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Wave-packet continuum discretization for quantum scattering

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ABSTRACT

A general approach to a solution of few- and many-body scattering problems based on a continuum-discretization procedure is described in detail. The complete discretization of continuous spectrum is realized using stationary wave packets which are the normalized states constructed from exact non-normalized continuum states. Projecting the wave functions and all scattering operators like t-matrix, resolvent, etc. on such a wave-packet basis results in a formulation of quantum scattering problem entirely in terms of discrete elements and linear equations with regular matrices. It is demonstrated that there is a close relation between the above stationary wave packets and pseudostates which are employed often to approximate the scattering states with a finite L_2 basis. Such a fully discrete treatment of complicated few- and many-body scattering problems leads to significant simplification of their practical solution. Also we get finite-dimensional approximations for complicated operators like effective interactions between composite particles constructed via the Feshbach-type projection formalism. As illustrations to this general approach we consider several important particular problems including multichannel scattering and scattering in the three-nucleon system within the Faddeev framework.

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1. Introduction

The formulation and practical solution for scattering problems in few- and many-body systems entails on many difficulties caused by several reasons: (i) complicated boundary conditions, especially above the breakup thresholds; (ii) separation of the proper physical solution from unphysical ones (e.g. forbidden by the symmetry requirements, etc.); (iii) high dimension of resulting integral or integro-differential scattering equations; (iv) presence of complicated moving singularities in the kernels of few-body scattering equations.

All these difficulties have resulted in the current situation in the field when we are able to treat rather accurately many-body bound states in very complicated systems consisting of tens or hundred particles while we are still unable to treat accurately even three- or four-body systems with Coulomb interactions or the scattering of particles with inner degrees of freedom, e.g. the collision of a few molecules in quantum theory of chemical reactions, or a triple collisions of three- or four nuclei, etc. Moreover, even a solution of conventional three-nucleon scattering problem with realistic interactions requires an extensive usage of supercomputers [1]. It hampers strongly the further progress in this important area. Thus, one can formulate an important goal: it is not only to simplify greatly the solution of some few- and many-body scattering problems, but also to develop a new method in scattering theory which would be quite similar in a spirit to the bound-state problem solving. So that the whole treatment of few- and many-body scattering would be close to the routine bound-state calculations in quantum chemistry or in nuclear physics.

On this way, many L_2-type methods have been suggested and widely developed in the past and even now they are actively progressing. Among these the following methods can be mentioned: the R-matrix type approaches [2], the equivalent quadrature technique [3,4] and the Stieltjes–Tchebyshev moment-theory approach [5,6], the Lorentz integral transform [7], the harmonic oscillator representation [8] and the J-matrix approach [9], the continuum-discretized coupled-channel method (CDCC) [10–12], the pseudochannel extension of the coupled-reaction-channel approach [13], the convergent close coupling approach [14], different realizations of the complex scaling method [15] and others (see also the recent review [16]). All these approaches are utilized rather actively in atomic, chemical and nuclear physics.

In this paper we suggest another general approach for solving a few-body scattering problem based on the usage of special normalized states, the so-called stationary wave packets (WPs) or eigendifferentials. The concept of eigendifferentials was introduced long ago by pioneers of quantum physics: H. Weyl [17], E. Wigner [18], H. Bethe [19] and others to treat non-normalizable continuum states (which do not belong to a Hilbert space) in a framework of the standard theory of Hermitian operators in a Hilbert space. The idea of stationary wave packets turned out to be very fruitful at early stages of the quantum theory development (see e.g. the detailed discussion in the classical textbooks [20,21]).

In our previous papers [22–30] we proposed to employ such normalized WP states as a very convenient discrete basis, onto which one can project out all the scattering operators and wave functions. Because WPs are related explicitly to exact scattering wave functions, many complicated operators such as free or channel resolvents have analytical finite-dimensional approximations in the WP representation. This leads immediately to a replacement of the scattering operators by finite matrices, so that a solution of a few-body scattering problem is reduced to solving simple matrix equations with regular matrix elements instead of multi-dimensional integral equations with singular kernels in a conventional formulation. In addition, our approach results in a very effective numerical scheme for a practical solution. Thus, in the present paper we report the main results of the general WP approach and describe how to reformulate complicated singular few-body scattering equations into a form which allows to solve them straightforwardly on a serial personal computer in a rather short time.

The work has the following structure. Section 2 is dedicated to the description of the eigendifferentials (stationary wave packets) and their interrelation to conventional non-normalized scattering wave functions, on the one hand, and discrete pseudostates resulting from a standard diagonalization procedure for the Hamiltonian matrix, on the other. Section 3 includes a detailed description of different properties and features of the stationary wave packets. In Section 4 we present a discrete

version of the scattering theory based on the WP representation for the scattering operators and wave functions. Section 5 is devoted to the multichannel scattering while Section 6 contains a general description of the three-body wave-packet formalism. In Section 7 a solution of the composite particle scattering off a target-nucleus is discussed. A formulation of the Faddeev equations in a discrete form and their practical solution are given in Section 8. We summarize our main results in Section 9. For the reader's convenience we added the Appendix which contains explicit formulas for the channel resolvent eigenvalues in the WP representation.

2. Discrete representation for the scattering states

Let us introduce some notations. We start here with two-body scattering problem in a stationary formulation. Assume that the potential v is local and spherically symmetrical, so that the angular momentum is conserved and the total Schroedinger equation is reduced to radial equations for a fixed value of the angular momentum l. Below we will deal mainly with the radial parts of the wave functions which justify the partial Schroedinger equation:

$$\left(\frac{1}{2\mu}\left[-\frac{d^2}{dr^2}+\frac{l(l+1)}{r^2}\right]+v(r)\right)\psi^l(r,E)=E\psi^l(r,E), \tag{1}$$

where we use units with $\hbar=1$ and μ is the reduced mass. We will omit also the index l wherever possible until Section 6 and also other indices related to spin, isospin, etc. until the cases they are to be detailed.

The operator in the left-hand side of Eq. (1) is the total Hamiltonian h, which can be written in the form:

$$h=h_0+v, \tag{2}$$

where h_0 is a free motion Hamiltonian. Further we will write all the relationships in an operator form using the Dirac notations, without specifying the representation. It is assumed that the Hamiltonians h_0 and h are Hermitian operators[1] (in an appropriate Hilbert space) and have a simple continuous spectrum $[0,\infty)$.

The total Hamiltonian h may also have a discrete spectrum describing bound states of the system. The corresponding bound-state wave functions of h are denoted as $\{|\psi_n^b\rangle\}_{n=1}^{N_b}$ while the continuum functions are denoted as $|\psi(E)\rangle$. They satisfy the Schroedinger equation (an operator form of Eq. (1))

$$h|\psi(E)\rangle=E|\psi(E)\rangle \tag{3}$$

and the usual orthogonality condition

$$\langle\psi(E)|\psi(E')\rangle=\delta(E-E'). \tag{4}$$

In our study, we also need the scattering wave functions $|\psi_q\rangle=\sqrt{\frac{q}{\mu}}|\psi(E)\rangle$ normalized to the delta-function of momentum $q=\sqrt{2\mu E}$:

$$\langle\psi_q|\psi_{q'}\rangle=\delta(q-q'). \tag{5}$$

2.1. Description of a continuous spectrum in terms of eigendifferentials

A description of continuum meets some difficulty in a stationary formulation of a quantum mechanical problem. As is well known, continuum wave functions for the total and free Hamiltonians, h and h_0, do not have a finite normalization unlike to bound-state wave functions and thus they do not belong to a Hilbert space. Strictly speaking, such non-normalizable states are not eigenfunctions of h

[1] The case of a non-Hermitian total Hamiltonian h with a complex potential will be discussed separately in Section 4.

and h_0 and some basic properties of Hamiltonians (the Hermiticity property) or even an orthogonality of continuum wave functions could not be proven in a normal manner with such non-normalizable set [18,20,21].

Nowadays this formal problem is avoided by using the Dirac delta-function (4) and by generalization of a Hilbert space to a rigged Hilbert space. However, in the past, physicists often employed another formal trick (see e.g. [18–21]) based on the Weyl's eigendifferential concept developed when studying the spectral theory for singular differential operators [17].

The idea is to introduce an interval with a small width ΔE for each value E from the continuum and then to construct the so-called eigendifferential, i.e. integral of the continuum wave function $|\psi(E)\rangle$ over the interval:

$$|\psi(E, \Delta E)\rangle = \int_E^{E+\Delta E} dE|\psi(E)\rangle. \tag{6}$$

It is easy to see that such state is normalizable (due to an integration) and belongs to a Hilbert space. In this way, one can generalize the conventional definition of a state normalization: the state $|\psi(E)\rangle$ is treated as normalizable if its eigendifferential has a finite norm [19].

To treat a whole continuum, it should be divided into non-overlapping intervals (i.e. it should be discretized). The system of eigendifferentials forms the orthonormal set [21]:

$$\langle\psi(E', \Delta E')|\psi(E, \Delta E)\rangle = \begin{cases} \Delta E, & \text{for the same intervals,} \\ 0, & \text{for different intervals.} \end{cases} \tag{7}$$

It is important to stress that the set of such eigendifferentials gives a diagonal representation for the Hamiltonian:

$$\frac{\langle\psi(E', \Delta E')|h|\psi(E, \Delta E)\rangle}{\Delta E} = \begin{cases} E + \dfrac{1}{2}\Delta E, & \text{for the same intervals,} \\ 0, & \text{for different intervals.} \end{cases} \tag{8}$$

Besides this, they have a finite overlap with initial (non-normalized) states

$$\langle\psi(E')|\psi(E, \Delta E)\rangle = \begin{cases} 1, & E' \in (E, E + \Delta E), \\ 0, & E' \notin (E, E + \Delta E). \end{cases} \tag{9}$$

A complete system of eigenfunctions for the Hermitian Hamiltonian h in the eigendifferential formalism is built from bound-state wave functions $|\psi_n^b\rangle$ and eigendifferentials [18,21]. In other words, for an arbitrary wave function $|\Phi\rangle$ one can write down the following expansion:

$$|\Phi\rangle = \sum_{n=1}^{N_b} C_n|\psi_n^b\rangle + \sum C(E)|\psi(E, \Delta E)\rangle, \tag{10}$$

where the sum over an infinite but accountable set of eigendifferentials has rather a symbolic meaning. However further one can pass to a limit $\Delta E \to 0$ which leads immediately to a conventional expansion of the arbitrary function $|\Phi\rangle$ over the bound-states and functions of the continuum:

$$|\Phi\rangle = \sum_{n=1}^{N_b} C_n|\psi_n^b\rangle + \int_0^{\infty} dE\tilde{C}(E)|\psi(E)\rangle. \tag{11}$$

The discrete sum in Eq. (10) goes to the integral expansion in Eq. (11) over continuum wave functions $|\psi(E)\rangle$ in the sense of a Riemann–Stieltjes integral [21]. Also it can be shown [21] that the finite normalization condition for eigendifferentials (7) leads just to a delta-function normalization of continuum states (4).

Today such a way of definition of the Hamiltonian eigenfunctions for a continuous spectrum is not used practically, as was noted above. But in our approach one employs such eigendifferentials as basis states to treat a scattering problem in a discrete representation. Below we demonstrate that this "classical" way is turned out to be extremely fruitful for practical calculations in few-body scattering problems.

There is also the another very popular concept for a treatment of a discretized continuum: the pseudostates. It will be demonstrated below that these two ways of discretization: via eigendifferentials and via pseudostates are closely interrelated.

2.2. Pseudostates and L_2 discretization of a continuum

As is known, pseudostates arise in an approximate treatment of continuous spectrum of a quantum system based on a projection of scattering wave functions into an orthogonal L_2 basis set $\{|\phi_n\rangle\}_{n=1}^N$ with a finite dimension N.

If one substitutes the expansion of a Hamiltonian eigenfunction in the basis functions $|\psi\rangle = \sum_{n=1}^N C_n|\phi_n\rangle$ into the Schroedinger equation (3) one gets the following system of algebraic linear equations for the expansion coefficients $\{C_n\}_{n=1}^N$

$$\sum_{k=1}^{N}[h_{nk} - E\delta_{nk}]C_k = 0, \quad n = 1, \ldots, N, \tag{12}$$

which corresponds to the eigenvalue problem for the Hamiltonian matrix with the elements $h_{nk} \equiv \langle\phi_n|h|\phi_k\rangle$. After a diagonalization of the Hamiltonian matrix one gets a set of eigenvalues[2] $\{\epsilon_n^*\}_{n=1}^N$ and eigenfunctions $|\psi_n\rangle = \sum_{k=1}^N C_k^n|\phi_k\rangle$ $(n = 1, \ldots, N)$. This discrete set can be divided into two groups: the eigenfunctions with lower eigenvalues describe the system bound states if they exist (in the case of a short-range potential their number is finite) while the remained eigenstates correspond to the continuum wave functions at discrete energies ϵ_n^*. Unlike to the exact continuum functions these discrete eigenstates have a finite norm and their eigenvalues define the discretized continuum. That is why they are usually referred to as *pseudo*states of the Hamiltonian h.

For the above pseudostates, the conditions similar to those given in Eqs. (7)–(8) for eigendifferentials are valid:

$$\begin{aligned}&\langle\psi_n|\psi_k\rangle = \delta_{nk},\\ &\langle\psi_n|h|\psi_k\rangle = \epsilon_n^*\delta_{nk}.\end{aligned} \tag{13}$$

An employment of pseudostates instead of exact scattering functions in practical scattering calculations meets the well known difficulty related to the difference in their normalization. The functions of pseudostates behave in some inner region like the scattering wave functions but, in sharp contrast with the latter, they vanish in the asymptotic region. Nevertheless, the functions of pseudostates together with bound-state wave functions form a complete set of basis functions, and this set can be used to approximate the spectral expansions of the scattering operators or scattering wave functions.

2.3. The equivalent quadrature concept

Very often it is necessary to find not operator itself, but only its matrix elements with normalized functions $|\Phi\rangle$. The example for such an employment is the calculation of transition probabilities between the bound states of subsystem via the intermediate continuum states, in particular, the calculation of response functions in the Lorentz integral transform (LIT) method [7] or the calculation of t-matrix elements on the basis of spectral expansion of the total resolvent of the system [6].

Let us consider a matrix element of some operator $B = f(h)$ which is a function of the Hamiltonian h using the spectral expansion of the operator B in a complete set of the Hamiltonian eigenfunctions:

$$\langle\Phi|B|\Phi\rangle = \sum_{n=1}^{N_b} f(\epsilon_n^*)|\langle\Phi|\psi_n^b\rangle|^2 + \int_0^\infty dEf(E)|\langle\Phi|\psi(E)\rangle|^2. \tag{14}$$

[2] Below we denote eigenvalues by an upper asterisk index to distinguish them from discretization interval end-points.

As is evident, the spectral expansion (14) includes not wave functions themselves but their quadratic forms $|\langle\Phi|\psi(E)\rangle|^2$. Such quantities are of L_2 type, so that there is no problem with a normalization of scattering wave functions. Moreover, these quadratic forms are finite and positive definite functions of energy. Therefore, the integral over continuous spectrum can be approximated by a discrete sum over respective pseudostates:

$$\langle\Phi|B|\Phi\rangle \approx \sum_{n=1}^{N_b} f(\epsilon_n^*)|\langle\Phi|\psi_n^b\rangle|^2 + \sum_{n=N_b+1}^{N} f(\epsilon_n^*)|\langle\Phi|\psi_n\rangle|^2 \tag{15}$$

and such a "spectral expansion" over pseudostates can be treated as some effective quadrature for the integral over continuum in Eq. (14). This approach has been suggested earlier for solution of different particular problems in atomic physics [3–6] using finite-dimensional approximations for Green functions. E.g., a conception of an equivalent quadrature (EQ) was introduced within the framework of the moment-theory approach for calculation of non-negative spectral densities [3,5]. The mesh points of the EQ coincide with pseudostate energies and corresponding weights are determined formally from relations between discrete and continuous quantities:

$$|\langle\Phi|\psi_n\rangle|^2 = \omega_n|\langle\Phi|\psi(\epsilon_n^*)\rangle|^2, \quad n = N_b + 1, \ldots, N \tag{16}$$

which are valid at discrete pseudostate energies ϵ_n^*.

One important result of the equivalent quadrature technique is the fact the quadrature weights do not depend upon the function $|\Phi\rangle$ and are determined actually by pseudostate wave functions and by the spectral density of the particular system. So that, the values ω_n can be treated as the coefficients for transformations from normalizable states $|\psi_n\rangle$ to non-normalizable functions $|\psi(\epsilon_n^*)\rangle$.

In general, finding the weights of the equivalent quadrature is highly non-trivial problem because the exact scattering wave functions $|\psi(E)\rangle$ are still unknown. However, for many problems when one needs only complete spectral sum, knowledge of these weights is not required. For example, the pseudostate functions are used for inclusion of intermediate continuum states for excitations of projectile or target in description of composite particle scattering in atomic [14] and nuclear [10] physics. In these cases, as a rule, the pseudostates are employed in expansion of a total wave function of the system to perform a coupled channel reduction of the initial many-body problem.

However, it is still possible to find scattering observables just from individual pseudostate wave functions if the EQ is known. In fact, if to write down an expression for the elastic scattering amplitude:

$$A(E) = \langle\psi_0(E)|v|\psi(E)\rangle, \tag{17}$$

it is easy to see that the function $v|\psi_0(E)\rangle$, where $|\psi_0(E)\rangle$ is a free motion function, is square-integrable in case of a short-range potential v. So that, one can employ the properly normalized pseudostate instead of the exact scattering wave function:

$$\bar{A}_n \approx \langle\psi_0(\epsilon_n^*)|v|\psi_n\rangle. \tag{18}$$

To find direct relation between "continuous" $A(E)$ and "discrete" $\bar{A}_n$ amplitudes, one can use the EQ definition (16) which results in:

$$A(\epsilon_n^*) \approx \frac{\bar{A}_n}{\sqrt{\omega_n}}. \tag{19}$$

Actually, the problem of evaluation of ω_n is related to finding a spectral density in the continuous spectrum of h. One of the methods is to evaluate moments of the energy distribution using spectral expansion in pseudostates. Then, the equivalent quadrature weights can be found from a solution of complicated set of nonlinear algebraic equations [6]. However, to find the EQ, the eigendifferential formalism can be used.

