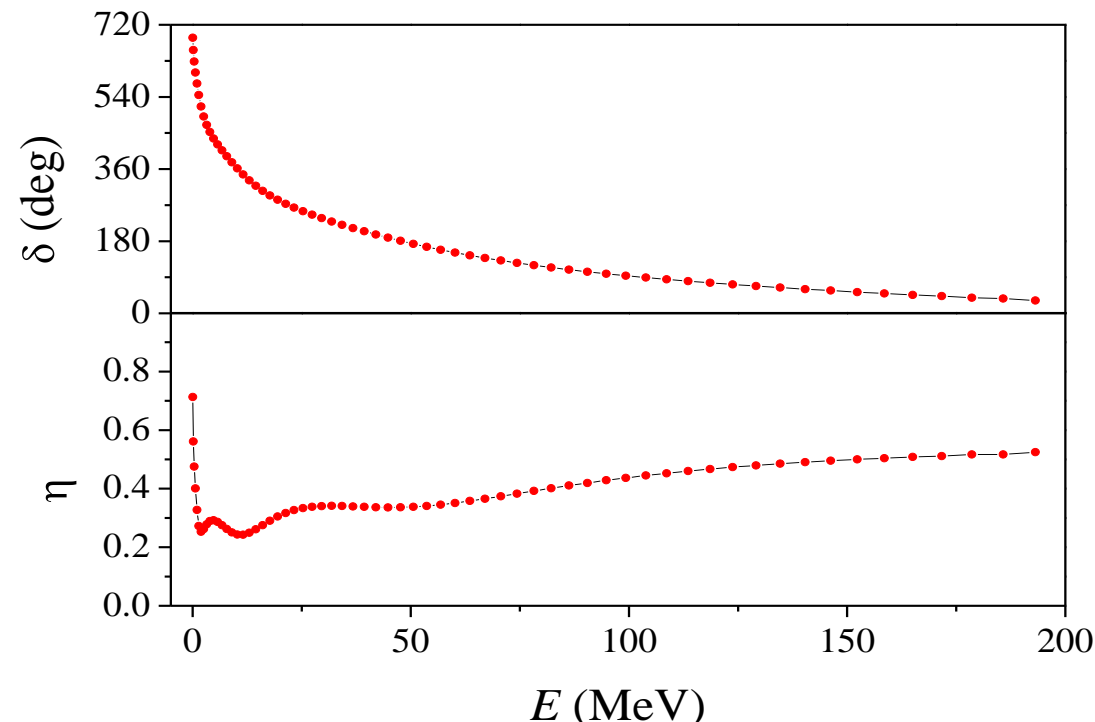
discretized spectrum of the kinetic-energy operator
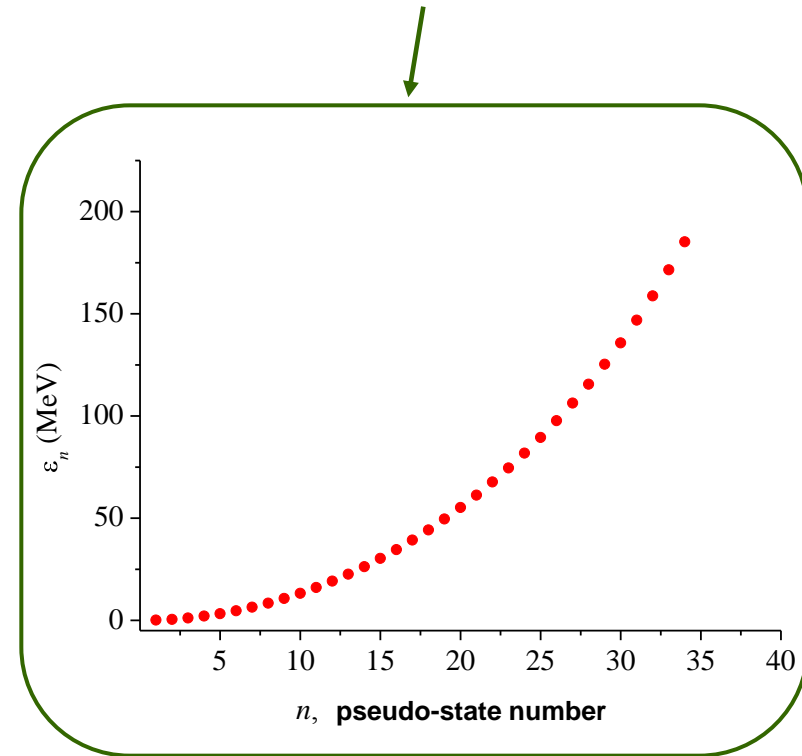
To summarize:

We presented in this *first part* of the *Lecture 1* some basic notions and formalism for wave-packet discretization of continuum and finding the S-matrix for various types of interactions.

Part II:

Description of Composite-Particles Scattering by a Stable Target

Contents

1. Formulation of the problem for scattering of a composite particle by a structureless target.

2. Johnson and Soper method.

3. Multichannel scattering problems.

4. Continuum-discretized coupled-channels (CDCC) method.

5. Application of the wave-packet discretization method to the problem.

6. Detailed comparison of the CDCC-and wave-packet solutions.

7. Impact of closed channels to the elastic-scattering cross section.

8. Construction of effective potentials for composite particle interaction.

Let's consider the scattering of a composite particle {bc} by a structureless target A.

This is a three-body problem. In order to find the observables, one should solve a Schrödinger equation for the wavefunction of the entire system taking into account the boundary conditions in different asymptotic channels…

b   A

R_1

r_1

c

b   A

r_2

R_2

c

b   A

R_3

r_3

c
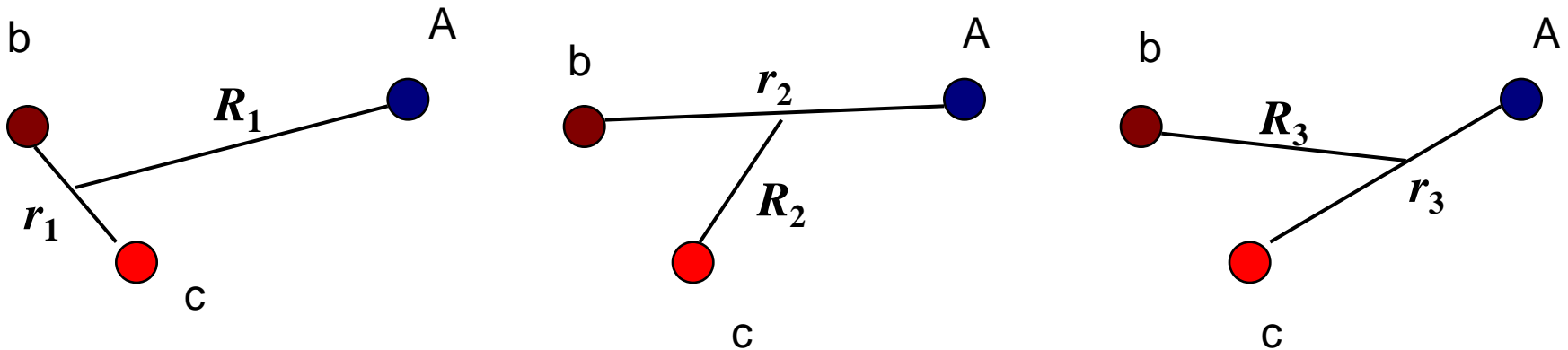
…or solve a system of Faddeev equations.

We shall consider a simplified scheme, in which boundary conditions in one asymptotic channel only are taken into account. Herewith we neglect the rearrangement processes, when a fragment of the system {bc} is picked up by the target A. This approximation is justified if there are no bound states in subsystems {bA} and {cA}.
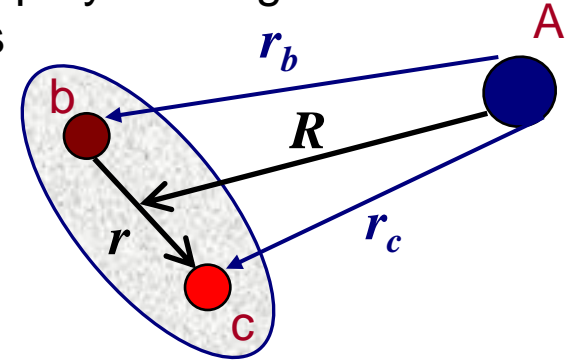
The total Hamiltonian has the form:

$$H = h_0(\mathbf{R}) + h_0^{bc}(\mathbf{r}) + v_{bc}(r) + v_{bA}(r_b) + v_{cA}(r_c) = H_{bc} + V^{ext}$$

The channel Hamiltonian defines asymptotic states of the system:

$$H_{bc} = h_0(\mathbf{R}) \oplus (h_0^{bc}(\mathbf{r}) + v_{bc}(r))$$
$$= h_0(\mathbf{R}) \oplus h_{bc}(\mathbf{r}).$$

Coordinates:

$$\mathbf{r} = \mathbf{r}_b - \mathbf{r}_c,$$ **coordinate of relative motion of particles b and c**

$$\mathbf{R} = \frac{1}{2}\ \mathbf{r}_b + \mathbf{r}_c$$ **center-of-mass coordinate of subsystem {bc}**

(for equal masses of particles b and c)

The external interaction:

$$V^{ext}(\mathbf{r}, \mathbf{R}) = v_{bA}\left(\left|\mathbf{R} + \frac{1}{2}\mathbf{r}\right|\right) + v_{cA}\left(\left|\mathbf{R} - \frac{1}{2}\mathbf{r}\right|\right)$$

