PHYSICAL REVIEW C **89**, 064008 (2014)

New general approach in few-body scattering calculations: Solving discretized Faddeev equations on a graphics processing unit

V. N. Pomerantsev,* V. I. Kukulin,† and O. A. Rubtsova‡
Institute of Nuclear Physics, Moscow State University, Leninskie Gory, Moscow 119991, Russia
(Received 22 April 2014; published 30 June 2014)

Background: The numerical solution of few-body scattering problems with realistic interactions is a difficult problem that normally must be solved on powerful supercomputers, taking a lot of computer time. This strongly limits the possibility of accurate treatments for many important few-particle problems in different branches of quantum physics.
Purpose: To develop a new general highly effective approach for the practical solution of few-body scattering equations that can be implemented on a graphics processing unit.
Methods: The general approach is realized in three steps: (i) the reformulation of the scattering equations using a convenient analytical form for the channel resolvent operator, (ii) a complete few-body continuum discretization and projection of all operators and wave functions onto an L_2 basis constructed from stationary wave packets, and (iii) the ultrafast solution of the resulting matrix equations using a graphics processor.
Results: The whole approach is illustrated by a calculation of the neutron-deuteron elastic scattering cross section below and above the three-body breakup threshold with a realistic NN potential that is performed on a standard PC using a graphics processor with an extremely short runtime.
Conclusions: The general technique proposed in this paper opens a new way for a fast practical solution of quantum few-body scattering problems in both nonrelativistic and relativistic formulations in hadronic, nuclear, and atomic physics.

DOI: 10.1103/PhysRevC.89.064008 PACS number(s): 21.45.−v, 02.60.−x, 03.65.Nk

I. INTRODUCTION

It is well known that a sharp contrast exists today in the quantum-mechanical treatment of few- and many-body systems between very effective and fast bound-state calculations on the one hand and very time-consuming few-particle scattering calculations on the other hand. Practical solutions for a discrete spectrum may incorporate many hundreds or even thousands of particles with simple Coulomb-like interactions in atomic or molecular physics, or up to 20–25 nucleons with complicated realistic NN interactions in nuclear physics, while even the solution of the four-nucleon scattering problem with realistic NN interactions, especially above the three-body breakup threshold, represents a strong challenge for modern theorists [1]. There are at least two reasons for such a strong contrast. First, the few-body scattering problem includes complicated boundary conditions, especially above the three- or four-body breakup thresholds, and second, the multiparticle Hamiltonian has a degenerate continuous spectrum, so that each pair or triple of particles can be in an infinite number of states at the same energy.

The first problem has been solved mathematically by formulation of the Faddeev-Yakubovsky equations whose full solution satisfies, as has been strictly proved [2], all of the necessary boundary conditions. However, the price for this correct formulation is a very sophisticated form of these integral equations, whose kernels have complicated moving singularities. Therefore, in the previous four decades a lot of exact and approximate methods for solving the Faddeev-Yakubovsky equations have been proposed. However, due to the complexity of realistic few-body scattering problems, practical solutions usually require a massively parallel implementation, so that even now exact Faddeev-like scattering calculations are performed mainly on powerful supercomputers (see, e.g., the recent $3N$ calculations [3]). The complexity of the few-body equations leads to the fact that an accurate numerical treatment for realistic few-body scattering problems remains available only to a limited number of experts.

The most effective way to treat the second key problem related to degeneracy of few-body continuous spectra of the total and channel Hamiltonians is their discretization by one or another method and usage of L_2 normalized states as approximations for exact continuum states. Nowadays, many such discretization methods exist (see, for example, a recent comprehensive review [1]). However, it is still not clear whether these particular discretization methods give a discrete form of scattering equations, which permit a high degree of parallelism in a numerical solution. The last point is crucially important for further progress in few-body scattering calculations because even powerful supercomputers cannot give essential acceleration of the calculations if the solution method does not permit an effective parallelization for all parts of the algorithm.

Quite recently, a new computational technique has been introduced based on the general-purpose graphics processing unit (GPGPU). This technique utilizes a graphics processing unit (GPU) that has been initially designed to carry out computations for computer graphics. Nowadays, GPUs are

*pomeran@nucl-th.sinp.msu.ru
†kukulin@nucl-th.sinp.msu.ru
‡rubtsova@nucl-th.sinp.msu.ru

specialized to perform ultrafast general-purpose computations and they can replace a supercomputer realization in many particular cases. Also, special extensions of standard programming languages are developed to use GPU facilities in tedious scientific calculations (see, e.g., Ref. [4]).

This technique has been actively pursued and successfully used in quantum chemistry [5], lattice QCD calculations [6], Monte-Carlo simulations, etc. Recently, *ab initio* nuclear structure GPU calculations [7] have been performed as well as GPU treatments of Faddeev equations for quantum trimer systems [8]. It is of great interest to apply such GPU techniques to realistic few-body scattering calculations. This would open new possibilities for accurate few-body studies in general and could make them more accessible to a wider number of researchers. However, the GPU realization requires an appropriate and specific formulation for scattering problems because this realization is most effective for algorithms with a high degree of parallelism and minimal interdependence between data processing in parallel threads.

The present authors have suggested in previous years the wave-packet continuum discretization technique [9,10], which has been tested carefully for the model NN interactions and found to be very efficient. One of the important features of the above discrete approach is that the resulting discretized form of the scattering equations is well suited for such a parallel realization. Below we show that such a massively parallel implementation of the whole solution can be made on a standard PC with a modern graphics processor that can perform all of the calculations using many thousands of parallel threads.

In the present paper we have also made a generalization of the wave-packet approach to few-body equations with a fully realistic NN interaction, which is not a trivial problem and requires a new determination for the multichannel resolvent in an analytical form. So we included a section with this description in the present paper.

The paper is organized as follows. In Sec. II we summarize the main features of the wave-packet approach and describe how it is used to solve the three-body scattering problem. In Sec. III the case of the coupled-channel two-body input interaction is discussed and formulas for the three-body channel resolvent are given. The results for the nd elastic scattering problem are represented in Sec. IV. Section V is dedicated to a description of our first GPU tests for the problem in question and a comparison of the corresponding computational efficiency of the CPU and GPU realizations on the same PC. The main results of the paper are summarized in the conclusion.

II. NEW GENERAL APPROACH IN FEW-BODY SCATTERING CALCULATIONS

The present work discusses the solution of few- and many-body scattering problems in atomic, molecular, nuclear, and hadronic physics. Here we discuss in detail all of the steps needed to implement our new approach and we illustrate the whole technique using a nontrivial example—the solution of the Faddeev equations for nd scattering below and above the three-body breakup threshold with a realistic NN interaction.

A. The basic features of the approach

In our approach, we change all of the steps used in the conventional procedure for solving the Faddeev equations in momentum space.

(i) The first step is to replace the conventional form of the Faddeev integral equation, e.g., for a transition operator U describing elastic nd scattering [11],

$$U = PG_0^{-1} + Pt_1G_0U, \tag{1}$$

with the half-shell equivalent form

$$U = Pv_1 + Pv_1G_1U. \tag{2}$$

Here v_1 is the two-body interaction, t_1 is the two-body t matrix, G_0 is the resolvent of the free three-body Hamiltonian H_0, $P = P_{12}P_{23} + P_{13}P_{23}$ is the particle permutation operator, and $G_1 = [E + i0 - H_1]^{-1}$ is the resolvent of the channel Hamiltonian

$$H_1 = h_1 \oplus h_0^1, \tag{3}$$

where $h_1 = h_0 + v_1$ is the two-body NN sub-Hamiltonian and h_0^1 is the sub-Hamiltonian describing free motion of the third nucleon relative to the NN subsystem. The index 1 is the Jacobi-set index of the initial state.

One of the main purposes for such a replacement is to change the required two-body input: instead of fully off-shell two-body t matrices at many energies, we suggest employing two-body interactions v_1 in combination with the channel resolvent G_1. However, in such a replacement, one has to evaluate additionally the channel resolvent operator G_1. Fortunately, in the wave-packet approach, the finite-dimensional approximation for this operator is calculated easily in a closed analytical form [9].

Moreover, the whole energy dependence appears now in the channel resolvent operator (rather than in the off-shell t matrix, as in the conventional formulation), which is calculated explicitly. So that, with such a replacement, we can find a solution of few-body scattering equations *at many energies almost with the same computational effort that is needed for a single energy*.

