NOVEL TECHNIQUES FOR ULTRAFAST FEW-BODY SCATTERING CALCULATIONS

V. I. Kukulin,
Moscow State University, Russia

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Lecture 2

Quantum Scattering Theory in Discrete Representation — Effective Way Towards Ultra-Fast Scattering Calculations

There is a sharp contrast between rather simple and direct few-body BOUND-STATE CALCULATIONS and very tedious SCATTERING CALCULATIONS even for a three-body case.

The theoretical groups of Bochum and Hannover are nearly the unique in the world who are able to make fully realistic 3*N* scattering calculations above 3*N*-breakup threshold at energies E_N~30-300 MeV using completely realistic 2*N* and 3*N* interactions.

Why?

There are several reasons, but the main one is a very complicated way in numerical treatment of Faddeev equations with proper account of 3*N* forces well above the 3*N*-breakup threshold.

Let's illustrate this by Faddeev equations for three identical bosons

(from H. Liu, Ch. Elster and W. Gloeckle)

Faddeev equation in Jacobi momenta variables has the form

$$\begin{aligned}\langle \mathbf{pq}|T|\varphi_d \mathbf{q}_0\rangle &= \varphi_d\left(\mathbf{q}+\frac{1}{2}\mathbf{q}_0\right) t_s\left(\mathbf{p},\frac{1}{2}\mathbf{q}+\mathbf{q}_0, E-\frac{3}{4m}q^2\right) \\ &+ \int d^3q'' t_s\left(\mathbf{p},\frac{1}{2}\mathbf{q}+\mathbf{q}'', E-\frac{3}{4m}q^2\right) \frac{\left\langle \mathbf{q}+\frac{1}{2}\mathbf{q}'', \mathbf{q}''\,|T|\,\varphi_d\mathbf{q}_0\right\rangle}{E-\frac{1}{m}(q^2+q''^2+\mathbf{q}\cdot\mathbf{q}'')+i\varepsilon}. \end{aligned} \tag{0.1}$$

Here $t_s(\mathbf{p}',\mathbf{p}) = t(\mathbf{p},\mathbf{p}') + t(-\mathbf{p}',\mathbf{p})$ is the symmetrized t matrix and E is the total energy in the center of mass (c.m.) system

$$E = E_d + \frac{3}{4m}q_0^2 = E_d + \frac{2}{3}E_{lab}. \tag{0.2}$$

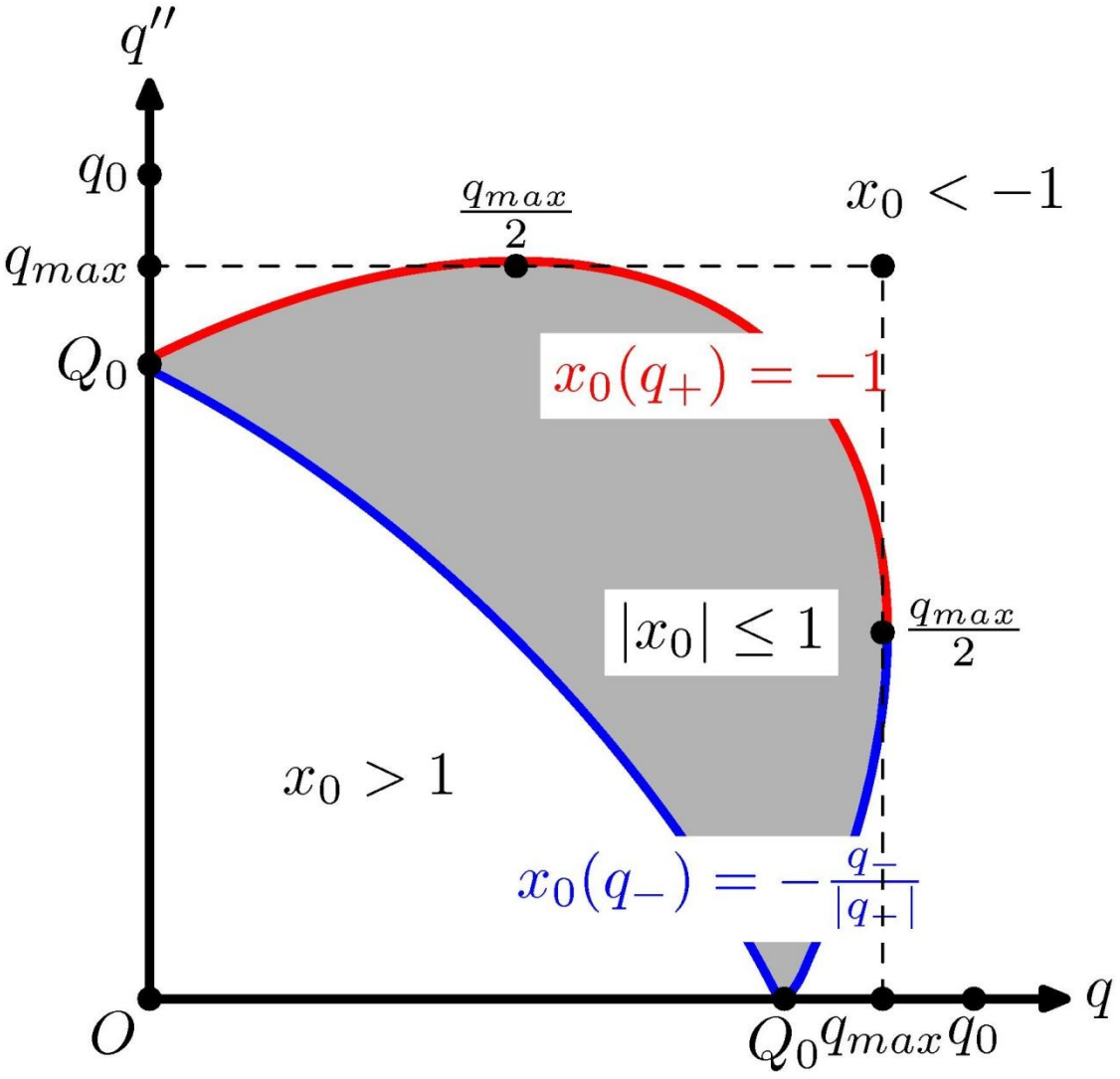
$t_s(z)$ has a pole at $z = E_d$. Extracting the residue explicitly by defining

$$t_s(\mathbf{p}',\mathbf{p},z) \equiv \frac{\hat{t}_s(\mathbf{p}',\mathbf{p},z)}{z-E_d} \tag{0.3}$$

and similarly for T, Eq. (0.1) can be rewritten as

$$\begin{aligned}\langle \mathbf{pq}|\hat{T}|\varphi_d \mathbf{q}_0\rangle &= \varphi_d\left(\mathbf{q}+\frac{1}{2}\mathbf{q}_0\right) \hat{t}_s\left(\mathbf{p},\frac{1}{2}\mathbf{q}+\mathbf{q}_0, E-\frac{3}{4m}q^2\right) \\ &+ \int d^3q'' \frac{\hat{t}_s\left(\mathbf{p},\frac{1}{2}\mathbf{q}+\mathbf{q}'', E-\frac{3}{4m}q^2\right)}{E-\frac{1}{m}(q^2+q''^2+\mathbf{q}\cdot\mathbf{q}'')+i\varepsilon} \frac{\left\langle \mathbf{q}+\frac{1}{2}\mathbf{q}'', \mathbf{q}''|\hat{T}|\varphi_d\mathbf{q}_0\right\rangle}{E-\frac{3}{4m}q''^2-E_d+i\varepsilon}. \end{aligned} \tag{0.4}$$

Area of q''-integration in the plane q''-q



For clear illustration we consider the case of simple s-wave interactions using the reduction scheme of Ahmadzadeh and Tjon:

$$\Psi_s(p,q) = \Phi(p,q) + \frac{1}{\pi q} \int_0^\infty dp_2^2 \int_0^\infty dq_2^2 \int_{-1}^{1} d(\cos\theta_{22})$$

$$\times \delta(q^2 - q_1^2)\, t(p^2, p_1^2, s-q^2)\, \frac{p_2^2 q_2^2}{p_2^2 + q_2^2 - s}\, \Psi_s(p_2, q_2) \qquad (24)$$

where

$$\begin{cases} q_1^2 = \frac{1}{4}\left(3p_2^2 + q_2^2 - 2\sqrt{3}\, p_2 q_2 \cos\theta_{22}\right) \\ p_1^2 = \frac{1}{4}\left(p_2^2 + 3q_2^2 + 2\sqrt{3}\, p_2 q_2 \cos\theta_{22}\right) \end{cases} \qquad (25)$$

Rewriting the δ-function in terms of $\cos\theta_{22}$:

$$\delta(q^2 - q_1^2) = \begin{cases} \frac{2}{\sqrt{3}\,p_2 q_2}\,\delta\left[\cos\theta_{22} + \left(\frac{4q^2 - 3p_2^2 - q_2^2}{2\sqrt{3}\,p_2 q_2}\right)\right] \text{ at} \\ \qquad \frac{1}{3}(2q - q_2)^2 < p_2^2 < \frac{1}{3}(2q + q_2)^2 \\ 0, \quad \text{in any other case.} \end{cases}$$

Now, we'll make the integration over $\cos\theta_{22}$ in eq. (24) and find the equation

$$\Psi_s(p,q) = \Phi(p,q) + \frac{2}{\sqrt{3}\pi q} \int_0^{\infty} dq_2^2 \int_A^B dp_2^2\, t(p^2, p_1^2, s - q^2) \times \left(\frac{1}{p_2^2 + q_2^2 - s}\right) \Psi_s(p_2, q_2) \qquad (22)$$

where $A = \frac{1}{3}(2q + q_2)^2$; $B = \frac{1}{3}(2q - q_2)^2$

and $p_1^2 = p_2^2 + q_2^2 - q^2$

It follows from the Eq. (27) that three-body wave functions Ψ_s in right- and left-hand sides are given in different sets of coordinates:

$$\Psi_s \quad p_2, q_2 \quad \text{v.s.} \quad \Psi_s \quad p, q$$

So, when iterating the Eq. (27) we must interpolate at each iteration step:

$$\Psi_s \quad p, q \quad \Rightarrow \quad \Psi_s \quad p_2, q_2$$

at every coordinate mesh-point! This leads to many thousands, or even many hundred thousands multi-dimensional interpolations at every interpolation step!!

These difficulties get much worse when treating the general three-nucleon case of many coupled partial waves.

Partial-wave reduction for the three-body Faddeev equations

(E.P. Harper, Y.E. Kim, A. Tubis, PRC, **2**, 877 (1970).)