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The way of solution

The total three-body wavefunction can be represented in the form of expansion on the complete set of two-body Hamiltonian h_{bc} states:

(it is assumed for simplicity that there is only one bound state in the subsystem $\{bc\}$)

$$\Psi(\mathbf{r}, \mathbf{R}) = \phi_0(\mathbf{r})\chi_0(\mathbf{R}) + \sum_\alpha \int_0^\infty \phi_\alpha(\varepsilon, \mathbf{r})\chi_{\varepsilon\alpha}(\mathbf{R})d\varepsilon \quad (1)$$

bound-state wavefunction

continuous-spectrum wavefunctions

α — possible quantum numbers

After substituting this expansion into three-body Schrödinger equation

$$H|\Psi\rangle = E|\Psi\rangle,$$

one obtains an infinite system of coupled equations. Solution of this system is practically impossible, therefore, different approximations are generally used rather than total expansion (1).
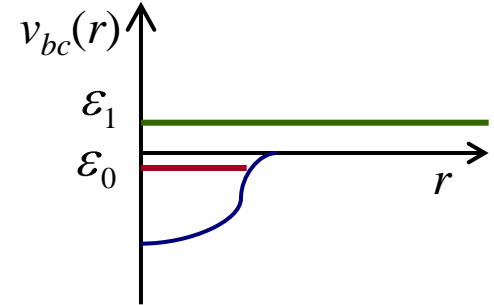
For example, in the Johnson and Soper method the entire continuous spectrum of the Hamiltonian h_{bc} is replaced by one pseudo-state ϕ_1 with the energy ε_1.

Johnson and Soper method (*R.C. Johnson & P.J.R. Soper, 1970*)

The approximation to the total wavefunction of a system is

$$\Psi(\mathbf{r}, \mathbf{R}) = \phi_0(\mathbf{r})\chi_0(\mathbf{R}) + \phi_1(\mathbf{r})\chi_1(\mathbf{R})$$

$$\langle\phi_0|h_{bc}|\phi_0\rangle = \varepsilon_0, \quad \langle\phi_1|h_{bc}|\phi_1\rangle = \varepsilon_1$$

After substituting this expression into Schrödinger equation and projecting onto the states ϕ_0 and ϕ_1, the system of two coupled equations is obtained:

$$\langle\phi_0|H - E|\Psi\rangle = 0$$
$$\langle\phi_1|H - E|\Psi\rangle = 0$$

$$\Rightarrow$$

$$\langle\phi_0|H|\phi_0\rangle\chi_0(\mathbf{R}) - E\chi_0(\mathbf{R}) = -\langle\phi_0|H|\phi_1\rangle\chi_1(\mathbf{R})$$
$$\langle\phi_1|H|\phi_1\rangle\chi_1(\mathbf{R}) - E\chi_1(\mathbf{R}) = -\langle\phi_1|H|\phi_0\rangle\chi_0(\mathbf{R})$$

Or, in more detail,

$$\langle\phi_i|H|\phi_i\rangle = \langle\phi_i|h_0(\mathbf{R}) + h_{bc} + V^{\text{ext}}|\phi_i\rangle = h_0(\mathbf{R}) + \varepsilon_i + V_{ii}^{\text{ext}}(\mathbf{R}), \ i = 0,1$$

$$\langle\phi_0|H|\phi_1\rangle = \langle\phi_0|h_0(\mathbf{R}) + h_{bc} + V^{\text{ext}}|\phi_1\rangle = V_{01}^{\text{ext}}(\mathbf{R}), \quad \langle\phi_1|H|\phi_0\rangle = V_{10}^{\text{ext}}(\mathbf{R})$$

The following notation for channel-coupling potentials has been introduced here:

$$V_{ij}^{\text{ext}}(\mathbf{R}) = \int\phi_i(\mathbf{r})V^{\text{ext}}(\mathbf{r}, \mathbf{R})\phi_j(\mathbf{r})d\mathbf{r}$$

So, the wavefunctions for elastic scattering and for excited two-body pair in a continuum state can be found from the coupled equations:

$$\left[h_0(\mathbf{R}) + V_{ii}^{\text{ext}}(\mathbf{R}) - (E - \varepsilon_i) \right] \chi_i(\mathbf{R}) = -V_{ij}^{\text{ext}}(\mathbf{R}) \chi_j(\mathbf{R}), \ j \neq i, \ i = 0,1 \qquad (1)$$

Asymptotic boundary conditions:

$$\chi_i(R) \underset{R \to \infty}{\longrightarrow} u^{(-)}(K_i, R)\delta_{i,0} - \sqrt{\frac{K_i}{K_0}} S_{i,0} u^{(+)}(K_i, R), \quad K_i = \sqrt{\frac{2m(E - \varepsilon_i)}{\hbar^2}}, \ i = 0,1 \qquad (2)$$

$S_{i,0}$ – the S-matrix elements, defining the probability of elastic scattering ($i=0$) and excitation into continuum ($i=1$).

The Johnson-Soper model represents a simple example of the reduction of three-body scattering problem to multichannel (two-channel one in the present case) scattering problem.

The peculiarity of such problems consists in the fact, that the continuous spectrum of the Hamiltonian is degenerate at the energies above the second channel threshold (ε_1 in the model). Therefore, the system (1) at these energies has, besides the solution satisfying the boundary conditions (2), an additional linearly independent solution corresponding to an incident wave in the second channel 1.
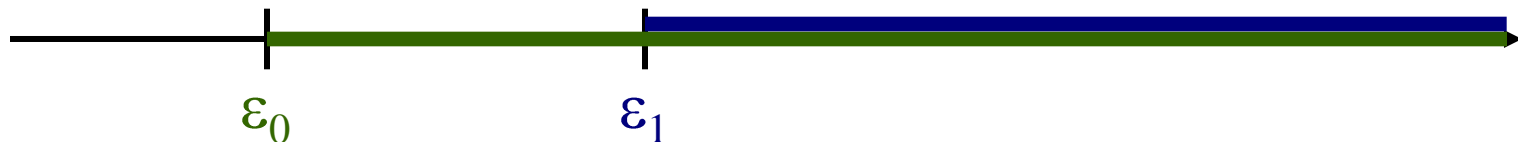
The two-body coupled-channel Hamiltonian for two-channel system can be represented in the matrix form

$$\mathbf{H} = \begin{pmatrix} h_0^0 + \varepsilon_0 & 0 \\ 0 & h_0^1 + \varepsilon_1 \end{pmatrix} + \begin{pmatrix} V_{00} & V_{01} \\ V_{10} & V_{11} \end{pmatrix}$$

free Hamiltonian

coupling potentials

Spectrum of two-channel free Hamiltonian

ε_0 ε_1

The continuous spectrum starts from the first threshold ε_0.

In the region $\varepsilon_0 < E < \varepsilon_1$, for each energy, there exists the unique solution of Schrödinger equation for the wavefunction, corresponding to an incident wave in the first channel. Herewith, the second channel is closed.

In the region $E > \varepsilon_1$ the spectrum is doubly degenerate. For each energy there exist two linearly independent solutions, each of them being related to an incident wave in the respective channel.

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Multichannel scattering problems can also be solved via multichannel Lippmann-Schwinger equation for the wavefunction.

In our two-channel case this equation takes the form

$$\begin{pmatrix} \chi_0 \\ \chi_1 \end{pmatrix} = \begin{pmatrix} \psi_0^1 \\ 0 \end{pmatrix} + \begin{pmatrix} V_{00} & V_{01} \\ V_{10} & V_{11} \end{pmatrix} \underbrace{\begin{pmatrix} [(E-\varepsilon_0)+i0-h_0^0]^{-1} & 0 \\ 0 & [(E-\varepsilon_1)+i0-h_0^1]^{-1} \end{pmatrix}}_{\text{two-channel free resolvent}} \begin{pmatrix} \chi_0 \\ \chi_1 \end{pmatrix}$$

two-channel free resolvent

The elastic-scattering amplitude is obtained from the expression

$$A_{\text{el}} \sim \begin{pmatrix} \psi_0^1 & 0 \end{pmatrix} \begin{pmatrix} V_{00} & V_{01} \\ V_{10} & V_{11} \end{pmatrix} \begin{pmatrix} \chi_0 \\ \chi_1 \end{pmatrix} = \left\langle \psi_0^1 \middle| V_{00} \middle| \chi_0 \right\rangle + \left\langle \psi_0^1 \middle| V_{01} \middle| \chi_1 \right\rangle$$