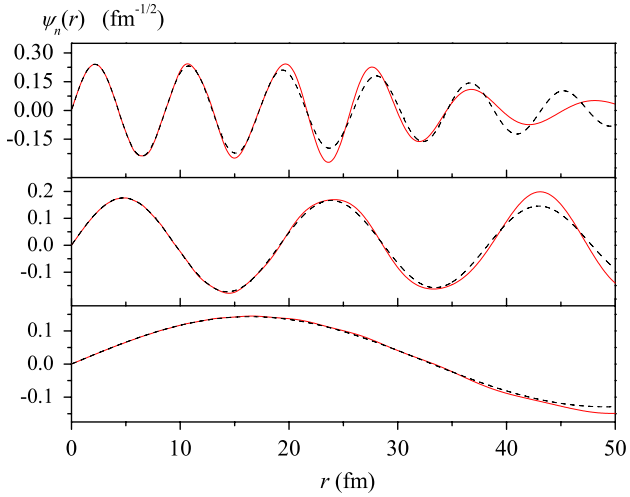

Fig. 1. Comparison of pseudostates (solid curves) of the free motion Hamiltonian obtained in a basis of Gaussians with exact eigendifferentials (dashed curves) constructed for the same distribution of eigenenergies of the Hamiltonian discretized continuum.

2.4. Pseudostates as approximations for eigendifferentials

In our previous works [23,24,27] the following way for finding the coefficients of transformation from normalizable functions to non-normalizable ones has been suggested. This method is based on the observation that pseudostate wave functions are very similar to eigendifferentials. In particular, both types of functions behave in the inner region like an exact scattering wave function, whereas in the asymptotic area they vanish differently in accordance with their own properties. Moreover, functions from both sets are normalized and the Hamiltonian matrices in both sets are diagonal.

It means one can treat pseudostates as approximations just for eigendifferentials rather than for exact non-normalizable scattering wave functions.[3] Of course, this approximation is valid only when eigenenergies of both states (8) and (13) are coincided.

In Fig. 1 we compare pseudostates of the free Hamiltonian found in the Gaussian basis (see details in Ref. [27]) with exact eigendifferentials (normalized to unity) constructed for the same distribution of eigenenergies ϵ_n^*. It is clear that both type functions are nearly coincide in some inner domain.

Further, it is easy to see that the coefficients of transformation to non-normalizable states (see the definition (6)) are given simply by the widths ΔE in the discretization procedure for eigendifferentials:

$$A(E) \approx \frac{\langle \psi_0(E)|v|\psi(E,\Delta E)\rangle}{\Delta E}. \tag{20}$$

Using the direct correspondence between eigendifferentials (with the normalization factor) and pseudostates (here the discretization width ΔE may depend on the index n)

$$\frac{\langle \psi_0(\epsilon_n^*)|v|\psi(\epsilon_n^*,\Delta E_n)\rangle}{\sqrt{\Delta E_n}} \approx \langle \psi_0(\epsilon_n^*)|v|\psi_n\rangle, \tag{21}$$

and comparing Eqs. (19) and (20), one gets an approximate relation:

$$\omega_n \approx \Delta E_n. \tag{22}$$

[3] It is worth noting that the interrelation of pseudostates and eigendifferentials has been also proved in Refs. [10,11] on the basis of the CDCC method. In this approach these two types of states are considered to treat a composite particle scattering off heavy target. However, direct relations between them have been established for the equidistant discretization distribution only.

So that, we find an amazing result: the coefficients of transformation from pseudostates to exact continuum wave functions are determined, first of all, by the distribution of discrete pseudostates energies ϵ_n^* rather than by the form of basis functions $|\phi_n\rangle$ themselves. Actually the form of basis functions determines implicitly the pseudostate energy distribution: it will be different for various basis sets.

It would be very appropriate to give here some clear example. Let us consider a free particle motion in a spherical box with radius R. The solution of a radial Schroedinger equation for S-wave in this case is an infinite set of wave functions (normalized to unity)

$$\psi_{0n}(r) = \sqrt{\frac{2}{R}} \sin q_n^* r, \quad q_n^* = \frac{\pi n}{R}, \; n = 0, \ldots, \tag{23}$$

instead of exact free motion states:

$$\psi_{0q}(r) = \sqrt{\frac{2}{\pi}} \sin qr. \tag{24}$$

For this case the weights of the EQ do not depend on the index n and can be found explicitly:

$$\omega_n = \frac{\pi}{R}. \tag{25}$$

It is clear that this quantities coincide *exactly* to the discrete momentum differences $d_n = q_{n+1}^* - q_n^*$ (momentum analog of the energy widths in (6)). In other words, one can determine the weights of the EQ directly via the discretization width

$$\omega_n = d_n \tag{26}$$

rather than via the size of the box R (although they are interrelated).

When we are dealing with an L_2-discretization using an arbitrary basis, this can be treated as a solution of the scattering problem in a box with blurred boundaries but these boundaries are difficult to determine explicitly. However they do impact on a discrete energy distribution which is used for finding approximate weights or widths of discretization intervals. So that, eventually in order to derive the values of scattering observables from the discrete energy distribution one should determine the spectral partition parameters using eigenvalues ϵ_n^* of pseudostates obtained from the Hamiltonian matrix diagonalization. In general case, the energy interval widths ΔE_n would be different for different n.

Thus, our main idea here is that pseudostates are approximations for exact eigendifferentials. Surely, the above argumentation is not strict but plausible. It is also necessary to have similarity between pseudostates and eigendifferentials at least within the interaction range. It means that the size of the pseudostate basis should be rather large and the interval widths to be rather small. Unfortunately, it is difficult to give more strict conditions for such a replacement here. Some estimates can be found in Ref. [29].

Below we formulate a fully discrete version of a stationary scattering theory using the eigendifferential (wave-packet) formalism, while in practical realizations we replace often exact eigendifferentials with pseudostates found from the Hamiltonian matrix diagonalization on an appropriate basis. Both these points make it possible to simplify greatly the practical solving of few-body scattering problems.

3. Stationary wave packets and their properties

In the approach which will be used everywhere in this work, the eigendifferentials will be employed as primary basis functions upon which all wave functions and operators will be expanded. In other words, we will treat scattering problems in a discrete representation.

We rename eigendifferentials as stationary wave packets because the name seems to us more physical and clear for understanding. The approach developed – we refer to it as the wave-packet continuum discretization method (WPCD) – takes the advantages of the above L_2 techniques and simultaneously gives an accurate solution of few-body equations.

3.1. Basic definition of stationary wave packets

The stationary wave packets are constructed from exact wave functions of continuous spectrum as their eigendifferentials (normalized to unity). But WPs are considered here as ordinary functions and thus the details of a partition procedure for a continuous spectrum have to be defined.

Let us restrict the continuous spectrum of the free Hamiltonian h_0 $[0, \infty)$ with some maximal value of energy $E_{\max}$ and then divide the whole interval $[0, E_{\max}]$ into finite number of non-overlapping intervals $[\mathcal{E}_{i-1}, \mathcal{E}_i]_{i=1}^N$ (where $\mathcal{E}_0 = 0$ and $\mathcal{E}_N = E_{\max}$) which we recall, according to Ref. [10], as discretization bins. We assume here that the value $E_{\max}$ is finite although sufficiently large in order to provide convergence to the exact solution of the problem to be treated. Every such an energy bin corresponds to the interval $[q_{i-1}, q_i]$ on the momentum axis q where $q = \sqrt{2\mu E}$ and μ is the reduced mass. For the sake of convenience we will denote both the momentum and the energy bins by a symbol $\mathfrak{D}_i$ (i is an interval number). Also we denote widths of momentum and energy intervals as follows:

$$d_i = q_i - q_{i-1}, \qquad D_i = \mathcal{E}_i - \mathcal{E}_{i-1}. \tag{27}$$

Further we consider the complete set of continuous spectrum states $|\psi_{0q}\rangle$ for the free Hamiltonian h_0 (for each partial wave l) normalized as in Eq. (5). Now we define the free stationary wave packets as integrals of free motion wave functions over the discretization bins as in Eq. (6):

$$|x_i\rangle = \frac{1}{\sqrt{B_i}} \int_{\mathfrak{D}_i} dq f(q) |\psi_{0q}\rangle, \quad i = 1, \ldots, N, \tag{28}$$

where $f(q)$ is some weight function and B_i is a normalization coefficient related to each other by the formula:

$$B_i = \int_{\mathfrak{D}_i} dq |f(q)|^2. \tag{29}$$

By modifying the weight function $f(q)$ one can get different types of WPs. In particular, the case $f(q) = \sqrt{q/\mu}$ corresponds to the energy wave-packets which coincide with eigendifferentials (6) up to normalization factors. The case $f(q) = 1$ leads to momentum WPs, etc. However it is important to note that when the partition used is sufficiently dense (i.e. for small bin widths) the particular form of the weight function does not matter. Moreover in practical calculations one can replace energy WPs with momentum ones (for the same partition) and errors related to this replacement are very small.

According to the definition (28) it is easy to show that the states $|x_i\rangle_{i=1}^N$ form an orthonormalized set [23]:

$$\langle x_i | x_j \rangle = \delta_{ij}, \quad i, j = 1, \ldots, N. \tag{30}$$

Then it is straightforward to get a formula for the overlap integral between WP states and initial plane waves:

$$\langle x_i | \psi_{0q} \rangle = \begin{cases} \dfrac{f(q)}{\sqrt{B_k}}, & q \in \mathfrak{D}_i, \\ 0, & q > q_N. \end{cases} \tag{31}$$

The free Hamiltonian matrix (and also the matrix of any operator depending upon h_0 or just commuting with it) is *diagonal* in such a basis while the respective eigenvalues depend on the weight function:

$$\langle x_i | h_0 | x_j \rangle = \frac{\delta_{ij}}{B_i} \int_{\mathfrak{D}_i} |f(q)|^2 \frac{q^2}{2\mu} dq. \tag{32}$$

In the case of energy WPs, the eigenvalues of h_0 are just the bin midpoints:

$$\langle x_i | h_0 | x_i \rangle \equiv \mathcal{E}_i^* = \frac{1}{2}(\mathcal{E}_{i-1} + \mathcal{E}_i), \tag{33}$$

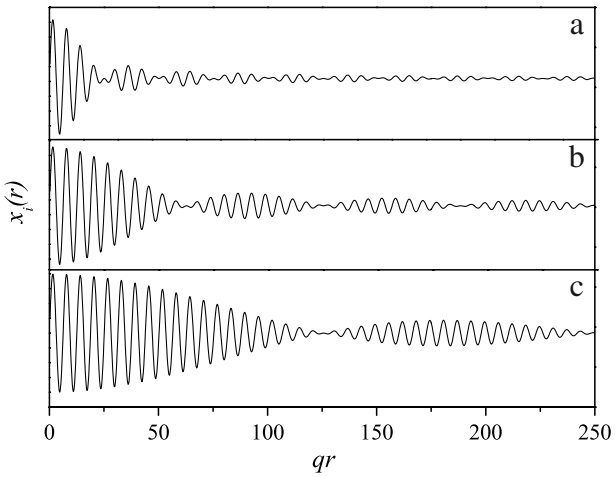

Fig. 2. Coordinate behavior of s-wave WP states $x_i(r)$ for different values of bin width d_i in ratio to momentum value q: $d_i/q = 0.25$ (a), $d_i/q = 0.1$ (b) and $d_i/q = 0.05$ (c).

and in the case of momentum WPs, the eigenvalues are:

$$\mathcal{E}_i^* = \frac{1}{6\mu}(q_{i-1}^2 + q_{i-1}q_i + q_i^2). \tag{34}$$

Such WP states will be used to carry out all our calculations. From practical point of view the wave-packet set can be used in any scattering calculations on the same footing as usual discrete L_2 bases like the harmonic oscillator basis or a basis of Gaussians. However, in contrast to those, such WP basis states give a diagonal representation for a Hamiltonian matrix and have a direct relation (31) to exact continuum wave functions.

3.2. Behavior of wave-packet functions in configuration and momentum spaces

The WP functions have an interesting behavior both in coordinate and momentum spaces. Consider for simplicity the case of $f(q) = 1$. It is easy to show [23,27] that in coordinate space WP functions behave as follows (here we use the reduced radial part of a wave function for s-wave):

$$x_i(r) = \sqrt{\frac{2d_i}{\pi}}\sin(q_i^* r)\frac{\sin(d_i r/2)}{d_i r/2}, \tag{35}$$

where $q_i^* = \frac{1}{2}(q_{i-1} + q_i)$ is a midpoint of the interval $\mathfrak{D}_i$. So that, free WPs nearly coincide with non-normalized continuum wave functions in the area $r \ll r_i = \frac{2}{d_i}$. As is seen from Eq. (35), the "packetting" procedure defined in Eq. (28) results in an additional decreasing factor which just provides the wave function with finite normalization.

In Fig. 2 the coordinate behavior of three WP states (35) are compared for different ratios of bin width d_i and its midpoint value q_i^*. It follows from the figure that the radial behavior of the WPs resemble the characteristic picture of beats (i.e. dual-frequency oscillations) and the smaller ratio d_i/q_i^* corresponds to the slower decay of the WP function. Therefore such functions can be employed to approximate the non-normalized continuum wave functions on longer distances. This property is crucially important for few-body scattering calculations because the Faddeev components of the total wave function have a specific long-range asymptotic behavior which must be reproduced correctly.

In the momentum representation, the free WP functions are simple step-like functions: they do not vanish only for the momentum interval coinciding with their bin, i.e. only for the on-shell region.

In this area they are fully determined by the weight function $f(q)$:

$$x_i(q) = \frac{f(q)(\theta(q - q_{i-1}) - \theta(q - q_i))}{\sqrt{B_i}}, \tag{36}$$

where the θ is the Heaviside step-like function.[4] When $f(q) = 1$ all the wave functions in the momentum WP representation take a histogram form. Being generalized onto a few-body case, the free few-body WP basis functions are built as direct products of step-like functions along every independent momentum variable. In this way, the whole momentum space is replaced by a finite momentum lattice. In this sense we will refer to this basis as *a lattice basis*.

3.3. Wave packets as a basis

For further investigations, the important questions are: does the WP set form a basis and how one can prove a convergence of the results with increasing a basis dimension. It should be noted here that for the set of pseudostates the problem of completeness does not exist because the pseudostates jointly with the bound states form the same linear span as the initial L_2 basis set. So that, the set of the pseudostates and bound states form a basis which becomes complete in the limit $N \to \infty$.

It is clear that, unlike to the eigendifferential case when $\Delta E \to 0$, the WP set does not form a complete basis in a full Hilbert space if bin widths are kept to be finite. But one can introduce the WP subspace $\mathcal{H}_P$ in which the orthonormal set $\{|x_i\rangle\}_{i=1}^N$, of course, forms a basis. The projection operator onto WP subspace is defined as usually:

$$\mathfrak{p} = \sum_{i=1}^{N} |x_i\rangle \langle x_i|. \tag{37}$$

Thus we will refer below to the WP set as a WP basis keeping in mind it is the basis in a subspace $\mathcal{H}_P$.

One has to make here some estimates concerning the convergence of the results obtained in $\mathcal{H}_P$ to exact scattering solutions with increasing the basis dimension.

The exact unit operator I, which can be written in the following form:

$$I \equiv \sum_{i=1}^{N} I_i + I_\mathrm{r} = \sum_{i=1}^{N} \int_{\mathfrak{D}_i} |\psi_{0q}\rangle \langle\psi_{0q}| dq + \int_{q_N}^{\infty} |\psi_{0q}\rangle \langle\psi_{0q}| dq, \tag{38}$$

is replaced in the WP approach with the wave-packet projection operator $\mathfrak{p}$ given by the Eq. (37). This replacement implies two following approximations:

(i) the infinite continuous spectrum is truncated with the maximal momentum value q_N and the residual spectral integral I_r is neglected;
(ii) exact partial spectral projection operators I_i are replaced with the WP partial projectors $|x_i\rangle\langle x_i|$.

Surely, these approximations are not valid in a full Hilbert space. But keeping in mind numerical applications of the method one can compare the mean values of operators I and $\mathfrak{p}$ in some L_2 normalized state $|\Phi\rangle$ having an effective range r_0. To satisfy the following conditions (corresponding to the above points (i) and (ii))

$$\langle\Phi|\mathfrak{p}|\Phi\rangle \approx \langle\Phi| \sum_{i=1}^{N} I_i |\Phi\rangle, \qquad \langle\Phi|I_r|\Phi\rangle \ll \langle\Phi| \sum_{i=1}^{N} I_i |\Phi\rangle \tag{39}$$

[4] Here the θ-function is defined as follows:

$$\theta(q) = \begin{cases} 1, & q \geq 0 \\ 0, & q < 0. \end{cases}$$

one has to have sufficiently small bin widths d_i and sufficiently high maximal momentum value q_N [27]:

$$d_i \ll \frac{1}{r_0} \ll q_N, \quad i = 1, \ldots, N. \tag{40}$$

With these restrictions one can choose for the practical realization the proper conditions for the momentum bin partition $\{\mathfrak{D}_i\}_{i=1}^N$. Then one can check the convergence of the results with increasing a wave-packet basis dimension, when the bin widths become smaller and the maximum value q_N becomes higher. This procedure simulates changes in eigenvalue $\{\epsilon_n^*\}$ distributions for pseudostates with increasing a basis dimension N.

One can employ, for example, distributions (grids) transforming a finite interval to whole numerical axis of a momentum variable, e.g. the Tchebyshev grid [28]:

$$q_i = q_{\mathrm{m}} \tan\left[\frac{2i-1}{4N}\pi\right], \quad i = 1, \ldots, N, \tag{41}$$

where q_{m} is a common scale parameter.

The usage of such grid points is convenient because this makes it possible to study the convergence of the results with increasing the basis dimension as in the usual L_2-basis case. One can expect that the result obtained in the WP representation approaches the exact solution with increasing the basis dimension N.

3.4. Construction of WP states for the total Hamiltonian

Similarly to the free Hamiltonian (h_0) case, one can build a WP set for the total Hamiltonian $h = h_0 + v$. For this purpose, a partition of continuum for the total Hamiltonian (for a given partial wave) into non-overlapping bins $\{\Delta_k = [\epsilon_{k-1}, \epsilon_k]\}_{k=1}^M$ with $\epsilon_0 = 0$ and $\epsilon_M = E_{\max}$ (or $\Delta_k = [q_{k-1}, q_k]$) is introduced. In general, this partition might be different from that for the free WPs $\{\mathfrak{D}_i\}$. The *scattering wave-packets* are defined as integrals of exact scattering wave functions $|\psi_q\rangle$ over the intervals chosen:

$$|z_k\rangle = \frac{1}{\sqrt{C_k}} \int_{\Delta_k} dq\, w(q) |\psi_q\rangle, \tag{42}$$

where C_k and $w(q)$ are the normalization coefficients and weight functions respectively. They have the same properties as free WPs. However, the total Hamiltonian may have also a discrete spectrum. In this case one has to add bound-state wave functions of h to the scattering WP set to obtain complete WP set corresponding to the total Hamiltonian h.