The nonrelativistic three-particle scattering matrix T for particles of mass m_1, m_2, and m_3 can be decomposed as[1,8]

$$T = T^{(1)} + T^{(2)} + T^{(3)} . \qquad (2.1)$$

The $T^{(i)}$'s satisfy the Faddeev equations

$$T^{(i)}(s) = T_i(s) - \sum_{j \neq i} T_i(s) G_0(s) T^{(j)}(s), \quad i = 1, 2, 3 . \qquad (2.2)$$

$G_0(s)$ is the three-particle Green's function

$$G_0(s) = (H_0 - s)^{-1}, \qquad (2.3)$$

(H_0 being the three-particle kinetic energy operator), s is the total energy of the three-particle system, the T_i's are the off-shell two-body T-matrices

Partial-wave expansion for three-body plane waves:

$$|p, q, \alpha\rangle_i = |p, q, \alpha(i, jk)\rangle_i = |[p(LS)J, q(ls)j]\mathcal{J}\mathcal{J}_z; (Tt)\mathcal{T}\mathcal{T}_z\rangle_i$$
$$= \sum_{m_J, m_j} \langle Jm_J jm_j | \mathcal{J}\mathcal{J}_z\rangle \, |p(LS)Jm_J; q(ls)jm_j\rangle_i \, |(Tt)\mathcal{T}\mathcal{T}_z\rangle_i$$

with

$$|p(LS)Jm_J; q(ls)jm_j\rangle_i = \sum_{m_L, m_S} \sum_{m_l, m_s} \langle Lm_L Sm_S | Jm_J\rangle \langle lm_l sm_s | jm_j\rangle \, |pLm_L; qlm_l\rangle |Sm_S\rangle_i |sm_s\rangle$$

and

$$|Sm_S\rangle_i = |(s_j s_k)Sm_S\rangle_i = \sum_{m_{s_j}, m_{s_k}} \langle s_j m_{s_j} s_k m_{s_k} | Sm_S\rangle \, |s_j m_{s_j}\rangle \, |s_k m_{s_k}\rangle \quad (ijk \text{ cyclic}),$$

The Faddeev equation, in the J-j coupling scheme, becomes

$$\psi_s^{(1)}(p,q,\alpha) = \varphi_s^{(1)}(p,q,\alpha) - 2\sum_{\alpha_2}\int_0^\infty p_2^{\,2}dp_2 \int_0^\infty q_2^{\,2}dq_2 \frac{{}^{(1)}K_2}{p_2^{\,2}+q_2^{\,2}-s}\ \psi_s^{(1)}(p_2,q_2,\alpha_2),$$

where

$$\psi_s^{(1)}(p,q,\alpha) = {}_1\langle p,q,\alpha|T^{(1)}(s)|\psi\rangle_A,$$

$$\psi_s^{(1)}(p_2,q_2,\alpha_2) = {}_1\langle p_2,q_2,\alpha_2|T^{(1)}(s)|\psi\rangle_A,$$

$$\varphi_s^{(1)}(p,q,\alpha) = {}_1\langle p,q,\alpha|T_1(s)|\psi\rangle_A,$$

and

$${}^{(1)}K_2 = {}_1\langle p,q,\alpha|T_1(s)|p_2,q_2,\alpha_2\rangle_2 .$$

Using (4.4) in (4.9), we obtain

$${}^{(1)}K_2 = \sum_{\substack{\text{(all magnetic numbers}\\ \text{except } \mathcal{J}_z,\ \mathcal{J}_{2z})}} \langle \mathcal{J}\mathcal{J}_z|Jm_J jm_j\rangle \langle Jm_J|Lm_L Sm_S\rangle \langle jm_j|lm_l\, sm_s\rangle \langle J_2 m_{J_2} j_2 m_{j_2}|\mathcal{J}_2\mathcal{J}_{2z}\rangle$$

$$\times \langle L_2 m_{L_2} S_2 m_{S_2}|J_2 m_{J_2}\rangle \langle l_2 m_{l_2} s_2 m_{s_2}|j_2 m_{j_2}\rangle \int d\hat{p}\int d\hat{q}\int d\hat{p}_2\int d\hat{q}_2\, Y^*_{Lm_L}(\hat{p})Y^*_{lm_l}(\hat{q})Y_{L_2,m_{L_2}}(\hat{p}_2)Y_{l_2 m_{l_2}}(\hat{q}_2)$$

$$\times {}_1\langle \vec{p},\vec{q};Sm_S,sm_s;\,(Tt)\mathcal{T}\mathcal{T}_z\,|\,T_1(s)\,|\,\vec{p}_2,\vec{q}_2;\,S_2m_{S_2},\,s_2m_{s_2};(T_2t_2)\mathcal{T}_2\mathcal{T}_{2z}\rangle_2 .$$

The final result for the integral part of the Faddeev equation (4.6) is

$$\int_0^\infty p_2^2 dp_2 \int_0^\infty q_2^2 dq_2 \frac{{}^{(1)}K_2}{p_2^2 + q_2^2 - s}\, \psi_s^{(1)}(p_2, q_2, \alpha_2)$$

$$= \tfrac{1}{2} \sum_{S_1, J_1} \delta_{JJ_1} \delta_{SS_1} \delta_{\mathcal{T}_z \mathcal{T}_{2z}} (-1)^{t_2 - T_2 - \mathcal{T}_2} \hat{T}\hat{T}_2 W(t_1 t_3 \mathcal{T}_2 t_2; T_2 T) \sum_{T_z, t_z} \langle T T_z t t_z | \mathcal{T} \mathcal{T}_z \rangle \langle T T_z t t_z | \mathcal{T}_2 \mathcal{T}_{2z} \rangle$$

$$\times \sum_{L_1} \bar{\delta}_{L_1, L} \sum_{\lambda \Lambda r r_1 r_2} \binom{2l+1}{2\lambda}^{1/2} \binom{2L_1+1}{2\Lambda}^{1/2} (\alpha_{12})^{l-\lambda+\Lambda-1} (\beta_{12})^{\lambda+L_1-\Lambda-1} (-1)^{L_1+l-\lambda} (2L_2+1)^{1/2} (2l_2+1)^{1/2}$$

$$\times (2r_1+1)(2r_2+1)[2(L_1-\Lambda)+1]^{1/2}[2(l-\lambda)+1]^{1/2} \hat{r}^2 \begin{pmatrix} L_2 & r & r_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \Lambda & \lambda & r_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} r & l_2 & r_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L_1 - \Lambda & l-\lambda & r_2 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times G_{J-j}\, \frac{1}{q^{l+1}} \int_0^\infty dq_2 q_2^{L_1 - \Lambda + l - \lambda + 1} \int_{|\alpha_{12} q_2 - q|/\beta_{12}}^{(\alpha_{12} q_2 + q)/\beta_{12}} dp_2 p_2^{\Lambda + \lambda + 1} \frac{\tau_{L_1, L}^{J_1 S T T_z}(p^2, p_2^2 + q_2^2 - q^2; s - q^2)}{(p_2^2 + q_2^2 - s)(p_2^2 + q_2^2 - q^2)^{L_1/2}}$$

$$\times P_r \left(\frac{\beta_{12}^2 p_2^2 + \alpha_{12}^2 q_2^2 - q^2}{2\alpha_{12}\beta_{12} p_2 q_2} \right) \psi_s^{(1)}(p_2, q_2, \alpha_2) .$$

The τ function is related to the two-body t matrix for $S = 0$ and $T = 0$ or 1 by the relation

$$\tau_{L, L}^{L 0 T T_z}(p^2, p_1^2; s - q^2) = -\frac{2}{\pi} t_L(p, p_1; (s - q^2)^{1/2}) ,$$

where G_{J-j} is the geometrical factor given by

$$G_{J-j} = \frac{1}{2\mathcal{J}+1} \sum_{\substack{\text{all } m\text{'s}, \\ J_z}} (-1)^{m_r} \delta_{\mathcal{J}\mathcal{J}_2} \delta_{\mathcal{J}_z \mathcal{J}_{2z}} \delta_{m_{L_1}+m_{S_1},\, m_L+m_S} \delta_{m_\Lambda+m_\lambda,\, m_{L_2}-m_r} \delta_{m_r+m_{l_2},\, m_{L_1}+m_l-m_\Lambda-m_\lambda}$$

$$\times \langle \mathcal{J}\mathcal{J}_z | Jm_J jm_j \rangle \langle Jm_J | Lm_L Sm_S \rangle \langle jm_j | lm_l sm_s \rangle \langle J_2 m_{J_2} j_2 m_{j_2} | \mathcal{J}_2 \mathcal{J}_{2z} \rangle \langle L_2 m_{L_2} S_2 m_{S_2} | J_2 m_{J_2} \rangle$$

$$\times \langle l_2 m_{l_2} s_2 m_{s_2} | j_2 m_{j_2} \rangle \langle Lm_L Sm_S | J_1 m_L + m_S \rangle \langle L_1 m_{L_1} S_1 m_{S_1} | J_1 m_{L_1} + m_{S_1} \rangle \langle s_3 m_{s_3} s_1 m_{s_1} | S_2 m_{S_2} \rangle$$

$$\times \langle s_2 m_{s_2} s_3 m_{s_3} | S_1 m_{S_1} \rangle \langle \lambda m_\lambda l - \lambda\, m_l - m_\lambda | lm \rangle \langle \Lambda m_\Lambda L_1 - \Lambda\, m_{L_1} - m_\Lambda | L_1 m_{L_1} \rangle$$

$$\times \begin{pmatrix} L_2 & r & r_1 \\ m_{L_2} & m_r & m_r - m_{L_2} \end{pmatrix} \begin{pmatrix} \Lambda & \lambda & r_1 \\ m_\Lambda & m_\lambda & -m_\lambda - m_\Lambda \end{pmatrix} \begin{pmatrix} r & l_2 & r_2 \\ m_r & m_{l_2} & -m_r - m_{l_2} \end{pmatrix} \begin{pmatrix} L_1 - \Lambda & l - \lambda & r_2 \\ m_{L_1} - m_\Lambda & m_l - m_\lambda & m_\Lambda + m_\lambda - m_{L_1} - m_l \end{pmatrix}.$$

(4.19)

Thus, let's summarize the numerical problems in solving FEqs.

1. Variable integration limits.
2. Moving branching points in equation kernels.
3. Complex deformation for path of integration.
4. Multi-dimensional interpolations.

How to avoid these problems?

It is evident that these problems cannot be avoided by the conventional approach. We need to use essentially different representation for scattering operators and wavefunctions.

So, we need a principally new way!!

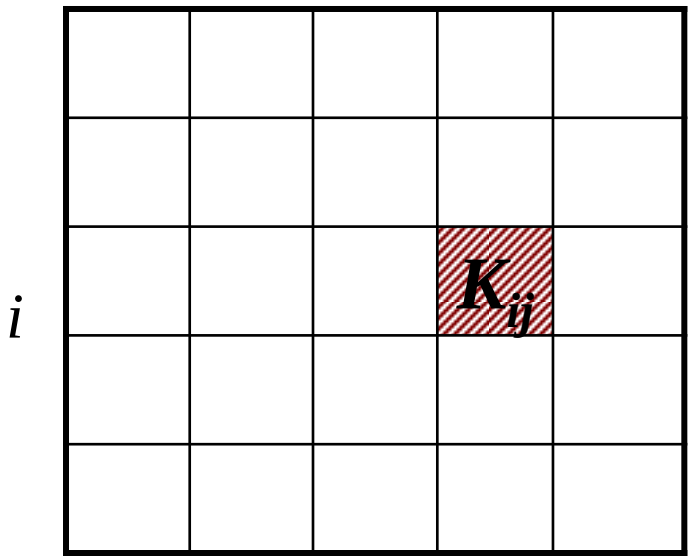
In this new way we want to use the highly effective and very fast GPU-computations (i.e. computations via ultrafast graphical processors).

So, we should transform the multi-dimensional integral equations into a form convenient for graphical-processor treatment, i.e. to a pixel-like form.

We may use a transformation which is similar to well-known transformation from analog to discrete (pixel) digital images, e.g. in a movie production.

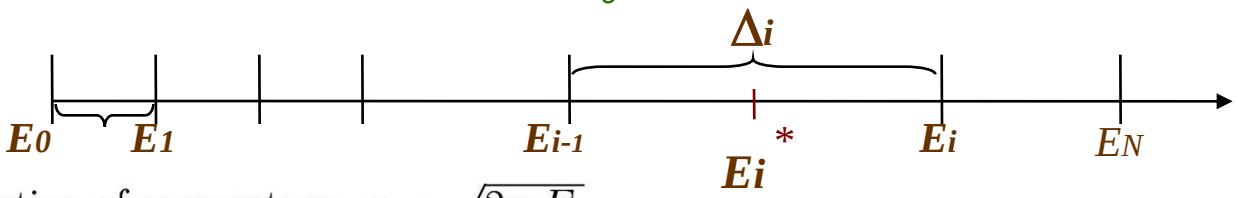
Thus, in our discrete scattering theory, we have discrete matrix functions K_{ij} instead of original continuous kernel function $K(p,q)$.

The value of every 'pixel' K_{ij} is a result of integration and some averaging for initial integral kernel around the point (p_i,q_j).



Stationary wave packets and their properties

Discretization of the free Hamiltonian H_0 continuum



Discretization of momentum: $q_i = \sqrt{2mE_i}$.