Another important advantage of our approach is a new treatment of three-body breakup. Contrary to the conventional approach, we treat three- or many-body breakup processes as particular cases of inelastic excitations (into states of the discretized continuum) [10]. Such a treatment strongly facilitates breakup calculations.

(ii) The second step is to project the integral kernels of the reformulated Faddeev equations and the solution onto a special orthogonal basis of the stationary wave packets (WPs), which corresponds to a formulation of the scattering problem on a momentum lattice. Such a basis is very appropriate for constructing normalized analogs of continuum states for the channel Hamiltonian H_1. It follows that the solution of the three-body scattering problem is described in

the terms of asymptotic channel states, in contrast to the conventional approach, which employs free three-body states (the plane waves).

Such a projection of the three-body scattering equations onto a three-body WP basis results in matrix equations that allow us to circumvent the main difficulties that arise in the conventional solution of the initial singular integral equation. First, the use of a finite matrix for the permutation operator in a discrete WP basis eliminates the need for the very numerous multidimensional interpolations of a given solution into the "rotated" Jacobi set during iterations. Further, all singularities of the Faddeev kernel (in the form Pv_1G_1) are isolated now in the channel resolvent G_1 and thus can be easily smoothed and averaged when using the WP representation [9]. At last, the resulting matrix equations can be solved directly at real energies without any contour rotations or deformations onto complex planes, which are often employed in the solution of singular integral equations.

The resulting matrix equation (of high dimension) obtained in the WP approach is solved by simple iterations when they converge or otherwise by applying an additional Pade-approximant summation. The computational scheme turns out to be very efficient and thus the whole calculation can be performed even on a standard PC.

Following these steps, in our previous papers, [9,10], we studied elastic scattering and breakup cross sections in a $3N$ system with a central NN potential. However it was still unclear if the advantages of the above computational scheme remain valid for realistic NN interactions including tensor, spin-orbit, etc., components and in particular when the number of contributing spin-orbital partial channels is large.[1] To investigate this question we apply our approach to a three-nucleon system interacting with a realistic NN interaction, including a tensor component (the Nijmegen NN potential [12]), at energies below and above the three-body breakup threshold.

(iii) To further extend the complexity of scattering problems that can be treated accurately, it is desirable to develop a highly parallel algorithm for the solution of the resulting matrix equations of large dimension. *The third step* is to parallelize the algorithm to adapt it for computations by a GPU. Such a GPU realization is shown in the present paper to make the solution of the resulting matrix equations (derived from a multichannel system of integral Faddeev equations) extremely fast even on a standard PC.

[1] In particular, the authors of the recent review [1] expressed some doubts in the full applicability of the present WP approach to realistic interactions.

B. Discrete form of the Faddeev equation in wave-packet representation

Here we briefly describe our approach based on a continuum discretization using the stationary WPs. We illustrate this using the example of the Faddeev equation (2) for the transition operator U for nd scattering (for further details, see Refs. [9,10]).

1. Definition of momentum lattice basis functions

To construct the three-body WP basis functions, we start from the two-body case and introduce partitions of the continua of two free sub-Hamiltonians, h_0 and h_0^1, onto nonoverlapping intervals $\{\mathfrak{D}_i \equiv [\epsilon_{i-1},\epsilon_i]\}_{i=1}^{M}$ and $\{\bar{\mathfrak{D}}_j \equiv [\mathcal{E}_{j-1},\mathcal{E}_j]\}_{j=1}^{N}$, respectively. These sub-Hamiltonians describe the free motion of particles 2 and 3 with relative momentum p and the free motion of particle 1 with momentum q relative to the center of mass of the pair {23}, respectively. Thus the free stationary wave packets $|\mathfrak{p}_i\rangle$ and $|\mathfrak{q}_j\rangle$ are built as integrals of the free solutions $|p\rangle$ and $|q\rangle$ over the discretization bins:

$$|\mathfrak{p}_i\rangle = \frac{1}{\sqrt{B_i}}\int_{\mathfrak{D}_i} f(p)|p\rangle dp, \quad |\mathfrak{q}_j\rangle = \frac{1}{\sqrt{\bar{B}_j}}\int_{\bar{\mathfrak{D}}_j} \bar{f}(q)|q\rangle dq, \tag{4}$$

where B_i and $\bar{B}_j$ and $f(p)$ and $\bar{f}(q)$ are normalization factors and weight functions, respectively [9,10]. Here and below we denote the functions and values corresponding to the q variable with an additional bar mark to distinguish them from the functions corresponding to the p variable.

When constructing the three-body WP basis one should take into account spin and angular parts of the basis functions. We use the following quantum numbers for the subsystems and the whole three-body system according to the (jj)-coupling scheme:

$$\alpha = \{l,s,j\}, \quad \beta = \{\lambda,I\}, \quad \Gamma = \{J,\pi,T\}, \tag{5}$$

where l, s, and j are NN quantum numbers: l is the orbital momentum, s is the spin, and $\mathbf{j} = \mathbf{l} + \mathbf{s}$ is the total angular momentum of the subsystem (the interaction potential depends on the value of j). 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, $\mathbf{J} = \mathbf{j} + \mathbf{I}$ is a total angular momentum of the three-body system, T is the total isospin, and π is the parity, all of them are conserved. Let's 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 free WP states should be defined for each partial wave l and λ and further they are multiplied by the appropriate spin-angular states. Thus the three-body basis function can be written as

$$\left|X_{ij}^{\Gamma\alpha\beta}\right\rangle = \left|\mathfrak{p}_i^l\right\rangle \otimes \left|\mathfrak{q}_j^\lambda\right\rangle |\alpha,\beta:\Gamma\rangle, \tag{6}$$

where $|\alpha\rangle$ is a spin-angular state of the NN pair, $|\beta\rangle$ is a spin-angular state of the third nucleon, and $|\Gamma\rangle$ is a set of three-body quantum numbers.

The state (6) is the WP analog of the exact plane wave state in the three-body continuum $|p,q;\alpha,\beta:\Gamma\rangle$ for the three-body free Hamiltonian $H_0 = h_0 \oplus h_0^1$.

The free stationary wave packets defined in Eq. (4) with unit weights are steplike functions in the momentum representation [9,10] while the three-body free WP basis functions are constant inside the cells of the lattice built by a convolution of two one-dimensional cells, $\{\mathfrak{D}_i\}_{i=1}^M$ and $\{\bar{\mathfrak{D}}_j\}_{j=1}^N$. We refer to the free WP basis as *a lattice* basis. We denote the two-dimensional bins (i.e., the lattice cells) by $\mathfrak{D}_{ij} = \mathfrak{D}_i \otimes \bar{\mathfrak{D}}_j$.

2. The wave-packet basis for the channel Hamiltonian

In the case of a single-channel two-body input interaction (e.g., the central one), we have demonstrated [9,10] that it is possible to define *scattering WPs* corresponding to the exact scattering wave functions $|\psi_p\rangle$ of the sub-Hamiltonian h_1:

$$|z_k\rangle = \frac{1}{\sqrt{C_i}} \int_{\Delta_i} w(p)|\psi_p\rangle dp, \tag{7}$$

where Δ_i are partition intervals and C_i and $w(p)$ are a normalization factor and a weight function.

To use the states (7) practically, one can approximate them with the pseudostates of the sub-Hamiltonian h_1 in some L_2 bases [9,10]. Also it has been shown that the free WP basis is very appropriate to approximate scattering states because the respective functions have a very long-range behavior in configuration space. Therefore we can calculate the eigenstates (the bound and pseudostates) of the sub-Hamiltonian h_1 matrix in the two-body WP basis $\{|\mathfrak{p}_i\rangle\}_{i=1}^M$ via a diagonalization procedure. As a result one gets the eigenstates of the h_1 sub-Hamiltonian expanded in the free WP basis (for each partial wave l):

$$\left|z_k^l\right\rangle \approx \sum_{i=1}^{M} O_{ki}^l \left|\mathfrak{p}_i^l\right\rangle. \tag{8}$$

For the case of a central interaction, the three-body quantum numbers for the channel Hamiltonian H_1 are the same as those for the three-body free Hamiltonian H_0, so that total three-body WP states corresponding to the channel Hamiltonian H_1 (three-body scattering wave packets—SWPs) are built as direct products of the two-body WPs with the same spin-angular quantum numbers α, β, and Γ:

$$\left|Z_{kj}^{\Gamma\alpha\beta}\right\rangle \equiv \left|z_k^l\right\rangle \otimes \left|\mathfrak{q}_j^\lambda\right\rangle |\alpha,\beta:\Gamma\rangle. \tag{9}$$

The main advantage of the basis constructed from the SWP (9) is that one gets *an explicit analytical* and even *diagonal form* for the matrix of the three-body channel resolvent G_1 [9,10].