In practical solution, the basic problem arises, i.e. how to construct these scattering WPs without solving the initial scattering problem. Here one exploits an idea of similarity between eigendifferentials (WPs) and pseudostates discussed in Section 2. So that, free WPs can be used as a basis to construct scattering WPs for the total Hamiltonian h as its pseudostates. For this purpose we apply a diagonalization procedure for the total Hamiltonian matrix in a free WP basis. As a result we get a discrete sets of eigenvalues ϵ_k^* and respective eigenvectors $|\tilde{z}_k\rangle$.

Since the free WP basis functions (in the momentum space) are step-like functions, the momentum dependence of all functions expressed via such a basis have also a histogram-like form. An example of the momentum dependence for the bound state (deuteron) function in such step-like basis in comparison with the exact function for the Yamaguchi s-wave triplet NN potential is displayed in Fig. 3.

All the eigenstates corresponding to the area of continuous spectrum obtained in such a WP-representation can be treated as approximations for scattering wave packets $|z_k\rangle$ defined above, provided the eigenvalues of Hamiltonian matrix coincide with eigenvalues of the exact wave-packets. This condition can be easily satisfied because a bin partition for exact scattering WPs is built "by hands".

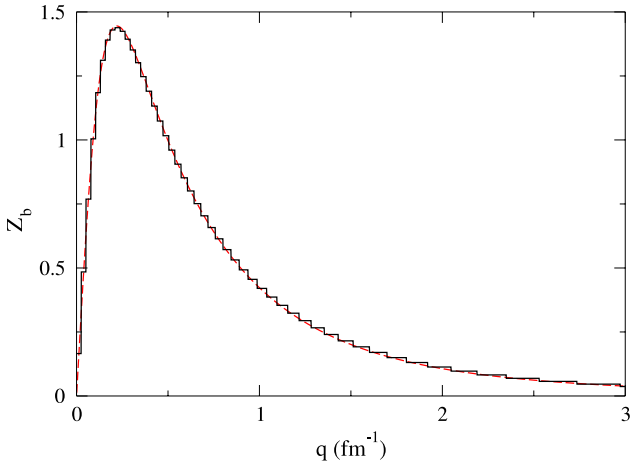

Fig. 3. Comparison of the exact deuteron wave function in the momentum representation for the Yamaguchi potential (dashed curve) with its approximation in the free WP basis (solid line) found from the Hamiltonian matrix diagonalization.

As a result, one derives a very convenient discrete representation for the scattering WPs using a superposition of free wave packets:

$$|z_k\rangle \approx |\tilde{z}_k\rangle = \sum_{i=1}^{N} O_{ki}|x_i\rangle. \tag{43}$$

The validity of this WP-representation is illustrated by the same particular example of the Yamaguchi potential for which both exact scattering wave functions and also exact scattering WPs are constructed in an explicit form and thus can be compared with approximations given by Eq. (43).

In Fig. 4, wave functions of two pseudostates in momentum representation (with indices $k = 6$ and 11) obtained in the free WP basis are compared to the corresponding exact scattering wave packets. It is important to stress here that these exact scattering WPs (42) (dashed curves in the figure) are still square-integrable functions, despite the fact that they have logarithmic singularities on the boundaries of the "on-shell" interval, i.e. in the interval to which the WP energy ϵ_k^* belongs. It is clear from the above comparison that the pseudostates composed from step-like WPs reproduce quite reasonably the structure of exact scattering wave packets "on average".

Such a discrete approximation for the scattering WPs is extremely useful for few-body scattering studies where one is able to build a few- and many-body WP basis not only for a free motion Hamiltonian but also for a few-body channel Hamiltonian. Moreover, in this approach one finds a very convenient analytical form for the resolvent and off-shell t-matrix operators for a two-body subsystem by a straightforward Hamiltonian diagonalization procedure (see e.g. Section 5).

Furthermore, we will demonstrate henceforth how to generalize this convenient way to a multichannel scattering case and how to treat multichannel pseudostates (see Section 5). However, in a general case of a few-particle scattering one has to take into account a specific behavior of scattering wave functions in different asymptotic channels. In such cases one should formulate discrete versions for the Faddeev and many-body Lippmann–Schwinger integral equations (see Sections 6–8).

3.5. Coulomb wave packets

One of the big advantages of an employment of L_2 normalized WP states for a continuum treatment is a possibility to consider long-range potentials like the Coulomb one quite similarly to short-range ones. It is because the essential singularities at small momentum q peculiar to wave functions and transition operators for the Coulomb potential are somehow averaged out and then smoothed in the WP representation.

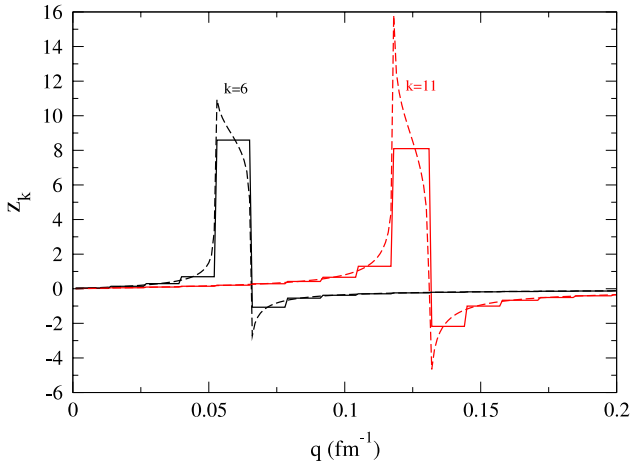

Fig. 4. The functions of pseudostates (with numbers $k = 6, 11$) obtained in the free WP basis (solid lines) in comparison with respective exact scattering wave-packets (dashed lines) for the *NN* spin–triplet Yamaguchi potential.

As a vivid illustration we consider here two-body scattering with repulsive Coulomb Hamiltonian[5]

$$h_C = h_0 + \frac{z_1 z_2 e^2}{r}, \tag{44}$$

where z_1 and z_2 are the particle charges, r is the distance between them. So, one can introduce here *Coulomb wave packets* $|x_i^C\rangle$ as basis functions. Such Coulomb WPs are built from the regular Coulomb wave functions $F_l(q, r)$ (for each partial wave l) by the integration over discretization bins [22] quite similarly to the general case:

$$|x_i^C\rangle = \frac{1}{\sqrt{B_i}} \int_{\mathfrak{D}_i} dq f(q) |F_l(q)\rangle. \tag{45}$$

These WP states (45) are normalized, so that they can be built practically using pseudostates of the Coulomb Hamiltonian (44) on some L_2 basis. Thus, in such a discrete representation one gets an interesting result when one can represent accurately Coulomb WPs via a finite set of free-motion WPs.

This non-trivial statement is illustrated in Fig. 5 where the exact Coulomb WPs for *pp* system are compared to the respective Coulomb pseudostates found via diagonalization of the Coulomb Hamiltonian on the free WP basis, and the free WPs themselves at the same energy. It is clearly seen from the figure the Coulomb WP $|x_i^C\rangle$ can be very accurately approximated by free WPs. This interesting result leads to many far going consequences in few- and many-body scattering problems for charged particles.

4. Discrete version of the scattering theory

The direct relationship between continuum wave functions and their WPs makes it possible to develop a closed wave-packet formalism to treat a few- and many-body scattering in a convenient fully discrete representation. The complete formalism has been described in detail in our previous papers [23,27] so that we present here for the reader's convenience only the extract of the basic results.

[5] The Coulomb attraction can be also treated in the WP approach, however it needs a separate study.

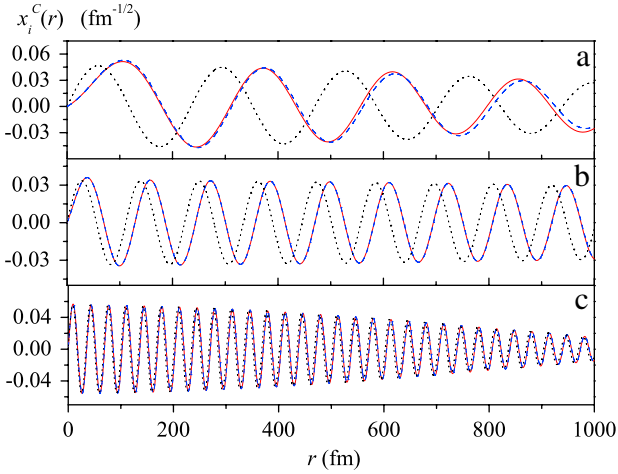

Fig. 5. The exact s-wave Coulomb WPs (dashed curves), the pseudostates found via the free WP basis (solid curves) and the free WPs at the same energy (dotted curves) for pp system at three center of mass energies: $E_{\text{c.m.}} = 0.03$ MeV (a), $E_{\text{c.m.}} = 0.133$ MeV (b) and $E_{\text{c.m.}}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

4.1. The wave packet space

Let us call the linear shell spanned on basis of free WPs $\{|x_i\rangle_{i=1}^N\}$ as an eigen wave-packet space of the Hamiltonian h_0. The projection operator onto this space $\mathfrak{p}$ is defined in Eq. (37).

The property (31) allows one to find a finite-dimensional representation for any operator $A = R(h_0)$ which depends on Hamiltonian h_0 or just commutes with it:

$$\mathfrak{A} \equiv \mathfrak{p}A\mathfrak{p} = \sum_{i=1}^{N} |x_i\rangle A_i \langle x_i|, \tag{46}$$

where the corresponding eigenvalues A_i are given in an explicit form:

$$A_i = \frac{1}{B_i} \int_{\mathfrak{D}_i} dq R\left(\frac{q^2}{2\mu}\right) |f(q)|^2. \tag{47}$$

E.g., discrete eigenvalues of the free Hamiltonian are given via Eq. (32).

So that, using these properties one can build finite-dimensional analogs for different scattering operators in the free WP basis. In particular, the resolvent of the free Hamiltonian $g_0(E) = [E + \mathrm{i}0 - h_0]^{-1}$ is diagonal in the free WP representation:

$$\mathfrak{g}_0(E) \equiv \mathfrak{p}g_0(E)\mathfrak{p} = \sum_{i=1}^{N} |x_i\rangle g_i(E) \langle x_i|. \tag{48}$$

Here the complex eigenvalues $g_i(E)$ are determined according to the general formula (47). It should be mentioned that the resolvent of the total Hamiltonian $g(E) = [E + \mathrm{i}0 - h]^{-1}$ has the same diagonal representation in the scattering WP set [23].

For the charged particle scattering, one may easily build the finite-dimensional approximation for the Coulomb resolvent $g_C = [E + \mathrm{i}0 - h_C]^{-1}$ in the Coulomb WP basis:

$$\mathfrak{g}_C(E) = \sum_{i=1}^{N} |x_i^C\rangle g_i(E) \langle x_i^C|. \tag{49}$$

The Coulomb resolvent eigenvalues $g_i(E)$ are found from the same Eq. (47) as for the free resolvent. The explicit formulas for these eigenvalues are given in the Appendix.

The eigenvalues $g_i(E)$ incorporate logarithmic singularities at the bin endpoints. To smooth such undesirable singularities and to convert our scheme to be completely discrete, one can employ an additional averaging procedure over the "on-shell" energy bin to represent the energy dependence of the resolvent. As a result, we get *a purely finite-dimensional representation for the free resolvent* which is now free of any singularities at real energies. In other words, instead of the operator $\mathfrak{g}_0(E)$ which continuously depends on energy one obtains the discrete set of operators

$$\mathfrak{g}_0^k \equiv \frac{1}{D_k}\int_{\mathfrak{D}_k} \mathfrak{g}_0(E)dE, \quad k = 1, \ldots, N, \tag{50}$$

each of which is the averaged resolvent operator on the "on-shell" energy bin $\mathfrak{D}_k$ where D_k is its energy width.

4.2. Correspondence between "continuous" and "discrete" quantities

Within the WP-formalism the discretization procedure involving three steps is introduced:

(i) Division of continuous spectrum of the free Hamiltonian onto non-overlapping intervals and introduction of free WPs.
(ii) Projection of the scattering (and also bound-state) wave functions and operators onto the above WP space.
(iii) An additional energy-averaging procedure for energy dependent operators.

It would be very useful to demonstrate how this discretization procedure works in practical calculations by the example of solving the Lippmann–Schwinger equation for the transition operator $t(E)$:

$$t(E) = v + vg_0(E)t(E). \tag{51}$$

After application of the above three steps (i)–(iii) one gets a discrete set of operators $\mathfrak{t}^k$ at $E \in \mathfrak{D}_k$ (instead of continuous operator $t(E)$). The matrix elements of $\mathfrak{t}^k$ in the WP basis are related directly to off-shell elements of t-matrix:

$$t(q, q', E) \approx \frac{[\mathfrak{t}^k]_{ij}}{\sqrt{D_i D_j}}, \quad \begin{pmatrix} q \in \mathfrak{D}_i \\ q' \in \mathfrak{D}_j \\ E \in \mathfrak{D}_k \end{pmatrix}. \tag{52}$$

These operators $\mathfrak{t}^k$ satisfy simple matrix equations

$$\mathfrak{t}^k = \mathfrak{v} + \mathfrak{v}\mathfrak{g}_0^k\mathfrak{t}^k, \quad E \in \mathfrak{D}_k \tag{53}$$

where we denote by Gothic letters the WP projections of the respective operators. From Eq. (53), one can get any on- and off-shell t-matrix elements whose energy and momentum dependencies are represented by histograms. It should be emphasized that t-matrix constructed in the WP representation satisfies exactly the unitarity relation [27].

Let us note that to find an elastic amplitude at energy $E \in \mathfrak{D}_k$ one has to solve Eq. (53) for one column of t-matrix only, i.e. $[\mathfrak{t}^k]_{ik}$, $i = 1, \ldots, N$.

Finally, the S-matrix (and partial phase shift) can be found from the relation:

$$S(E) \approx 1 - 2\pi \mathrm{i}\frac{[\mathfrak{t}^k]_{kk}}{D_k}, \quad E \in \mathfrak{D}_k, \tag{54}$$

where D_k is the bin energy width.

By similar derivation one can build the WP analogs for the Möller wave operators, total Hamiltonian resolvent, etc. [27].

Table 1 shows the one-to-one correspondence between "discrete" and initial "continuous" quantities. As a good illustration of such a fully discrete technique for finding the transition operator we present here the solution of α–α scattering problem where interaction includes both nuclear and Coulomb potentials [22]. The basic s-, d- and g- partial α–α phase shifts found using the above WP-technique with additional energy averaging are displayed in Fig. 6.

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

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

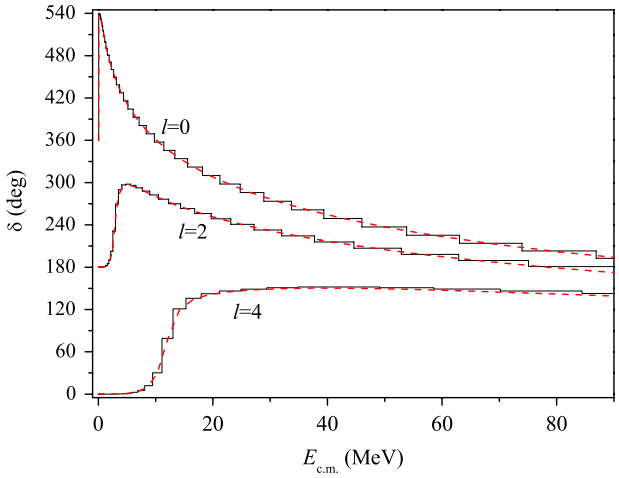

Fig. 6. s-, d- and g-wave partial phase shifts of $\alpha - \alpha$ scattering found via the WP approach (solid curve) and derived from a direct solution of the Schroedinger equation by the Numerov method (dashed curve).

4.3. A case of a complex-valued interaction potential

Although the above technique has been suggested initially for the case of Hermitian Hamiltonians it is straightforwardly generalized for a complex interaction v case as well.

For a complex potential case, an accurate treatment [31] requires an introduction of biorthogonal sets of the scattering states corresponding to incoming and outgoing boundary conditions:

$$\begin{aligned} |\psi^{(+)}(E)\rangle &= |\psi_0(E)\rangle + g_0^{(+)}(E) v |\psi^{(+)}(E)\rangle, \\ |\psi^{(-)}(E)\rangle &= |\psi_0(E)\rangle + g_0^{(-)}(E) v^\dagger |\psi^{(-)}(E)\rangle. \end{aligned} \tag{55}$$

In the wave-packet approach, one can introduce respective sets of stationary wave packets and further construct discrete analogs of the above Lippmann–Schwinger equations. This technique is discussed in Ref. [23].

However, to evaluate the scattering t-matrix and corresponding S-matrix it is sufficient to solve the matrix equations (53) in a free WP representation similarly to a case of Hermitian interaction [28]. The only difference here is that the projected potential $\mathfrak{v}$ and its matrix are complex-valued now.