Singularities of two-channel resolvent

ε_0 ε_1

cuts
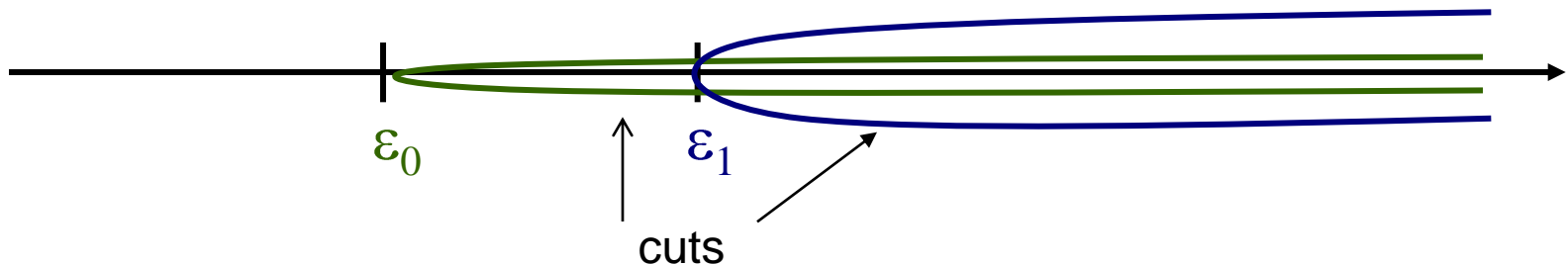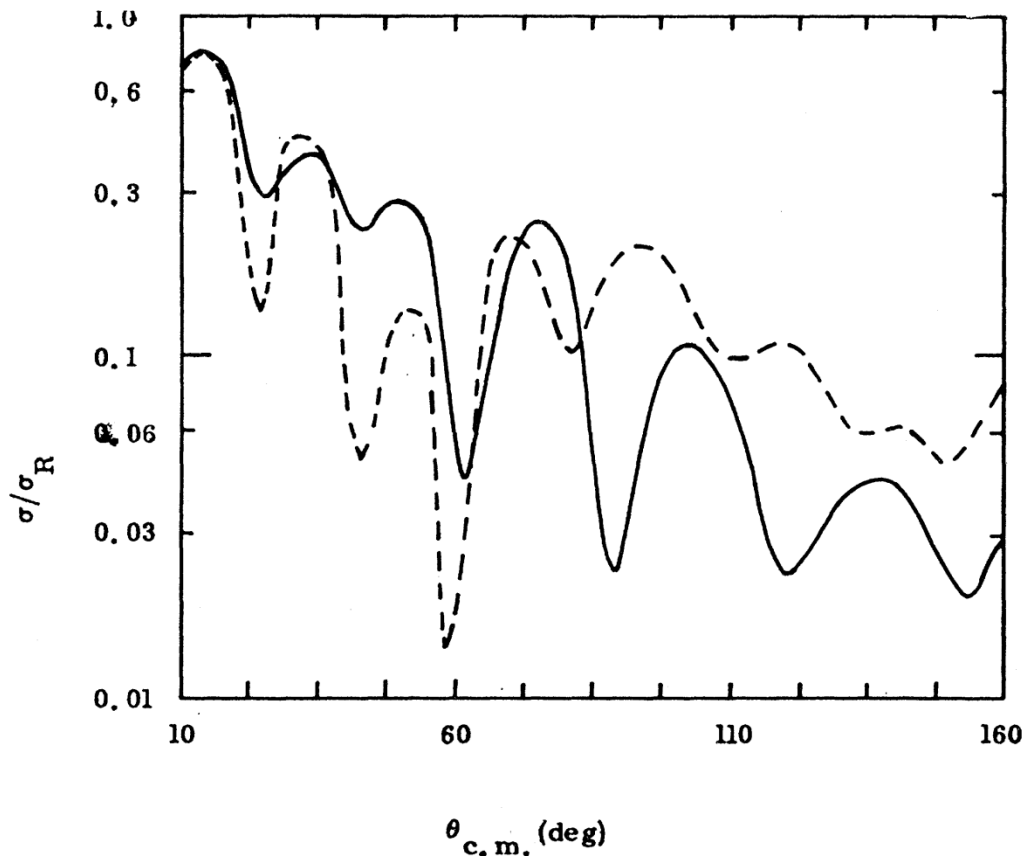
Differential cross section for elastic scattering of deuterons by ^{58}Ni nuclei at the energy 21.6 MeV, calculated with taking the intermediate continuum excitation into account (solid curve), and also on the basis of the folding model, i.e. without taking this effect into account (dashed curve).
(*Johnson & Soper, PRC, 1970*)

The method of Johnson and Soper provides a good qualitative description for the influence of intermediate breakup on the elastic-scattering process. For a good quantitative description of this effect the continuum-discretized coupled-channels method was developed.

Continuum-discretized coupled-channels (CDCC) method

The CDCC method is based on discretization of the continuous spectrum of the Hamiltonian h_{bc}. Herewith, the expansion for the total three-body wavefunction of the system takes the form of a finite sum

$$\Psi(\mathbf{r}, \mathbf{R}) = \phi_0(\mathbf{r})\chi_0(\mathbf{R}) + \sum_\alpha \sum_i \phi_{\alpha i}(\mathbf{r})\chi_{\alpha i}(\mathbf{R}). \quad (2)$$

Here $\phi_{\alpha i}(\mathbf{r})$ denote the states of the discretized spectrum with energies ε_i.

The CDCC system of equations takes the same form as the Johnson-Soper system:

$$\left[h_0(\mathbf{R}) + V_{ii}^{\text{ext}}(\mathbf{R}) - (E - \varepsilon_i) \right] \chi_i(\mathbf{R}) = -\sum_{j \neq i} V_{ij}^{\text{ext}}(\mathbf{R}) \chi_j(\mathbf{R}), \quad i = 0,..,N$$

$$\chi_i(R) \underset{R \to \infty}{\longrightarrow} u^{(-)}(K_i, R)\delta_{i,0} - \sqrt{\frac{K_i}{K_0}} S_{i,0} u^{(+)}(K_i, R), \quad K_i = \sqrt{\frac{2m(E - \varepsilon_i)}{\hbar^2}}, \quad i = 0,..,N$$

In the expansion (2) the open channels with energies $\varepsilon_i < E$ are only taken into account. For inclusion of the closed channels into consideration the form of boundary conditions should be modified.
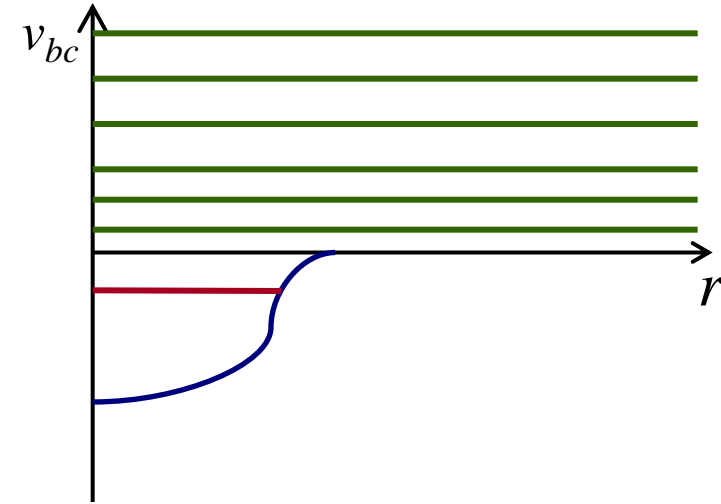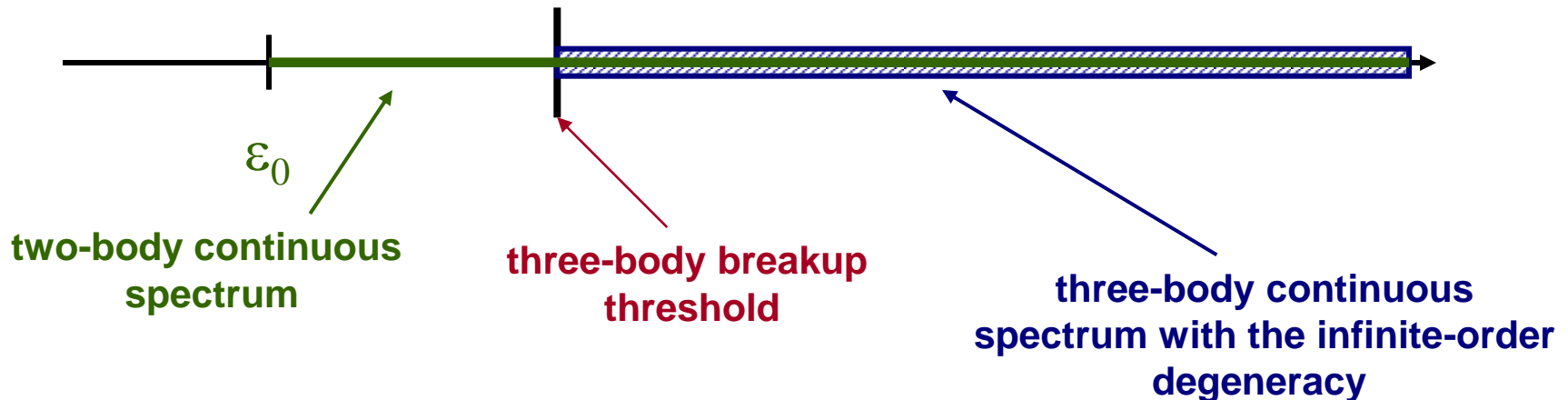
Spectrum of the multichannel Hamiltonian being used in CDCC approach

$$\varepsilon_0 \quad\quad \varepsilon_1 \quad \varepsilon_2 \quad \varepsilon_3 \quad \varepsilon_4 \quad \varepsilon_5$$
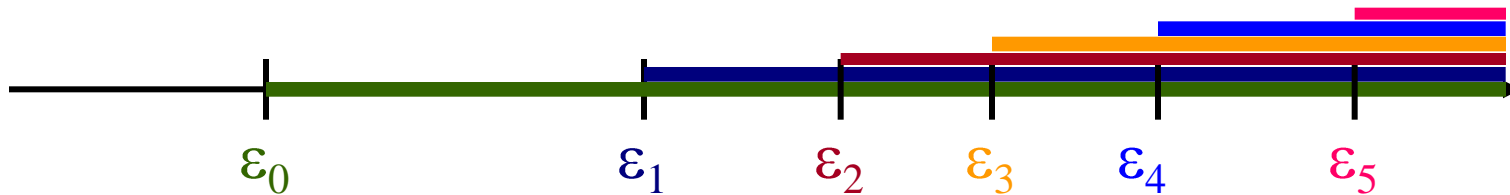
After crossing every new threshold, the degeneracy degree (of continuous spectrum) is increased by unity.