Stationary wave packets:

$$|x_i\rangle = \frac{1}{\sqrt{B_i}} \int_{q_{i-1}}^{q_i} f_i(q)|\psi_{0q}\rangle \mathrm{d}q, \quad i = 1, \ldots, N.$$

$f_i(q)$ — weight functions. $B_i = \int_{q_{i-1}}^{q_i} |f_i(q)|^2 \mathrm{d}q.$

Wave packets form an orthonormalized set:

$$\langle x_i|x_j\rangle = \delta_{ij}, \quad \hat{P} = \sum_{i=1}^{N} |x_i\rangle\langle x_i| \text{— the projector.}$$

Matrix of any operator $R(H_0)$ is diagonal:

$$\langle x_i|R(H_0)|x_j\rangle = \frac{\delta_{ij}}{B_i} \int_{q_{i-1}}^{q_i} R\left(\frac{q^2}{2m}\right) |f(q)|^2 \mathrm{d}q.$$

Plane waves:

$$\langle \psi_{0q}|\psi_{0q'}\rangle = \delta(q - q')$$

‘Energy’ packets

$$\left.\begin{array}{c} f(q) = \dfrac{q}{m} \\ B_i = E_i - E_{i-1} \equiv \Delta_i \end{array}\right\} \quad \text{E-packets } |X_i\rangle.$$

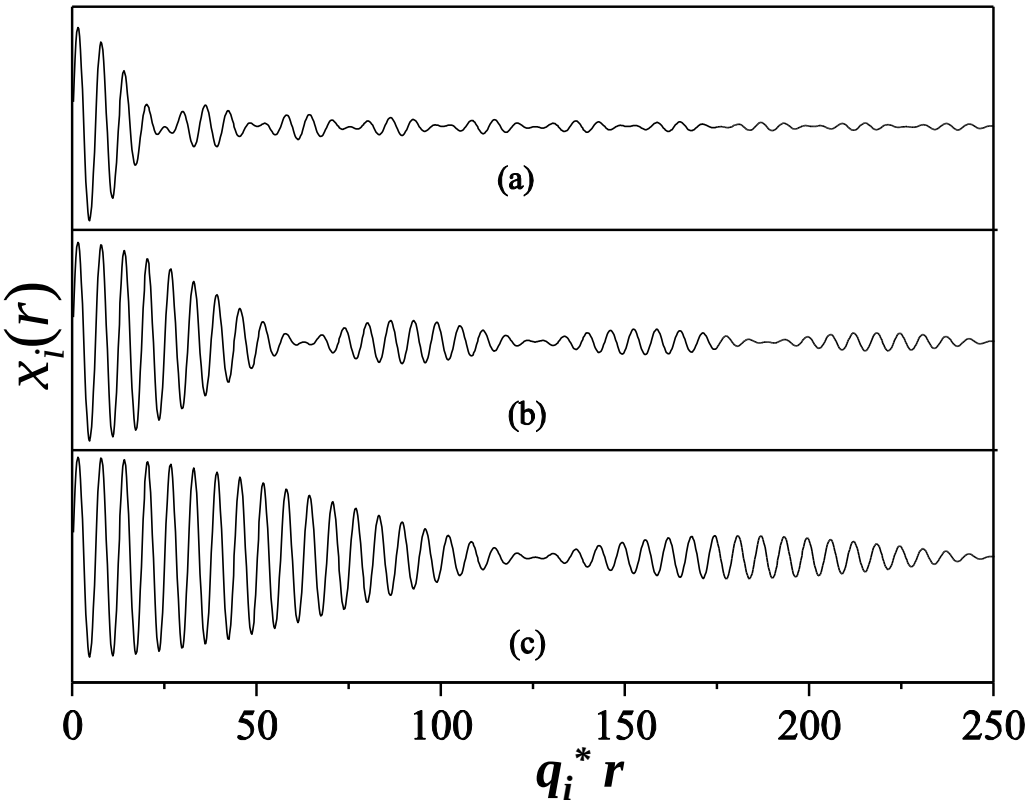
‘Momentum’ packets

$$\left.\begin{array}{c} f(q) = 1 \\ B_i = q_i - q_{i-1} \equiv d_i \end{array}\right\} \quad \text{q-packets } |x_i\rangle.$$

Behavior of WPs in configuration space

$$x_i(r) = \sqrt{d_i}\,\psi_0(q_i^*, r)\,\frac{\sin\ d_i r/2}{d_i r/2}$$

Coordinate behavior of wave packets for different ratios of their widths to their momentum eigenvalues d_i/q_i^*



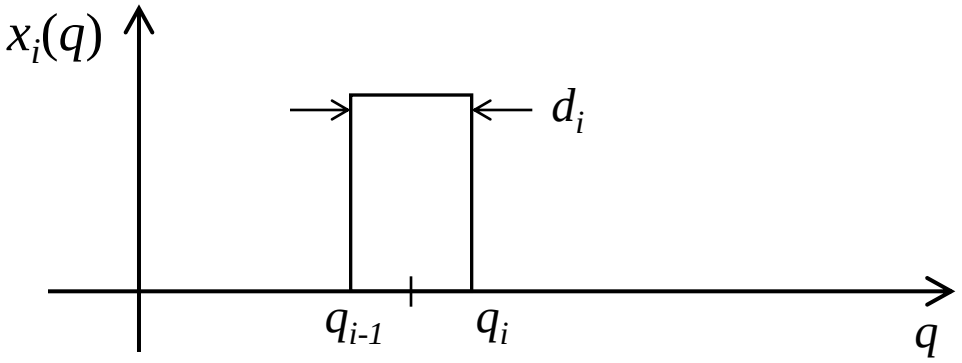
$$\frac{d_i}{q_i^*} = \begin{cases} 0.25 \text{ (a)}; \\ 0.1 \text{ (b)}; \\ 0.05 \text{ (c)}. \end{cases}$$

The smaller wave-packet width corresponds to slower decrease of its wavefunction at the asymptotics.

Momentum representation

$$x_i(q) = \frac{\theta(q - q_{i-1}) - \theta(q - q_i)}{\sqrt{d_i}}, \quad i = 1, \ldots, N.$$

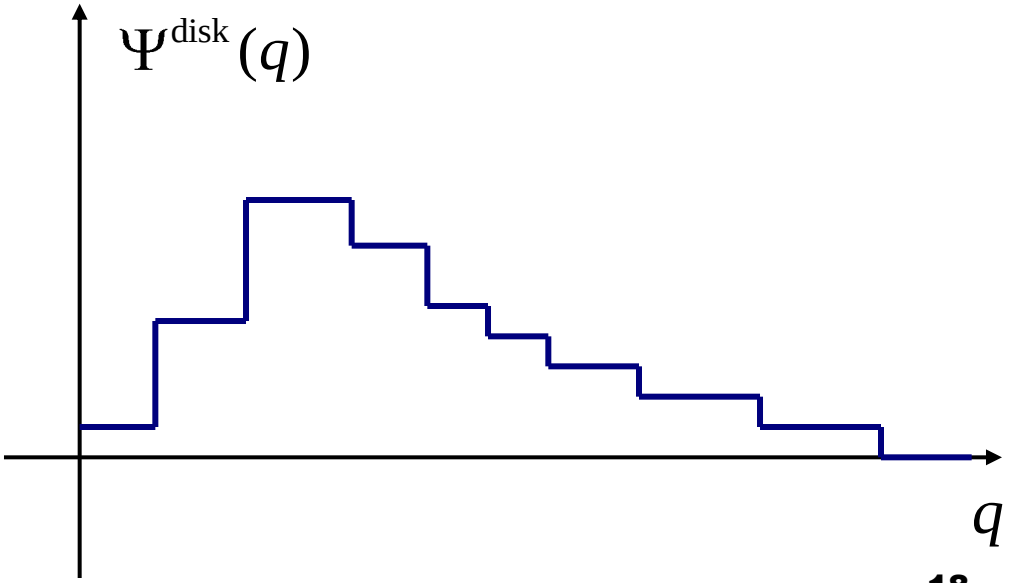
The basis element x_i looks like a rectangular impulse.



By applying the projector $\mathbb{P} = \sum_{i=1}^{N} |x_i\rangle\langle x_i|$ to any function continuous over q,

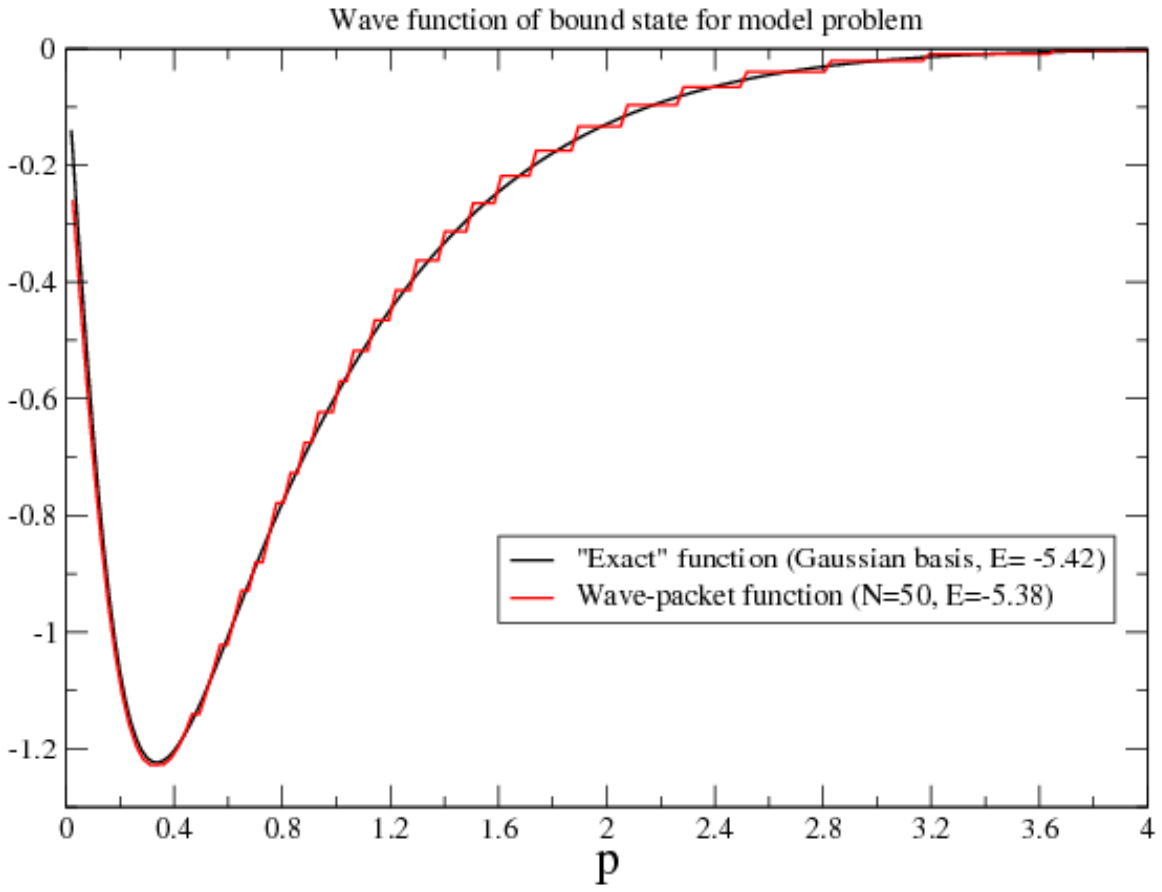
one obtains

$$|\Psi^{\text{disk}}\rangle \equiv \mathbb{P}|\Psi\rangle = \sum_{i=1}^{N} C_i |x_i\rangle$$



Now one can project the Schroedinger equation onto such a lattice space and come to purely matrix problem

$$\mathbb{H}\left|\Psi_k^{\text{disk}}\right\rangle = E_k^{\text{disk}}\left|\Psi_k^{\text{disk}}\right\rangle, \text{ где } \mathbb{H} = \mathbb{P}H\mathbb{P}, \left|\Psi_k^{\text{disk}}\right\rangle = \mathbb{P}\left|\Psi\right\rangle$$