As a practical example we consider here the case of neutron–nucleus scattering with the optical complex-valued non-local potential introduced by Perey and Buck [32]

$$U(\mathbf{r}, \mathbf{r}') = V\left(\frac{1}{2}|\mathbf{r} + \mathbf{r}'|\right) \cdot W(|\mathbf{r} - \mathbf{r}'|), \tag{56}$$

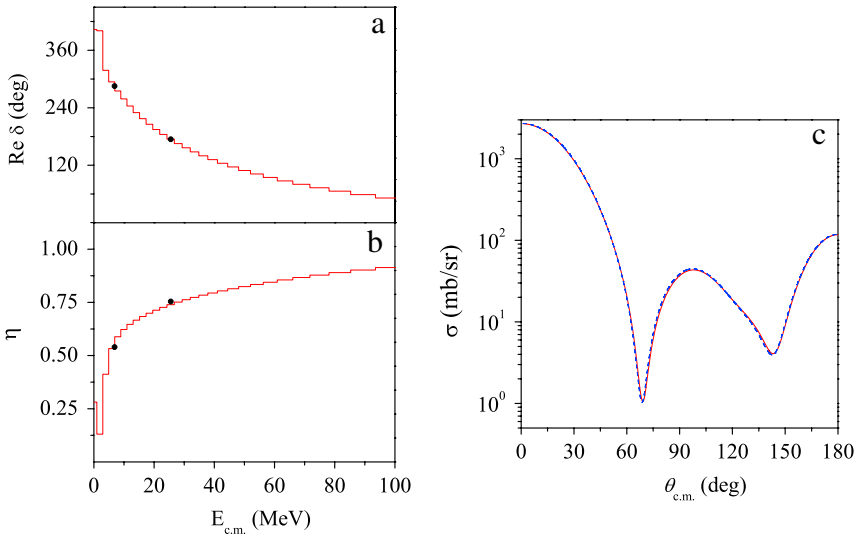

Fig. 7. The real parts of s-wave phase shifts Re δ (a), inelasticity parameter η (b), and the differential cross section for neutron scattering off ^{56}Fe at $E_n = 7$ MeV (for the non-local optical-model potential) obtained with the WP approach (solid curve). The black circles in Figs. (a) and (b) and the dashed curve in Fig. (c) correspond to the results for local phase equivalent potentials obtained by the direct numerical integration of the Schroedinger equation.

where $V(x)$ is a usual complex Woods–Saxon optical model potential of the argument $x = \frac{1}{2}|\mathbf{r} + \mathbf{r}'|$ and the non-locality W is of the Gaussian type

$$W(|\mathbf{r} - \mathbf{r}'|) = \frac{\exp[-(|\mathbf{r} - \mathbf{r}'|/\beta)^2]}{\pi^{3/2}\beta^3} \tag{57}$$

with the scale parameter β. This nonlocal potential is energy independent in contrast to ordinary energy dependent local potentials used in the optical model. However in the WP approach, we meet not any additional difficulty associated with this non-locality because one employs only a matrix of an interaction potential in the free WP basis in a practical solution. Thus the whole numerical scheme remains just the same as in Hermitian and local potential cases.

By this approach, we have found partial phase shifts and differential cross sections for a neutron scattering off ^{56}Fe using the complex-valued non-local potential given by Eq. (56) (see further details in Ref. [28]). In Fig. 7(a) and (b) the real parts of s-wave phase shifts $\delta(E)$ and inelasticity parameter $\eta \equiv |S| = |\exp(2i\delta(E))|$ are displayed. In Fig. 7(c), the differential cross section for the neutron scattering off ^{56}Fe at the incident neutron energy $E_n = 7$ MeV calculated by means of the WP technique for all necessary partial waves (up to $l_{\max} = 10$) is shown. To demonstrate an accuracy of our method we employ a direct numerical solution of the Schroedinger equation (with the conventional Numerov method) for local phase-shift equivalent potentials of Woods–Saxon type, which provide the same differential cross sections as the initial non-local ones at two incident neutron energies $E_n = 7$ and 26 MeV [32]. The results for nonlocal potential nearly coincide with those for direct numerical solution with the local energy dependent interaction.

So that, the wave-packet approach for the solution of the typical optical-model scattering problems with complex-valued and non-local potentials is also fully applicable. Below in Section 7, we will use this result in a solution of a three-body problem of a composite particle scattering on a structureless target.

It should be mentioned that we do not study the pseudostates corresponding to non-Hermitian interactions in the present paper. Generalization of the pseudostate treatment as approximations to stationary wave packets for a non-Hermitian interaction case requires a separate study (see also

our discrete approach towards solving scattering problems without any scattering equations via the spectral shift formalism [29]).

5. Multichannel scattering problem

Very often many-body scattering problem in atomic, nuclear and molecular physics can be reduced to a multichannel scattering although the number of channels to be incorporated may be very large. Also a multichannel problem arises in a simple two-body case when an interaction potential is not spherically symmetrical.

The total multichannel Hamiltonian of the system can be written in a matrix form (in the channel indices ν, ν')

$$h_{\nu\nu'} = h_{0\nu}\delta_{\nu\nu'} + v_{\nu\nu'}, \quad \nu, \nu' = 1, \ldots, K, \tag{58}$$

where $h_{0\nu}$ is the free-motion Hamiltonian in the channel ν with simple continuous spectrum $[\Omega_\nu, \infty)$, Ω_ν is the ν-channel threshold, and $v_{\nu\nu'}$ are the coupling potentials. Further we will denote the operator matrices by the bold characters. The matrix of the free multichannel Hamiltonian $\mathbf{h}_0$ is diagonal and therefore the continuous spectrum of $\mathbf{h}_0$ is the union of spectra of $h_{0\nu}$. Thus, the continuous spectrum of the multichannel Hamiltonian is degenerate (in contrast to a single-channel case), and the multiplicity of the degeneracy η being equal to the number of open channels and hence depends upon energy. This means that there are η independent scattering wave functions corresponding to different boundary conditions at each energy.

5.1. The free WP basis for a multichannel scattering

Now one has to define free WP sets for each free motion channel Hamiltonian $h_{0\nu}$. We found that it is very convenient to make the bin partitions for continuous spectra in various channels by such a way that bins in different channels would be coinciding. So in this case, the interval endpoints will be placed at the same energies in all open channels. By this way one gets a degenerated discretized spectrum of the multichannel free Hamiltonian $\mathbf{h}_0$. Such a discretization procedure, as will be demonstrated below, allows to treat multichannel pseudostates and also to determine multichannel t-matrix even without solving any scattering equations [29].

So that, in the multichannel problem, one makes a partition of the total continuum as usual: the region $[\Omega_1, E_{\max}]$ is divided into finite number of energy bins $\mathfrak{D}_i \equiv [\mathcal{E}_{i-1}, \mathcal{E}_i]_{i=1}^N$. Hereby an energy threshold Ω_ν of the channel ν should coincide with left end of some bin which we denote as i_ν. Thus, for bins with indices $i < i_\nu$ there exist only $\nu - 1$ open channels. We assume that channels are enumerated in order of increasing their threshold energies Ω_ν and $i_1 = 1$. Fig. 8 demonstrates how the discretized three-channel spectrum is constructed.

Using such partitions, the corresponding set of free WPs in each initial channel ν:

$$|x_i^\nu\rangle = \frac{1}{\sqrt{D_i}} \int_{\mathfrak{D}_i} dE |\psi_0^\nu(E)\rangle, \quad \nu = 1, \ldots, K, \; i = i_\nu, \ldots, N \tag{59}$$

can be constructed from the exact wave functions $|\psi_0^\nu(E)\rangle$ of the free Hamiltonian $h_{0\nu}$ continuum.

After the introduction of multichannel WPs it is straightforward to build a finite dimensional representation for all the channel resolvents $g_0^\nu(E) = [E + \mathrm{i}0 - h_{0\nu}]^{-1}$ in fully analogous way with a single-channel case. The channel resolvents g_0^ν enter the expansion for the multichannel free resolvent. So that, this operator has the following finite-dimensional approximation in the WP basis:

$$\mathfrak{g}_0(E) = \sum_{\nu=1}^{K} \sum_{i=i_\nu}^{N} |x_i^\nu\rangle g_i^\nu(E) \langle x_i^\nu|, \tag{60}$$

where the complex eigenvalues are defined by the formulas similar to the single-channel ones.

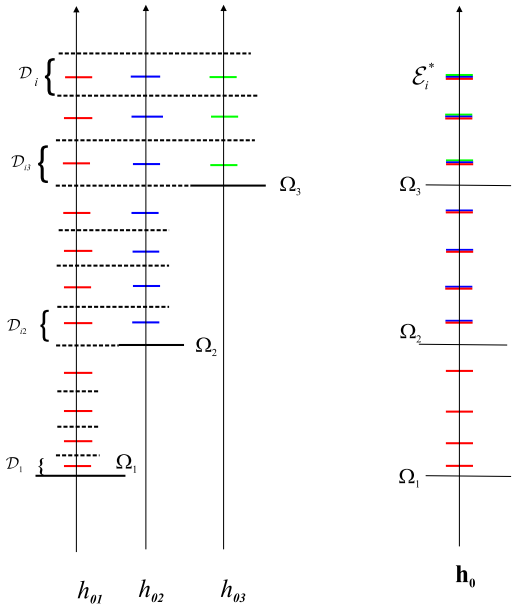

Fig. 8. The structure of the discretized spectra for the separate branches of the free motion Hamiltonians $h_{0\nu}$, $\nu = 1, 2, 3$, (on the left) and the resulting degenerate discretized spectrum of the total free Hamiltonian $\mathbf{h_0}$ (on the right). The dashed lines represent bin boundaries while the solid lines inside bins correspond to free WP eigenvalues $\mathcal{E}_i^*$.

Further one can project the basic scattering operators onto such multichannel WP-basis similarly to the single-channel case treated above. In particular, the transition matrix elements for multichannel scattering problem is defined from the multichannel Lippmann–Schwinger equation:

$$t_{\nu\nu'}(E) = v_{\nu\nu'} + \sum_{\mu=1}^{K} v_{\nu\mu} g_0^{\mu}(E) t_{\mu\nu'}(E), \quad \nu, \nu' = 1, \ldots, K. \tag{61}$$

So that, a solution for the multichannel scattering problem is found by solving the matrix WP analog of the above equation which is a direct generalization of the single-channel equation (53).

However, there is another way by which one can solve the multichannel problem in the WP representation using properties of multichannel pseudostates.

5.2. Eigenchannel representation and a multichannel resolvent

To study the resolvent of the total multichannel Hamiltonian **h**, we shall employ the multichannel formalism in the so called Eigenchannel Representation (ER). The ER is the representation in which the multichannel S-matrix takes a diagonal form with respect to the channel indices [33]. More definitely, one can introduce at each energy E two orthogonal sets of the scattering functions for the Hamiltonian **h**:

- wave functions $\{|\psi^{\nu}(E)\rangle\}_{\nu=1}^{\eta}$ corresponding to the incoming waves in the channel ν (the so called experimental channel representation) and
- wave-functions $\{|\tilde{\psi}^{\varkappa}(E)\rangle\}_{\varkappa=1}^{\eta}$ defined in the eigenchannel representation.

The ER states differ from the experimental channel states by a rotation in the channel space with the rotation matrix being dependent on the energy E [29,33].

Then using just the above ER formalism one defines multichannel *scattering* wave-packets and derives an analytical finite-dimensional representation for the total multichannel resolvent (similarly to a one-channel case).

It is convenient to construct multichannel scattering WP's as integrals of the exact scattering wave functions for the total Hamiltonian **h** defined in the ER:

$$|z_k^{\varkappa}\rangle = \frac{1}{\sqrt{C_k^{\varkappa}}} \int_{\Delta_k^{\varkappa}} w(E)|\tilde{\psi}^{\varkappa}(E)\rangle dE, \quad k = k_{\varkappa}, \ldots, N^{\varkappa}, \tag{62}$$

where $\Delta_i^{\varkappa} \equiv [\epsilon_{i-1}^{\varkappa}, \epsilon_i^{\varkappa}]$ are new set of the total Hamiltonian bins whose parameters might be different for different $\varkappa$.

Now we have to derive a spectral expansion of the total multi-channel resolvent using multi-channel scattering states defined in the ER. The spectral expansion of the resolvent in the "ordinary" set of the initial eigenfunctions of h can be written as the sum of bound-state and continuum parts of the total resolvent, viz. $g(E) = g^{\mathrm{B}}(E) + g^{\mathrm{C}}(E)$, where

$$g^{\mathrm{B}}(E) = \sum_{n_b=1}^{N_b} \frac{|\psi_{n_b}\rangle\langle\psi_{n_b}|}{E - E_{n_b}}, \qquad g^{\mathrm{C}}(E) = \sum_{\nu=1}^{K} \int_{\Omega_\nu}^{\infty} dE' \frac{|\psi^{\nu}(E')\rangle\ \langle\psi^{\nu}(E')|}{E + \mathrm{i}0 - E'}. \tag{63}$$

It is easy to show that the following relation is valid:

$$\sum_{\nu=1}^{\eta} |\psi^{\nu}(E')\rangle\ \langle\psi^{\nu}(E')| = \sum_{\varkappa=1}^{\eta} |\tilde{\psi}^{\varkappa}(E')\rangle\ \langle\tilde{\psi}^{\varkappa}(E')|, \tag{64}$$

which corresponds to a rotation between experimental channel and eigenchannel representations.

Thus, we arrive at the spectral expansion of the continuum part of the total resolvent in the Hamiltonian eigenfunctions defined in ER:

$$g^{\mathrm{C}}(E) = \sum_{\varkappa=1}^{K} \int_{\Omega_\varkappa}^{\infty} dE' \frac{|\tilde{\psi}^{\varkappa}(E')\rangle\ \langle\tilde{\psi}^{\varkappa}(E')|}{E + \mathrm{i}0 - E'}, \tag{65}$$

where the thresholds $\Omega_\varkappa$ in the ER coincide with thresholds of the initial experimental channels ν.

Applying the projection onto the multichannel basis (62) one gets the following finite-dimensional representation for the total multichannel resolvent expressed via the multichannel scattering WP basis

$$\mathfrak{g}^{\mathrm{C}}(E) = \sum_{\varkappa=1}^{K} \sum_{k=k_\varkappa}^{N} |z_k^{\varkappa}\rangle g_k^{\varkappa}(E) \langle z_k^{\varkappa}|, \tag{66}$$

where complex eigenvalues $g_k^{\varkappa}(E)$ are defined as integrals over discretization bins, similar to the single-channel ones.

Now the key question arises, how to construct the states (62) without solving the scattering problem as we have done in a one-channel case. For this purpose we will employ here a new treatment of multichannel pseudostates.

5.3. Multichannel pseudostates and a solution of multichannel scattering problems without any scattering equations

The continuous spectrum of the total multichannel Hamiltonian **h** coincides with the spectrum of $\mathbf{h}_0$, so that at each energy there should exist η independent solutions corresponding to different boundary conditions for the scattering problem. Therefore, the usual L_2 discretization procedure becomes rather unclear here, because when the total Hamiltonian is represented by a respective matrix in some arbitrary finite L_2-basis the required multiplicity of the spectrum disappears and one has only one pseudostate at every discrete energy value which can hardly be treated properly. So, it seems a one-to-one correspondence between the continuous spectrum (which is multiply degenerated) and its discretized analog is lost in the multichannel case.

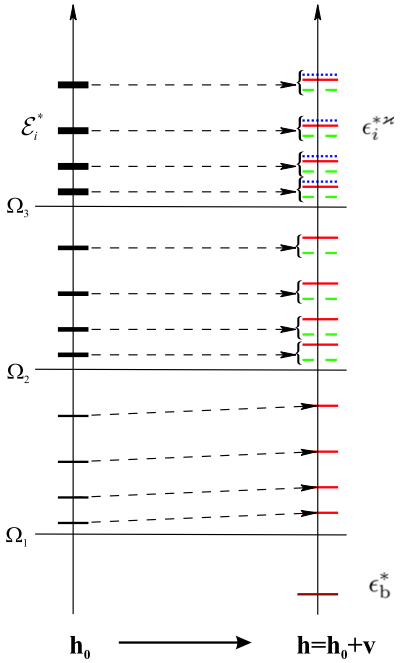

Fig. 9. The splitting of the eigenvalues in the degenerated discretized spectrum of the multichannel Hamiltonian $\mathbf{h_0}$ caused by addition of the interaction $\mathbf{v}$. Ω_ν are the channel thresholds while ϵ_b^* is the isolated eigenvalue corresponding to the single (in this example) bound state of the total Hamiltonian $\mathbf{h}$. Sublevels inside each split set corresponding to the same eigenchannel number $\varkappa$ are shown by the same lines (i.e. solid, dashed and dotted).

However, the problem still can be solved if the discretized spectrum of the free multichannel Hamiltonian is degenerate with necessary multiplicity as we constructed above. As was shown in Ref. [29], the application of the perturbation $\mathbf{v}$ to the unperturbed operator $\mathbf{h_0}$ with degenerate discretized spectrum leads to a splitting of each η-fold degenerate eigenvalue $\mathcal{E}_i^*$ into the set of η perturbed eigenvalues $\{\epsilon_i^{*\varkappa}\}_{\varkappa=1}^{\eta}$ of the total Hamiltonian $\mathbf{h}$ as is schematically shown in Fig. 9. The very important property of the perturbed spectrum was shown in [29] (on the basis of results from Ref. [34]), namely, these split sublevels form different intermittent sets in the energy domain between thresholds (i.e. the domain with fixed multiplicity η) $\{\epsilon_i^{*\varkappa}\}_{i=i_\eta}^{i_{\eta+1}-1}$ each of which corresponds to the $\varkappa$-th branch of the continuum spectrum. So that the split levels are arranged in the same order (see Fig. 9):

$$\epsilon_i^{*\varkappa+1} > \epsilon_i^{*\varkappa}, \quad i = i_\eta, \ldots, i_{\eta+1} - 1.$$

Moreover, this means that bands of split sublevels corresponding to different initial bins i are not overlapped with each other, which allows us to extract different $\varkappa$ branches from multichannel pseudostate spectrum.

Thus, one can select the new set of eigenvalues $\{\epsilon_i^{*\varkappa}\}_{i=i_\varkappa}^{N^\varkappa}$ (and corresponding functions of pseudostates) for each value $\varkappa$ which can be treated as the $\varkappa$-th branch of the discretized multichannel continuum and be confronted with the ER scattering states for respective branch of the continuous spectrum of the total Hamiltonian [29]. So, in this way, we can establish a one-to-one correspondence between the discretized spectrum of the multichannel Hamiltonian matrix and the continuous spectrum of the initial multichannel Hamiltonian. Due to such a classification of branches in the discretized spectrum, one can treat multichannel pseudostates on the same footing as the one-channel pseudostates. Now we can make the next step—consider multichannel pseudostates as approximations to multichannel WPs defined in the ER (62) (we have done the same step in a one-channel case).

In this way, we get the multichannel scattering WP which is expressed from the free WPs by a simple orthogonal transformation quite similarly to a one-channel case:

$$|z_k^\varkappa\rangle \approx \sum_{\nu=1}^{K}\sum_{i=i_\nu}^{N} O_{ki}^{\varkappa\nu}|x_i^\nu\rangle. \tag{67}$$

Now one can construct the WP approximation for the total multichannel resolvent via the relation (66) and get a final solution of the multichannel scattering problem.