Initial spectrum of three-body channel Hamiltonian

$$\varepsilon_0$$

two-body continuous spectrum

three-body breakup threshold

three-body continuous spectrum with the infinite-order degeneracy

The approximation of initial infinite-order degenerate spectrum by the multichannel spectrum of a finite-order degeneracy works generally quite well and is, therefore, commonly used.

However, the energy dependency of the observables can have some superfluous unphysical singularities in the vicinity of threshold points of multichannel spectrum.

Example: The modulus of the elastic-channel S-matrix for the 11-channel problem has singularities near the threshold values of energy.

at the opening of the second channel
S-matrix becomes inelastic

singularities (cusps) near the threshold points

$|S_{0,0}|$

1,00
0,95
0,90
0,85
0,80
0,75
0,70
0,65

1   10   100

$E - \varepsilon_0$ (MeV)
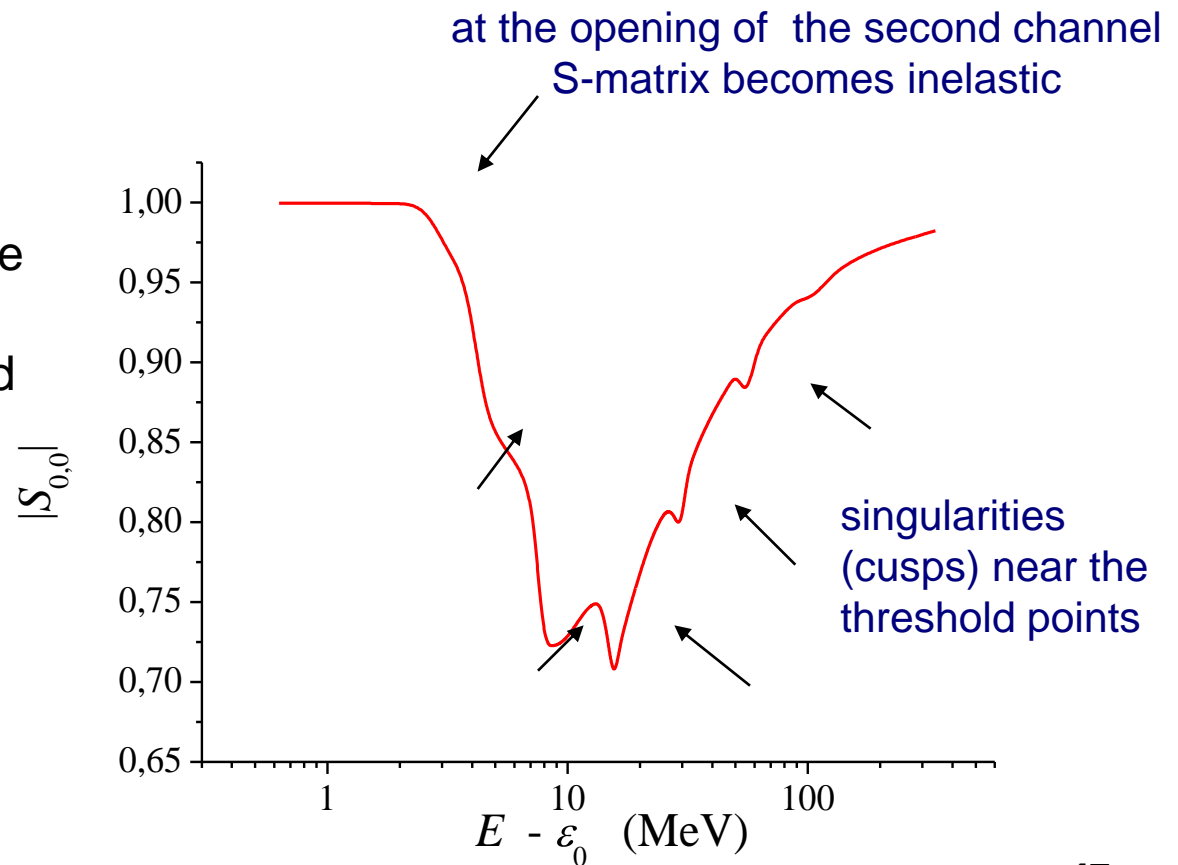
Total discretization of three-body continuum

The solution of initial three-body problem can be built by using total discretization of the channel-Hamiltonian (H_{bc}) spectrum on the basis of the Wave-Packet Continuum-Discretization method (WPCD) .

$$H_{bc} = h_0(\mathbf{R}) \oplus h_{bc}(\mathbf{r}).$$

Elements of the three-body wave-packet basis are constructed here as products of wave-packet states of two-body Hamiltonians h_0 and h_{bc}: $\quad \left| Z_{ik} \right\rangle = \left| z_i, x_k \right\rangle$

We shall use the states with fixed values of pair angular momenta l and L, and also total orbital angular momentum Λ and its projection M:

$$\left\langle \mathbf{r}, \mathbf{R} \middle| z_i^l, x_j^L, \Lambda \mathrm{M} \right\rangle \equiv z_i^l(r) x_j^L(R) \mathcal{Y}_{lL}^{\Lambda \mathrm{M}} \left(\hat{\mathbf{r}}, \widehat{\mathbf{R}} \right)$$

The state z_0 of two-body wave-packet basis corresponds to the bound state $\phi_0(r)$ in the subsystem {bc} (we assume for simplicity that it is an s-wave state).

The matrix of the channel Hamiltonian (and also of any operator, functionally depending on it) is diagonal on the constructed basis:

$$\left\langle z_i, x_j \middle| H_{bc} \middle| z_{i'}, x_{j'} \right\rangle = \left\langle z_i \middle| h_{bc} \middle| z_{i'} \right\rangle \left\langle x_j \middle| x_{j'} \right\rangle + \left\langle x_j \middle| h_0 \middle| x_{j'} \right\rangle \left\langle z_i \middle| z_{i'} \right\rangle = \left(\varepsilon_i + E_j^* \right) \delta_{i,i'} \delta_{j,j'}.$$

The resolvent of the channel Hamiltonian

$$G_{bc}^{(+)}(E) = [E + i0 - H_{bc}]^{-1}$$

This operator is represented by the convolution of two-body resolvents:

$$G_{bc}^{(+)}(E) = \frac{1}{2\pi i} \int\limits_{-\infty}^{+\infty} g_{bc}^{(+)}(E - \varepsilon) g_0^{(+)}(\varepsilon) d\varepsilon$$

Using spectral expansions for the operators, we obtain the following expression for G_{bc}:

$$G_{bc}^{(+)}(E) = G_{bc}^{BC}(E) + G_{bc}^{CC}(E),$$

where bound-continuum (BC) and continuum-continuum (CC) parts have the forms

$$G_{bc}^{BC}(E) = \int\limits_0^\infty \frac{\left| \phi_0^0, \psi_0^\Lambda(E_2), \Lambda M \right\rangle \left\langle \phi_0^0, \psi_0^\Lambda(E_2), \Lambda M \right|}{E + i0 - \varepsilon_0 - E_2} dE_2$$

$$G_{bc}^{CC}(E) = \sum_{L=|\Lambda-l|}^{|\Lambda+l|} \sum_l \int\limits_0^\infty \int\limits_0^\infty \frac{\left| \psi^l(E_1), \psi_0^L(E_2), \Lambda M \right\rangle \left\langle \psi^l(E_1), \psi_0^L(E_2), \Lambda M \right|}{E + i0 - E_1 - E_2} dE_1 dE_2$$

Finite-dimensional approximation of the channel resolvent

Projecting exact expressions for BC and CC parts of the channel resolvent onto the states from three-body wave-packet basis, we obtain the following finite-dimensional representations for these operators:

$$\mathbb{G}_{bc}^{BC} = \sum_{j=1}^{N_\Lambda} \left| z_0^0, x_j^\Lambda, \Lambda M \right\rangle G_{0j}^{0\Lambda} \left\langle z_0^0, x_j^\Lambda, \Lambda M \right|, \quad \boxed{G_{0j}^{0\Lambda} = \frac{1}{\Delta_j^\Lambda} \int_{E_{j-1}^\Lambda}^{E_j^\Lambda} \frac{dE_2}{E + i0 - \varepsilon_0 - E_2}}$$

the resolvent eigenvalues

$$\mathbb{G}_{bc}^{CC} = \sum_{L,l} \sum_{i=1}^{K_l} \sum_{j=1}^{N_L} \left| z_i^l, x_j^L, \Lambda M \right\rangle G_{ij}^{lL} \left\langle z_i^l, x_j^L, \Lambda M \right|, \quad \boxed{G_{ij}^{lL} = \frac{1}{\Delta_i^l \Delta_j^L} \int_{E_{i-1}^l}^{E_i^l} \int_{E_{j-1}^L}^{E_j^L} \frac{dE_1 dE_2}{E + i0 - E_1 - E_2}}$$

Total channel resolvent in the wave-packet representation:

$$\mathbb{G}_{bc} = \mathbb{G}_{bc}^{BC} + \mathbb{G}_{bc}^{CC}$$

The observables can be found from the finite-dimensional analog of three-body Lippmann-Schwinger equation for the transition operator:

$$\mathbb{T} = \mathbb{V} + \mathbb{V}\mathbb{G}_{bc}\mathbb{T}$$

Here the matrix analog of the external-interaction operator has been used:

$$\mathbb{V} = \sum_{l,L}\sum_{l',L'}\sum_{i,i'}\sum_{j,j'}\left|z_i^l, x_j^L, \Lambda M\right\rangle\underbrace{\left\langle z_i^l, x_j^L, \Lambda M\left|V_{bA} + V_{cA}\right|z_{i'}^{l'}, x_{j'}^{L'}, \Lambda M\right\rangle}\left\langle z_{i'}^{l'}, x_{j'}^{L'}, \Lambda M\right|$$

matrix element in three-body
wave-packet basis

The elastic-scattering amplitude is proportional to the diagonal matrix element of the wave-packet *T*-matrix:

$$A_{\mathrm{el}}(E) \approx \frac{\mathbb{T}_{0j,0j}}{\Delta_j^\Lambda}, \;\; E - \varepsilon_0 \in \left[E_{j-1}^\Lambda, E_j^\Lambda\right]$$

The non-diagonal matrix elements of the wave-packet *T*-matrix define the breakup amplitudes.