Having the WP basis for the channel Hamiltonian (9) at our disposal, it is possible to project all of the constituents of the integral equation (2) and find its finite-dimensional, i.e., matrix, analog. As an important result of the projecting of the channel operator $G_1 v_1$ onto the SWP basis, one gets the main part of the Faddeev kernel matrix in a convenient analytical form, with a completely analytical energy dependence, in sharp contrast to a conventional approach with a fully off-shell t matrix in a numerical form.

3. The matrix of the permutation operator

The permutation operator matrix $\mathbb{P}$ in the three-body SWP basis $|Z_{kj}^{\Gamma\alpha\beta}\rangle$ can be expressed through the overlap matrix $\mathbb{P}^0$ in the free WP basis $|X_{ij}^{\Gamma\alpha\beta}\rangle$ using the rotation matrices $\mathbb{O}$ from the expansion (8):

$$\left\langle Z_{kj}^{\Gamma\alpha\beta}\middle|P\middle|Z_{k'j'}^{\Gamma\alpha'\beta'}\right\rangle \approx \sum_{ii'} O_{ki}^l O_{k'i'}^{l'*} \left\langle X_{ij}^{\Gamma\alpha\beta}\middle|P\middle|X_{i'j'}^{\Gamma\alpha'\beta'}\right\rangle. \tag{10}$$

A matrix element of the operator P in the free WP basis is equal to the overlap between basis functions defined in different Jacobi sets. Such a matrix element can be calculated by integration with the basis functions over the momentum lattice cells:

$$\begin{aligned}&\left\langle X_{ij}^{\Gamma\alpha\beta}\middle|P\middle|X_{i'j'}^{\Gamma\alpha'\beta'}\right\rangle \\ &\quad= \int_{\mathfrak{D}_{ij}} p^2 dp q^2 dq \int_{\mathfrak{D}'_{i'j'}} (p')^2 dp' (q')^2 dq' \\ &\qquad\times \frac{f^*(p)\bar{f}^*(q) f(p')\bar{f}(q')}{\sqrt{B_i B_{i'} \bar{B}_j \bar{B}_{j'}}} \langle pq,\alpha\beta:\Gamma|P|p'q',\alpha'\beta':\Gamma\rangle,\end{aligned} \tag{11}$$

where the prime on the lattice cell $\mathfrak{D}'_{i'j'}$ indicates that the cell belongs to the other Jacobi set while $\langle pq,\alpha\beta:\Gamma|P|p'q',\alpha'\beta':\Gamma\rangle$ is the kernel of the particle permutation operator in momentum space. This kernel, as is well known [11], is proportional to the product of a Dirac δ and a Heaviside θ function. However, due to integration in Eq. (11), these singularities get averaged over the momentum lattice cells and, as a result, the elements of the permutation operator matrix in the WP basis are finite and regular.

The matrix element in Eq. (11) can be calculated using a double numerical integration. The practical technique of such a calculation is described in the Appendix.

4. Matrix analog of the Faddeev equation for elastic nd scattering and breakup

Having evaluated the matrix of the permutation operator P, the calculation of the kernel Pv_1G_1 matrix becomes fast and straightforward.

As a result of projecting the integral equation (2) onto the three-body SWP basis, one gets its matrix analog (for each set of three-body quantum numbers Γ):

$$\mathbb{U} = \mathbb{P}\mathbb{V}_1 + \mathbb{P}\mathbb{V}_1\mathbb{G}_1\mathbb{U}. \tag{12}$$

Here $\mathbb{P}$, $\mathbb{V}_1$, and $\mathbb{G}_1$ are matrices of the permutation operator, the pair interaction, and the channel resolvent, respectively, defined in the SWP basis.[2]

The on-shell elastic amplitude for the nd scattering in the WP representation is defined by a diagonal matrix element of

[2] A similar reduction to the discrete matrix form can be done also for Lippmann-Schwinger, Faddeev-Yakubovsky, and relativistic Faddeev equations.

the $\mathbb{U}$ matrix [9,10]:

$$A_{\rm el}^{\Gamma\alpha_0\beta}(q_0) \approx \frac{2m}{3q_0}\frac{\langle Z_{0j_0}^{\Gamma\alpha_0\beta}|\mathbb{U}|Z_{0j_0}^{\Gamma\alpha_0\beta}\rangle}{\bar{d}_{j_0}}, \tag{13}$$

where m is the nucleon mass, q_0 is the initial two-body momentum, and $|Z_{0j_0}^{\Gamma\alpha_0\beta}\rangle = |z_0^{\alpha_0},\mathfrak{q}_{j_0}^{\lambda};\alpha_0,\beta:\Gamma\rangle$ is the SWP basis state corresponding to the initial scattering state. Here $|z_0^{\alpha_0}\rangle$ is the bound state of the pair (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 the momentum width of this bin.

It should be noted here that in our discrete WP approach *the three-body breakup is treated as a particular case of an inelastic scattering* [10] (defined by the transitions to the specific two-body discretized continuum states), so that the breakup amplitude can be defined in terms of *the same matrix* $\mathbb{U}$ determined from Eq. (12).

For the case of the tensor components of the NN interaction (or other coupled-channel two-body interactions v_1), the generalization of the whole formalism is straightforward. However, it is necessary to take into account some new aspects related to the discretized spectrum of the two-body *multichannel* Hamiltonian h_1 to build the correct approximation for the discretized resolvent G_1.

III. CHANNEL RESOLVENT IN THE CASE OF A COUPLED-CHANNEL INTERACTION

A. Construction of the SWP basis for a coupled-channel sub-Hamiltonian

The three-body SWP states corresponding to the channel Hamiltonian H_1 can be defined similarly to the one-channel two-body interaction case, i.e., as direct products of two-body WP states for the h_0^1 and h_1 sub-Hamiltonians (jointly with the bound state of h_1) multiplied by spin-angular functions of the system. However, here the possible spin-angular couplings in the {23} subsystem due to the tensor component in a pairwise interaction v_1 should be taken into account.

Recently, the present authors have developed a convenient approach for solving multichannel scattering problems via a straightforward diagonalization of the multichannel Hamiltonian in a WP basis—the discrete spectral-shift (DSS) formalism [13]. In this approach, the multichannel Hamiltonian pseudostates have been shown to correspond to scattering wave functions defined in the so-called eigenchannel representation (ER) [14] for which the multichannel S matrix is diagonal.

Let's introduce two types of scattering states of the sub-Hamiltonian h_1: the scattering states $|\psi_p^l\rangle$ (which include radial and angular parts) corresponding to the initial wave with a definite orbital momentum l and the scattering states defined in the ER $|\psi_p^{\varkappa}\rangle$, where $\varkappa$ is an eigenchannel index. In the case of a tensor NN interaction, the scattering states $|\psi_p^{\varkappa}\rangle$ are linear combinations of the states $|\psi_p^l\rangle$, e.g., the coupled pairs $^3S_1$-$^3D_1$, $^3P_2$-$^3F_2$, etc.

The main advantage of the ER formalism is that one gets the following spectral expansion for the resolvent of the pair sub-Hamiltonian $g_1(E) \equiv [E + i0 - h_1]^{-1}$ (see, e.g., Ref. [15]):

$$g_1(E) = \frac{|z_0\rangle\langle z_0|}{E-\epsilon_0} + \sum_{\varkappa}\int_0^{\infty}\frac{|\psi_p^{\varkappa}\rangle\langle\psi_p^{\varkappa}|}{E+i0-\frac{p^2}{m}}dp, \tag{14}$$

which is *diagonal* in the eigenchannel index $\varkappa$. In Eq. (14), ϵ_0 is an energy of the bound state $|z_0\rangle$ and m is the nucleon mass.