Two faces of the wave-packet basis

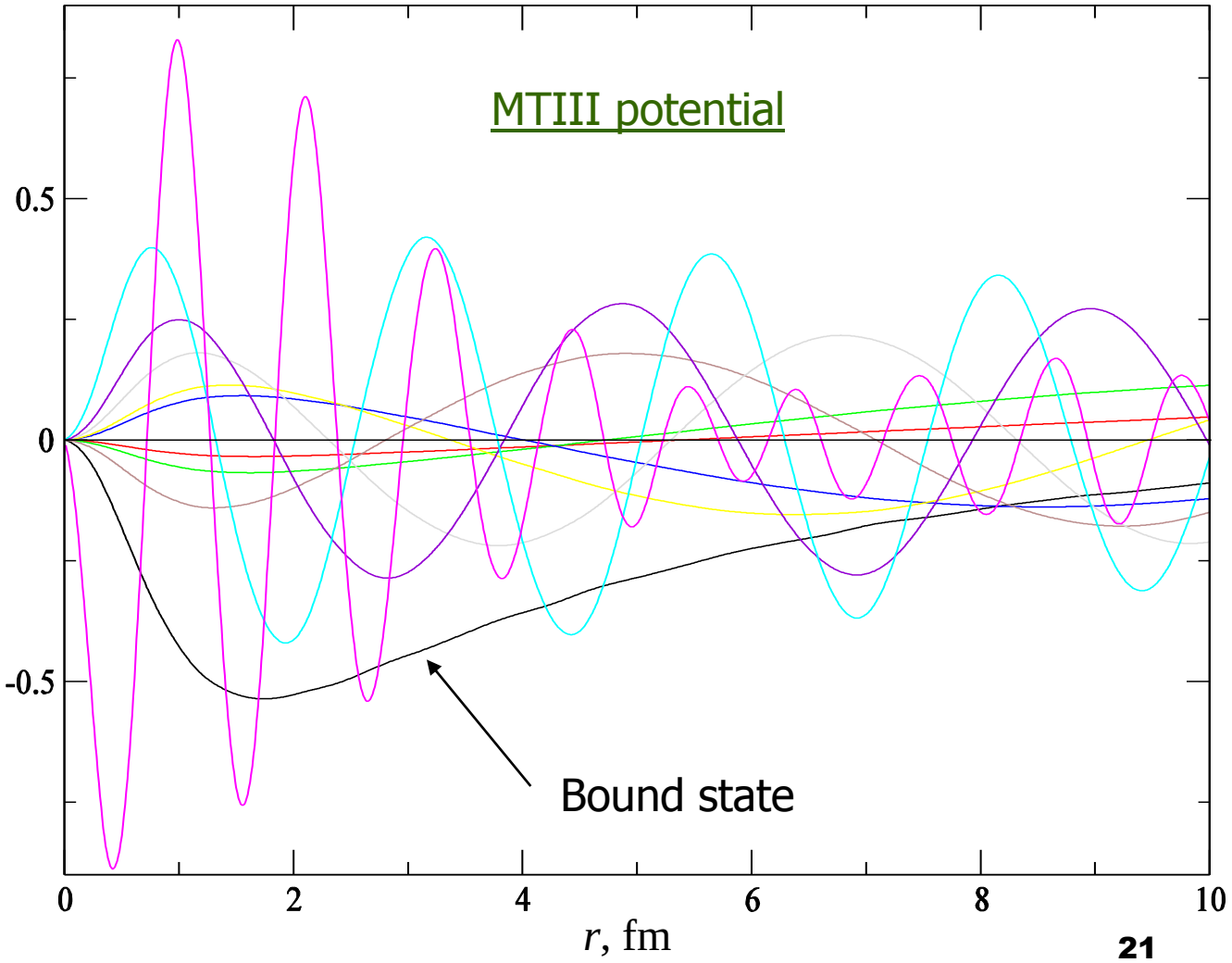
- The WPB can be considered as orthonormalized ‘localized’ plane-wave basis which is ideally suited for scattering calculations.

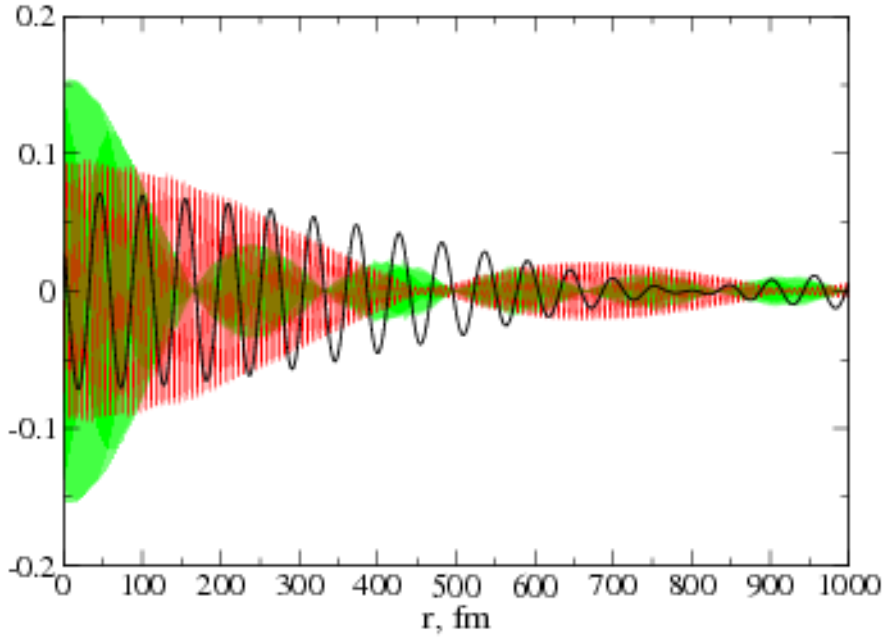
- On the other hand, we can consider this complete L_2-basis as appropriate basis for conventional variational calculations like Harmonic oscillator or Gaussian bases.

Wave packets as a basis for variational solution

Diagonalization procedure: $|z_p\rangle = \sum_{n=1}^{N} C_{pn}|x_n\rangle$ → $\det||H_{nn'} - E\delta_{nn'}|| = 0 \mapsto \{C_{pn}, E_p\}_{p=1}^{N}$

Wave-packet pseudo-states with positive energies are very close to exact scattering wave packets (corresponding to the total Hamiltonian). This property takes place in asymptotic region as well.





The coordinate behavior of several wave-packet states for the MT-III NN potential found by the diagonalization of the Hamiltonian matrix on the free wave-packet basis.

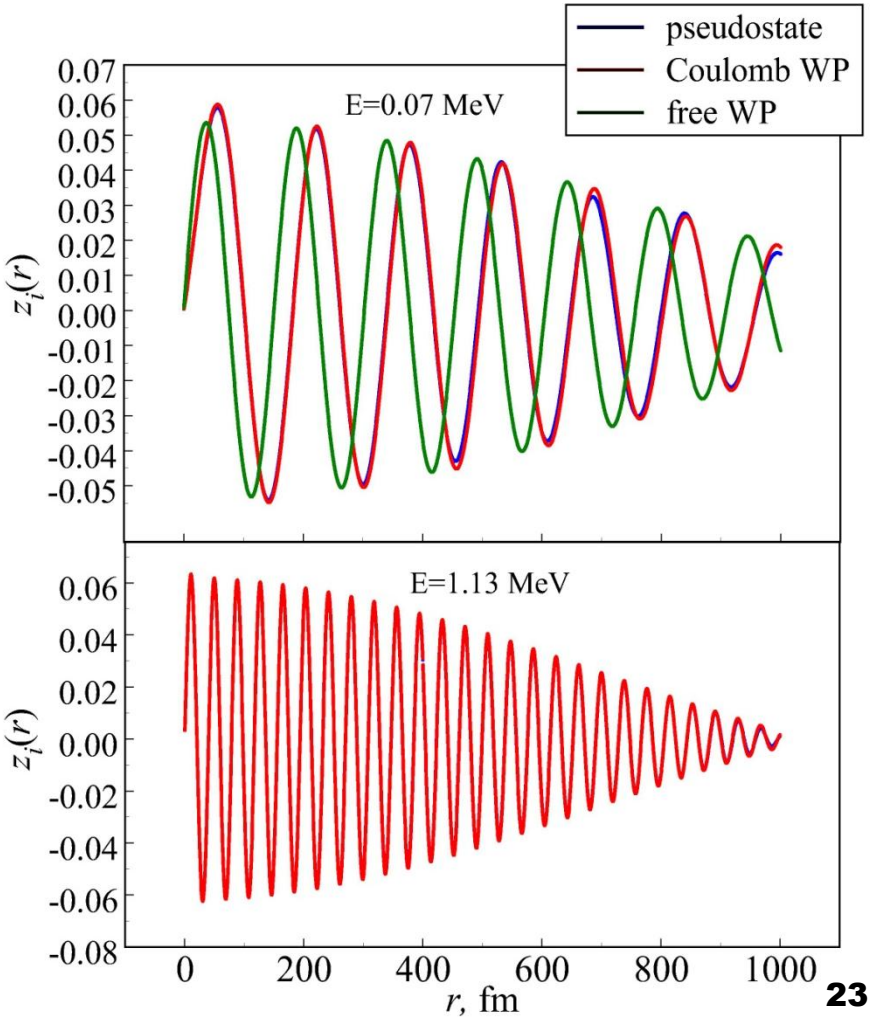
Wave-packet basis in the Coulomb scattering problem

Wave-packet functions decrease very slowly, so this basis is ‘long-ranged’ and thus is very convenient for approximation of continuum states.
This is also valid for the long-range potentials.

It is well known that exact wave functions of the Coulomb Hamiltonian continuum cannot be expanded over exact plane waves because of the infinite radius of the Coulomb force.

But we found that Coulomb wave-packets can be expanded over finite set of free wave packets!

Thus, the projection onto the wave-packet representation is an effective way for the regularization of the Coulomb singularities.



Formulation and solution of three- and few-body scattering problems in the wave-packet representation

(All formulations and calculations in this part have been done jointly with my coathors: O.Rubtsova and V.Pomerantsev)

Total Hamiltonian:

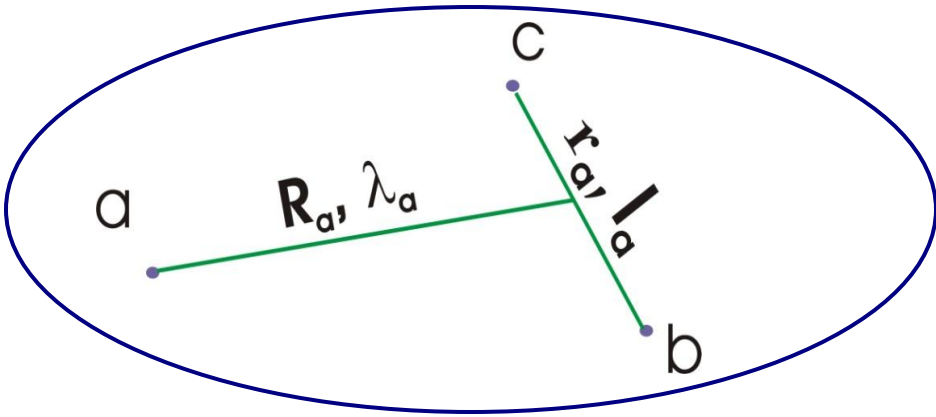
$$H = H_0 + V_a + V_b + V_c.$$

Channel Hamiltonian:

$$H_a = H_0 + V_a = h_a \oplus h_0^a.$$

Channel wave-packet basis:

$$|S_a, \Lambda M\rangle \equiv |Z_i^{l_a}, X_j^{\lambda_a}, \Lambda M\rangle.$$



In general few-body case, WP basis should be constructed in each Jacobi coordinate set via direct production of each subsystem WP bases. Such a basis consists of eigenstates of each channel Hamiltonian.

Lattice representation leads to a complete few-body continuum discretization.

This original approach includes a few basic moments.

— Discretization of the whole momentum space (in two Jacobi momenta) into rectangular cells.

— The set of such two-dimensional step-like functions forms a complete discrete basis which we use to expand the unknown solution and also the integral-equation kernels.

— As a result of such wave-packet discretization we get one simple matrix equation with regular matrix elements.

— In this approach the matrix elements for the multi-channel resolvent entering the integral kernels are expressed via simple analytical formulas.