With the use of approximations for two-body wave-packet states of Hamiltonians $h_0(\mathbf{R})$ and $h_{bc}(\mathbf{r})$ through pseudo-states in appropriate L_2 bases, it is possible to obtain analytic expressions for matrix elements of the external-interaction operator.

Thus, exploring the expansions

$$\left| z_i^l \right\rangle = \sum_n C_{in} \left| \varphi_i^l \right\rangle, \quad \left| x_j^L \right\rangle = \sum_k B_{jk} \left| \chi_k^L \right\rangle,$$
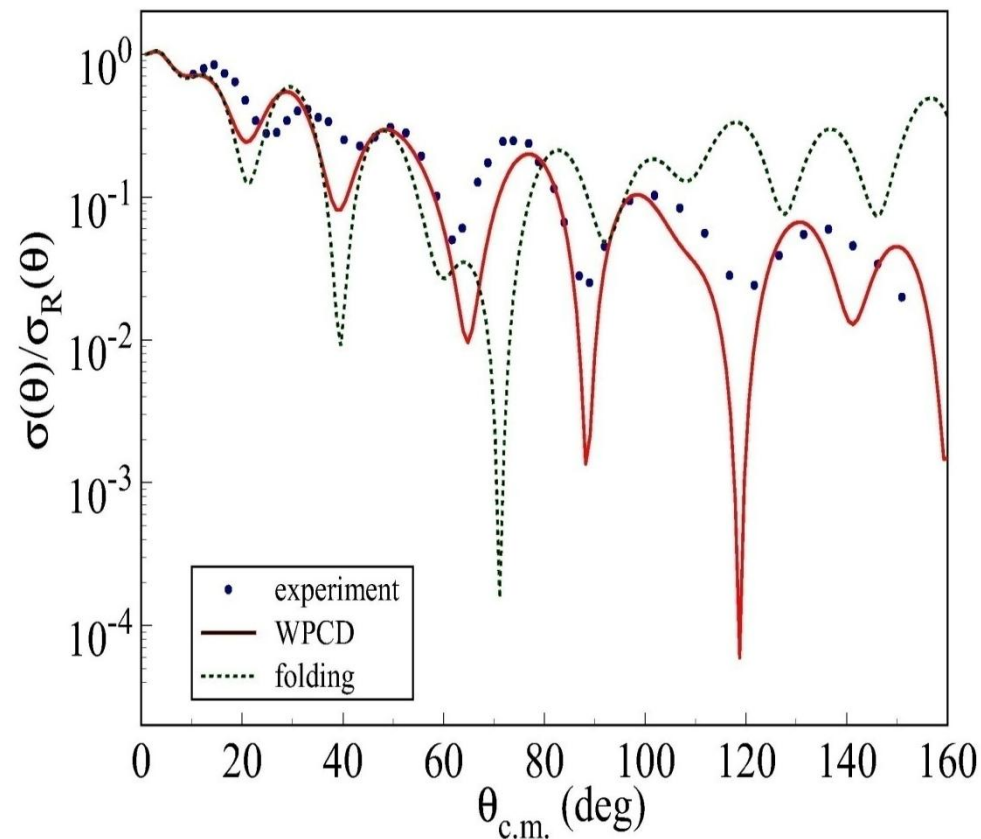
we obtain the following formula for matrix elements of interaction potential:

$$\left\langle z_i^l, x_j^L, \Lambda M \left| V_{bA} + V_{cA} \right| z_{i'}^{l'}, x_{j'}^{L'}, \Lambda M \right\rangle =$$

$$= \sum_{n,k} \sum_{n',k'} C_{in} C_{i'n'} B_{jk} B_{j'k'} \left\langle \varphi_n^l, \chi_k^L, \Lambda M \left| V_{bA} + V_{cA} \right| \varphi_{n'}^{l'}, \chi_{k'}^{L'}, \Lambda M \right\rangle$$
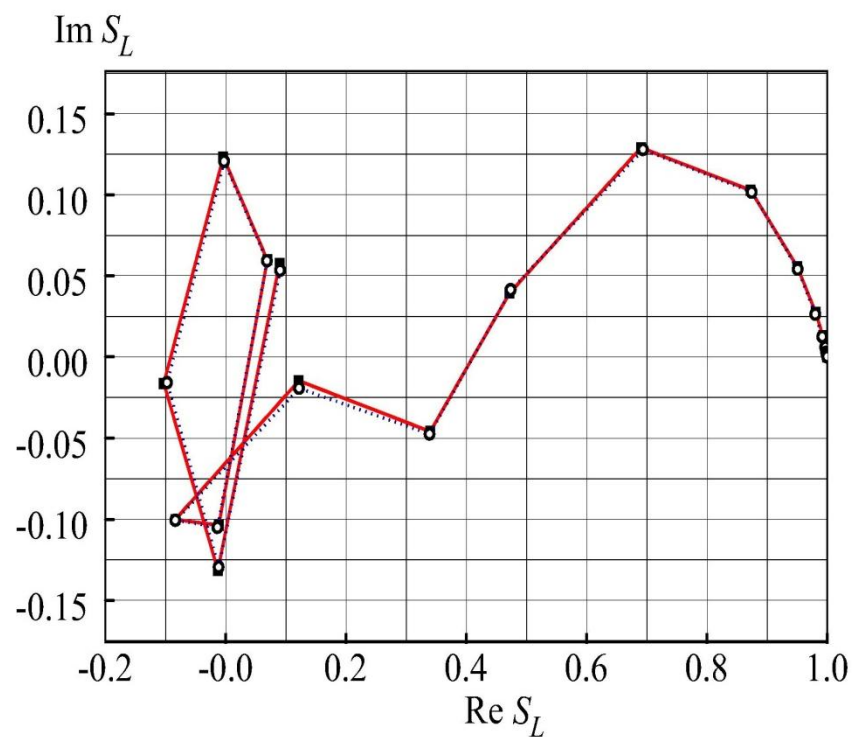
these matrix elements can be calculated
analytically for a wide class of interactions

Results for d+^{58}Ni elastic scattering at the incident energy E_{d} = 21.6 MeV

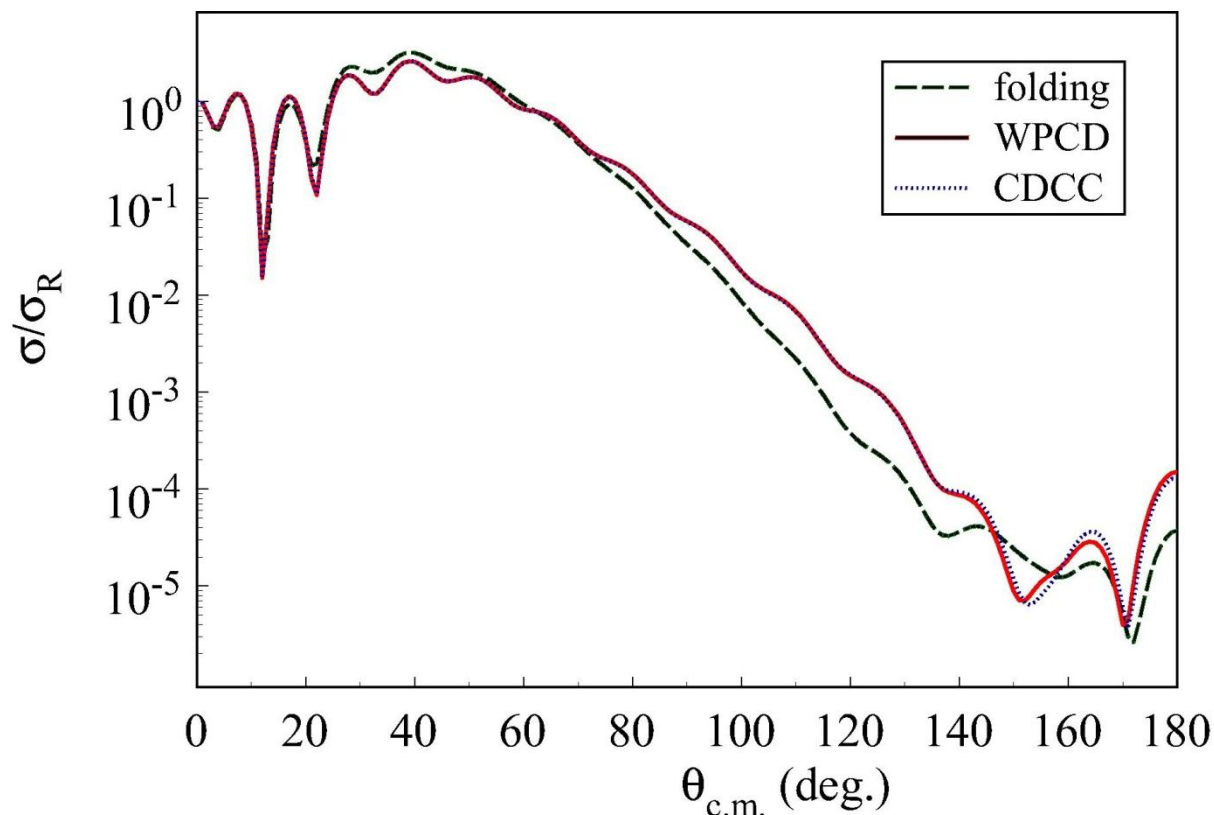## Differential cross section for elastic scattering

Argand-plot for partial S-matrix elements

Comparative analysis of results obtained within wave-packet continuum discretization and CDCC approaches

Differential cross section for elastic scattering of deuterons by $^{58}\mathrm{Ni}$ nuclei at the incident-deuteron energy $E_{\mathrm{d}} = 80$ MeV.