Thus, it is convenient to construct multichannel two-body SWPs as integrals of exact scattering wave functions of the sub-Hamiltonian h_1 defined in the ER:

$$|z_{\varkappa,i}\rangle = \frac{1}{\sqrt{C_i^{\varkappa}}}\int_{\Delta_i^{\varkappa}} w(p)|\psi_p^{\varkappa}\rangle dp, \quad i = 1,\ldots,M^{\varkappa}, \tag{15}$$

where $\Delta_i^{\varkappa} \equiv [E_{i-1}^{\varkappa}, E_i^{\varkappa}]$ are new partition intervals whose parameters might be different for different $\varkappa$.

The crucial feature of the DSS formalism defined in Ref. [13] is that these multichannel SWPs can be constructed (jointly with the deuteron bound-state wave function) as pseudostates of the Hamiltonian h_1 matrix in the multichannel free WP basis $|\mathfrak{p}_i^l\rangle$ (where radial and angular parts of wave functions are included). Because l is not conserved, for each value of total momentum j, the two-channel h_1 sub-Hamiltonian states are constructed from free WP bases $\{|\mathfrak{p}_i^l\rangle\}_{l=l_1,l_2}$ defined for both possible values of l_1 and l_2.

Finally, we have at our disposal the multichannel SWP basis functions that are related to the free WPs by a simple orthogonal transformation like in the one-channel case (8):

$$|z_{\varkappa_{\tilde{\alpha}},k},\tilde{\alpha}\rangle = \sum_{i=1}^{M}\sum_{l} O_{ki}^{\varkappa_{\tilde{\alpha}}l}|\mathfrak{p}_i^l,\alpha\rangle, \tag{16}$$

where the spin-angular parts of wave functions are taken into account as well and the multi-index $\tilde{\alpha} = \{\varkappa_{\tilde{\alpha}}, s, j\}$ related to the ER is introduced. Below we do not detail the index $\varkappa_{\tilde{\alpha}}$, which is a part of the multi-index $\tilde{\alpha}$.

In this way, we construct the three-body SWP basis functions for the channel Hamiltonian H_1 as direct products of the two-body ones for the h_0^1 and h_1 sub-Hamiltonians:

$$|Z_{kj}^{\Gamma\tilde{\alpha}\beta}\rangle \equiv |z_{\varkappa_{\tilde{\alpha}},k}^{\tilde{\alpha}}\rangle \otimes |\mathfrak{q}_j^{\beta}|\tilde{\alpha},\beta:\Gamma\rangle. \tag{17}$$

These states are WP analogs of the three-body ER scattering states $|\psi_p^{\varkappa_{\tilde{\alpha}}},q;\tilde{\alpha},\beta:\Gamma\rangle$ of the channel Hamiltonian H_1.

Hence, starting from free WP bases for each two-body sub-Hamiltonian one gets a set of basis states for both the three-body free and channel Hamiltonians, H_0 and H_1, respectively, which are related to each other by a simple matrix rotation.

B. Resolvent of the channel Hamiltonian

The spectral expansion of the three-body channel resolvent G_1 in the ER can be found straightforwardly by making a convolution of the multichannel subresolvent g_1 with the resolvent $g_1^0(E) = [E + i0 - h_0^1]^{-1}$ for the free sub-Hamiltonian h_0^1 of the third nucleon:

$$G_1(E) = \frac{1}{2\pi i}\int_{-\infty}^{\infty} d\varepsilon g_1(\varepsilon)g_0^1(E-\varepsilon). \tag{18}$$

This leads to the following representation for the multichannel three-body resolvent operator G_1 via the scattering

eigenfunctions of the NN subsystem defined in the ER:

$$G_1(E) = \sum_{\Gamma,\tilde{\alpha}_0,\beta} \int_0^\infty dq \frac{|z_0,q,\tilde{\alpha}_0\beta:\Gamma\rangle\langle z_0,q,\tilde{\alpha}_0\beta:\Gamma|}{E+i0-\epsilon_0-\frac{3q^2}{4m}} + \sum_{\Gamma,\tilde{\alpha},\beta} \int_0^\infty dpdq \frac{\left|\psi_p^{\varkappa_{\tilde{\alpha}}},q;\tilde{\alpha},\beta:\Gamma\right\rangle\left\langle\psi_p^{\varkappa_{\tilde{\alpha}}},q;\tilde{\alpha},\beta:\Gamma\right|}{E+i0-\frac{p^2}{m}-\frac{3q^2}{4m}}. \quad (19)$$

The first term (the bound-continuum part) in Eq. (19) is a spectral sum over three-body states corresponding to the free motion of the third nucleon relative to the deuteron. The second term (the continuum-continuum part) in Eq. (19) for the channel resolvent includes channel three-body states with NN pair interacting in the continuum (in the ER) and its imaginary part is defined by a discontinuity across the three-body cut on the Riemann energy surface.

By projecting the channel resolvent operator onto the three-body SWP basis defined in Eq. (17), one can find analytical formulas for matrix elements of operator G_1 in such a basis. The respective matrix is diagonal in all wave-packet and spin indices:

$$\left\langle Z_{kj}^{\Gamma\tilde{\alpha}\beta}\middle|G_1(E)\middle|Z_{k'j'}^{\Gamma\tilde{\alpha}'\beta'}\right\rangle = \delta_{kk'}\delta_{jj'}\delta_{\tilde{\alpha}\tilde{\alpha}'}\delta_{\beta\beta'}G_{kj}^{\Gamma\tilde{\alpha}\beta}(E). \quad (20)$$

Here the diagonal matrix elements $G_{kj}^{\Gamma\tilde{\alpha}\beta}(E)$ depend, in general, on the spectral partition parameters (i.e., $\Delta_k^{\varkappa_{\tilde{\alpha}}}$ and $\bar{D}_j$ values) and total energy E only. These matrix elements do not depend explicitly on the interaction potential v_1.

The matrix elements $G_{kj}^{\Gamma\tilde{\alpha}\beta}(E)$ are defined as integrals over the respective momentum intervals for the bound-continuum part of the whole operator,

$$G_{0j}^{\Gamma\tilde{\alpha}_0\beta}(E) = \frac{1}{\bar{B}_j}\int_{\bar{\mathfrak{D}}_j} \frac{|\bar{f}(q)|^2 dq}{E+i0-\epsilon_n^\alpha-\frac{3q^2}{4m}}, \quad (20a)$$

and for the continuum-continuum part,

$$G_{kj}^{\Gamma\tilde{\alpha}\beta}(E) = \frac{1}{C_k^{\varkappa_{\tilde{\alpha}}}\bar{B}_j}\int_{\Delta_k^{\varkappa_{\tilde{\alpha}}}}\int_{\bar{\mathfrak{D}}_j} \frac{|w(p)|^2|\bar{f}(q)|^2 dpdq}{E+i0-\frac{p^2}{m}-\frac{3q^2}{4m}}. \quad (20b)$$

If the solution of the scattering equations in the finite-dimensional WP basis converges with increasing the basis dimension, the final result turns out to be *independent* of the particular spectral partition parameters.

Representations (20a) and (20b) for the channel resolvent are the basis of the wave-packet approach, because, after a straightforward analytical evaluation of the integrals[3] in Eqs. (20a) and (20b), one gets explicit formulas for the three-body resolvent and thus a drastic simplification of the solution of a general three-body scattering problem. These analytical expressions can be used directly to solve the matrix Faddeev equation in Eq. (12).

[3]We have found previously [16] the explicit formulas for the resolvent matrix elements (20a) when one uses the WPs with the weight functions $w(p) \sim \sqrt{p}$ and $\bar{f}(q) \sim \sqrt{q}$.

IV. SOLUTION OF THE *nd* SCATTERING PROBLEM WITH A REALISTIC *NN* INTERACTION

In this section the effectiveness of the new approach in few-body calculations is illustrated by solving the Faddeev equations for *nd* scattering with the realistic Nijmegen NN potential [12].