General three-body problem in the Faddeev framework

Faddeev expansion of the total scattering wave function:

$$|\Psi(E)\rangle = |\psi^{(1)}\rangle + |\psi^{(2)}\rangle + |\psi^{(3)}\rangle.$$

Faddeev equations for the components:

$$|\psi^{(a)}\rangle = |\Phi_{01}\rangle\delta_{a1} + G_a V_a \sum_{b\neq a} |\psi^{(b)}\rangle, \quad a = 1, 2, 3.$$

F.-d. approximation for each Faddeev component:

$$|\hat{\psi}^{(a)}\rangle = \sum_{ik} O^a_{ik} |S^{(a)}_{ik}\rangle, \quad a = 1, 2, 3.$$

F.-d. equations for the 'packetted' Faddeev components

$$|\hat{\psi}^{(a)}\rangle = |S^{(1)}_0\rangle\delta_{a1} + \mathbb{G}_a \mathbb{V}_a \sum_{b\neq a} \mathbb{P}_{ab} |\hat{\psi}^{(b)}\rangle, \quad a = 1, 2, 3.$$

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

$$\mathbf{G}_a = \sum_{S_a}^{N} G_a(E)_{S_a} \left|S_a\right\rangle\left\langle S_a\right|$$

The permutation operators in the wave-packet basis

The permutation operators can be expressed in our complete three-body wave-packet basis as:

$$\mathbb{P}_{ab} = \sum_{ik,i'k'} |S_{ik}^{(a)}\rangle [\langle S_{ik}^{(a)} | S_{i'k'}^{(b)}\rangle] \langle S_{i'k'}^{(b)}|.$$

where $\langle S_{ik}^{(a)} | S_{i'k'}^{(b)}\rangle \equiv \langle z_i, x_k, (a) | z_{i'}, x_{k'}, (b)\rangle.$

Using expansion of scattering WPs on a free wave-packet basis

$$|z_i^{(a)}\rangle = \sum_j C_{ij}^{(a)} |x_j^{(a)}\rangle.$$

one gets: $\langle S_{ik}^{(a)} | S_{i'k'}^{(b)}\rangle = \sum_{j,j'} C_{ij}^{(a)} C_{i'j'}^{*(b)} \underbrace{\langle x_j, x_k, (a) | x_{j'}, x_{k'}, (b)\rangle}.$

these matrix elements are independent on energy and interaction

Computation of the permutation operator in the wave-packet basis

The wave function of the three-nucleon system is expanded in partial waves, using (jj)-coupling. For fixed values of the total J and parity, this expansion leads to a system of N coupled equations for channel Faddeev components of the wave function (or amplitudes) with $N = 5 - 34$.

Each channel is characterized by the following quantum numbers:

$$\alpha = \{l, s, j, \lambda, I, t, T, J\},$$

where l is orbital angular momentum of a nucleon pair; s is spin of the pair; $\vec{j} = \vec{l} + \vec{s}$ is the total angular momentum of the pair; λ is the orbital angular momentum of the third nucleon with respect to the center of mass of the pair; $\vec{I} = \vec{\lambda} + 1/2$ is the total angular momentum of the third nucleon; t is isospin pair ($l + s + t$ is odd); T is the total isospin and J is the total angular momentum of the system.

One of the main difficulties in solving the FEs related to the structure of the matrix elements of the permutation operator P. In the plane-wave basis this matrix element is:

$$\langle p'q'\alpha'|P|pq\alpha\rangle = \int_{-1}^{+1} \frac{\delta(p'-\pi_1)}{(p')^{l'+2}} \frac{\delta(p-\pi_2)}{(p)^{l+2}} G_{\alpha'\alpha}(q',q,x)\,\mathrm{d}x, \qquad (1)$$

where

$$\pi_1 = \sqrt{q^2 + q'^2/4 + qq'x}, \qquad \pi_2 = \sqrt{q'^2 + q^2/4 + qq'x}; \qquad (2)$$

$$G_{\alpha'\alpha}(q',q,x) = \sum_{l_1,l_1',k} q^{l_2+l_2'} q'^{l_1+l_1'} P_k(x) g_{\alpha'\alpha}^{l_1'l_1k}, \qquad l_1+l_2=l; \qquad l_1'+l_2'=l'; \qquad (3)$$

x is the angle between the vectors $\mathbf{q}$ and $\mathbf{q}'$, P_k is the Legendre polynomial and $g_{\alpha'\alpha}^{l_1'l_1k}$ are geometrical coefficients.

Using the equation $\delta(p-z) = 2p\delta(p^2-z^2)$ and removing the integral over x in (1) one gets the following representation for the permutation operator:

$$\langle p'q'\alpha'|P|pq\alpha\rangle = \frac{4}{qq'pp'}\delta(p'^2+3/4q'^2-(p^2+3/4q^2))\,\vartheta(1-|x|) \quad (4)$$

$$\times \sum_{l_1,l_1',k} F^{l_1'l_1k}(p,p',q,q')g^{l_1'l_1k}. \quad (5)$$

Here, the angle x is a function of three momenta, e.g., p, q, q':

$$x = \frac{p^2-q'^2-q^2/4}{qq'}. \quad (6)$$

Functions $F^{l_1'l_1k}(p,p',q,q')$ are the homogeneous functions of momenta and can be reduce to the following form:

$$F^{l_1'l_1k}(p,p',q,q') = \left(\frac{q'}{p'}\right)^{l'}\left(\frac{q}{p}\right)^{l}\left(\frac{q'}{q}\right)^{l_1+l_1'-l'} P_k(x). \quad (7)$$

The algebraic coefficients $g^{l_1' l_1 k}_{\alpha' \alpha}$ look like (W. Gloeckle):

$$
\begin{aligned}
g^{l_1' l_1 k}_{\alpha' \alpha} \;=\; & -\sqrt{\hat{l}\hat{s}\hat{j}\hat{t}\hat{\lambda}\hat{I}\hat{l}'\hat{s}'\hat{j}'\hat{t}'\hat{\lambda}'\hat{I}'}
\left\{ \begin{array}{ccc} \frac{1}{2} & \frac{1}{2} & t \\ \frac{1}{2} & T & t' \end{array} \right\}
\sum_{LS} (\hat{L}\hat{S})
\left\{ \begin{array}{ccc} \frac{1}{2} & \frac{1}{2} & s \\ \frac{1}{2} & S & s' \end{array} \right\}
\left\{ \begin{array}{ccc} l & s & j \\ \lambda & \frac{1}{2} & I \\ L & S & J \end{array} \right\} \\
& \times \left\{ \begin{array}{ccc} l' & s' & j' \\ \lambda' & \frac{1}{2} & I' \\ L & S & J \end{array} \right\}
\hat{k} \left(\frac{1}{2}\right)^{l_2 + l_1'}
\sqrt{\frac{(2l+1)!}{(2l_1)!(2l_2)!}}
\sqrt{\frac{(2l'+1)!}{(2l_1')!(2l_2')!}}
\sum_{f f'} \left\{ \begin{array}{ccc} l_1 & l_2 & l \\ \lambda & L & f \end{array} \right\} \\
& \times \left\{ \begin{array}{ccc} l_2' & l_1' & l' \\ \lambda' & L & f' \end{array} \right\}
\langle l_2 0 \lambda 0 | f 0 \rangle \langle l_1' \lambda' 0 | f' 0 \rangle
\left\{ \begin{array}{ccc} f & l_1 & L \\ f' & l_2' & k \end{array} \right\}
\langle k 0 l_1 0 | f' 0 \rangle \langle k 0 l_2' 0 | f 0 \rangle
\end{aligned}
$$

Overlap matrix elements in the free wave-packet basis for S-waves

In our approach we use a lattice basis, i.e. the wave-packet basis built from the momentum free-motion packets. Two-dimensional (three-body) free wave-packet in momentum representation is a step-like function:

$$\langle p,q|x_i y_j\rangle \equiv \langle p,q|\Delta\rangle = \frac{1}{\sqrt{\Delta p \Delta q}} \frac{\vartheta(p\in\Delta p)}{p} \frac{\vartheta(q\in\Delta q)}{q}, \qquad (8)$$

where variables p and q are defined on the intervals $\Delta p = (p_{i-1}, p_i)$ and $\Delta q = (q_{j-1}, q_j)$ (we use the same notation for the interval widths, i.e. $\Delta p = p_i - p_{i-1}$ and $\Delta q = q_j - q_{j-1}$) and the function $\vartheta(p \in \Delta p) = 1$, if $p \in \Delta p$, and 0 otherwise. Such wave packets are normalized to unity with the weight $p^2 dp q^2 dq$ and form an orthonormal basis (if the intervals are not overlapped to each other).

To find the matrix elements of the permutation operator P over the free wave-packets (8), one has to integrate the function (4) (we denote here $\langle p'q'\alpha'|P|pq\alpha\rangle \equiv P^{\alpha'\alpha}(p',q',p,q)$) over rectangular cells $\Delta p, \Delta p', \Delta q, \Delta q'$:

$$\langle \Delta', \alpha'|P|\Delta, \alpha\rangle = \frac{1}{\sqrt{\Delta p \Delta p' \Delta q \Delta q'}} \int_{\Delta p \Delta p' \Delta q \Delta q'} P^{\alpha'\alpha}(p', q', p, q)\, p dp\, q dq\, p' dp'\, q' dq'. \tag{9}$$

Assuming that the size of the cells is sufficiently small, the smooth function $F^{l_1' l_1 k}(p, p', q, q')$ (7) can be taken out of the integral in (9):

$$P^{\alpha'\alpha}(p', q', p, q) \approx \sum_{l_1, l_1', k} F^{l_1' l_1 k}(p^*, p^{*\prime}, q^*, q^{*\prime}) g^{l_1' l_1 k} P^{00}(p', q', p, q), \tag{10}$$

where the quantities labeled with asterisks are the values of momenta at the midpoint of the overlap of the pair of cells $(\Delta p, \Delta q)$ and $(\Delta p', \Delta q')$, and P^{00} is "nonsmooth" part of the overlap function (4):

$$P^{00}(p', q', p, q) = \frac{4}{qq'pp'} \delta(p'^2 + 3/4 q'^2 - (p^2 + 3/4 q^2))\, \vartheta(1 - |x|). \tag{11}$$

Now one should evaluate the integral over the non-smooth part:

$$\langle\Delta'|P^{00}|\Delta\rangle = \frac{4}{\sqrt{\Delta p\Delta p'\,\Delta q\Delta q'}}\int_{\Delta p\Delta p'\,\Delta q\Delta q'} \delta(p'^2+3/4q'^2-(p^2+3/4q^2))\,\vartheta(1-|x|)\,dp\,dq\,dp'\,dq',$$

which is equal to the overlap area for two cells, viz. (Δp,Δq) and (Δp',Δq').

For this purpose it is convenient to use the polar coordinates. Let us introduce the "aligned" momentum variables p and $\tilde{q} = \sqrt{(3/4)}q$ for which the law of energy conservation takes the form $p^2 + \tilde{q}^2 = p'^2 + \tilde{q}'^2$. Polar coordinates Q, α are introduced as:

$$\tilde{q} = Q\sin\alpha, \quad p = Q\cos\alpha, \quad Q^2 = p^2 + \tilde{q}^2. \qquad (12)$$

The ratio p/q, the angle x and the functions F can be expressed in terms of $\{Q, \alpha\}$ as follows:

$$p/q = \frac{\sqrt{3/4}}{\tan\alpha}, \quad x = \frac{3}{4\tan^2\alpha}\frac{1}{R} - R - \frac{1}{4R}, \text{ where } R = \frac{\sin\alpha'}{\sin\alpha}, \qquad (13)$$

$$F^{l_1' l_1 k}(p, p', q, q') = (4/3)^{(l+l')/2}(\tan\alpha')^{l'}(\tan\alpha)^{l} R^{l_1+l_1'-l'} P_k(x). \qquad (14)$$

The area of overlap region for two 'boxes' (Δp,Δq) and (Δp',Δq') can be calculated in polar coordinates as:

$$\begin{aligned}
&\int \delta(p'^2 + 3/4q'^2 - (p^2 + 3/4q^2))\vartheta \, dp\, dq\, dp'\, dq' \\
&= (4/3) \int \delta(Q^2 - Q'^2)\vartheta \, Q dQ d\alpha Q' dQ' d\alpha' \\
&= (1/3) \int \delta(Q^2 - Q'^2)\vartheta \, d(Q^2) d\alpha d(Q'^2) d\alpha' \\
&= (1/3) \int \vartheta(1 - |x|) \, d(Q^2) d\alpha d\alpha' \equiv 1/3\Pi(\Delta,'\Delta), \qquad (15)
\end{aligned}$$

where $\Pi(\Delta, \Delta') = \int \vartheta(1 - |x|) dQ^2 d\alpha d\alpha'$.