At rather high collision energies the results of two methods, based on total and partial discretizations of continuous spectrum, almost coincide.

However, the results obtained in calculations at lower collision energies were initially different for these two methods.

The origin of these discrepancies was in the fact that the contribution of closed channels in discretized spectrum of the subsystem {bc} was usually neglected in CDCC approach.

n-p discretized spectrum

$\varepsilon_K = E_{max}$
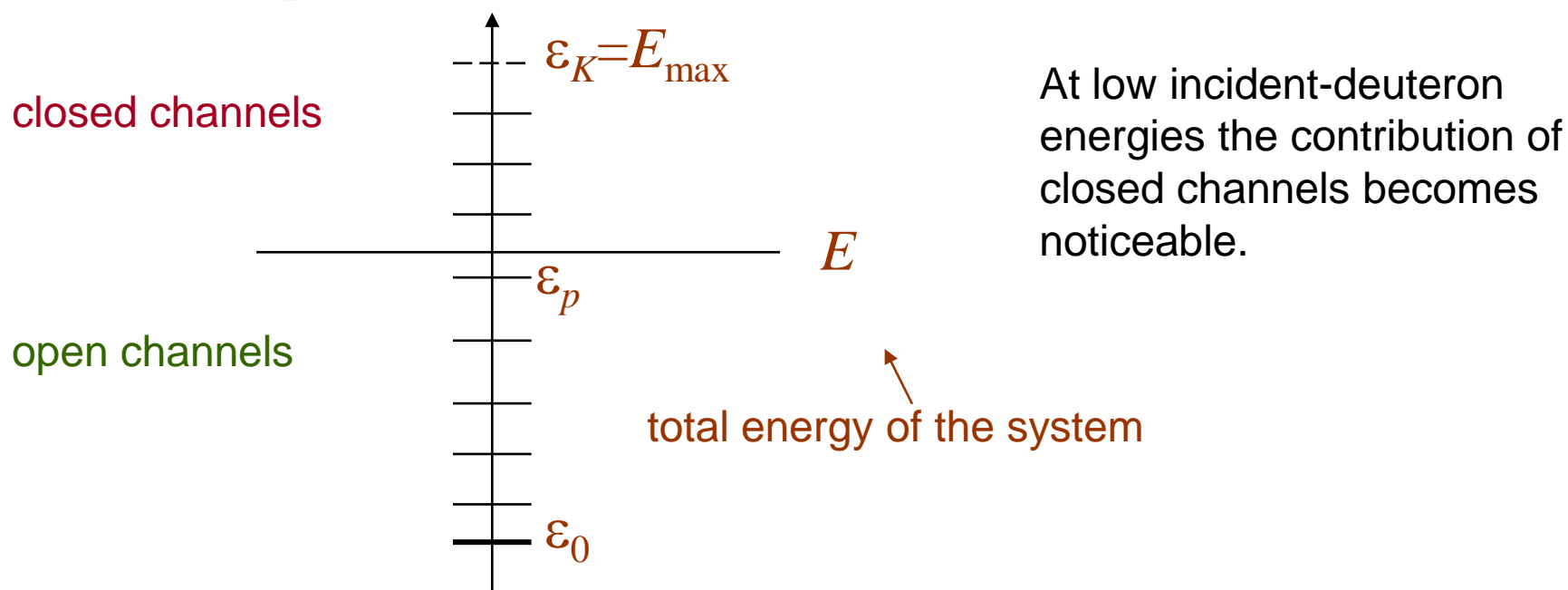
closed channels

At low incident-deuteron energies the contribution of closed channels becomes noticeable.

E

ε_p

open channels

total energy of the system

ε_0

In the wave-packet approach the closed "deuteron" channels are taken into account in exactly the same way as open channels.

In constrast, in the CDCC-method the modification of boundary conditions for the wavefunction components, corresponding to the closed channels, is required.

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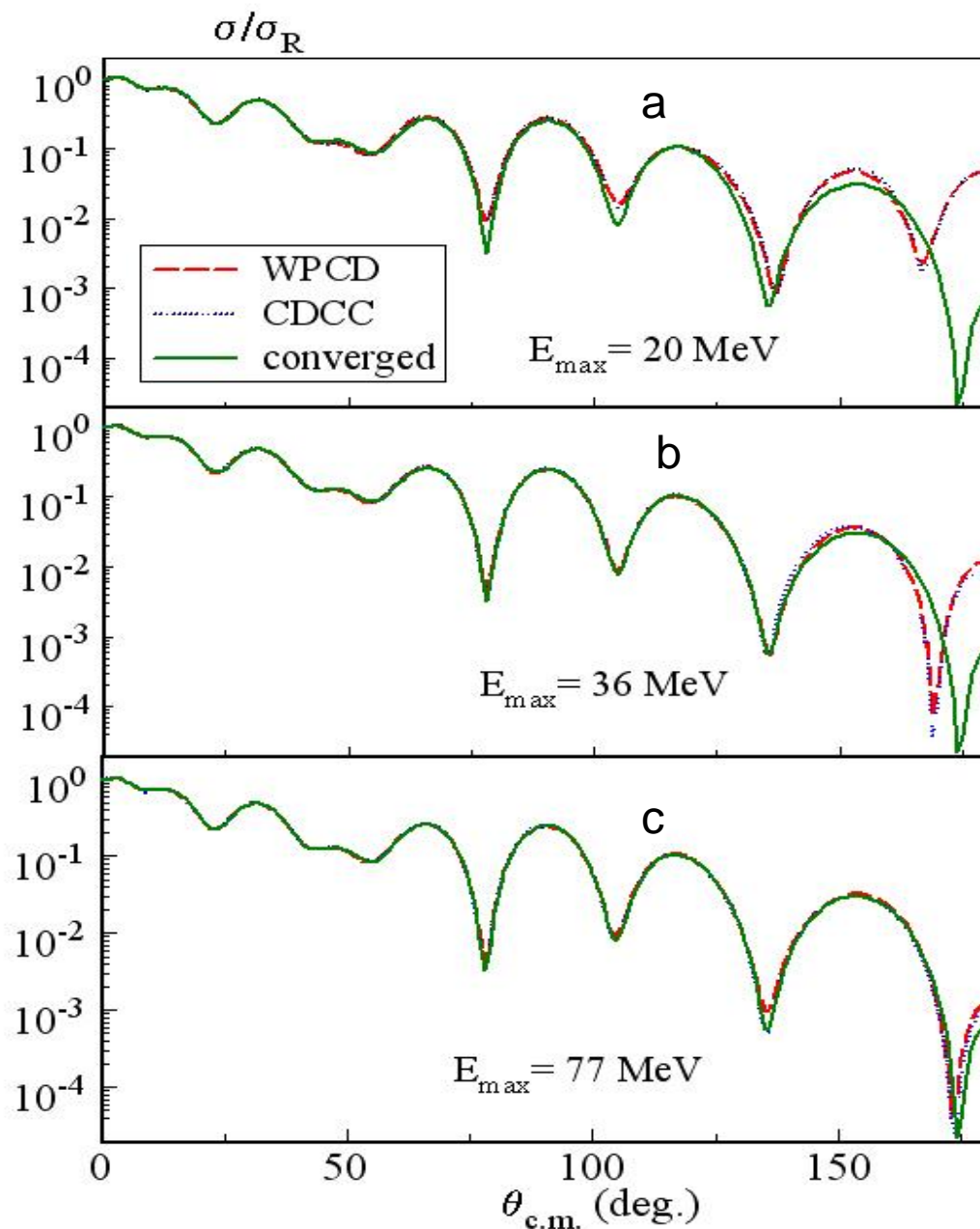
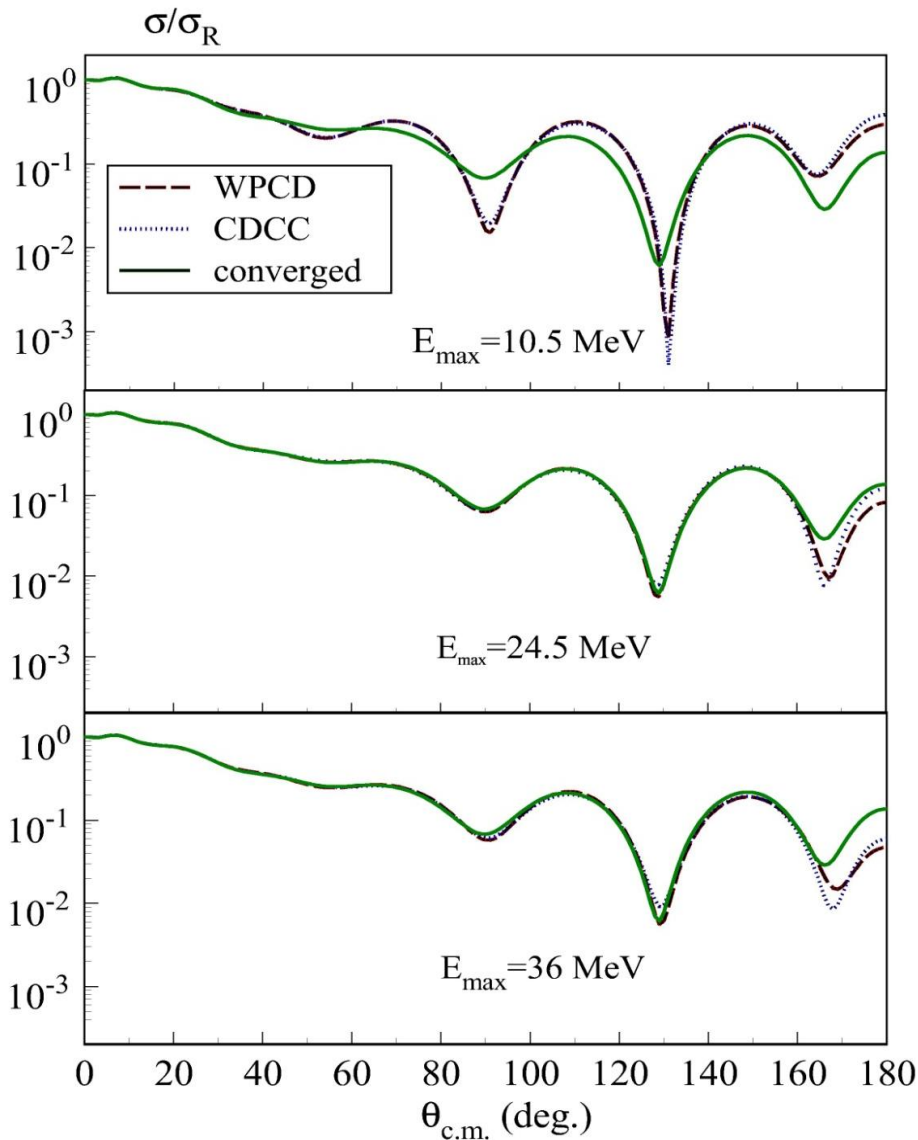Results of calculations at the incident energy $E_d = 21.6$ MeV.