The S matrix of elastic *nd* scattering is usually parametrized by the eigen phase shifts and mixing angles in the total channel spin $\mathbf{\Sigma} = \mathbf{s} + \boldsymbol{\sigma}$ representation (here s is the NN pair spin and σ is a spin of the third nucleon). Unitary transformation between amplitudes defined in the representation of the total angular momentum of the third nucleon I and the Σ representation is given by the following matrix [11]:

$$U^J_{\lambda'\Sigma',\lambda\Sigma} = \sum_{I,I'} \sqrt{\hat{I}'\hat{\Sigma}'}(-1)^{J-I'} \begin{Bmatrix} \lambda' & 1/2 & I' \\ j & J & \Sigma' \end{Bmatrix} \times \sqrt{\hat{I}\hat{\Sigma}}(-1)^{J-I} \begin{Bmatrix} \lambda & 1/2 & I \\ j & J & \Sigma \end{Bmatrix} U^J_{\lambda' I',\lambda I}. \quad (21)$$

In Figs. 1–3 the results of our fully discrete calculations for elastic *nd* scattering with the Nijm I NN interaction performed within the WP approach are compared with the results of the conventional Faddeev calculations of the Bochum-Krakow group [11].

In the example, we restricted ourselves to the total isospin value $T = 1/2$ and took into account all of the pairwise NN channels with a two-body total angular momentum $j \leqslant 3$ (this gives up to 54 spin-angular channels).

In Fig. 1 the results for the lowest even partial phase shifts $\delta_{\Sigma\lambda}^{J\pi}$ of elastic *nd* scattering both below and above a three-body breakup threshold are shown. In the example, we employed WP bases with dimensions $M = N = 144$ along two Jacobi coordinates. This gives a matrix system with the dimension $144\times144 = 20\,736$, which has been handled easily on an ordinary PC in contrast to typical conventional calculations for similar Faddeev systems that require supercomputer facilities

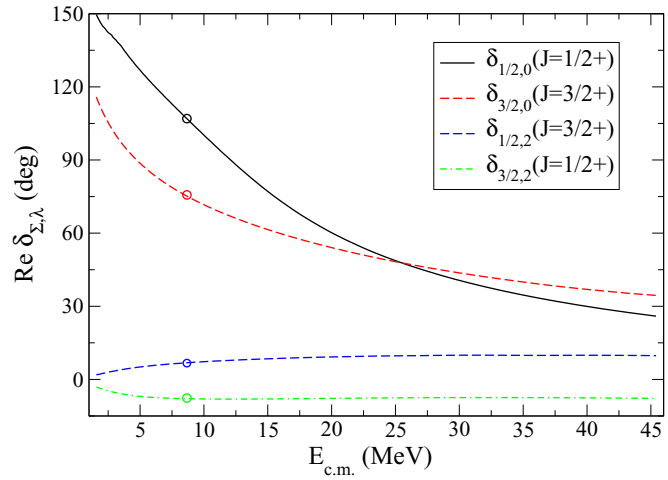

FIG. 1. (Color online) Some of S- and D-wave partial phase shifts of the elastic *nd* scattering obtained within the WP approach (solid lines) and within the standard Faddeev calculations (circles) [11].

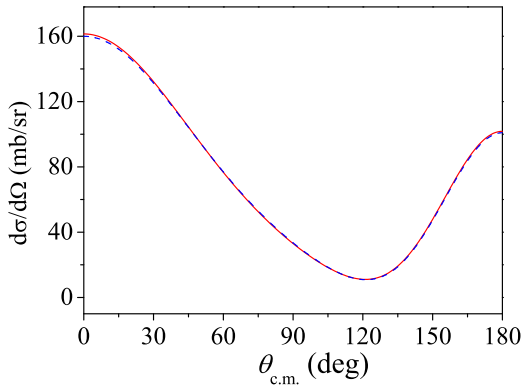

FIG. 2. (Color online) The differential cross section for elastic *nd* scattering at 13 MeV obtained via the WP technique (solid line) and within the standard Faddeev calculations [11] (dashed line).

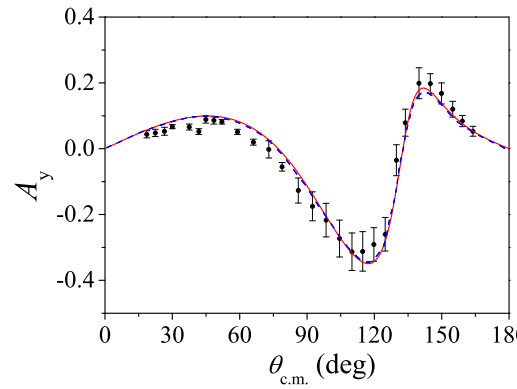

FIG. 3. (Color online) The neutron vector analyzing power A_y for the elastic *nd* scattering at 35 MeV obtained within the WP approach (solid line) compared to the results from Ref. [11] (dashed line) and the experimental *pd* data [17].

(see, e.g., Ref. [3]).[4] It should be especially emphasized that the calculation of the phase shifts at 100 different energy values displayed in Fig. 1 takes, in our approach, only about twice as much time as the calculation for a single energy because for all energies we employ the same permutation matrix $\mathbb{P}$, which is calculated only once.

In Fig. 2 our results for the differential cross section for elastic *nd* scattering at 13 MeV are compared to the results of conventional Faddeev calculations[5] [11], while in Fig. 3 the same 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 $M \times N = 100 \times 100$ has been used and the partial waves with the total angular momentum up to $J \leqslant 17/2$ have been taken into account.

It is clear from all of the above illustrative examples that one can achieve almost perfect agreement between our results and the results of the standard Faddeev calculations [11] performed on a powerful supercomputer.

The present calculations were performed on the serial PC with an Intel i7-3770K (3.50 GHz) processor with 32 GB of RAM. The real CPU computational time (which includes the permutation matrix evaluation), i.e., the total calculation that starts from the two-body interaction potential and ends with partial three-body amplitudes for a 54-channel calculation with the basis dimension 10^4 for a single value of the total angular momentum J and parity takes about 7 min.

Although the whole calculation for many partial waves will take a longer time, there is the possibility within the present approach to accelerate the whole calculation and thus solve more complicated scattering problems already using an ordinary PC. So, keeping in mind our general aim to simplify and accelerate drastically realistic many-body scattering calculations in nuclear, atomic, molecular, etc., studies by using a discrete matrix reduction of the integral scattering equations in the WP scheme, we propose to employ the ultrafast GPGPU technique to further optimize the solution of the resulting matrix equations.

V. SOLUTION OF THE FADDEEV MATRIX EQUATION USING GPU

In this section, we demonstrate a high efficiency of using a graphics processor in the numerical solution of the above matrix equation for the three-body scattering problem.

A. Parallelization of a numerical algorithm

First we describe the overall numerical scheme for solving the three-body scattering problem in the WP formalism, paying particular attention to those aspects that are important for an efficient parallelization.

The use of a fixed matrix for the permutation operator completely eliminates the necessity of the numerous and time-consuming interpolations of a current solution in the iterations. These computations take the majority of the computing time in the standard integral approach.[6] Contrary to this, in our approach, the main computational effort (in the case of CPU calculations) is spent on a calculation of the permutation matrix $\mathbb{P}^0$ in the lattice WP basis. However, the matrix $\mathbb{P}^0$ is independent of energy, and therefore, being calculated once, it can be used to solve the scattering problem at many energies, as well as for various two-particle input interactions, while in the standard approach the whole calculation must be repeated for each energy and for each type of two-body interaction.

The main difficulty that is met in the practical solution of the matrix equation (12) is its large dimension. So, it is impossible even to store the entire matrix of the kernel $\mathbb{K} = \mathbb{P}\mathbb{V}_1\mathbb{G}_1$ in the RAM of a computer. However, one can effectively employ

[4]Although the matrix dimension in our approach is much higher than that in the conventional approach, our kernel contains a very sparse permutation matrix with only ca. 1% of nonvanishing matrix elements.

[5]For this comparison we employed the partial phase shifts and mixing angles given in the Ref. [11] for values of the total angular momentum at $J \leqslant 7/2$.

[6]Note that such very numerous multidimensional interpolations at every step of the iterations seem to be hardly realizable via highly parallel execution.

the fact that the matrix $\mathbb{K}$ can be represented as a product of four matrices: a very sparse matrix $\mathbb{P}^0$ (only about 1% of its matrix elements are nonzero [10]), a diagonal matrix G_1, and two block matrices. Therefore, it is sufficient to store only factors of the matrix $\mathbb{K}$ instead of all its matrix elements (only the nonzero elements of the sparse matrix are stored). In this way, the required memory can be reduced by about 100 times. This eliminates the need for an external memory in the process of iteration, which in turn reduces the computational time by an order of magnitude even for a conventional CPU realization.