Thus we get:

$$\langle \Delta', \alpha' | P | \Delta, \alpha \rangle = \frac{4}{3} \frac{A^{\alpha' \alpha}}{\sqrt{\Delta p \Delta p' \Delta q \Delta q'}} \Pi(\Delta,'\Delta), \qquad (16)$$

where

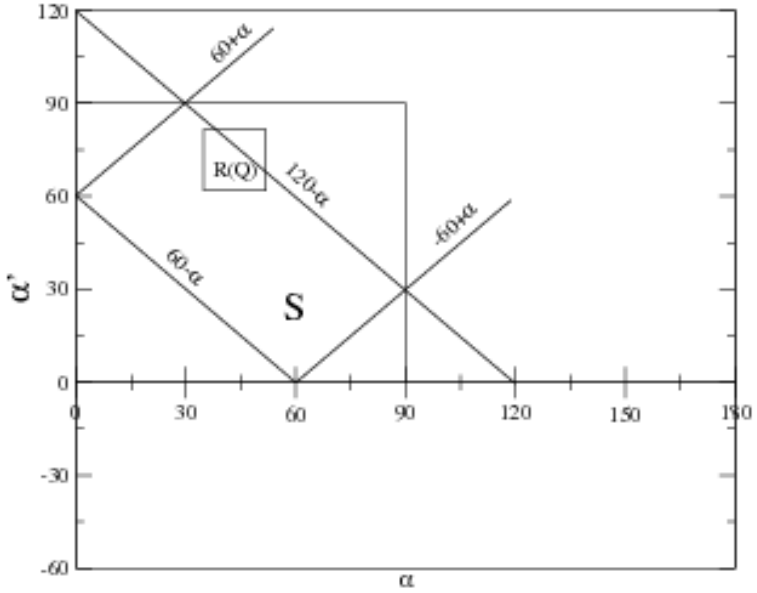
$$A^{\alpha' \alpha} = \sum_{l_1, l_1', k} F^{l_1' l_1 k}(p^*, p^{*\prime}, q^*, q^{*\prime}) g^{l_1' l_1 k}. \qquad (17)$$

See eq. (14) for the meaning of symbols.

Region of integration in the plane (α, α')

The condition $|x| < 1$ can be expressed through the polar angles α, α'. The overlap region $S(\alpha, \alpha')$, determined by the condition $|x| < 1$ is a rectangle bounded by four straight lines (see Figure):

$$\begin{aligned} \alpha' &> 60 - \alpha \\ \alpha' &< 120 - \alpha \\ \alpha' &> -60 + \alpha \\ \alpha' &< 60 + \alpha \end{aligned}$$



The region of integration in the plane (α,α') is the intersection of the large rectangle S restricted by the above four straight lines corresponding to four inequalities (the region of admissible values of α and α') and a small rectangle R(Q) whose vertices depend on Q-value.

The area of intersection between the large rectangles S and small box R(Q) can be evaluated analytically by formulas of elementary geometry.

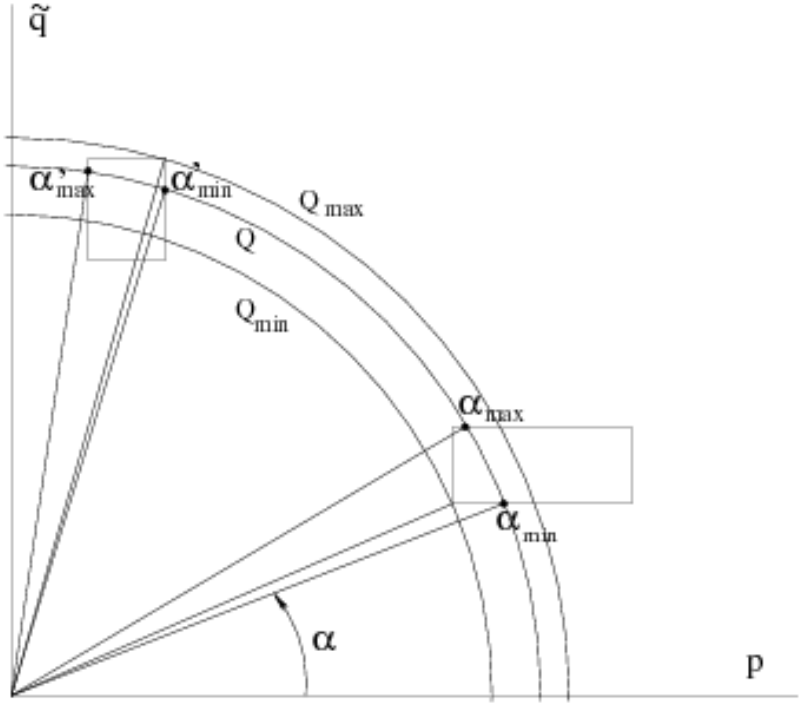
Rectangular cells $\Delta p \otimes \Delta q$, $\Delta p' \otimes \Delta q'$ are transformed to the areas of $S(Q^2, \alpha)$, $S(Q^2, \alpha')$ respectively, so that the integral (15) equals to the volume of a three-dimensional body V bounded by the intersection of three mutually perpendicular cylindrical surfaces $S(\alpha, \alpha')$, $S(Q^2, \alpha)$ and $S(Q^2, \alpha')$:

$$\Pi = \int \vartheta(|x|)\, d(Q^2) d\alpha d\alpha' = \int_{S(\alpha,\alpha') \cup S(Q^2,\alpha) \cup S(Q^2,\alpha')} dQ^2 d\alpha d\alpha'. \quad (18)$$

In practice, this integral is calculated as the external integral over Q^2 in the range $(Q^2_{\text{min}}\, Q^2_{\text{max}})$ from the intersection area of two rectangles in the plane (α, α'): $S(\alpha, \alpha')$ and $R(\alpha_{\text{min}}, \alpha_{\text{max}}, \alpha'_{\text{min}}, \alpha'_{\text{max}})$

$$\Pi = \int_{Q^2_{\text{min}}}^{Q^2_{\text{max}}} d(Q^2) \int \int_{S \cap R(Q)} d\alpha d\alpha'. \quad (19)$$

The integration limits over Q^2 and the vertices of the rectangle R are computed directly:



$Q_{\min}$ – lower left corner of the cell Δ;
$Q_{\max}$ – upper right corner of the cell Δ';

$$\alpha_{\min}(Q) = \max(\arcsin\frac{\tilde{q}_{i-1}}{Q}, \arccos\frac{p_i}{Q});$$

$$\alpha_{\max}(Q) = \min(\arcsin\frac{\tilde{q}_i}{Q}, \arccos\frac{p_{i-1}}{Q});$$

$$\alpha'_{\min}(Q) = \max(\arcsin\frac{\tilde{q}'_{j-1}}{Q}, \arccos\frac{p'_j}{Q});$$

$$\alpha'_{\max}(Q) = \min(\arcsin\frac{\tilde{q}'_j}{Q}, \arccos\frac{p'_{j-1}}{Q}).$$

On the definition of the integration limits in the variables Q, α, α'. The cells Δ and Δ' in the plane $(p\tilde{q})$ and their polar coordinates $(\alpha_{\min}, \alpha_{\max})$ and $(\alpha'_{\min}, \alpha'_{\max})$ are shown.

To summarize: we have evaluated the matrix elements $\langle \Delta', \alpha' | P | \Delta, \alpha \rangle$ for the permutation operator *P* between the wave-packet basis states (see Eq. (16)). These elements are expressed in a simple almost analytical formula.

Wave-packet form of Faddeev equations for *nd* scattering

Now, having the permutation operators and channel resolvents expressed in a simple way in the wave-packet basis, the system of integral equations for the partial Faddeev amplitudes can be reduced to a simple matrix equation:

$$\mathbf{X} = -\mathbf{P}\mathbf{v}_1 - \mathbf{P}\mathbf{v}_1\mathbf{G}_1\mathbf{X}, \tag{20}$$

where $\mathbf{P}$, $\mathbf{v_1}$ and $\mathbf{G_1}$ are the matrices of the permutation operator P, pairwise NN interaction v_1 and channel resolvent $G_1(E) = (E - H_0 - v_1)^{-1}$ correspondingly, and $\mathbf{X}$ is the matrix analog for partial amplitude.

We use the perturbed wave-packet lattice basis:

$$|S_{ij}\rangle = |z_i, y_j\rangle, \tag{21}$$

where $|z_i\rangle$ are the wave packets constructed from the exact scattering functions for two-particle subsystem (the perturbed two-particle packets), and $|y_i\rangle$ are the free wave packets corresponding to the free motion of the third particle.

Just employment of such a perturbed-packet basis is a distinctive feature of our approach, because in this basis the channel-resolvent matrix $\mathbf{G_1}$ is diagonal and its elements are defined by explicit expressions including only the values of the cell endpoints and the total energy of the system.

The perturbed wave packets $|z_i\rangle$ can be approximated by **pseudostates** obtained from a diagonalization of the two-particle Hamiltonian in the free wave-packet basis $\{x_i\}$:

$$|z_i\rangle \approx |\tilde{z}_i\rangle = \sum O_{ik}|x_k\rangle, \tag{22}$$

where the matrix O_{ik} resulting from diagonalization defines the transition from free wave packets to perturbed ones. Then the matrix elements of the permutation operator $\mathbf{P}$ can be simply expressed in terms of its matrix elements $P^0_{kj,k'j'}$ taken in free wave-packet basis:

$$P_{ij,i'j'} \equiv \langle z_i y_j|P|z_{i'}y_{j'}\rangle \approx \sum_{kk'} O_{ik}O^*_{i'k'}P^0_{kj,k'j'}. \tag{23}$$

As a result, we have simple formulas and algorithms to compute all the elements included to the matrix analog (20) of the FE.

The three-body amplitudes

On-shell partial amplitudes of the elastic nd scattering are associated with certain "singular" elements of the matrix $\mathbf{X}$, which is a solution of the system (20):

$$U^J_{\lambda' I',\lambda I}(E) = \frac{2m}{3q_0}\frac{X^{\alpha'\alpha}_{i_0 j_0, i_0 j_0}}{d_{j_0}}, \qquad (24)$$

where the index i_0 corresponds to a bound state in pair subsystem (deuteron with binding energy ϵ_d), and the index j_0 denotes the "singular" interval along the second Jacobi momentum variable q, which the on-shell momentum $q_0 = \sqrt{\frac{4}{3}m(E-\epsilon_d)}$ belongs to.

The breakup amplitude A(p,q) can be defined from the same matrix $\mathbf{X}$, viz.

$$A(p,q) \sim e^{i\delta_{NN}(p)} \frac{X_{0 j_0, ij}}{\sqrt{d_{j_0} d_i d_j}}, \quad \begin{matrix} p \in d_i \\ q \in d_j \\ q_0 \in d_{j_0} \end{matrix}$$

To summarize: we have formulated the new framework for solving few- and many-body scattering equations (e.g. the Faddeev ones) in the wave-packet form. This clear matrix form makes it possible to simplify enormously the whole solution of any few-body scattering equation as compared to its conventional form in the following points:

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

• Due to this smoothing, there is no need in deformation of the integration path when solving the singular equation.