As a good illustration of this approach we have calculated the coupled-channel S-matrix and the partial phase shifts and the mixing angle ε for the Nijmegen I NN potential [35] in coupled triplet ${}^3S_1 - {}^3D_1$ channels for the total spin $S = 1$ and isospin $I = 0$. The two-channel t-matrix has been obtained from the total resolvent using the well known formula

$$\mathbf{t}(E) = \mathbf{v} + \mathbf{v}\mathbf{g}(E)\mathbf{v},$$

where finite-dimensional representation for the resolvent (66) in the two-channel pseudostate basis is used. More definitely, the multichannel t-matrix for $E \in \mathfrak{D}_i$ is defined by the relation:

$$t_{\nu\nu'}(E) \approx \frac{\langle x_i^\nu|v|x_i^{\nu'}\rangle}{D_i} + \frac{\langle x_i^\nu|v|z_\mathrm{b}\rangle\langle z_\mathrm{b}|v|x_i^{\nu'}\rangle}{D_i(E-\epsilon_\mathrm{b}^*)} + \sum_{\varkappa=1}^{K}\sum_{k=k_\varkappa}^{N^\varkappa}\frac{\langle x_i^\nu|v|z_k^\varkappa\rangle}{\sqrt{D_i}} g_k^\varkappa(E)\frac{\langle z_k^\varkappa|v|x_i^{\nu'}\rangle}{\sqrt{D_i}}, \tag{68}$$

where $|z_\mathrm{b}\rangle$ is a WP approximation for the bound-state wave function with energy ϵ_b^* (the deuteron wave function) and matrix elements of the interaction potential $\mathbf{v}$ between free and scattering WP states can be written using expansion (67) as follows:

$$\langle x_i^\nu|v|z_k^\varkappa\rangle = \sum_{\mu=1}^{K}\sum_{j=j_\mu}^{N} O_{kj}^{\varkappa\mu}\langle x_i^\nu|v|x_j^\mu\rangle. \tag{69}$$

Thus, in the developed approach we can find the accurate multichannel t-matrix using only the diagonalization of the respective multichannel Hamiltonian with appropriate L_2-basis, i.e. *without solving any scattering equations at all.*

In Fig. 10 the partial phase shifts $\delta_0(E)$, $\delta_2(E)$, and mixing parameter $\varepsilon(E)$ (i.e. those which determine NN differential scattering cross sections—in the Stapp parametrization) are shown in very wide energy range $0 < E_\mathrm{lab} < 800$ MeV. They are found from just a single diagonalization of the respective two-channel Hamiltonian of the NN interaction using a two-channel free WP-basis. We compare these quantities in the figure to those obtained from direct numerical integration of the two-channel Lippmann–Schwinger integral equation at many energies in the above energy range. The agreement seems to be almost perfect.

This comparison shows that one can derive the accurate multichannel t-matrix or total resolvent for general multichannel case using only a single diagonalization of the total multichannel Hamiltonian matrix. It opens a new way in complicated coupled-channel calculations in atomic, molecular and nuclear physics. Moreover, this approach allows to construct finite-dimensional representations for few-body channel resolvents in a case of coupled-channel interaction in subsystems of total few-body system, e.g. to account some inner degrees of freedom.

6. Stationary wave packets in a three-body problem

Let us consider now a general three-body scattering problem for particles 1, 2 and 3, interacting via pairwise short-range potentials v_a ($a = 1, 2, 3$). It is convenient to use here three Jacobi momentum sets $(\mathbf{p}_a, \mathbf{q}_a)$ corresponding to three channel Hamiltonians H_a ($a = 1, 2, 3$) which define the asymptotic states of the system. The symbol p_a denotes the relative momentum of b and c particles while q_a is the momentum of the third particle relative to the c.m. of the pair $\{bc\}$. In a general case of different particles the respective wave-packet bases should be constructed independently for each Jacobi set [23,27]. Below we show how to built one of those.

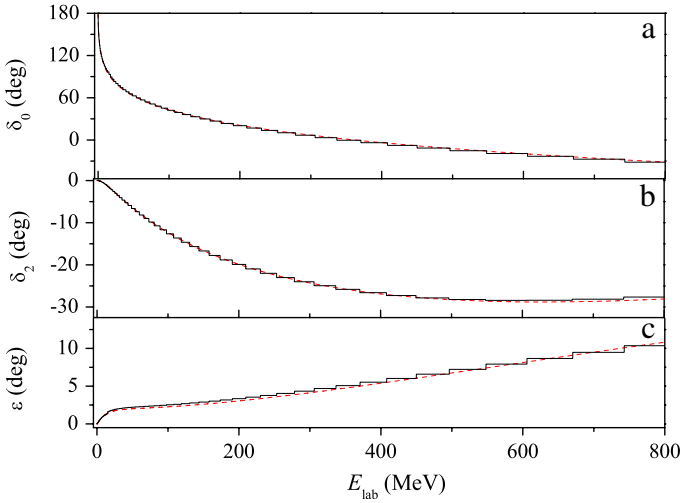

Fig. 10. The $^3S_1 - {}^3D_1$ partial phase shifts δ_0 (a), δ_2 (b) and the mixing parameter ε (c) for the Nijmegen *NN* potential found from two-channel Hamiltonian diagonalization in the WP basis (solid curves) and from the direct numerical solution of the two-channel Lippmann–Schwinger equation (dashed curves).

The channel Hamiltonian (e.g. H_1 for $a = 1$) takes the form of a direct sum of two sub-Hamiltonians

$$H_1 \equiv h_1 \oplus h_0^1, \tag{70}$$

where sub-Hamiltonian $h_1 = h_0 + v_1$ includes the interaction v_1 in the {23}-subsystem and the sub-Hamiltonian h_0^1 corresponds to a free relative motion of the center of mass for particles 2 and 3 and the spectator particle 1.

6.1. The lattice three-body basis

The three-body wave-packet basis should be constructed at first for the three-body free Hamiltonian defined in the same Jacobi set:

$$H_0 = h_0 \oplus h_0^1. \tag{71}$$

So that the three-body free-motion wave-packet states are built as direct products of the respective two-body wave-packet states. To construct the three-body free WP basis functions, we introduce partitions of the continua of two free-motion sub-Hamiltonians, h_0 and h_0^1, onto non-overlapping intervals $\{\mathfrak{D}_i \equiv [\mathcal{E}_{i-1}, \mathcal{E}_i]\}_{i=1}^N$ and $\{\bar{\mathfrak{D}}_j \equiv [\bar{\mathcal{E}}_{j-1}, \bar{\mathcal{E}}_j]\}_{j=1}^{\bar{N}}$ respectively and introduce two-body free WPs as in Eq. (28):

$$|x_i\rangle = \frac{1}{\sqrt{B_i}} \int_{\mathfrak{D}_i} f(p)|\psi_{0p}\rangle dp, \qquad |\bar{x}_j\rangle = \frac{1}{\sqrt{\bar{B}_j}} \int_{\bar{\mathfrak{D}}_j} \bar{f}(q)|\psi_{0q}\rangle dq, \tag{72}$$

where p and q are Jacobi momenta and B_i, $\bar{B}_j$ and $f(p)$, $\bar{f}(q)$ are normalization factors and weight functions respectively. Here and below we denote functions and values corresponding to the variable q with additional bar mark to distinguish them from functions corresponding to the variable p.

When constructing the three-body WP basis one should take into account spin and angular parts of the basis functions. Thus the three-body basis function can be written as:

$$|X_{ij}^{\Gamma\alpha\beta}\rangle \equiv |x_i^\alpha, \bar{x}_j^\beta; \alpha, \beta : \Gamma\rangle = |x_i^\alpha\rangle \otimes |\bar{x}_j^\beta\rangle\, |\alpha, \beta : \Gamma\rangle, \tag{73}$$

where $|\alpha\rangle$ is a spin-angular state for the {23} pair, $|\beta\rangle$ is a spin-angular state for the third particle, and $|\Gamma\rangle$ is a set of three-body quantum numbers. The state (73) is the WP analog of the exact free motion state in three-body continuum $|p, q; \alpha, \beta : \Gamma\rangle$ for the three-body free Hamiltonian H_0 [36].

The three-body free WP basis functions (73) are constant inside the cells of the momentum lattice built from two one-dimensional cells $\{\mathfrak{D}_i\}_{i=1}^{N}$ and $\{\bar{\mathfrak{D}}_j\}_{j=1}^{\bar{N}}$ in momentum space. Therefore we refer to *a free WP* basis as *a lattice* basis and denote the respective two-dimensional bins (i.e. the lattice cells) by $\mathfrak{D}_{ij} = \mathfrak{D}_i \otimes \bar{\mathfrak{D}}_j$.

Such multi-dimensional wave-packet basis is an "eigenbasis" for the free Hamiltonian H_0 and has the same properties with respect to this operator as two-body free WPs with respect to the two-body free Hamiltonian h_0. In particular, every operator which functionally depends on H_0 has an explicit finite-dimensional representation in the lattice basis discussed [27]. So that, it is straightforward to obtain *a diagonal representation* for the three-body free resolvent G_0 and to use it further for solving few-body scattering equations. This is a way to develop the wave-packet matrix scheme which is a finite-dimensional form of the initial scattering equations.

However, the above discrete representation has a remarkable advantage in comparison with the continuous one: one can construct and employ a few-body wave-packet basis directly for the three-body channel Hamiltonian H_1. This allows to simplify a solution of scattering problems drastically.

6.2. The WP basis for the channel three-body Hamiltonian

Let us introduce a WP basis for two-body sub-Hamiltonian h_1. Assume as above that there are N_b bound states in the {23} subsystem with corresponding bound-state wave functions $\{|z_n^\alpha\rangle\}_{n=1}^{N_b}$ and eigenenergies $\{\epsilon_n^{*\alpha}\}_{n=1}^{N_b}$. One defines the partition $\{\Delta_k\}_{k=N_b+1}^{N^\alpha}$ of the continuous spectrum of h_1 and constructs the set of scattering wave packets $|z_k^\alpha\rangle$ from the respective exact scattering wave functions $|\psi_p^\alpha\rangle$ according to Eq. (42). The complete WP basis $\{|z_k^\alpha\rangle\}_{k=1}^{N^\alpha}$ for the h_1 sub-Hamiltonian includes bound state functions and scattering wave packets and its functions may depend on possible spin-angular quantum numbers.

Now one can build the three-body wave-packets (3WP) for the channel Hamiltonian H_1 just as products of two types of WP states for h_1 and h_0^1 sub-Hamiltonians whose spin-angular parts are combined to the respective three-body states with quantum numbers Γ:

$$|Z_{kj}^{\Gamma\alpha\beta}\rangle \equiv |z_k^\alpha, \bar{x}_j^\beta; \alpha, \beta : \Gamma\rangle, \quad k = 1, \ldots, N^\alpha, \; j = 1, \ldots, \bar{N}. \tag{74}$$

The properties of the 3WP constructed in this way are the same as properties of the two-body wave packets viz. they form an orthonormal set and any operator functionally dependent on the channel Hamiltonian H_1 has a diagonal matrix representation in the subspace spanned on this basis. It allows us to construct a finite-dimensional approximation for the three-body channel resolvent $G_1(E) \equiv [E + \mathrm{i}0 - H_1]^{-1}$ in a very convenient analytical form.

Indeed, the exact three-body channel resolvent is a convolution of the two-body subresolvents $g_1(E) = [E + \mathrm{i}0 - h_1]^{-1}$ and $g_0^1(E) = [E + \mathrm{i}0 - h_0^1]^{-1}$ [23–25,27]:

$$G_1(E) = \frac{1}{2\pi\,\mathrm{i}} \int_{-\infty}^{\infty} d\epsilon g_1(\epsilon) g_0^1(E - \epsilon). \tag{75}$$

Using spectral expansions for these two-body resolvents and making the integration, one gets an explicit expression for the exact channel resolvent G_1 as a sum of two terms $G_1(E) = G_1^{\mathrm{BC}}(E) + G_1^{\mathrm{CC}}$, where the bound-continuum (BC) part takes the form [27]:

$$G_1^{\mathrm{BC}}(E) = \sum_{\Gamma,\alpha,\beta} \sum_{n=1}^{N_b} \int_0^\infty dq \frac{|z_n^\alpha, \psi_{0q}^\beta; \alpha, \beta : \Gamma\rangle \langle z_n^\alpha, \psi_{0q}^\beta; \alpha, \beta : \Gamma|}{E + \mathrm{i}0 - \epsilon_n^{*\alpha} - \frac{q^2}{2M}}, \tag{76}$$

where M is the reduced mass in the $\{23\}+1$ channel. While the continuum–continuum (CC) part of G_1 takes the form:

$$G_1^{\mathrm{CC}}(E)=\sum_{\Gamma,\alpha,\beta}\int_0^\infty dp\int_0^\infty dq\frac{|\psi_p^\alpha,\psi_{0q}^\beta;\alpha,\beta:\Gamma\rangle\langle\psi_p^\alpha,\psi_{0q}^\beta;\alpha,\beta:\Gamma|}{E+\mathrm{i}0-\frac{p^2}{2\mu}-\frac{q^2}{2M}},\tag{77}$$

where μ is the reduced mass in the $\{23\}$ subsystem.

Projecting further the exact channel resolvent onto the three-body channel 3WP basis defined in Eq. (74), one can find analytical formulas for the matrix elements of the G_1 operator. The respective matrix is diagonal in all wave-packet indices:

$$\mathfrak{G}_1=\sum_{\Gamma,\alpha,\beta}\sum_{k,j}|Z_{kj}^{\Gamma\alpha\beta}\rangle G_{kj}^{\Gamma\alpha\beta}(E)\langle Z_{kj}^{\Gamma\alpha\beta}|.\tag{78}$$

The matrix elements $G_{kj}^{\Gamma\alpha\beta}$ are defined as integrals over the respective momentum bins for the BC part:

$$G_{kj}^{\Gamma\alpha\beta}=\frac{1}{\bar{B}_j}\int_{\bar{\mathfrak{D}}_j}\frac{|\bar{f}(q)|^2dq}{E+\mathrm{i}0-\epsilon_k^{*\alpha}-\frac{q^2}{2M}},\quad k=1,\ldots,N_{\mathrm{b}},\ j=1,\ldots,\bar{N}\tag{78a}$$

and for the CC-one:

$$G_{kj}^{\Gamma\alpha\beta}=\frac{1}{C_k^\alpha\bar{B}_j}\int_{\Delta_k^\alpha}\int_{\bar{\mathfrak{D}}_j}\frac{|w(p)|^2|\bar{f}(q)|^2dpdq}{E+\mathrm{i}0-\frac{p^2}{2\mu}-\frac{q^2}{2M}},\quad k=N_{\mathrm{b}}+1,\ldots,N^\alpha,\ j=1,\ldots,\bar{N}.\tag{78b}$$

These elements depend on the spectral partition parameters (i.e. Δ_k^α and $\bar{\mathfrak{D}}_j$ bin endpoints) and total energy E only. They do not depend explicitly on the interaction potential v_1. When solving the scattering equations in the finite-dimensional WP basis the corresponding solution converges with increasing the basis dimension, the final result turns out to be *independent* of the particular spectral partition parameters. Explicit formulas for the resolvent matrix elements (78a) and (78b) are given in the Appendix.

The explicit analytical representation (78) for the channel three-body resolvent is a basic feature for the wave-packet approach since it allows us to simplify solution of the general three-body scattering problem drastically. In particular, this representation has been used to solve the finite-dimensional analog for the Faddeev equations [28,30]. This representation has been employed also to solve some particular three-body scattering problems using the three-body Lippmann–Schwinger equation [24–26] for composite projectile scattering off nuclear target (see below).

To use the states (74) practically, one can approximate them with the pseudostates of the sub-Hamiltonian h_1 in some L_2 basis. As has been shown earlier in Section 3, the free WP basis is very appropriate to approximate scattering states because the respective functions have a very long-range behavior in configuration space which makes it possible to describe properly an asymptotical behavior of Faddeev wave function components at large distances. So one can calculate the eigenstates (the bound and pseudostates) of the sub-Hamiltonian h_1 matrix in the two-body WP-basis $\{|x_i\rangle\}_{i=1}^N$ via a straightforward diagonalization procedure. As a result one gets the eigenstates of the h_1 sub-Hamiltonian expanded in the free WP basis (for each quantum number α) similar to Eq. (43).

Hence, starting from the free WP bases for each two-body sub-Hamiltonian one gets a set of three-body basis states both for free and channel Hamiltonians, H_0 and H_1 respectively, which are related to each other by a simple matrix rotation. Using projection of operators and wave functions onto these 3WP bases it is possible to solve three-body scattering problems via matrix formalism.

It should be mentioned that in a general few-body case, the free and the channel wave-packet bases can be constructed by a very similar procedure using a continuum discretization for every subsystem. In the bases constructed in this way, it is straightforward to find explicit finite-dimensional representations for channel and free resolvents and furthermore to solve the resulting scattering equations in a very convenient matrix form. Sections 7 and 8 will be devoted to vivid illustrations of the wave-packet continuum discretization technique to solve three-body scattering problems.

7. Composite particle scattering on a nuclear target

As an example of application of the three-body WP approach based on the finite-dimensional representation for the channel resolvent, we consider a particular three-body problem of a composite particle elastic scattering on a target when rearrangement channels are neglected while intermediate excitations into continuum are taken into account.

7.1. Solution of the Lippmann–Schwinger equation

The total Hamiltonian for the two-fragment projectile plus target system can be written as follows:

$$H = h_{\rm int} + h_C + V_{\rm ext}, \tag{79}$$

where $h_{\rm int} = h_0 + v_{12}(r_{12})$ is the internal sub-Hamiltonian including an interaction v_{12} between the projectile fragments 1 and 2, while $h_C(R)$ is the sub-Hamiltonian of projectile asymptotic motion including the center-of-mass Coulomb interaction, and $V_{\rm ext} = V_1(r_1) + V_2(r_2)$ is a sum of the fragment–target external interactions $V_{1(2)}$. Here r_1 and r_2 are the fragment positions and r_{12} is their relative distance.

The potentials $V_{1(2)}$ here are assumed to be complex.[6] As it has been shown in Section 4.3 the inclusion of a complex potential does not change the whole WP approach. Also we assume that there are bound states $\{|z_n\rangle\}_{n=1}^{N_b}$ with energies $\{\epsilon_n^*\}_{n=1}^{N_b}$ in $h_{\rm int}$ sub-Hamiltonian.