So, our overall numerical scheme should be quite suitable for parallelization and implementation on the multiprocessor systems, particularly on a GPU. The optimized algorithm for the solution of the realistic *nd* scattering problem consists of the following main steps:

(1) construction of the three-body SWP basis including preparation of two-body bases (via diagonalization of the pairwise NN sub-Hamiltonian matrix in the free WP basis); the calculation of the algebraic coefficients $g_{\gamma\gamma'}$ (A4) for the coupling of different spin-angular channels;

(2) selection of the nonzero elements of the overlap matrix $\mathbb{P}^0$;

(3) calculation of the nonzero elements of $\mathbb{P}^0$;

(4) calculation of the channel resolvent G_1; and

(5) solution of the resulting matrix equation by iteration using the Pade-approximant technique.

The runtimes for steps 1 and 4 are negligible in comparison with the total running time, so that we can leave these steps for sequential execution on the CPU. The main computational effort (in the CPU realization) is spent just on the calculation of the matrix elements of the $\mathbb{P}^0$ matrix (i.e., step 3), which are calculated independently of each other. So this step is ideal for parallelization and we primarily parallelized only the corresponding part of the computer code. However, since the matrix $\mathbb{P}^0$ is very sparse, to reach the high efficiency of its parallel computation, the preliminary selection of its nonzero elements should be carried out (step 2). The execution of the fifth step—iteration solution of the matrix equation—can certainly be accelerated using linear algebra routines implemented on the GPU, but as its execution time takes no more than 20% of the total time for solving the whole problem we did not optimize this step in the present study. Thus, in this calculation we have only parallelized the time-consuming steps 2 and 3 for the GPU.

B. Comparison of the GPU and CPU realizations

In this section we compare the runtimes for the CPU and GPU realizations of realistic *nd* elastic scattering calculations. For our GPU calculations we used an ordinary NVIDIA GTX-670 video card, which is not specialized for general-purpose computing.

First we compare the CPU and GPU realizations of the above algorithm for the case of the S-wave MT I-III NN interaction. This example clearly demonstrates the advantage of the GPU acceleration.

Figure 4 shows the dependence of the CPU- and GPU-computing times for the above steps 2, 3, and 5 and the complete solution for dimensions M and N of the WP bases chosen along both Jacobi variables. We take for simplicity

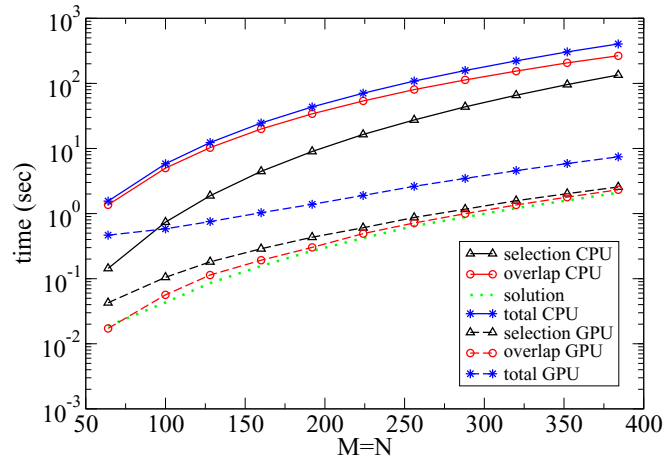

FIG. 4. (Color online) The dependence of the computing time on a CPU (solid lines) and a GPU (dashed lines) (for the full solution and separate steps) on the dimension of the basis $M = N$ for the *nd* scattering problem with S-wave NN interaction.

$M = N$ in all of our tests so that the total dimension of the matrix kernel is equal to M^2.

It is clear from Fig. 4 that the complete solution of the *nd* scattering problem in our approach for a basis of the large dimension[7] $M = 400$ takes only ca. 7 sec on a serial PC using a GPU. This ultrafast solution handles a huge matrix $160\,000 \times 160\,000$ including the calculation of the ca. $M^4/100 = 256$ millions of nonzero elements of matrix $\mathbb{P}^0$ where each matrix element is reduced to an integral of a rather complicated algebraic function. The integrals are calculated numerically with a 48-grid-point Gaussian quadrature.

From Fig. 4 it is seen that all of these 256 million integrals can be computed on the GPU in just 2.3 sec compared to 255 sec on the CPU. This demonstrates the real very high speed of GPU computations for the case discussed here.

In Fig. 5 we present the dependence of the GPU acceleration ratio $\eta = t(\text{CPU})/t(\text{GPU})$ on the dimension of the basis $M = N$ for the solution of the S-wave Faddeev problem. The total acceleration for the complete solution varies from 10 to 50 times depending on the basis dimension, while the time for calculating the nonzero elements of the matrix $\mathbb{P}^0$ (step 3), which takes the main part of the CPU computing time, is reduced by a factor of more than 100.

We now turn to the case of the realistic *nd* scattering problem with the Nijmegen NN potential. Taking into account higher partial waves leads to the system of coupled two-dimensional integral Faddeev equations. Now the calculation of each matrix element of $\mathbb{P}^0$ for partial waves with nonzero angular momenta includes several tens of double numerical integrals with some trigonometric functions and uses a large set of algebraic coefficients, $g^{l_1 l_1' k}_{\gamma\gamma'}$ (A4). The proper parallelization for this calculation with preselection of the nonzero matrix

[7]We take here a basis of this dimension just for a numerical test. To solve accurately the initial physical problem, the basis with $M = N = 100$ is quite enough.

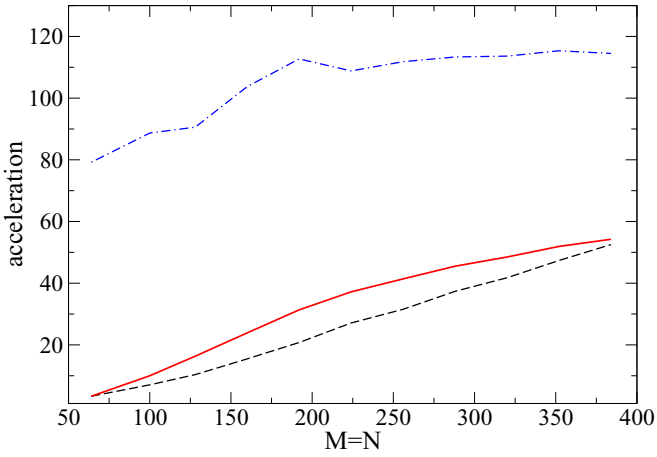

FIG. 5. (Color online) The dependence of the GPU-acceleration ratio η on the dimension of the basis $M = N$ in the calculation of the nd scattering problem with an S-wave NN interaction. The dashed line shows the acceleration for step 2 (selection), the dot-dashed line shows the acceleration for step 3 (calculation of $\mathbb{P}^0$), and the solid line shows the acceleration for the complete solution.

elements leads again to a rather fast algorithm realized on the GPU. Figure 6 demonstrates the GPU acceleration ratio $\eta = t(\text{CPU})/t(\text{GPU})$ for the complete solution (solid line) and for the steps 2 (dashed line) and 3 (dot-dashed) as a function of the basis dimension $M = N$ for the solution of the 18-channel Faddeev equations for the $J = \frac{1}{2}^+$ partial nd elastic amplitude.