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

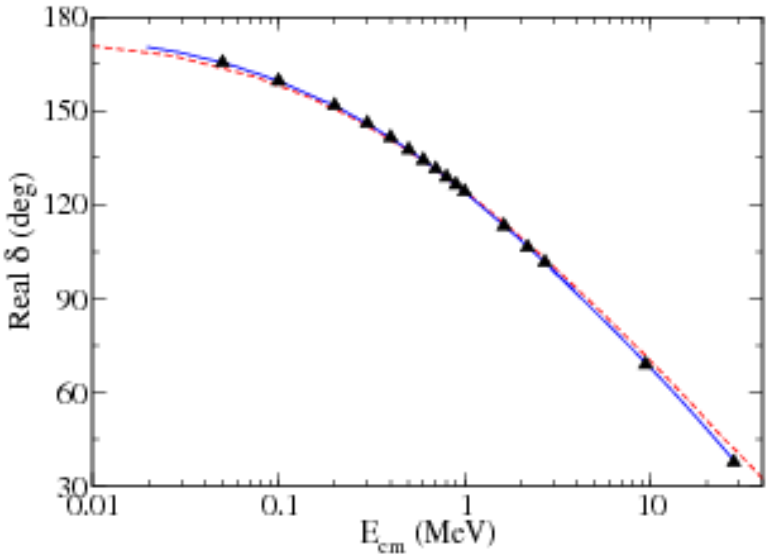
• Because of pixel-like form of the regular matrix which approximate the integral kernel one can parallelize the whole computation of all matrix elements via ultrafast graphical processor (which can operate with pixel-like data sets with ultrafast speed).

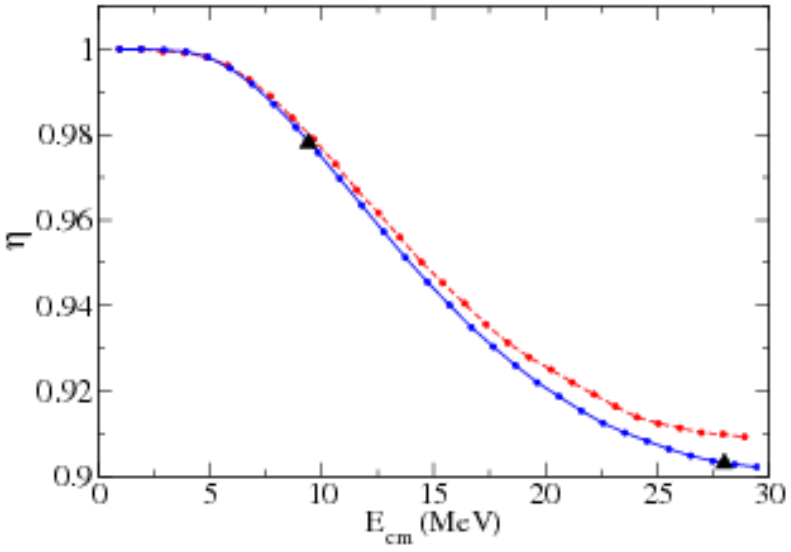
Thus, all these steps lead to fully new technology for scattering computations.

Illustrative examples

The benchmark calculation for n-d elastic scattering:

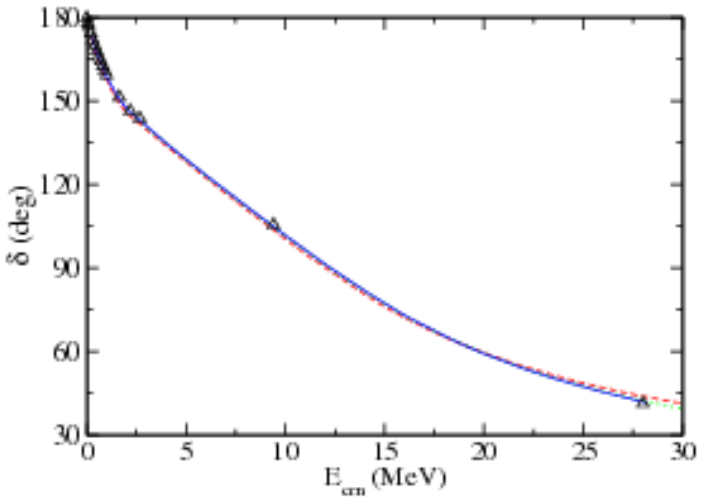
1) *s*-wave quartet channel (*S*=3/2)

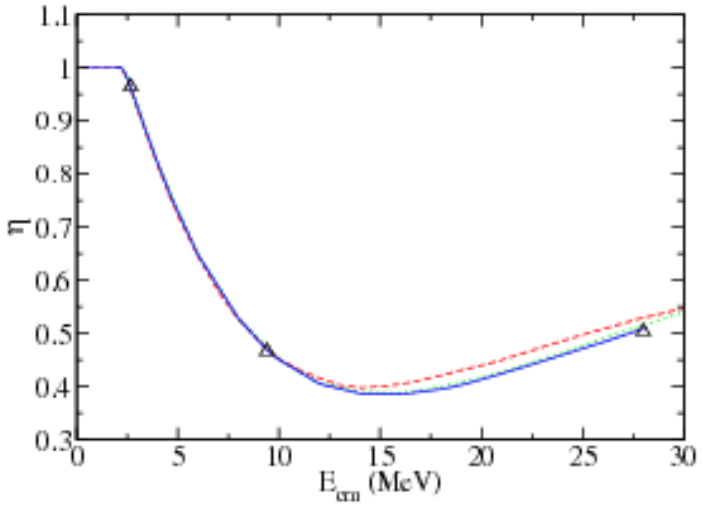




The real part of the s-wave partial phase shift (left panel) and the inelasticity parameter η (right panel) for $n-d$ quartet scattering found by the solution of matrix Faddeev-type reformulated equations on the three-body wave-packet basis at different basis dimensions $M \times N$: 100×100 (dashed curve), 200×200 (solid curve). The black triangles reflects the conventional Faddeev calculation results.

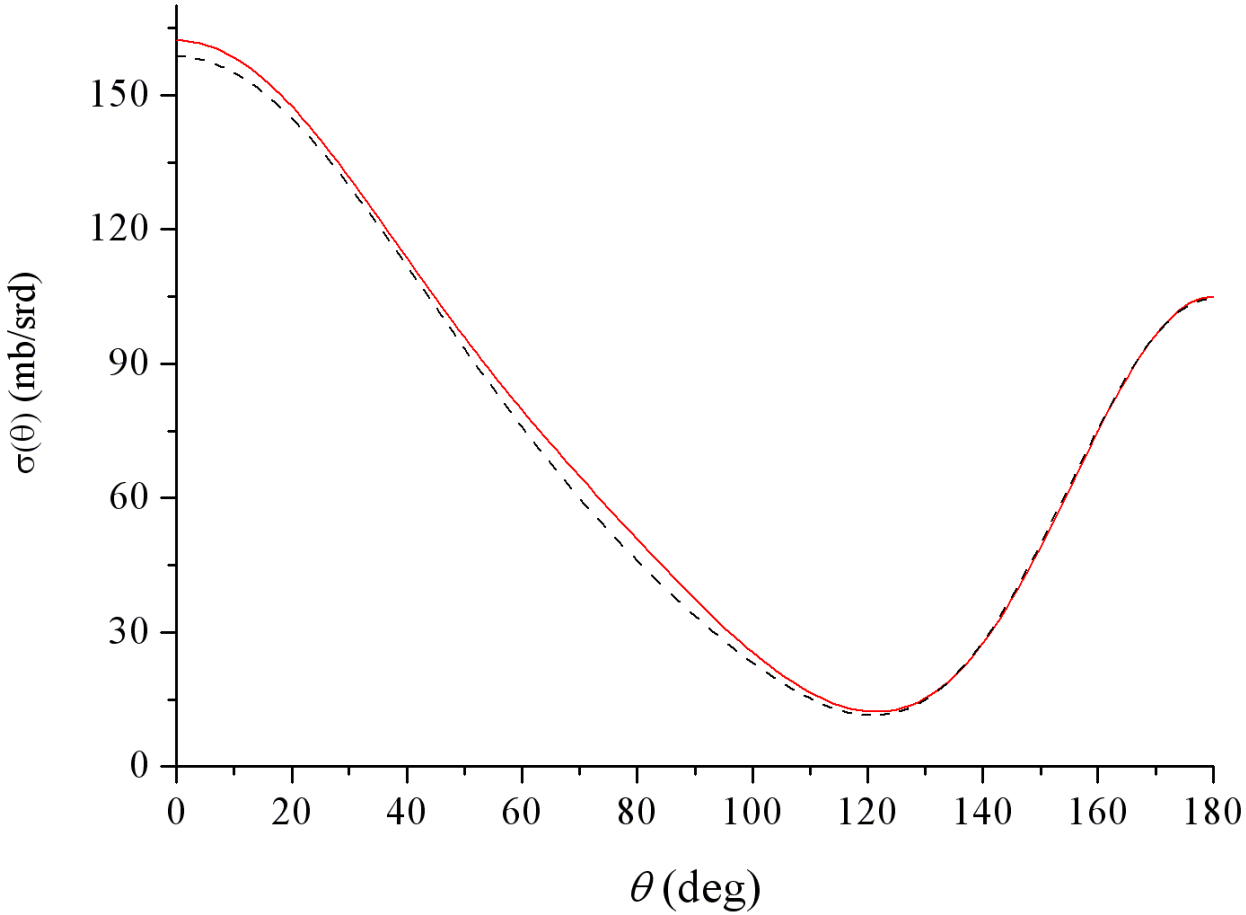
2) n-d elastic scattering: *s*-wave doublet channel (*S*=1/2)





The real part of the s-wave partial phase shift (left panel) and the inelasticity parameter η (right panel) for $n-d$ doublet scattering found by the solution of matrix Faddeev-type equations on the three-body wave-packet basis at different basis dimensions $M \times N$: $(50+50) \times 50$ (dashed curve), $(80+80) \times 80$ (dotted curve), $(100+100) \times 100$ (solid curve). The triangles show the conventional Faddeev calculation results.

Differential cross section of nd elastic scattering at E_{lab}=13 MeV (Nijm *NN* potential): comparison with the Bochum-group results.



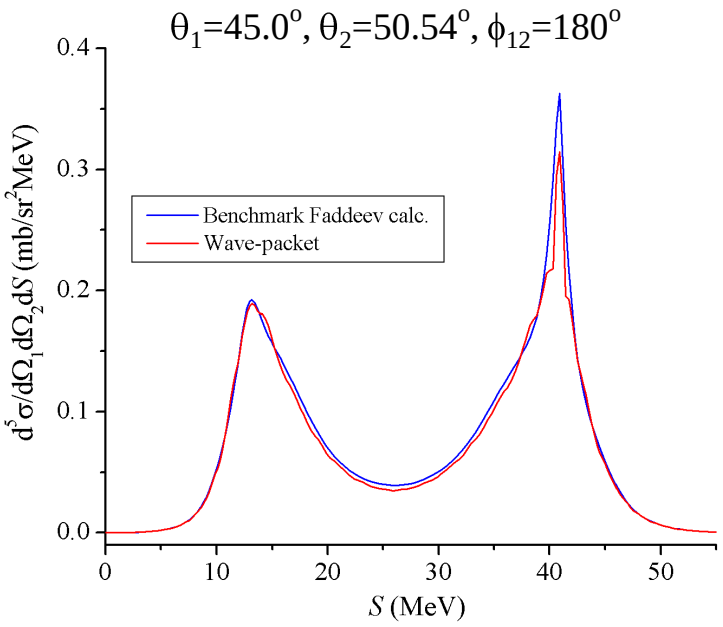
W. Gloeckle*

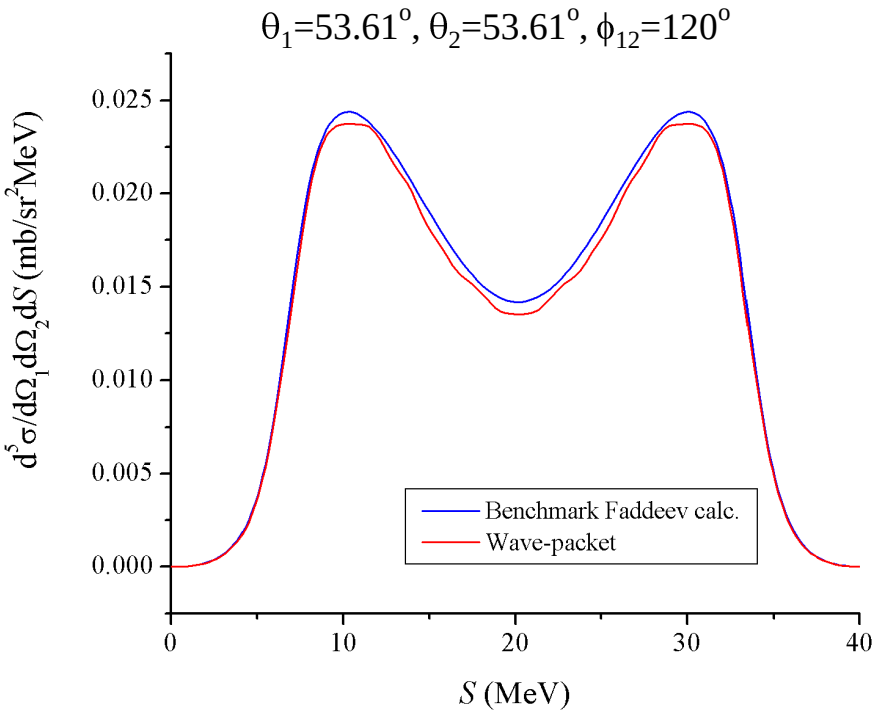
Wave-packet

(J_{max}=7/2)