The channel three-body Hamiltonian here is a direct sum of two sub-Hamiltonians:

$$H_{\rm ch} = h_{\rm int} \oplus h_C. \tag{80}$$

In our case the rearrangement channels can be neglected due to complex potentials of fragment–target interaction, so that, the transition operator T (which describes the elastic scattering of the projectile by the target nucleus as well as the projectile breakup) is found from *a single* Lippmann–Schwinger equation (LSE) [26]:

$$T(E) = V_{\rm ext} + V_{\rm ext} G_{\rm ch}(E) T(E), \tag{81}$$

where $G_{\rm ch} = [E + {\rm i}0 - H_{\rm ch}]^{-1}$ is the channel resolvent which determines the asymptotic states in the elastic channel.

Then, wave-packet basis states corresponding to a discretization of the channel Hamiltonian continuum are built as products of $h_{\rm int}$ and h_C sub-Hamiltonian WP basis states as defined in Eq. (74). The only difference in that we have to replace free WPs along the center of mass variable with Coulomb WPs for the sub-Hamiltonian h_C. Thus our WP basis in this case takes the form:

$$|Z_{kj}^{Ll\lambda}\rangle = |z_k^l, \bar{x}_j^{C\lambda}; l, \lambda : L\rangle, \tag{82}$$

where l and λ are subsystem orbital momenta while L is a total orbital momenta of the system which assumed to be conserved.

Thus, after a WP-projection of the three-body wave functions and scattering operators one gets respective vectors and matrices in the channel WP space. Such a wave-packet representation is eigen for the projected channel Hamiltonian and the basis states from Eq. (82) correspond to exact asymptotic states of the system. In particular, the initial state wave function of the system which defines the asymptotic free motion of the projectile corresponds to a single WP-state. For example, if one considers an elastic scattering of the projectile in its ground state (assume that $l = 0$), the initial state wave function $|\Psi_0^L(E)\rangle \equiv |z_1^0, \psi^L(E - \epsilon_1^*); L\rangle$ is represented by the WP-state $|Z_{1j_0}^L\rangle$ of the channel WP basis, where $E - \epsilon_1^* \in \bar{\mathfrak{D}}_{j_0}$.

[6] For this illustrative example, we use optical potentials of the fragment–target interaction at some fixed energy (see the details e.g. in Ref. [26]).

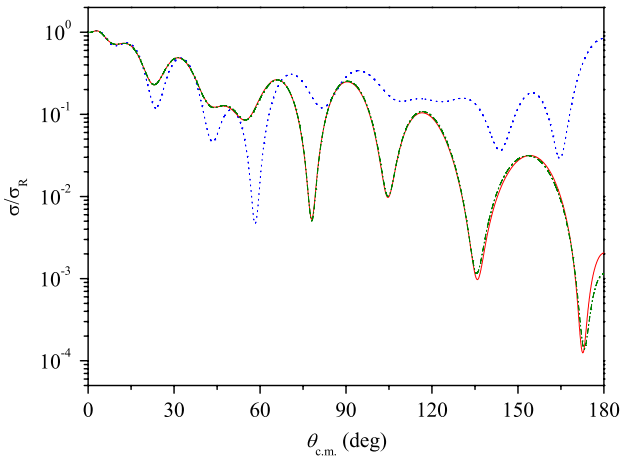

Fig. 11. The comparison of the elastic cross sections (in ratio to the Rutherford cross section σ_R) for the deuteron scattering on ^{58}Ni at $E_d = 21.6$ MeV calculated in the WPCD approach (solid curve) and the CDCC approach [26] (dash-dotted curve). The dotted curve reflects a result for the folding model which does not include the deuteron intermediate breakup channels.

Eventually, after the wave-packet projecting the scattering operators, all terms in the LSE (81) are reduced to a purely matrix form and thus the three-body T-matrix can be found from a single matrix equation:

$$\mathbb{T} = \mathbb{V} + \mathbb{V}\mathbb{G}_{\rm ch}\mathbb{T}, \tag{83}$$

where $\mathbb{V}$ is the external interaction matrix in the three-body wave-packet basis and $\mathbb{G}_{\rm ch}$ is a diagonal matrix of the channel resolvent (78) taken at the total energy E. It should be stressed that to find on-shell and half-shell T-matrix elements, it is sufficient to solve the matrix equation (83) only for one column $t_n \equiv T_{n,n_0},\ n = 1, \ldots, N \cdot \bar{N}$ (we use here the multi-index $n = (k, j)$, so that the label $n_0 = (1, j_0)$ corresponds to the initial state). In such a case, the respective solution is found from the equation

$$(\mathbb{I} - \mathbb{V}\mathbb{G}_{ch})t = v. \tag{84}$$

Here the elements of the vector v are defined as $v_n \equiv V_{n,n_0},\ n = 1, \ldots, N \cdot \bar{N}$, and $\mathbb{I}$ is the unit matrix. Finally, the S-matrix elements are interrelated to the vector of t-matrix elements by the relationship [26]:

$$S_{\rm el}(E) = 1 - 2\pi \mathrm{i} \frac{t_{n_0}}{\bar{D}_{j_0}}, \quad (E - \epsilon_1^*) \in \bar{\mathfrak{D}}_{j_0}. \tag{85}$$

As a particular example for such a scattering problem we consider the well known test case: the deuteron elastic scattering on ^{58}Ni target—see the respective results in Fig. 11. The details of a calculation and potential parameters used can be found in Ref. [26]. In this study we have shown that our discrete WP-solution for such a coupled-channel problem is in a very good agreement with that derived from the traditional CDCC approach in which one has to solve a large system of coupled differential equations in every partial wave.

It should be stressed that the above technique can be generalized for a case when a projectile consists of several fragments. In such a case, the internal Hamiltonian and external interaction in Eq. (79) take the form

$$h_{\rm int} = h_0 + \sum_{i<j} v_{ij}(r_{ij}), \qquad V_{\rm ext} = \sum_{i=1}^{K} V_i(r_i), \tag{86}$$

where v_{ij} are interactions between the projectile fragments, V_i are the fragment–target external interactions, r_i are fragments positions and r_{ij} are their relative distances.

If projectile–target interactions V_i are complex-valued the rearrangement channels can be neglected again, so that the transition operator can be found from the same Eq. (81) and the corresponding channel resolvent should be constructed using few-body pseudostates of the Hamiltonian $h_{\rm int}$ found in some appropriate L_2 basis. Further, the whole calculation scheme for the elastic amplitude remains the same as in the case of a two-fragment projectile discussed above. Also it is possible to include in consideration some inner degrees of freedom of the target (e.g. its excitation).

7.2. Construction of an effective projectile–target interaction

In many problems of quantum physics it is necessary to know an operator of effective interaction between a composite projectile and stable target or vice versa, which takes into account the virtual excitation of the incident particle (or target), i.e. its dynamic polarization in the scattering process. Such an operator of the effective interaction is replaced usually by some phenomenological optical potential between composite projectile and stable target (or vice versa) because its microscopic evaluation is often a very cumbersome problem. So the convenient approach for a theoretical calculation of the effective operator is a very good object for the theory.

The wave-packet discretization method allows us to construct such operators explicitly, using the finite-dimensional representation of the channel resolvent obtained above. In this solution it is convenient to apply the Feshbach projection operator formalism [37].

For the reader's convenience, we briefly recall a derivation of the effective operator of interaction within such projection approach for the case of composite particle scattering of a nucleus discussed in the previous subsection.

Consider the Schroedinger equation for the wave function of the system defined by the Hamiltonian (79)

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

Let, $|z_1\rangle$ be the projectile ground state with energy ϵ_1^*. Using the above projection operator technique, one defines two projection operators:

$$F = |z_1\rangle\langle z_1|, \qquad Q = 1 - F, \qquad QF = 0. \tag{87}$$

Here F is the projection operator onto the elastic channel, Q is the orthogonal projector onto all the inelastic channels. After application of the above projection operators to the Schroedinger equation for the total wave function it is split into two coupled equations for components $F|\Psi\rangle$ and $Q|\Psi\rangle$:

$$\begin{aligned}(FHF - E)F|\Psi\rangle &= -FHQ|\Psi\rangle,\\ (QHQ - E)Q|\Psi\rangle &= -QHF|\Psi\rangle.\end{aligned} \tag{88}$$

Further, we introduce the resolvent of the Hamiltonian projected onto Q-subspace: $G_{\rm Q}^{(+)}(E) = [E + {\rm i}0 - QHQ]^{-1}$. Then, substituting the second equation in (88) to the first one, the well known equation for the elastic scattering function $F|\Psi\rangle$ is derived:

$$(FHF + FU_{\rm eff}(E)F - E)F|\Psi\rangle = 0, \tag{89}$$

where

$$FU_{\rm eff}(E)F \equiv FHQG_{\rm Q}^{(+)}QHF \tag{90}$$

is an effective nonlocal and energy-dependent operator of interaction between a composite particle and the target taking into account all the inelastic channels. Since the operators F and $h_{\rm int} \oplus h_C$ commute, and the orthogonality condition $FQ = 0$ is valid, Eq. (89) takes the form of a conventional two-body Schroedinger equation for projection $|\chi_1\rangle = \langle z_1|\Psi\rangle$ of the total wave function onto the elastic channel:

$$[h_C + V_{\rm fold} + U_{\rm eff} - (E - \epsilon_1^*)]|\chi_1\rangle = 0. \tag{91}$$

Here we have introduced a folding potential $V_{\rm fold}$ describing the interaction of the projectile center of mass with the target nucleus when the inelastic channels corresponding to the excitation or breakup of the incident composite particle are fully neglected:

$$V_{\rm fold}(R) = \langle z_1|V_{\rm ext}|z_1\rangle. \tag{92}$$

Here the integration in the matrix element is carried out only over the internal variable. All inelastic (and breakup) effects are included into the non-local Feshbach potential:

$$U_{\rm eff}(E) = \langle z_1|V_{\rm ext}QG_Q(E)QV_{\rm ext}|z_1\rangle. \tag{93}$$

Despite the compact notation, the computation of this operator is in principle even more difficult problem than the solution of the original scattering problem. However, when using the wave-packet basis (82) consisted from eigenfunctions of the channel Hamiltonian the practical construction of operator $U_{\rm eff}(E)$ becomes clear and straightforward.

Indeed, using the wave-packet states for the channel Hamiltonian, one finds the finite-dimensional diagonal representation for the channel resolvent $G_{\rm ch}(E)$ obtained via formulas from Eq. (78).

In the WP-approach the Q-subspace is just orthogonal part of the WP subspace, so that the finite-dimensional representation for the projector Q can be written as (we omitted possible spin-angular indices):

$$\mathfrak{Q} = \sum_{k,j}{}' |z_k, \bar{x}_j^C\rangle\langle z_k, \bar{x}_j^C|, \tag{94}$$

where upper prime symbol means that the sum does not include the ground state of $h_{\rm int}$. Thus the matrix representation for the projected G_Q operator is straightforward:

$$\mathfrak{G}_Q(E) = \{[\mathfrak{G}_{\rm ch}^Q(E)]^{-1} - \mathfrak{V}_{\rm ext}^Q\}^{-1}, \tag{95}$$

where all operators are meant as being projected onto the Q-subspace.

After direct evaluation of the matrix for G_Q-operator from Eq. (95), the explicit formula for the effective potential in the wave-packet representation can be written in the form:

$$U_{\rm eff}(E,R,R') = \sum_{kj}{}' \sum_{k'j'}{}' B_{kj}(R)[\mathbb{G}_Q(E)]_{kj,k'j'}B^*_{k'j'}(R'), \tag{96}$$

where the form-factors are defined as the integrals:

$$B_{kj}(R) = \langle z_1|V_{\rm ext}|z_k, \bar{x}_j^C\rangle, \tag{97}$$

and an integration is meant over internal variable only. In practical calculations, all the necessary spin-angular parts of wave functions should be also taken into account.

Thus, the WP approach gives a direct and convenient way to calculate an effective optical potential for an interaction of a composite particle with a stable target. Also this formalism can be generalized for constructing an effective interaction between two colliding composite particles which may be excited or disintegrate in the scattering process.

In Fig. 12 the real and imaginary parts of the effective nonlocal optical potential for the deuteron and the ^{58}Ni nucleus interaction at incident deuteron energy $E_d = 80$ MeV calculated via the WP-approach are displayed for the total orbital angular momentum $L = 0$.

Besides the direct calculation of the complicated nonlocal interaction operator, the approach described above is very convenient in those cases where inelastic channels play a minor role of a correction to the elastic scattering when the main contribution comes from the folding potential. In such a case, one can employ the "inner" few-body WP basis of a rather small dimension for the calculation of the effective potential and the "external" two-body WP basis with a large dimension for the subsequent solution for the resulting two-body scattering problem with the total interaction including the folding potential and the above effective potential [24].

Just such a situation arises very often when the energy of collision of a composite particle with a stable target increases. The relative weight of the breakup channels decreases (after some

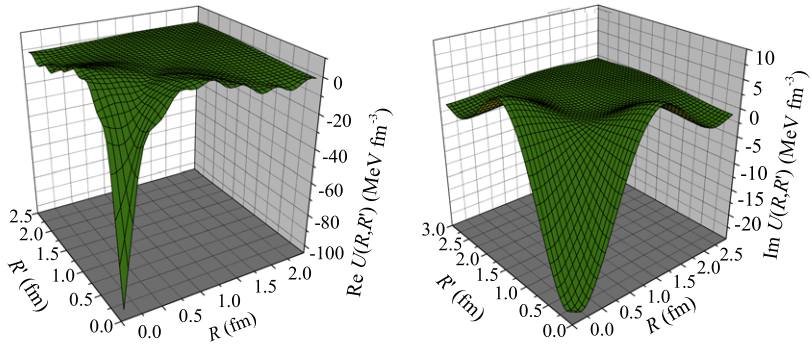

Fig. 12. The real (left) and imaginary (right) parts of the effective deuteron–^{58}Ni optical potential calculated at $E_d = 80$ MeV for the total angular momentum $L = 0$.

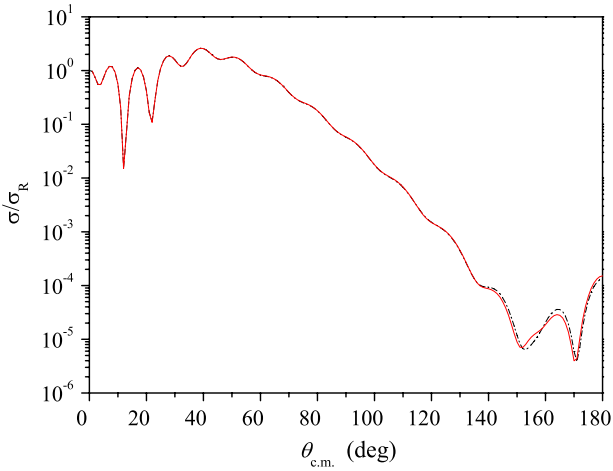

Fig. 13. The differential cross section for the elastic deuteron–^{58}Ni scattering at $E_d = 80$ MeV (in the ratio to the Rutherford cross section σ_R) calculated in the CDCC approach [26] (dash-dotted curve) and with the effective potential of the Feshbach type constructed in the WP approach (solid curve).

characteristic energy) and thus the contribution of the effective potential taking into account the projectile breakup is reduced as in our above example.

As an illustration for such an approach we present in Fig. 13 the differential cross section for elastic deuteron scattering off the nucleus ^{58}Ni at energy $E_d = 80$ MeV calculated using the above Feshbach potential. The result of such optical model calculation nearly coincides with the solution of a direct three-body problem found with the CDCC approach in Ref. [26]. We found in this study, the dimension of the Coulomb WP-basis $|\bar{x}_i^C\rangle$ used in Q projector is five times less than the dimension of the same Coulomb WP-basis used in "external" projector F.

Let us summarize, we are able rather easily to calculate with the described technique the theoretical non-local optical potentials for a scattering of composite projectiles on stable targets (or vice versa), or even for a collision of two composite particles.

8. Formulation and solution of the Faddeev equations in the wave-packet representation

The most rigorous and correct formulation for the few-body scattering problem can be attained using the Faddeev or Faddeev–Yakubovsky equations. We will demonstrate below that the wave-packet approach being applied to solving such equations gives the great advantages.

8.1. Formulation of Faddeev equations in momentum space and peculiar properties of their solution

Here we consider a solution of the Faddeev equations for a scattering of three identical particles 1, 2 and 3 with mass m (nucleons). In this case the elastic scattering observables can be found from a single Faddeev equation (FE) for the transition operator $\bar{U}$ (via the so-called AGS equation), e.g. in the following form [36]:

$$\bar{U} = PG_0^{-1} + PtG_0\bar{U}, \tag{98}$$

where t is the two-body off-shell t-matrix in three-body space, $G_0 = (E + \mathrm{i}0 - H_0)^{-1}$ is the free three-body resolvent and P is the permutation operator which changes the momentum variables from one Jacobi set to another one. For the case of three identical particles the operator P is defined as the sum of two cyclic permutations of particles:

$$P = P_{12}P_{23} + P_{13}P_{23}. \tag{99}$$

It should be emphasized that a similar permutation operator is included in kernels of the Faddeev equations in the case of various particles.

After the spin-angular expansion, the operator Eq. (98) for each value of the total angular momentum and parity is reduced to a system of two-dimensional integral equations in momentum space (or to coupled two-dimensional integro-differential equations in configuration space). Although Faddeev proved [38] that the kernels of these equations belong to the Fredholm type (i.e. the inhomogeneous equation has a unique solution), a practical solution of coupled two-dimensional integral equations is a very complicated and time-consuming task due to complicated singular structure of integral kernels and also the large number of coupled spin–orbital channels.

One of the problems is that kernels contain two-body off-shell t-matrices $t(q, q', E)$ for different values of the total orbital angular momentum and spin of the pair interacting particles, which should be calculated many times at different energies.

The second problem here is that the Faddeev-type kernel at real energy contains singularities of two types: two-particle cuts, corresponding to the presence of bound states in the subsystems, and the three-body logarithmic singularity (at the breakup threshold). The two-body singularities are easily eliminated by the technique of residues, while for a regularization of the three-body cut a number of special techniques have been suggested in the previous years. As a result, the whole solution procedure becomes rather complicated. Among such specific techniques the following are employed most often:

- choice of a special quadrature grid points for a momenta q' defined in one Jacobi set depending on a momentum q defined in another Jacobi set together with the spline interpolation of an unknown function at iteration method of solving;
- solution of the equations at the complex energy plane followed by an analytic continuation to the real axis;
- shift for an integration contour from the real axis to the complex momentum plane.