Studying the convergence over maximal energy E_{max} of the channels taken into account.

a – without considering closed channels

b,c – with taking different numbers of closed channels into account

The fully converged cross section is obtained only at $E_{max} = 110$ MeV.

Results of two approaches coincide at the same E_{max}!

σ/σ_R

WPCD
CDCC
converged

$E_{max}=10.5$ MeV

$E_{max}=24.5$ MeV

$E_{max}=36$ MeV

$\theta_{c.m.}$ (deg.)

Results of calculations at the incident energy $E_d=12$ MeV.

The fully converged cross section is reached only at $E_{max}= 77$ MeV

As the incident energy decreases, the contribution of closed channels to elastic-scattering amplitude gets more and more important.

Comparative study has shown that the results of wave-packet and CDCC methods almost coincide, if the all channels of discretized spectrum of subsystem {bc} up to the same values of the energy $E_{\max}$ are taken into account.

Herewith, the internal details of discretization (the distribution of pseudo-state energies, the number of discretization intervals, etc.) are not important.

However, the wave-packet continuum discretization method is connected with the integral formulation of scattering problems and has, therefore, substantial advantages.

In particular, this approach allows to construct finite-dimensional approximations of the three-body integral operators.

Construction of effective interaction potentials
for composite particles

With usage of the Feshbach's projection technique, the expression for effective two-body potential, describing the interaction of the subsystem {bc} with the target A and taking an intermediate breakup of this subsystem into account, can be obtained.

This so-called Feshbach's potential has non-local and energy-dependent form.

Let's introduce two projectors – the projector onto the bound state of the subsystem {bc} and its orthogonal complement:

$$F = \left| z_0 \right\rangle \left\langle z_0 \right|, \quad Q = 1 - F, \quad QF = 0.$$

The total three-body wavefunction of the system can be represented as the sum of its F- and Q-projections:

$$\left| \Psi(E) \right\rangle = F \left| \Psi(E) \right\rangle + Q \left| \Psi(E) \right\rangle$$

wavefunction component defining
the elastic-scattering part

wavefunction component defining
the subsystem-breakup part

Let's substitute the above two-component representation for the wavefunction into three-body Schrödinger equation and then apply F- and Q-projectors from the left:

$$H(F+Q)|\Psi\rangle = E|\Psi\rangle \qquad \Leftrightarrow \qquad \begin{array}{l} (FHF - E)|\Psi\rangle = -FHQ|\Psi\rangle \quad (1) \\ (QHQ - E)|\Psi\rangle = -QHF|\Psi\rangle \quad (2) \end{array}$$

The resolvent of the Hamiltonian QHQ is defined as $\;G_Q^{(+)}(E) = [E + i0 - QHQ]^{-1}$

The wavefunction component corresponding to the breakup is then expressed through the elastic-scattering component in the following way:

$$Q|\Psi\rangle = G_Q^{(+)}(E)QHF|\Psi\rangle$$

Substituting this expression into the equation (1), we obtain the equation for the wavefunction of elastic scattering:

$$(FHF - E)F|\Psi\rangle = -\left[FHQG_Q^{(+)}(E)QHF \right]F|\Psi\rangle$$

$$\underbrace{\qquad\qquad\qquad\qquad}_{U(E)}$$

effective non-local energy-dependent potential

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Simplifying further the left- and right-hand sides of the equation for elastic-scattering component, we obtain:

$$[h_0(\mathbf{R}) + V_0(R) - (E - \varepsilon_0)]F\left|\Psi\right\rangle = -U(E)F\left|\Psi\right\rangle,$$

where $V_0(R)$ is the so-called folding potential

$$V_0(R) = \int z_0(\mathbf{r})V^{\text{ext}}(\mathbf{r},\mathbf{R})z_0(\mathbf{r})d\mathbf{r},$$

and the effective interaction potential has the form

$$U(E) = FV^{\text{ext}}QG_Q^{(+)}(E)QV^{\text{ext}}F.$$

Finding this operator on the basis of conventional approaches is in general even more difficult problem that solution of the initial three-body problem.

However, within the wave-packet technique, this task can be easily done.

Let's introduce two-body wave-packet bases for the Hamiltonians h_0 and h_{bc}

$$\left\{\ \left|x_j^L\right\rangle_{j=1}^{N_L}\ {}_{L=0}^{L_{max}}\right\}\qquad\text{and}\qquad\left\{\left|z_0\right\rangle,\ \left|z_i^l\right\rangle_{i=1}^{K_l}\ {}_{l=0}^{l_{max}}\right\},$$

and construct from them the three-body wave-packet basis for the three-body channel Hamiltonian H_{bc}.

It is then apparent that projectors F and Q can be defined as parts of the total wave-packet projector:

$$\mathbb{F}=\sum_{j=1}^{N_\Lambda}\left|z_0,x_j^\Lambda,\Lambda M\right\rangle\left\langle z_0,x_j^\Lambda,\Lambda M\right|,\quad\mathbb{Q}=\sum_{L,l}\sum_{i=1}^{K_l}\sum_{j=1}^{N_L}\left|z_i^l,x_j^L,\Lambda M\right\rangle\left\langle z_i^l,x_j^L,\Lambda M\right|,\ \mathbb{P}=\mathbb{F}+\mathbb{Q}$$

The total resolvent G_Q can be found from the channel resolvent by solving Lippmann-Schwinger equation in the wave-packet Q-subspace:

$$\mathbb{G}_Q^{(+)}=\mathbb{G}_{bc}^{CC}+\mathbb{G}_{bc}^{CC}\mathbb{V}_Q^{ext}\mathbb{G}_Q^{(+)}$$

The channel resolvent in the Q-subspace is the usual CC part of the channel resolvent. The matrix of this operator is diagonal in the wave-packet basis.

After having obtained the operator G_Q in the wave-packet basis, the expression for the Feshbach operator takes the form

matrix elements of the operator $\mathbb{G}_Q^{(+)}$

$$U(E) = \left\langle z_0 \left| V^{\text{ext}} \mathbb{G}_Q^{(+)} V^{\text{ext}} \right| z_0 \right\rangle$$

$$= \sum_{L,l} \sum_{L',l'} \sum_{i,j} \sum_{i',j'} \left\langle z_0 \left| V^{\text{ext}} \right| z_i^l, x_j^L, \Lambda M \right\rangle G_{ij,i'j'}^{lL,l'L'} \left\langle z_{i'}^{l'}, x_{j'}^{L'}, \Lambda M \left| V^{\text{ext}} \right| z_0 \right\rangle$$

form factors

The form factors can be explicitly calculated from the formula

$$B_{ij}^{lL}(\mathbf{R}) = \left\langle z_0 \left| V^{\text{ext}} \right| z_i^l, x_j^L, \Lambda M \right\rangle =$$

$$= \int z_0(r) Y_0^0\left(\hat{\mathbf{r}}\right) V^{\text{ext}}(\mathbf{r},\mathbf{R}) z_i^l(r) \mathcal{Y}_{lL}^{\Lambda M}\left(\hat{\mathbf{r}}, \widehat{\mathbf{R}}\right) d\mathbf{r} \; x_j^L(R) \equiv B_{ij}^{lL}(R) Y_\Lambda^M\left(\widehat{\mathbf{R}}\right)$$

the angular part takes this form owing to conservation of the total angular momentum Λ