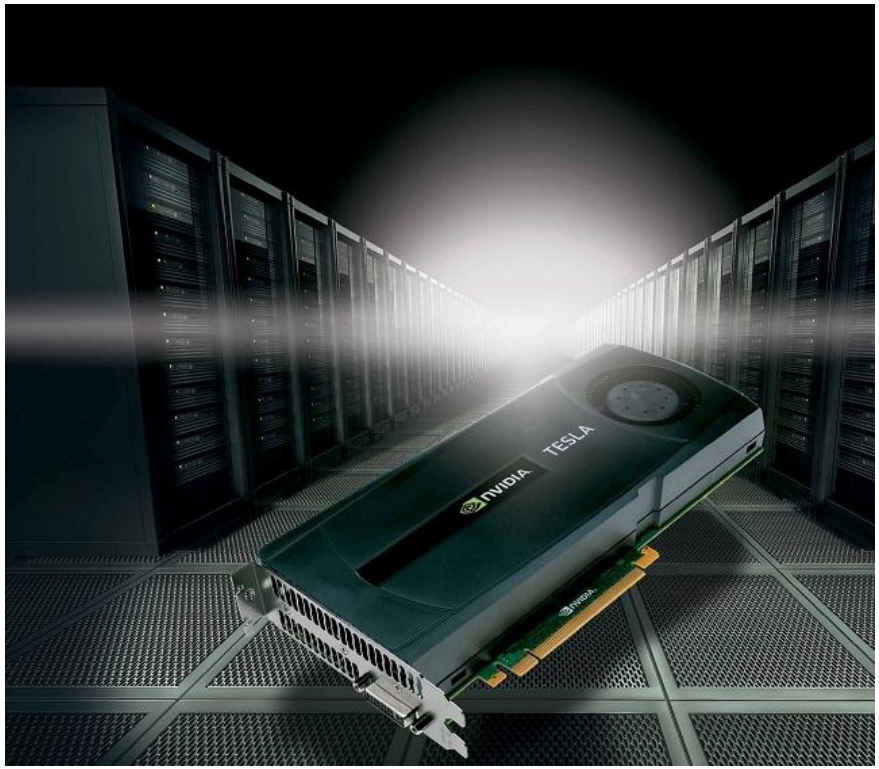
* Cross section is reconstructed from the partial-wave amplitudes (Phys. Rep. **274** (1996))

Three-body breakup n+d→n+n+p differential cross sections at E_{lab}=42 MeV





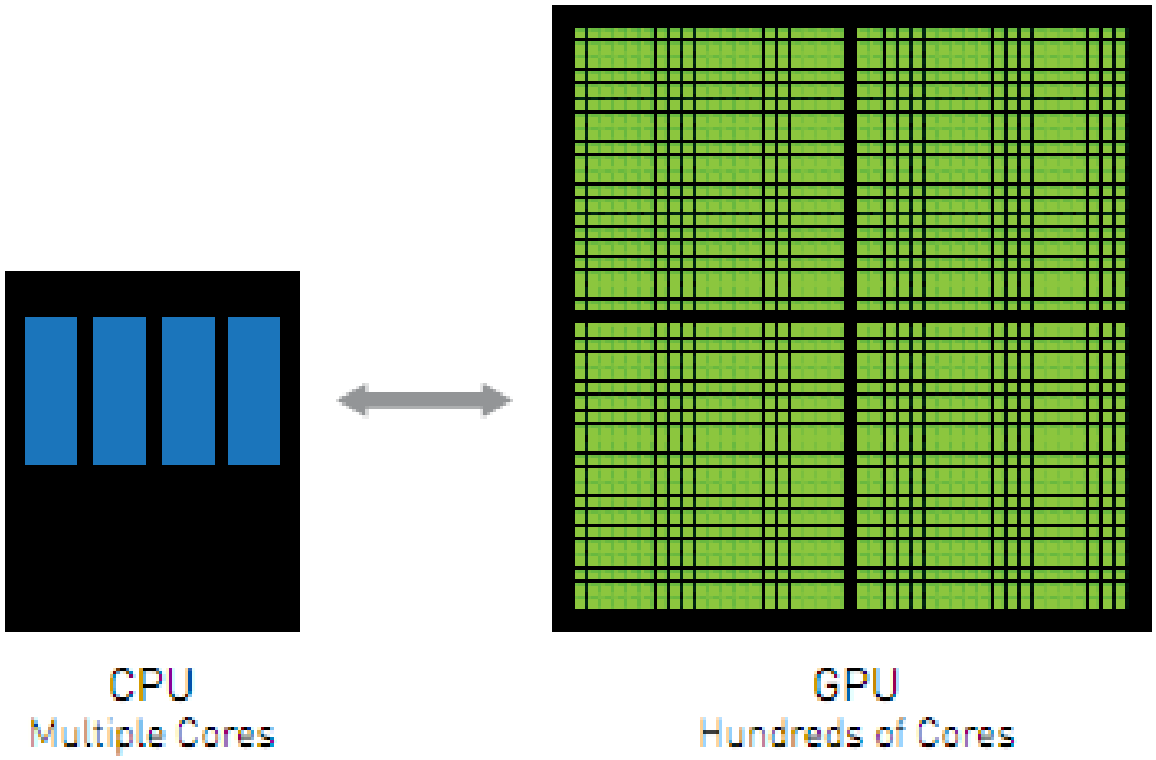
GPGPU-calculations for few-body scattering problems



Supercomputer Blue Gene in Juelich where all the calculations of the Bochum group have been performed

Large Supercomputer Kraken (Cray), University of Tennessee

Principal difference between CPU and GPU architectures

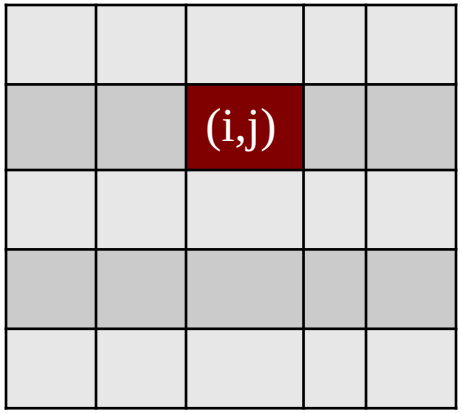


The basic problem in our case is how to reduce multi-dimensional integral equations of few- and many-body scattering to the form most appropriate for the massive-parallel realization, i.e. via quasi-independent parallel computations along many thousands threads.

New technology for solving multi-particle scattering problems

1. From the integral (continuous) kernels, we come to a purely discrete (pixel-like) form of the matrix kernel. So, we get two- (or more) dimensional histograms of high size.

$$K(p,q) \Rightarrow K_{ij} = \frac{1}{\Delta p \Delta q} \int K(p,q) dp dq$$



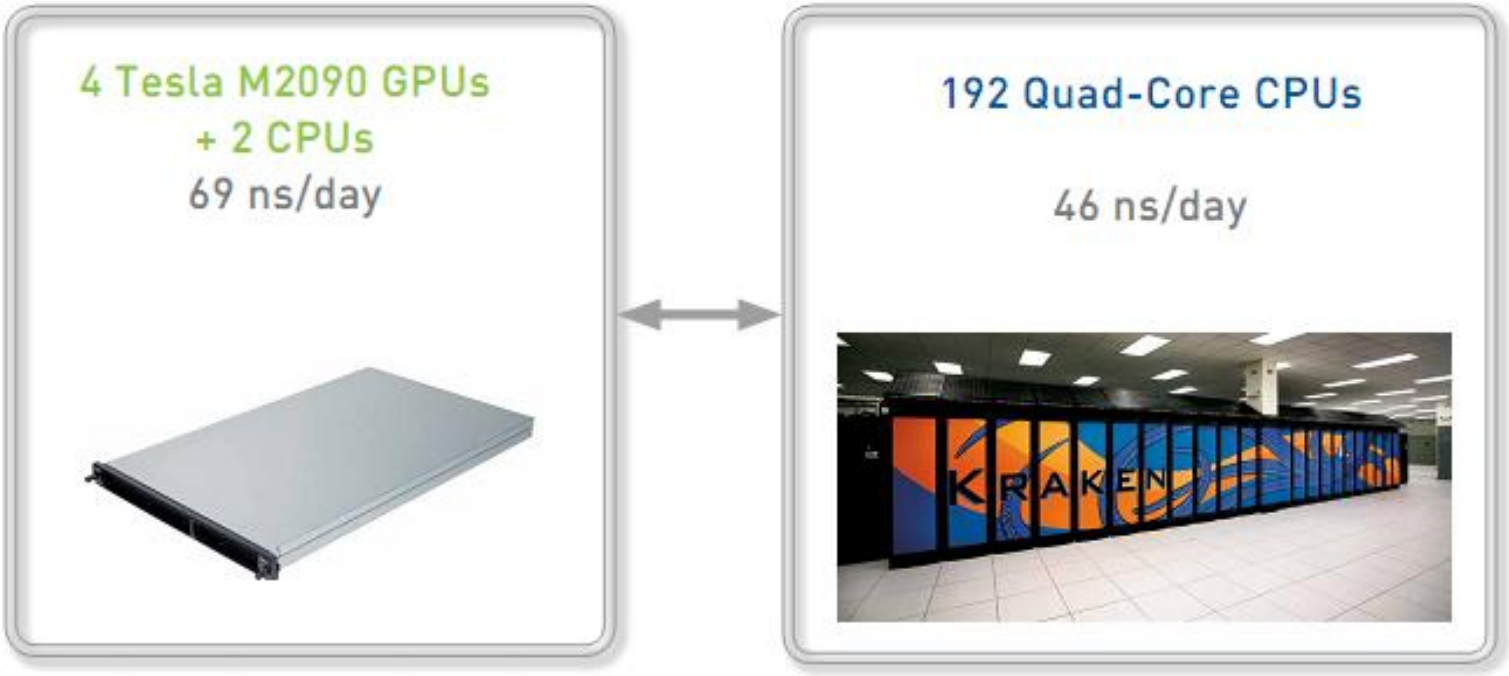
2. Usage of superfast graphical processors for fully parallel computation of the matrix kernels (pixels).

3. Development of parallel algorithms for all above calculations.

New era in computing: GPU computing

"The convergence of new, fast GPUs optimized for computation as well as 3D-graphics acceleration and vendor-neutral, industry-standard software development tools means the real beginning of the GPU computing era"

- Insight64 (NVIDIA)



Some examples for employment of GPU-computing with CUDA-medium in medicine, military applications, modeling the physical processes, etc.

- Air reconnaissance.
- Reconstruction of the detailed object structure on the basis of 3D USD-scanning (wide application in oncology).
- Modeling the blood flow in coronary arteries (application in angiography).
- Modeling the tsunami propagation over oceans and flood picture of the coast.
- Hydrodynamics of viscous fluid flows.
- Lattice QCD.
- Modeling the particle motion in particle accelerators.
- Oil- and gas prospecting.
- Etc., etc.

Air reconnaissance

Conclusion

Joining together the new methods for pixel-like discretization of multi-dimensional integral kernels with new GPGPU-computing in fully parallel mode using ultrafast graphical processors leads to new era in computations for multi-particle scattering problems.