However, the main characteristic feature of the Faddeev kernels is the presence of the particle permutation operator P. The kernel of this operator $P(p, q; p', q')$ as a function of the momenta contains δ-function and two θ-functions and this results in variable integration limits for integrals in the Faddeev kernels [36]. Therefore, when replacing the integrals with respective quadrature sums in numerical procedure it is necessary to apply an interpolation of the unknown solution depending on several variables at each step of an iterative procedure. As a result of such elaborated multi-dimensional interpolation on each iteration step, the interpolation procedure takes most of the computational time of the whole computation and requires an employment of powerful supercomputers [1].

On contrast to this, the WP method described here allows to circumvent completely the above difficulties in solving the Faddeev (and Faddeev–Yakubovsky) equations. First of all, instead of Eq. (98), one uses the equivalent form of the Faddeev equation for the transition operator U [30,39]:

$$U = Pv_1 + Pv_1G_1U. \tag{100}$$

In Eq. (100) G_1 is the three-body channel resolvent introduced in Section 6. Due to the identity $tG_0 \equiv v_1 G_1$ the kernels of Eqs. (98) and (100) are the same and their solutions $\bar{U}$ and U coincide on-shell and half-shell.

This form of the equation is especially useful in the WP representation with basis functions corresponding to the channel Hamiltonian H_1, because in this representation the resolvent G_1 has a simple analytical form and explicitly depends only on the partitions of the continuous spectra of the subsystems. Thereby the need for multiple estimations and multi-dimensional interpolation of the off-shell t-matrix is fully eliminated.

Further, all the singularities of the Faddeev kernel in the form (100) are concentrated in the channel resolvent G_1 and they are smoothed when projecting on the WP basis (averaged by the integration over the energy bins). Therefore the resulting matrix equation can be solved directly for real energies.

Finally, the use of the permutation matrix in the WP basis (as well as in any other fixed basis) completely eliminates the need for very numerous interpolations of the required solution at each iteration.

So, all these innovations taken together lead to great simplification in practical solution of the Faddeev-type few-body scattering equations.

8.2. Three-body wave-packet basis for 3N system

To illustrate this novel technique we consider the realistic Nd scattering problem, where one needs to particularize the three-body wave-packet basis for the case of three-nucleon system with tensor NN interactions. We use the following quantum numbers for the subsystems defined in Section 6 and in the whole three-body system according to the (jj)-coupling scheme:

$$\alpha = \{l, s, j_{23}\}; \qquad \beta = \{\lambda, I\}; \qquad \Gamma = \{J, \pi, T\}, \tag{101}$$

where l, s and j_{23} are the NN subsystem quantum numbers: l is an orbital momentum, s is a spin and $\mathbf{j}_{23} = \mathbf{l} + \mathbf{s}$ is a total angular momentum of the subsystem (the interaction potential depends, in general, on the value of j_{23}). The other quantum numbers are the following: λ is an orbital momentum and $\mathbf{I} = \boldsymbol{\lambda} + \boldsymbol{\sigma}$ is a total momentum of the third nucleon, where $\sigma = \frac{1}{2}$ is its spin. Finally, $\mathbf{J} = \mathbf{j}_{23} + \mathbf{I}$ is a total angular momentum of the three-body system, T is a total isospin and π is parity, all of them are being conserved. Let us also note that the pair isospin t can be defined by values of l and s, because the sum $l + s + t$ must be odd.

The two-body free WP states (72) should be defined for each partial waves l and λ and further they are multiplied by appropriate spin-angular states according to the notations in Eq. (101). Thus the free three-body basis function (73) can be written in the detailed form:

$$|X_{ij}^{\Gamma\alpha\beta}\rangle = |x_i^l, \bar{x}_j^\lambda; \alpha, \beta : \Gamma\rangle. \tag{102}$$

The three-body WP states corresponding to the channel Hamiltonian H_1 are defined here as in Section 6. However now one has to take into account all possible spin-angular couplings in {23} subsystem induced by tensor couplings in v_1 interaction, so the two-body scattering WPs of h_1 sub-Hamiltonian must be defined in the eigenchannel representation as in Eq. (62). Then, three-body channel WP states have the following form:

$$|Z_{kj}^{\Gamma\tilde{\alpha}\beta}\rangle \equiv |z_k^\varkappa, \bar{x}_j^\lambda; \tilde{\alpha}, \beta : \Gamma\rangle, \tag{103}$$

where the spin-angular quantum numbers $\tilde{\alpha}$ in {23} subsystem corresponds to the eigenchannel representation and differs from those, i.e. α, for the free WP basis. In particular, instead of an angular momentum value l this index contains eigenchannel value $\varkappa$, so that $\tilde{\alpha} = \{\varkappa, s, j_{23}\}$ while $\alpha = \{l, s, j_{23}\}$.

These states are the WP analogs for the three-body scattering states $|\psi_p^\varkappa, q; \tilde{\alpha}, \beta : \Gamma\rangle$ of the channel Hamiltonian H_1, where $|\psi_p^\varkappa\rangle$ is a scattering wave function of h_1 sub-Hamiltonian defined in the ER.

It has been shown in Section 5, that the pseudostates obtained via the diagonalization sub-Hamiltonian h_1 in a free WP basis are good approximations for the exact WPs $|z_k^\varkappa\rangle$ constructed from

the scattering wave functions for h_1. The exact WPs are related to the free WPs by a simple orthogonal transformation:

$$|z_k^{\varkappa}, \tilde{\alpha}\rangle = \sum_{i=1}^{N} \sum_{l} O_{ki}^{\varkappa l} |x_i^l, \alpha\rangle, \tag{104}$$

where spin-angular parts of wave functions are taken into account as well and the multi-index $\tilde{\alpha} = \{\varkappa, s, j_{23}\}$ related to the ER is used.

Now we have in our disposal the WP basis for the channel three-body Hamiltonian and can apply explicit formulas (78) for the channel resolvent G_1 which enters Eq. (100) (see also Ref. [39]).

8.3. Matrix analog for the Faddeev equation in the WP basis

In our approach, all the operators in Eq. (100) are projected onto 3WP basis corresponding to the channel Hamiltonian H_1. In other words, every operator, e.g. U, is replaced with its finite-dimensional WP representation:

$$\mathfrak{U}^{\Gamma} = \sum_{\tilde{\alpha},\beta,\tilde{\alpha}',\beta'} \sum_{k,j,k',j'} |Z_{kj}^{\Gamma\tilde{\alpha}\beta}\rangle \langle Z_{kj}^{\Gamma\tilde{\alpha}\beta}|U|Z_{k'j'}^{\Gamma\tilde{\alpha}'\beta'}\rangle \langle Z_{k'j'}^{\Gamma\tilde{\alpha}'\beta'}|. \tag{105}$$

As a result, one gets the matrix analog for the Faddeev equation (100) (for each value of Γ)

$$\mathbb{U} = \mathbb{P}\mathbb{V}_1 + \mathbb{P}\mathbb{V}_1\mathbb{G}_1\mathbb{U}. \tag{106}$$

Here $\mathbb{V}_1$ and $\mathbb{G}_1$ are the matrices of the pairwise interaction and the channel resolvent respectively, the matrix elements of which can be found in an explicit form.

Thus, to find the elastic scattering amplitude it is required: (1) to calculate matrix elements of $\mathbb{P}$, $\mathbb{V}_1$, $\mathbb{G}_1$ matrices and (2) to solve the system of algebraic equations (106).

The matrix $\mathbb{V}_1$ of the potential v_1 is diagonal in the indices j, j' of the wave-packet basis for the free sub-Hamiltonian h_0^1 and has the block form:

$$[\mathbb{V}_1]_{kj,k'j'}^{\tilde{\alpha}\beta,\tilde{\alpha}'\beta'} = \delta_{\beta\beta'}\delta_{jj'}\delta_{ss'}\delta_{j_{23}j'_{23}} \langle z_k^{\varkappa}|v_1|z_{k'}^{\varkappa'}\rangle_{j_{23}} \tag{107}$$

for $\tilde{\alpha} = \{\varkappa, s, j_{23}\}$. Here the subindex j_{23} in the potential v_1 matrix element means that it depends on the two-body total angular momentum value. The matrix elements (107) do not depend on index j and can be written with the usage of the rotation matrix $\mathbb{O}$ defined in Eq. (104) as:

$$\langle z_k^{\varkappa}|v_1|z_{k'}^{\varkappa'}\rangle_{j_{23}} = \sum_{i,i'} O_{ki}^{\varkappa l} O_{k'i'}^{\varkappa' l'} \langle x_i^l|v_1|x_{i'}^{l'}\rangle_{j_{23}},$$

where $\langle x_i^l|v_1|x_{i'}^{l'}\rangle_{j_{23}}$ are the potential matrix elements in the free WP basis.

The matrix of the operator P in the free three-body packet basis corresponds to the overlap between basis functions defined in different Jacobi sets:

$$[\mathbb{P}^0]_{ij,i'j'}^{\alpha\beta,\alpha'\beta'} \equiv \langle X_{ij}^{\Gamma\alpha\beta}|P|X_{i'j'}^{\Gamma\alpha'\beta'}\rangle = \langle X_{ij}^{\Gamma\alpha\beta}(1)|X_{i'j'}^{\Gamma\alpha'\beta'}(2)\rangle + \langle X_{ij}^{\Gamma\alpha\beta}(1)|X_{i'j'}^{\Gamma\alpha'\beta'}(3)\rangle, \tag{108}$$

where the argument 1 (or 2 and 3) in the basis functions denotes a respective Jacobi coordinate set. Such matrix elements are calculated by integration over the basis functions in momentum space:

$$[\mathbb{P}^0]_{ij,i'j'}^{\alpha\beta,\alpha'\beta'} = \int_{\mathfrak{D}_{ij}} dpdq \int_{\mathfrak{D}'_{i'j'}} dp'dq' \times \frac{P^{\Gamma}_{\alpha\beta,\alpha'\beta'}(p,q,p',q')}{\sqrt{d_i d_{i'} \bar{d}_j \bar{d}_{j'}}}, \tag{109}$$

where the prime at the lattice cell $\mathfrak{D}'_{i'j'}$ indicates that the cell belongs to the other (rotated) Jacobi set while the $P^{\Gamma}_{\alpha\beta,\alpha'\beta'}(p,q,p'q')$ is the kernel of particle permutation operator in a momentum space. This kernel, as is mentioned above, contains the product of a Dirac delta and two Heaviside theta functions. However, due to the integration over momentum bins in Eq. (109) these singularities are

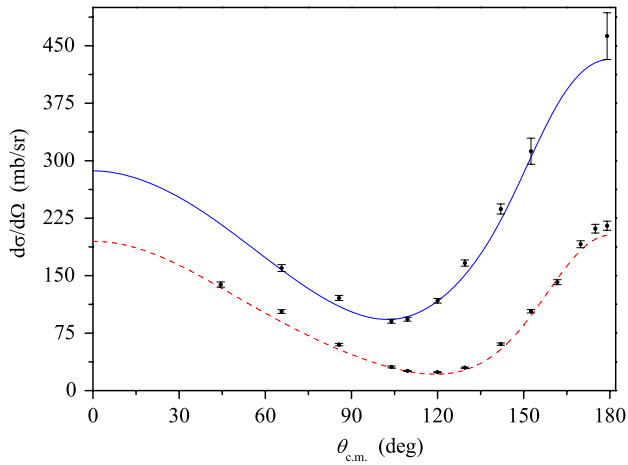

Fig. 14. The differential cross section for the elastic *nd* scattering calculated via the WPCD approach with the Nijmegen I *NN* potential for incident neutron energies $E_n = 3$ MeV (solid curve) and $E_n = 9$ MeV (dashed curve) in comparison with the experimental data (filled circles with error bars) [40].

averaged over the momentum lattice cells and, as a result, the elements of the permutation operator matrix in the WP basis become finite and non-singular.

The detailed technique for the calculation of the matrix element in Eq. (109) is presented in Ref. [39].

The permutation operator matrix $\mathbb{P}$ in the channel 3WP basis is expressed through the overlap matrix $\mathbb{P}^0$ for the lattice basis function of Eq. (109) with the help of the rotation matrices $\mathbb{O}$ if one uses the pseudostate approximation (104) for the scattering WPs $|z_k^s\rangle$:

$$\langle Z_{kj}^{\Gamma\tilde{\alpha}\beta}|P|Z_{k'j'}^{\Gamma\tilde{\alpha}'\beta'}\rangle \approx \sum_{ii'}\sum_{l,l'} O_{ki}^{\varkappa l} O_{k'i'}^{\varkappa' l'} [\mathbb{P}^0]_{ij,i'j'}^{\alpha\beta,\alpha'\beta'}. \tag{110}$$

So, we have a rather simple formulas and respective numerical algorithms to determine all the quantities entering the kernel of the matrix Faddeev equation (106).

8.4. Determination of observables in the WP approach

The elastic on-shell amplitude in the wave-packet representation is calculated as a diagonal (on-shell) matrix element of $\mathbb{U}$-matrix [30]:

$$A_{\rm el}^{\Gamma\tilde{\alpha}_0\beta}(q_0) \approx \frac{2m}{3q_0}\frac{\langle Z_{1j_0}^{\Gamma\tilde{\alpha}_0\beta}|\mathfrak{U}^\Gamma|Z_{1j_0}^{\Gamma\tilde{\alpha}_\beta}\rangle}{\bar{d}_{j_0}}, \tag{111}$$

where m is the nucleon mass, q_0 is the initial two-body momentum and $|Z_{1j_0}^{\Gamma\tilde{\alpha}_0\beta}\rangle = |z_1^{\tilde{\alpha}_0}, \bar{x}_{j_0}^{\lambda}; \tilde{\alpha}, \beta : \Gamma\rangle$ is the 3WP basis state corresponding to the initial scattering state. Here $|z_1^{\tilde{\alpha}_0}\rangle$ is the bound state of the *NN* pair in the initial state (the deuteron, in our case), the index j_0 denotes the bin $\bar{\mathfrak{D}}_{j_0}$ including the on-shell momentum q_0 and $\bar{d}_{j_0}$ is a momentum width of this bin.

In Fig. 14 the differential cross sections for *nd* elastic scattering found with the realistic Nijmegen I *NN* potential [35] in the WP approach are represented for different incident neutron energies in comparison with experimental data [40] (filled circles with error bars). It is evident from the figure that agreement with the data is very well.

In Fig. 15 the comparison is given for the neutron vector analyzing powers A_y for the elastic *nd* scattering at 35 MeV. Here the WP basis with dimension $N \times \bar{N} = 100 \times 100$ has been used and the partial waves with the total angular momentum up to $J \leq 17/2$ have been taken into account.

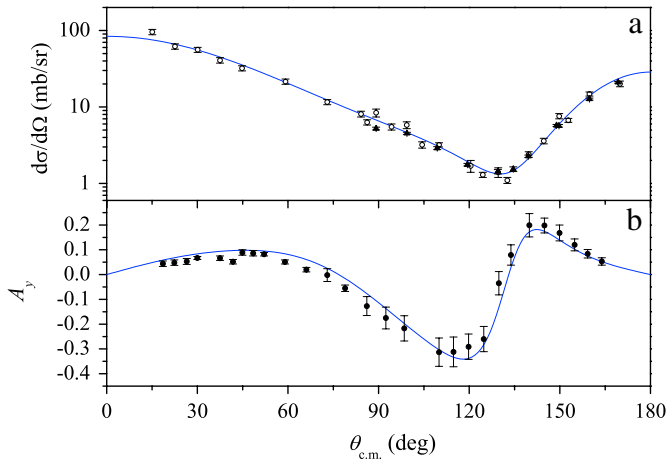

Fig. 15. The elastic *nd* scattering differential cross section (a) and the neutron vector analyzing power A_y (b) at 35 MeV obtained within the WP approach (solid line). The experimental sets are the following: *pd* data at 35 MeV [41] (filled circles), *nd* data at 36 MeV [42] (empty circles) and *nd* data at 35 MeV [43] (triangles) correspondingly.

8.5. Treatment of the three-body breakup in the WP-approach

Now let us pass to a treatment for the three-body breakup using the WP approach. One can show [30] that the breakup amplitude may be defined as a matrix element of *the same transition operator U* satisfying Eq. (100), not only as its diagonal element on initial states, but also for the transition to the continuum state of the channel Hamiltonian H_1:

$$T(p,q) \sim \frac{\langle z_1^{\tilde{\alpha}_0}, q_0; \tilde{\alpha}_0, \beta : \Gamma | U | \psi_p^{\tilde{\alpha}(+)}, q; \tilde{\alpha}, \beta : \Gamma \rangle}{pqq_0}, \tag{112}$$

where $|\psi_p^{\tilde{\alpha}(+)}\rangle$ is the scattering function for the Hamiltonian h_1 corresponding to the outgoing boundary condition, p, q are the final momenta of the subsystem {23} and the third nucleon respectively, q_0 is the initial momentum of the third nucleon. The momenta are related by the energy conservation $\epsilon_1^* + \frac{3q_0^2}{4m} = \frac{p^2}{m} + \frac{3q^2}{4m}$.

Thus, in the WP-approach, the breakup is treated as an inelastic scattering and corresponding amplitudes can be defined from matrix elements of the transition operator U with evident replacement of the *NN* bound-state wavefunction with the exact scattering WPs for the *NN* sub-Hamiltonian [30]. It should be mentioned that some similar treatment of the breakup process is used in the CDCC approach [11] where the authors replaced exact scattering wave functions with corresponding pseudostates. Also close ideas were discussed in the textbook [44] to evaluate the three-body breakup amplitudes.