Thus, the operator for effective interaction of a composite particle with a target in the wave-packet representation has the form

$$U^{\Lambda M}(E,\mathbf{R},\mathbf{R'}) = \sum_{L,l}\sum_{L',l'}\sum_{i,j}\sum_{i',j'} G^{lL.l'L'}_{ij,i'j'}(E) B^{lL*}_{ij}(R) B^{l'L'}_{i'j'}(R') Y^{M*}_{\Lambda} \widehat{\mathbf{R}}\ Y^{M}_{\Lambda}\ \widehat{\mathbf{R}}'$$
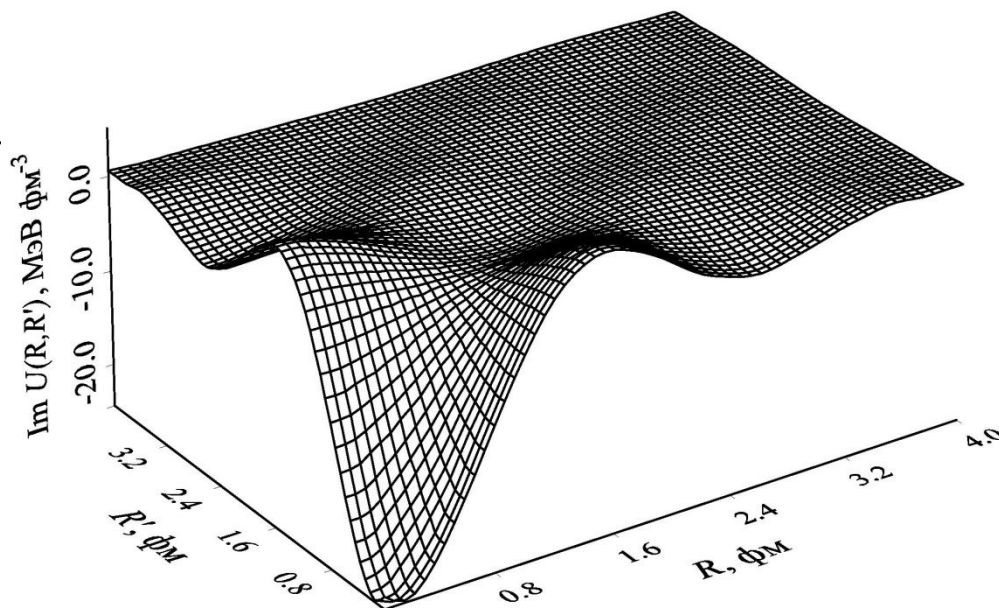
Real part
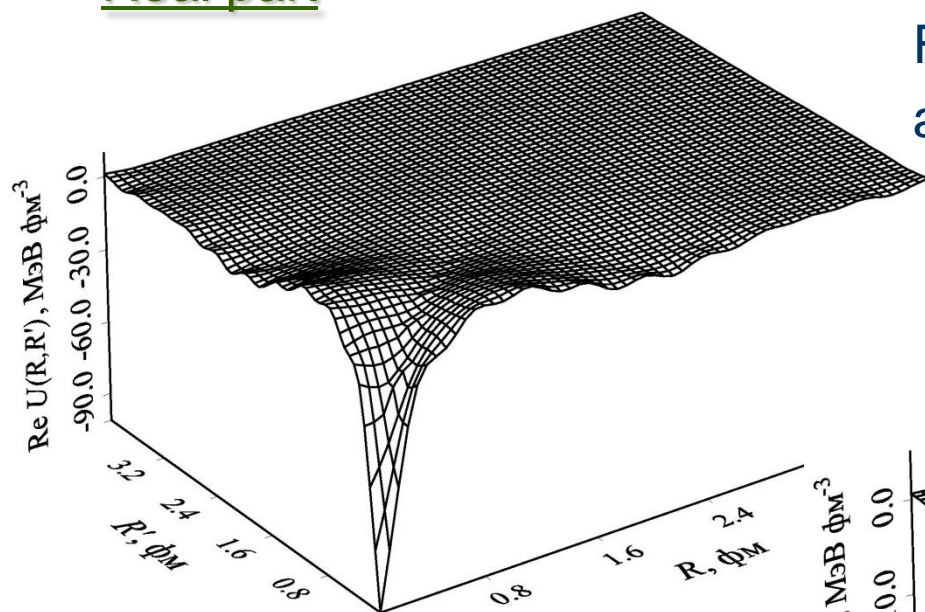
Feshbach potential for d+Ni scattering at the deuteron energy E_d = 80 MeV

Imaginary part

$\Lambda=0$

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The wave-packet form for the effective Feshbach potential can be used straightforwardly for treatment of composite-particles scattering by a target nucleus. Herewith, the discretization of the continuous spectrum of the free Hamiltonian $h_0(\mathbf{R})$ can be employed effectively.

It is important to emphasize, that parameters and size of such "external" wave-packet basis for the free Hamiltonian may be different from those for the "internal" wave-packet basis (for the same Hamiltonian), which has been taken for construction of the Feshbach potential.

The total potential of interaction of a composite particle with a target nucleus consists of the folding potential $V_0(R)$ and Feshbach potential $U(E,R,R')$. The non-local Feshbach potential generally has a shorter effective range and gives a smaller contribution to the elastic-scattering cross section, than the local folding potential.

Therefore, the "internal" basis of much smaller dimension (in 5-10 times), than the dimension of the "external" basis, may be utilized.

Thus, introducing Feshbach potential allows to essentially decrease the dimension of the three-body wave-packet basis, which is necessary for solving the total three-body problem of elastic scattering of a composite particle by a target nucleus.
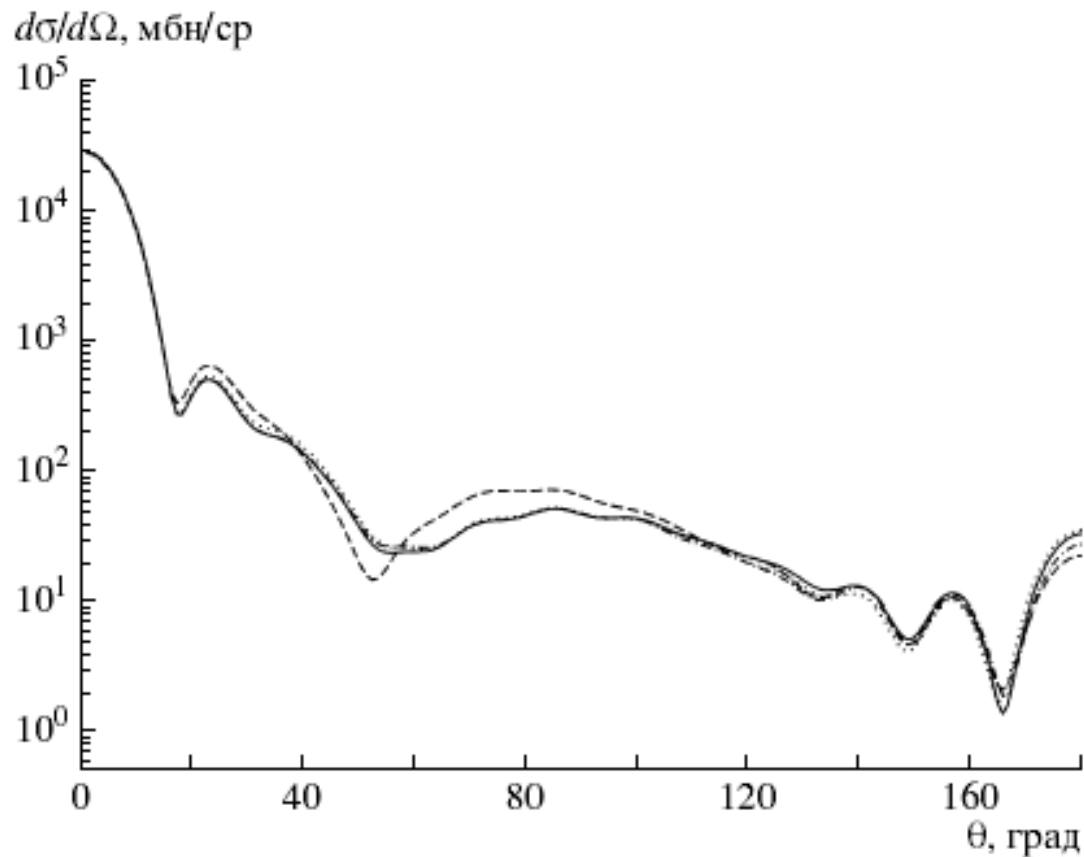
Differential cross sections for elastic scattering of deuterons by heavy nucleus, obtained on the basis of the wave-packet Feshbach potential at different dimensions of the internal basis: $N = 30$ (solid curve), $N = 50$ (dotted curve) and $N = 70$ (dash-dotted curve). The cross section corresponding to the folding potential is shown by the dashed curve. The external-basis dimension is $N_{ext} = 300$!

To summarize:

In the lecture we discussed some novel general formalism in quantum scattering theory based on total few-body continuum discretization with usage of the wave-packet basis of L_2-type.

The wave-packet continuum discretization technique has been demonstrated clearly to result in straightforward matrix equations with regular matrix elements instead of singular integral equations in a conventional approach.

This novel approach makes it possible to reformulate easily few-body scattering problems via effective non-local Feshbach potential between composite projectile and target, which fully takes into account the projectile (target) breakup.

In the next lecture we will discuss how to solve in such an approach the full Faddeev equations.