It is evident from the results presented that the passing from the CPU realization to the GPU realization *on the same PC* allows one to obtain a significant acceleration of the whole three-body calculation by an order of magnitude or higher. It is clear also that the use of a more powerful specialized graphics processor, like the Tesla K40, would lead even to a considerably

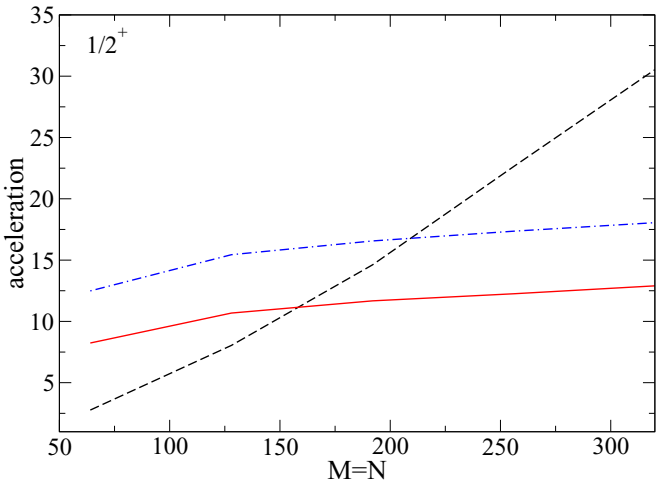

FIG. 6. (Color online) The dependence of the GPU acceleration ratio η on the dimension of the basis $M = N$ for the realistic nd scattering problem for $J = \frac{1}{2}^+$. The dashed line shows the acceleration for step 2 (selection), the dot-dashed line shows the acceleration for step 3 (calculation of $\mathbb{P}^0$), and the solid line shows the acceleration for the complete solution.

higher acceleration of calculations. However, it should be emphasized that the total acceleration that can be achieved by using a GPU depends crucially on the method used, the numerical scheme, and parallelization implementation.

VI. CONCLUSION

In conclusion, let us summarize the most important points of the proposed new general approach for the solution of few-body scattering problems.

(i) First, we rewrite the initial Faddeev equations, which include an off-shell t matrix, in a fully equivalent form that incorporates the product of the channel resolvent and the interaction operator. This allows us to simplify the required two-body input and also to fix all of the energy singularities in the channel resolvent operator. We note here that the four- and more particle integral Faddeev-Yakubovsky equations have, in principle, some similar structure as compared to three-body Faddeev equations (surely being more complicated and having a higher dimension). Therefore the discrete WP technique outlined in this paper can be employed for solving these general equations as well.

(ii) After that, we project out the transition and interaction operators onto a discrete wave-packet basis and employ a specific analytical form for one- and multichannel resolvent operators. This discrete form is extremely convenient for few-body calculations because we get a fixed matrix form (with fully regular matrix elements) for the scattering equations (of Lippmann-Schwinger, Faddeev, or Faddeev-Yakubovsky types). The most important improvement in such a WP projection is the fact that we can replace the permutation operators by fixed matrices, thus completely avoiding the numerous and time-consuming interpolations at every iteration step. Moreover, this matrix is both energy- and interaction independent and, being calculated once, can be used to solve various scattering problems with different potentials and at many energies.
These two steps lead to a rather effective numerical scheme which is realized on a standard PC for realistic $3N$ scattering calculations.

(iii) Last, we perform a proper parallelization of the solution and eventually we employ the ultrafast GPU technique to make very effective parallel calculations on a serial PC. This GPU realization for realistic scattering problems reduces the computational time by at least 1 order of magnitude (while for separate parts of the numerical scheme the total acceleration could reach 2 orders).

All of the above points open a new way for doing extensive many-body scattering calculations via continuum discretization, e.g., in quantum chemistry, nuclear reaction theory, solid state theory, etc.

There is little doubt that a similar (but surely more tedious) approach can also be applied to other scattering problems, e.g., to solve the relativistic Faddeev equations, Bethe-Salpeter equations, etc.

ACKNOWLEDGMENTS

The authors thank Dr. A.V. Boreskov for discussions of problems associated with the use of the GPU. The authors are also deeply grateful to Professor W. Polyzou for careful reading of the manuscript and valuable comments. This work has been supported partially by the Russian Foundation for Basic Research, Grants Nos. 12-02-00908 and No. 13-02-00399.

APPENDIX: CALCULATON OF PERMUTATION MATRIX ELEMENTS

The kernel of the permutation operator in momentum space has the form [11]

$$\langle pq\gamma|P|p'q'\gamma'\rangle = \int_{-1}^{1} dx \frac{\delta(p'-\pi_1)\delta(p-\pi_2)}{(p')^{l'+2}p^{l+2}} G_{\gamma\gamma'}(q,q',x), \tag{A1}$$

where the multi-indices γ and γ' include all possible spin-angular quantum numbers for the three-body states (as they are detailed in the Sec. II, i.e., $\gamma = l,s,j,\lambda,I,J,\pi,t,T$) and the following notations

$$\pi_1 = \sqrt{q^2 + \tfrac{1}{4}(q')^2 + qq'x}, \quad \pi_2 = \sqrt{\tfrac{1}{4}q^2 + (q')^2 + qq'x}, \tag{A2}$$

are used. The spin-angular coefficient G can be found from the formula

$$G_{\gamma\gamma'}(q,q',x) = \sum_{l_1,l_1',k} q^{l_2+l_2'}(q')^{l_1+l_1'} P_k(x) g_{\gamma\gamma'}^{l_1l_1'k}, \qquad \begin{matrix} l_1+l_2=l, \\ l_1'+l_2'=l', \end{matrix} \tag{A3}$$

where l and l' are two-body subsystem orbital momenta and the indices l_1, l_2, k, l_1', and l_2' arise from intermediate triangle sums. The sum in Eq. (A3) runs according to the triangle rules in the partial coefficient $g_{\gamma\gamma'}^{l_1l_1'k}$ which has the following explicit form [11]:

$$\begin{aligned} g_{\gamma\gamma'}^{l_1l_1'k} = {} & -\sqrt{\hat{I}\hat{s}\hat{j}\hat{t}\hat{\lambda}\hat{I}'\hat{s}'\hat{j}'\hat{t}'\hat{\lambda}'\hat{I}'} \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & t' \\ \frac{1}{2} & T & t \end{Bmatrix} \sum_{LS} (\hat{L}\hat{S}) \\ & \times \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & s' \\ \frac{1}{2} & S & s \end{Bmatrix} \begin{Bmatrix} l & s & j \\ \lambda & \frac{1}{2} & I \\ L & S & J \end{Bmatrix} \begin{Bmatrix} l' & s' & j' \\ \lambda' & \frac{1}{2} & I' \\ L & S & J \end{Bmatrix} \\ & \times \hat{k} \left(\frac{1}{2}\right)^{l_2'+l_1} \sqrt{\frac{(2l+1)!}{(2l_1)!(2l_2)!}} \sqrt{\frac{(2l'+1)!}{(2l_1')!(2l_2')!}} \\ & \times \sum_{ff'} \begin{Bmatrix} l_1' & l_2' & l' \\ \lambda' & L & f' \end{Bmatrix} \begin{Bmatrix} l_2 & l_1 & l \\ \lambda & L & f \end{Bmatrix} \\ & \times \langle l_2'0\lambda'0|f'0\rangle \langle l_10\lambda0|f0\rangle \\ & \times \begin{Bmatrix} f' & l_1' & L \\ f & l_2 & k \end{Bmatrix} \langle k0l_1'0|f0\rangle \langle k0l_20|f'0\rangle, \end{aligned} \tag{A4}$$

where the summation is done over all allowed intermediate quantum numbers. The projection of free three-body wave functions $|p,q\rangle$ (plane waves) onto the WP states can be found [for the case of unit weights $f(p)$ and $\bar{f}(q)$] from the following formula [10]:

$$\langle p,q|\mathfrak{p}_i\mathfrak{q}_j\rangle = \frac{1}{\sqrt{d_i\bar{d}_j}} \frac{\theta(p\in\mathfrak{D}_i)\theta(q\in\bar{\mathfrak{D}}_j)}{pq}. \tag{A5}$$

Here $d_i, \bar{d}_j$ are the widths of momentum intervals and function θ is the analog of the Heaviside step function: $\theta(p\in\mathfrak{D}_i)=1$ if p belongs to the interval $\mathfrak{D}_i$ and $\theta(p\in\mathfrak{D}_i)=0$ otherwise.