As an illustration, consider *nd* breakup amplitudes for the case of semi-realistic *s*-wave *NN* interactions MT III. In this illustrative calculation one takes $l = \lambda = 0$ and one has only *NN* spin quantum number s to distinguish different spin-angular channels: $\tilde{\alpha}_0 = s = 1$ for the initial channel, $\tilde{\alpha} = s = 0, 1$ for the final channels and the three body quantum number Γ is defined by the total spin value Σ. We show here the results for the hyperspherical breakup amplitude which defines an asymptotic behavior for a Faddeev component of the total wave function and is related to the breakup amplitude (112) as follows:

$$\mathcal{A}^{\Sigma s}(\theta) = \frac{4\pi m}{3\sqrt{3}} q_0 K^4 e^{i\pi/4} T^{\Sigma s}(p,q), \quad \theta = \arctan\left(\frac{\sqrt{3}q}{2p}\right) \tag{113}$$

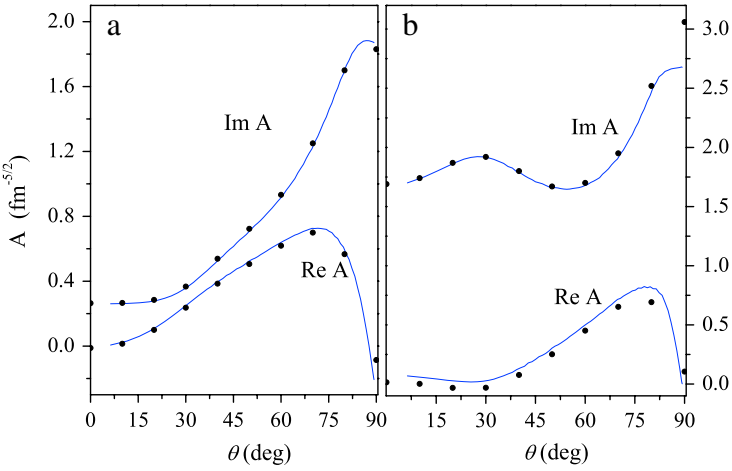

Fig. 16. A comparison of the hyperspherical breakup amplitudes $\mathcal{A}$ for the spin-quartet (a) and spin-doublet (b) channels obtained within WP technique (solid curves) and in the conventional Faddeev calculations [45] (full circles).

where θ is the hyperangle in momentum space. In the WP approach the breakup amplitude T is defined by non-diagonal elements of the transition operator $\mathfrak{U}$ (see details in Ref. [30]):

$$T^{\Sigma s}(p,q) \approx e^{i\delta(p_k^*)} \frac{\mathbb{T}^{\Sigma s}_{1j_0,kj}}{p_k^* q_j^* q_0},$$

$$\mathbb{T}^{\Sigma s}_{1j_0,kj} \equiv \frac{\langle Z^{\Sigma 1}_{1j_0} | \mathfrak{U}^{\Sigma} | Z^{\Sigma s}_{kj} \rangle}{\sqrt{\bar{d}_{j_0} d_k^s \bar{d}_j}}, \quad \begin{array}{l} q_0 \in \bar{\mathfrak{D}}_{j_0}, \\ q \in \bar{\mathfrak{D}}_j, \\ p \in \Delta_k^s, \end{array} \tag{114}$$

where $|Z^{\Sigma 1}_{1j_0}\rangle$ is the WP basis state corresponding to the initial state: index 1 denotes the bound state of the *NN* pair (deuteron) and index j_0 denotes the "on-shell" q-bin $\bar{\mathfrak{D}}_{j_0}$, while $|Z^{\Sigma s}_{kj}\rangle$ is a state of the channel Hamiltonian H_1. An 'excitation' to this state corresponds to a breakup process. Here $\delta(p_k^*)$ is the s-wave phase shift for the *NN* pair interaction at energy ϵ_k^{*s}, $p_k^* = \sqrt{m\epsilon_k^{*s}}$ and $q_j^* = \frac{1}{2}[q_{j-1} + q_j]$ are momenta corresponding to Δ_k^s and $\bar{\mathfrak{D}}_j$ bins respectively and the d_k^s is the momentum width of the Δ_k^s bin.

A comparison for the hyperspherical breakup amplitudes (113) defined in the WP approach with results for the benchmark solution of the Faddeev equation [45] is displayed in Fig. 16. The agreement is rather well except the hyperangle area near $\theta = 90^\circ$ which corresponds to small relative momenta p. The accurate treatment of this area requires some separate study [30].

8.6. Some important features of the algorithm for a solution of Faddeev equations in the WP approach. Realization through the GPU parallel computations

Using the WPCD approach, we have reduced the practical solution of the Faddeev equation to solving the system of algebraic equations (106). Thus, the WPCD algorithm for solving system consists of the following main steps:

1. Construction of free WP bases $\{|x_i\rangle, |\bar{x}_j\rangle\}$, calculation of the potential matrix $\langle x_i^\alpha | v_1 | x_{i'}^{\alpha'} \rangle$, diagonalization of two-particle sub-Hamiltonian matrices for each value of l and s and finding the energies of pseudostates and their functions in the WP representation, i.e. matrices O^{xl}_{ki}.
2. Calculation of the permutation matrix $\mathbb{P}^0$ in the lattice WP basis (109).

3. Calculation of the channel resolvent matrix $\mathbb{G}_1(E)$ in the WP basis corresponding to the channel Hamiltonian H_1 (the diagonal matrix).
4. Solution of the system of algebraic equations (106) and the determination of the elastic and breakup amplitudes.

Point 1 provides two-particle input for a solution of the three-body problem. In our WP approach, the input is obtained by a single (for each value of α) diagonalization of the two-particle Hamiltonian. The result of these diagonalizations can be used to solve the scattering problem at different energies E. Whereas in the standard approach to solve the Faddeev equations one has to calculate two-particle off-shell t-matrices many times for each value of E.

Point 2 is the key to simplify the whole solution of the Faddeev-type equations. Making use of a finite-dimensional approximation for the permutation operator, i.e. replacing it with a fixed matrix (in any basis), avoids the need for numerous and time-consuming multi-dimensional interpolations of a current solution during the iteration process. In the standard approaches, these interpolations take most of the computing time. Although the calculation of matrix elements of permutation operator in our approach also meets some difficulties—multiple integrals with variable limits, however these matrix elements are computed with simple functions. Nevertheless, the calculation of the permutation matrix $\mathbb{P}^0$ takes the major part of computing time in our algorithm in sequential execution on the CPU. But it should be stressed that the matrix $\mathbb{P}^0$ is independent of energy and therefore being calculated at once, it can be used to solve scattering problem at so many energies as we wish. Note also that due to energy conservation $p_1^2/m + 3q_1^2/(4m) = p_2^2/m + 3q_2^2/(4m)$, where subscripts 1 and 2 indicate the different Jacobi sets, the permutations matrix $\mathbb{P}^0$ is very sparse—only about 1 % its matrix elements are nonzero.

Point 3 is based on the main feature of the WP representation. It is just the advantage of the WP basis that the resolvent matrix $\mathbb{G}_1(E)$ for the channel Hamiltonian H_1 is diagonal, does not depend explicitly on interaction potentials and its elements are determined only by the distributions of two-dimensional bins and the total energy E using explicit formulas.

Thus, the only real difficulty in the practical solution of the matrix equation (106) is its high dimensionality—that is the price for the elimination of the basic difficulties of a standard approach to solving the Faddeev equation. Solution of an algebraic system of such high dimensionality is an untrivial problem even for a supercomputer. But in our approach we do not need in solution for the whole system. Indeed, to find the elastic and breakup amplitudes one needs only on-shell matrix elements of the transition operator. Each of these elements can be found by means of a simple iteration procedure (without completely solving the matrix equation (106)) with subsequent summation of the iterations via the Pade-approximant technique. Note that the same Pade-technique is used in the standard approach to the solution of the Faddeev equations [36].

As was mentioned earlier, the main computational effort in our case is spent on the calculation of the free WPs overlap matrix $\mathbb{P}^0$. Because these elements are computed independently from each other, the algorithm is very appropriate for parallelization and implementation on multiprocessor systems, in particular on a graphics processing unit (GPU).

We have adopted the multi-thread GPU algorithm for a fully realistic calculations for *nd* scattering above the breakup threshold and have attained the great (more than tenfold) acceleration in comparison with the calculation on the same PC without using GPU [39]. Fig. 17 illustrates dependence of the GPU-acceleration in the solution of the Faddeev equation with a realistic *NN* interaction on the dimension of the WP basis. The distinctive feature of the GPU-calculations is that the acceleration grows with increasing the basis dimension which is clearly seen in figure.

Thus, with this novel technology for a solution of few-body scattering problems, one can perform fully realistic calculations in 3*N* system on the serial PC for few minutes only.

8.7. Construction of an effective potential for nd scattering

It has been suggested [36], that the *nd* scattering problem can be solved by constructing an effective *nd* interaction potential.

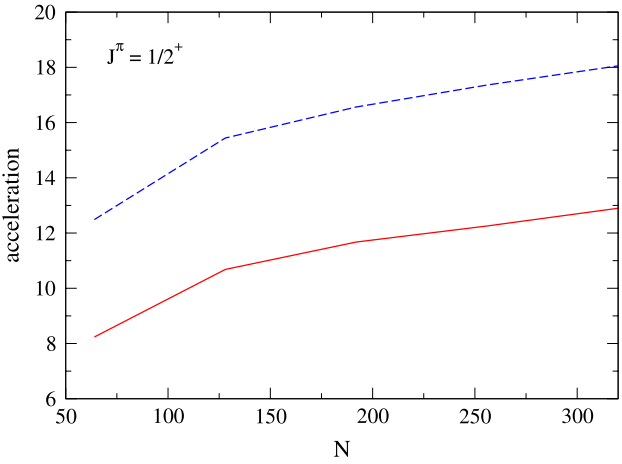

Fig. 17. The dependence of the GPU-acceleration on dimension of the basis $N \times \bar{N}$, here $\bar{N} = N$, for the realistic *nd* scattering problem with Nijmegen I *NN* potential at $J = \frac{1}{2}^+$: dashed line shows the acceleration for step 2 (calculation of the permutation matrix $\mathbb{P}^0$), solid line—the acceleration for the complete solution (see the main text).

Indeed, let us consider again the equation for the transition operator (100) and divide the channel resolvent G_1 into two parts (according to the projectors F and Q introduced in Section 7)

$$G_1 = G_{1F} + G_{1Q}. \tag{115}$$

It is evident that this division corresponds just to bound-continuum and continuum–continuum parts of the channel resolvent, i.e. $G_{1F} = G_1^{\mathrm{BC}}$ and $G_{1Q} = G_1^{\mathrm{CC}}$, where the first operator contains channel states including deuteron bound state $|z_1\rangle$.

Then, instead of a single Eq. (100), one can derive two equations:

$$U = Pv_1 + Pv_1 G_1^{\mathrm{BC}} \mathcal{V} \tag{116}$$

$$\mathcal{V} = Pv_1 + Pv_1 G_1^{\mathrm{CC}} \mathcal{V}. \tag{117}$$

It is easy to see that the first equation essentially determines the elastic amplitude and is an equation for two-particle scattering, while the second equation defines just the effective interaction potential of deuteron as a whole with an incident neutron and takes into account inelastic processes.

In the traditional approach, the solution of Eq. (117) is practically very hard, because it requires knowledge of the channel resolvent in the subspace orthogonal to the bound state (i.e. its continuum–continuum part). In the WP approach, the solution of this equation presents no difficulty, since the channel resolvent G_1^{CC} is well known here. Then the method for solving the problem of *nd* scattering by means of effective potentials can be represented schematically as follows:

(i) introduction of the 3WP basis for the channel Hamiltonian and construction of an analytical finite-dimensional representation for G_1^{CC} operator;
(ii) solution of Eq. (117) in the above WP representation;
(iii) solution of Eq. (116) in a two-body free WP basis using a matrix form of $\mathcal{V}$ operator obtained at the previous stage.

9. Summary

We described in the present paper a general technique for the continuum discretization in few-body scattering problem based on the projection of scattering operators and respective wave functions onto the discrete basis of stationary wave packets. The basic idea behind the approach is a similarity (within some restricted space) of exact non-normalized scattering states of the Hamiltonian and the

respective discrete and normalized wave-packet basis states. So that, such a WP projection allows us to transform the complicated singular multi-dimensional integral equations describing scattering (like general Lippmann–Schwinger or Faddeev–Yakubovsky equations) to regular matrix equations which can be solved directly within computational procedures similar to those used in bound-state calculations.

This novel approach has a few characteristic features which allow to simplify drastically the whole solution of few- and many-body scattering equations.

First, owing to some averaging the integral kernels over the momentum cells, all their complicated moving singularities are smoothed out and as a result one gets the simple matrix equations with finite matrix elements. This allows one to solve the resulting matrix equations directly on real energy axis without any contour deformation, continuation to complex energy plane or special interpolation procedures.

Second, instead of fully off-shell t-matrix at many energies entering the integral kernel in a conventional approach, one uses the initial potential (the matrix of which is calculated easily) and the matrix of the channel resolvent which is found by means of explicit formulas.

Third, the exact scattering wave packets in pair subsystems are treated as usual normalized excited states. This makes possible to consider a three-body breakup process as an inelastic scattering to normalized pseudostates. Such a replacement simplifies greatly the description of three- and few-body breakup processes.

Fourth, due to a specific matrix structure of resulting matrix equations one can organize the massively-parallel computing with use of the graphics processing unit. This makes it possible to carry out all the computations via thousands of threads on the GPU inside a desktop PC and leads to real ultra-fast calculations for the scattering problems in few-body systems.

The developed wave-packet approach to solving few-body scattering problems is universal and may be used in different branches of nuclear, atomic and chemical physics, in quantum statistics and nuclear matter theory. Also it can be directly generalized to a relativistic case.

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Appendix. Explicit formulas for the channel resolvent eigenvalues

A.1. Eigenvalues of two-body resolvent

Two-body free resolvent eigenvalues for the case of momentum WPs ($f(q) = 1$) are defined by the general formula (47) and thus they have the following form:

$$g_i(E) = \frac{\mu}{qd_i}\left\{\ln\left|\frac{q-q_{i-1}}{q-q_i}\right| + \ln\left|\frac{q+q_i}{q+q_{i-1}}\right| - \mathrm{i}\pi\left[\theta(q-q_{k-1}) - \theta(q-q_k)\right]\right\}, \tag{A.1}$$

where $q = \sqrt{2\mu E}$ and the combination of the Heaviside θ-functions means that the imaginary parts of the eigenvalues do not vanish only in a single interval to which the respective on-shell momentum value belongs: $q \in \mathfrak{D}_k$.

The energy averaged eigenvalues are defined by integral

$$g_i^k \equiv \frac{1}{D_k}\int_{\mathfrak{D}_k} g_i(E)\frac{q}{\mu}\mathrm{d}q, \quad E \in \mathfrak{D}_k. \tag{A.2}$$

Explicit formulas for the q-packet case now are the following:

$$g_i^k = \frac{1}{D_k d_i}\left[Q_{ki}^{(+)} - Q_{ki}^{(-)}\right] - \frac{\mathrm{i}\pi}{D_k}\delta_{ik}, \tag{A.3}$$

where

$$Q_{ki}^{(\pm)} = \sum_{k'=k-1}^{k} \sum_{i'=i-1}^{i} (-1)^{k-k'+i-i'} [q_{k'} \pm q_{i'}] \ln |q_{k'} \pm q_{i'}|.$$

In the case of the energy free WPs with the weight function $f(q) = \sqrt{\frac{q}{\mu}}$, the formula for the free resolvent eigenvalue becomes the following:

$$g_i(E) = \frac{1}{D_i} \ln \left| \frac{E - \mathcal{E}_{i-1}}{E - \mathcal{E}_i} \right| - \frac{\mathrm{i}\pi}{D_k} [\theta(E - \mathcal{E}_{k-1}) - \theta(E - \mathcal{E}_k)], \quad E \in \mathfrak{D}_k, \tag{A.4}$$

where $\mathcal{E}_i$ are bin endpoints. The eigenvalue for the averaged resolvent in the energy free WP basis takes the form:

$$g_i^k = \frac{1}{D_k D_i} W_{ki} - \frac{\mathrm{i}\pi}{D_k} \delta_{ik}, \tag{A.5}$$

where

$$W_{ki} = \sum_{k'=k-1}^{k} \sum_{i'=i-1}^{i} (-1)^{k-k'+i-i'} [\mathcal{E}_{k'} - \mathcal{E}_{i'}] \ln |\mathcal{E}_{k'} - \mathcal{E}_{i'}|.$$

A.2. Eigenvalues of three-body channel resolvent

The eigenvalues defined in (78a) for the BC part of indices in a case of energy WPs are the following

$$\left.\begin{aligned} \mathrm{Re}[G^{\Gamma\alpha\beta}(E)]_{kj} &= \frac{1}{\bar{D}_j} \ln \left| \frac{\mathcal{E}_{j-1} + \epsilon_k^{*\alpha} - E}{\mathcal{E}_j + \epsilon_k^{*} - E} \right|, \\ \mathrm{Im}[G^{\Gamma\alpha\beta}(E)]_{kj} &= -\frac{\pi}{\bar{D}_j} \left\{ \theta(\mathcal{E}_j + \epsilon_k^{*\alpha} - E) - \theta(\mathcal{E}_{j-1} + \epsilon_k^{*\alpha} - E) \right\} \end{aligned}\right\}. \tag{A.6}$$

These BC eigenvalues have the same functional form as eigenvalues of the two-body free resolvent given in (A.4). The only difference is that bound points $\mathcal{E}_j$ of partition of the free sub-Hamiltonian h_0^1 continuum are shifted to eigenvalues $\epsilon_k^{*\alpha}$ of the sub-Hamiltonian h_1.

The real parts of the CC-parts of the channel resolvent have the following form:

$$\begin{aligned} \mathrm{Re}[G^{\Gamma\alpha\beta}(E)]_{kj} = {} & \frac{1}{D_k^\alpha \bar{D}_j} \Big\{ (\Delta + \Delta_-) \ln |\Delta + \Delta_-| + (\Delta - \Delta_-) \ln |\Delta - \Delta_-| \Big\} \\ & - \frac{1}{D_k^\alpha \bar{D}_j} \Big\{ (\Delta + \Delta_+) \ln |\Delta + \Delta_+| + (\Delta - \Delta_+) \ln |\Delta - \Delta_+| \Big\}, \end{aligned} \tag{A.7}$$

where:

$$\Delta \equiv \epsilon_k^{*\alpha} + \mathcal{E}_j^* - E, \qquad \Delta_- \equiv \frac{D_k^\alpha - \bar{D}_j}{2}, \qquad \Delta_+ \equiv \frac{D_k^\alpha + \bar{D}_j}{2}$$

and $D_k^\alpha, \bar{D}_j$ are energy widths of bins for sub-Hamiltonians h_1 and h_0^1 respectively.

The imaginary parts of the CC-eigenvalues also have an explicit analytical form

$$\begin{aligned} \mathrm{Im}[G^{\Gamma\alpha\beta}(E)]_{kj} = {} & -\frac{\pi}{D_k^\alpha \bar{D}_j} \Big\{ (\Delta + \Delta_+)\theta(\Delta + \Delta_+) + (\Delta - \Delta_+)\theta(\Delta - \Delta_+) \\ & - (\Delta + \Delta_-)\theta(\Delta + \Delta_-) - (\Delta - \Delta_-)\theta(\Delta - \Delta_-) \Big\}. \end{aligned} \tag{A.8}$$

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