To obtain the permutation matrix elements in the lattice basis (11), one should integrate the kernel (A1) over the lattice cells $\mathfrak{D}_{ij}$ and $\mathfrak{D}_{i'j'}$. These matrix elements are defined by the following integrals:

$$\begin{aligned} [\mathbb{P}_0]_{ij,i'j'}^{\gamma\gamma'} \equiv \left\langle X_{ij}^{\gamma}\middle|P\middle|X_{i'j'}^{\gamma'}\right\rangle = {} & \sum_{kl_1l_1'} \frac{g_{\gamma\gamma'}^{kl_1l_1'}}{\sqrt{d_i\bar{d}_jd_{i'}\bar{d}_{j'}}} \int_{\mathfrak{D}_{ij}} dpdq \\ & \times \int_{\mathfrak{D}_{i'j'}} dp'dq' \int_{-1}^{1} dx \frac{q^{l_2+l_2'+1}(q')^{l_1+l_1'+1}}{(p')^{l'+1}p^{l+1}} \\ & \times \delta(p'-\pi_1)\delta(p-\pi_2)P_k(x). \end{aligned} \tag{A6}$$

Using the Dirac δ functions, the integrals over p and p' are evaluated analytically:

$$\begin{aligned} [\mathbb{P}_0]_{ij,i'j'}^{\gamma\gamma'} = {} & \sum_{kl_1l_1'} \frac{g_{\gamma\gamma'}}{\sqrt{d_i\bar{d}_jd_{i'}\bar{d}_{j'}}} \int_{\bar{\mathfrak{D}}_j} dq \int_{\bar{\mathfrak{D}}_{j'}} dq' \int_{-1}^{1} dx \\ & \times \frac{q^{l_2+l_2'+1}(q')^{l_1+l_1'+1}}{(\pi_1)^{l'+1}(\pi_2)^{l+1}} P_k(x)\theta(\pi_1\in\mathfrak{D}_{i'})\theta(\pi_2\in\mathfrak{D}_i). \end{aligned} \tag{A7}$$

Further, the residual integrals can be evaluated in polar coordinates:

$$q = Q\cos\phi, \quad q' = Q\sin\phi. \tag{A8}$$

Then the matrix element takes the form

$$[\mathbb{P}_0]_{ij,i'j'}^{\gamma\gamma'} = \sum_{kl_1l_1'} \frac{g_{\gamma\gamma'}}{\sqrt{d_i\bar{d}_jd_{i'}\bar{d}_{j'}}} I, \tag{A9}$$

where

$$\begin{aligned} I = {} & \int_{-1}^{1} dx\, P_k(x) \int_{\phi_1}^{\phi_2} d\phi \frac{(\cos\phi)^{l_2+l_2'+1}(\sin\phi)^{l_1+l_1'+1}}{(\zeta_1)^{l'+1}(\zeta_2)^{l+1}} \\ & \times \int_{Q_1(\phi)}^{Q_2(\phi)} QdQ\, \theta\left(Q\in\frac{\mathfrak{D}_{i'}}{\zeta_1}\right)\theta\left(Q\in\frac{\mathfrak{D}_i}{\zeta_2}\right), \end{aligned} \tag{A10}$$

and the following notations are employed:

$$\begin{aligned} \zeta_1 &= \sqrt{\cos^2\phi + \tfrac{1}{4}\sin^2\phi + x\cos\phi\sin\phi}, \\ \zeta_2 &= \sqrt{\tfrac{1}{4}\cos^2\phi + \sin^2\phi + x\cos\phi\sin\phi}. \end{aligned} \tag{A11}$$

The boundaries of the integral area in the (Q,ϕ) plane are defined by transformation of the rectangle in the (q,q') plane, so that

$$\phi_1 = \arctan\left(\frac{q'_{j'-1}}{q_j}\right), \quad Q_1(\phi) = \max\left(\frac{q_{j-1}}{\cos\phi}, \frac{q'_{j'-1}}{\sin\phi}\right),$$
$$\phi_2 = \arctan\left(\frac{q'_{j'}}{q_{j-1}}\right), \quad Q_2(\phi) = \min\left(\frac{q_j}{\cos\phi}, \frac{q'_{j'}}{\sin\phi}\right). \tag{A12}$$

Evaluating the Q integral analytically, one gets the following expression for the integral I:

$$I = \int_{-1}^{1} dx\, P_k(x) \int_{\phi_1}^{\phi_2} d\phi\, F_{ij,i'j'}(\phi,x) \frac{(\cos\phi)^{l_2+l'_2+1}(\sin\phi)^{l_1+l'_1+1}}{(\zeta_1)^{l'+1}(\zeta_2)^{l+1}}, \tag{A13}$$

where the following function is introduced:

$$F_{ij,i'j'}(\phi,x) = \frac{1}{2}\left[\min\left(\frac{q_j}{\cos\phi}, \frac{q'_{j'}}{\sin\phi}, \frac{p'_{i'}}{\zeta_1}, \frac{p_i}{\zeta_2}\right)\right]^2 - \frac{1}{2}\left[\max\left(\frac{q_{j-1}}{\cos\phi}, \frac{q'_{j'-1}}{\sin\phi}, \frac{p'_{i'-1}}{\zeta_1}, \frac{p_{i-1}}{\zeta_2}\right)\right]^2. \tag{A14}$$

Finally, one gets the eventual formula for the permutation matrix:

$$[\mathbb{P}_0]^{\gamma\gamma'}_{ij,i'j'} = \sum_{kl_1l'_1} \frac{g^{kl_1l'_1}_{\gamma\gamma'}}{\sqrt{d_i\bar{d}_j d_{i'}\bar{d}_{j'}}} \int_{-1}^{1} dx\, P_k(x) \int_{\phi_1}^{\phi_2} d\phi\, F_{ij,i'j'}(\phi,x) \frac{(\cos\phi)^{l_2+l'_2+1}(\sin\phi)^{l_1+l'_1+1}}{(\zeta_1)^{l'+1}(\zeta_2)^{l+1}}. \tag{A15}$$

In practical treatments these integrals are evaluated numerically.

[1] J. Carbonell, A. Deltuva, A. C. Fonseca, and R. Lazauskas, Progr. Part. Nucl. Phys. **74**, 55 (2014).

[2] L. D. Faddeev, Sov. Phys. JETP **12**, 1014 (1961); O. A. Yakubovsky, Sov. J. Nucl. Phys. **5**, 937 (1967).

[3] H. Witała and W. Glöckle, Phys. Rev. C **85**, 064003 (2012).

[4] https://developer.nvidia.com/cuda-zone

[5] K. A. Wilkinson, P. Sherwood, M. F. Guest, and K. J. Naidoo, J. Comp. Chem. **32**, 2313 (2011).

[6] M. A. Clark, R. Babich, K. Barrose, R. C. Brower, and C. Rebbi, Comp. Phys. Com. **181**, 1517 (2010).

[7] H. Potter *et al.*, in *Proceedings of NTSE-2013, Ames, IA, USA, May 13–17, 2013*, edited by A. M. Shirokov and A. I. Mazur (Khabarovsk, Russia, 2014), p. 263, http://www.ntse-2013.khb.ru/Proc/Sosonkina.pdf.

[8] E. Yarevsky, *Mathematical Modeling and Computational Science*, edited by A. Gheorghe, J. Buša, and M. Hnatic, Lecture Notes in Computer Science Vol. 7125 (Springer, New York, 2012), p. 290.

[9] O. A. Rubtsova, V. N. Pomerantsev, and V. I. Kukulin, Phys. Rev. C **79**, 064602 (2009); V. N. Pomerantsev, V. I. Kukulin, and O. A. Rubtsova, *ibid.* **79**, 034001 (2009).

[10] O. A. Rubtsova, V. N. Pomerantsev, V. I. Kukulin, and A. Faessler, Phys. Rev. C **86**, 034004 (2012).

[11] W. Glöckle, H. Witała, D. Hüber, H. Kamada, and J. Golack, Phys. Rep. **274**, 107 (1996).

[12] V. G. J. Stoks, R. A. M. Klomp, C. P. F. Terheggen, and J. J. de Swart, Phys. Rev. C **49**, 2950 (1994).

[13] O. A. Rubtsova, V. I. Kukulin, V. N. Pomerantsev, and A. Faessler, Phys. Rev. C **81**, 064003 (2010).

[14] M. Danos and W. Greiner, Phys. Rev. **146**, 708 (1966).

[15] O. A. Rubtsova, V. I. Kukulin, and V. N. Pomerantsev, Phys. At. Nucl. **77**, 486 (2014).

[16] V. I. Kukulin, V. N. Pomerantsev, and O. A. Rubtsova, Theor. Math. Phys. **150**, 403 (2007).

[17] S. N. Bunker *et al.*, Nucl. Phys. A **113**, 461 (1968).