Solving three-body scattering problems in the momentum lattice representation

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A brief description of the novel approach toward solving few-body scattering problems in a finite-dimensional functional space of the L_2 type is presented. The method is based on the complete few-body continuum discretization in the basis of stationary wave packets. This basis, being transformed to the momentum representation, leads to the cell-lattice-like discretization of the momentum space. So the initial scattering problem can be formulated on the multidimensional momentum lattice, which makes it possible to reduce the solution of any scattering problem above the breakup threshold (where the integral kernels include, in general, some complicated moving singularities) to convenient simple matrix equations that can be solved on the real energy axis. The phase shifts and inelasticity parameters for the three-body nd elastic scattering with MT I-III NN potential both below and above the three-body breakup threshold calculated with the proposed wave-packet technique are in a very good agreement with the previous accurate benchmark calculation results.

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I. MOTIVATION FOR THE WORK

The strictly proved integral equations for the solution of few-body scattering problems were developed many years ago by Faddeev and Yakubovsky [1,2]. After these pioneer works a lot of investigations of few-body quantum physics along these lines were carried out for the next few decades. Despite great progress in this field [3–9], the practical solution of few-nucleon scattering problems with realistic $2N$ and $3N$ interactions, especially above the three-body breakup threshold, remains a rather cumbersome computational problem that needs very powerful computer resources. Moreover, the practical solution of multidimensional four-nucleon Faddeev–Yakubovsky equations with realistic NN and $3N$ interactions is so problematic that even now $4N$ systems above the three-body threshold can be practically treated only with simple pairwise local interactions [6,9]. The reason of this is the very laborious numerical routines in the coordinate space and the complicated moving singularities in multidimensional kernels of the integral momentum-space equations.

At the same time, several efficient methods for the accurate approximation of few-body continuum wave functions in various L_2 bases have been developed [10–18]. These are the "moment T-matrix method" [10], the J-matrix approach [11–13], "the harmonic oscillator representation" [14], the Lorentz integral transform method [15], the continuum-discretized coupled-channel method (CDCC) [16–18], etc. However, most of them can be used for special cases of the few-body scattering only, e.g., for the so-called truly few-body scattering when there are no bound states in any two-body subsystems [14] or for the composite particle scattering off heavy target when stripping channels can be neglected [16–18]. In other cases one can describe the processes when few-body wave functions in the initial channel are of the bound-state type and the L_2 basis is used to approximate the final-state few-body continuum only [15], or one treats a three-body scattering at small energies below the three-body threshold only [13]. So that, with the above L_2-type methods no precise calculations for the basic three-body nd scattering case above the breakup threshold have been carried out to date.[1]

Thus, it would be very convenient to have at our disposal a sufficiently universal method for general continuum discretization in different two- and few-body scattering problems (in nuclear physics, atomic physics, hadronic physics, etc.), which operates with L_2 functions only and nonsingular matrix equations both below and above the breakup thresholds.

A few years ago the present authors developed a new approach to solving few-body scattering problems based on the discretization of the continuous spectrum of the total Hamiltonian [20–24]. The method uses stationary wave packets, which are L_2-type functions, instead of the exact scattering wave functions. In these works an original wave-packet formalism has been developed that allows one to construct finite-dimensional (f.-d.) approximations for basic scattering-theory operators and find the scattering observables using such approximations. The approach has recently been tested for the elastic scattering and breakup of composite projectiles scattered off heavy targets (neglecting the stripping processes), and perfect agreement with the conventional CDCC results has been found [23,24]. In the present article we extend our wave-packet approach much further, toward solving a general three-body scattering problem on the basis of the projected Faddeev equations, and illustrate the new technique using the

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[1]The realistic three-nucleon calculations for, e.g., nd (or pd) scattering below and above the three-body breakup threshold have been carried out with either the variational method [19] using the Schrödinger equation approach or the Faddeev equations in the momentum [8] or in the configuration space [5].

example of quartet and doublet nd scattering below and above the three-nucleon breakup threshold.[2]

II. FORMULATION OF THE APPROACH

Here we describe the three-body wave-packet discretization procedure for elastic nd scattering. The elastic amplitude X for the quartet case can be found from a single integral Faddeev equation [25]

$$X = -Pv_1 - Pv_1G_1X, \tag{1}$$

where v_1 is the triplet NN interaction potential, $G_1 = (E - H_1)^{-1}$ is the three-body resolvent of the channel Hamiltonian $H_1 = H_0 + v_1$, and P is the permutation operator. We emphasize here that this form of Faddeev equation (i.e., with kernel Pv_iG_i instead of the more standard form Pt_iG_0) is much more convenient for the wave-packet approach because of the fact that the channel three-body resolvent G_i in our approach can be calculated in a simple analytical form and has a diagonal matrix representation [see Eqs. (6)–(8)].

To solve the three-nucleon scattering equation [Eq. (1)], let us introduce the finite basis $\{|S_i\rangle\}_{i=1}^{\mathcal{N}}$ such that the projector $\Gamma_{\mathcal{N}}$ onto the f.-d. basis subspace can (in some not rigorous sense) approximate the unit operator $\Gamma_{\mathcal{N}} = \sum_{i=1}^{\mathcal{N}} |S_i\rangle\langle S_i| \to 1$. Then one can define the $\mathcal{N}$-dimensional approximation for any operator A as its projection onto the respective basis subspace: $\Gamma_{\mathcal{N}}A\Gamma_{\mathcal{N}} = \sum_{ij} |S_i\rangle A_{ij}\langle S_j|$, with corresponding matrix elements $A_{ij} \equiv \langle S_i|A|S_j\rangle$. Using such matrix approximations for the scattering operators, the initial integral equation can be reduced to the respective matrix equation. We denote the matrices of projected operators with corresponding bold letters. So, one finds the matrix equation instead of the integral equation (1):

$$\mathbf{X} = -\mathbf{P}\mathbf{v}_1 - \mathbf{P}\mathbf{v}_1\mathbf{G}_1\mathbf{X}. \tag{2}$$

Thus, it looks like it would be possible to find some approximate solutions of the initial integral equation using some appropriate L_2 bases through the simple matrix algebra. However, not every L_2 basis is suitable for this purpose. The integral kernel of the Faddeev equation includes the fixed-pole singularities and also the complicated moving singularities above the three-body breakup threshold. Only these singularities correspond to the proper boundary conditions in coordinate space and provide the correct physical solution of the Faddeev equations, but a construction of the appropriate basis for the projection of such kernels is a highly nontrivial problem. Another key problem here is the calculation of matrix elements for v_1, P, and especially G_1 operators in the chosen basis, which can appear, in general, to be a rather cumbersome task. The appropriate stationary wave-packet basis helps to overcome all the above difficulties and formulate the matrix equations whose solutions can really approximate with high accuracy the solutions of the initial integral equations. Such a basis will be demonstrated to provide a convenient analytical diagonal representation for the three-body channel resolvent matrix $\mathbf{G}_1$ and, on the other hand, this basis covers a sufficiently wide functional L_2 space to provide well converged results.

The channel Hamiltonian H_1 is the direct sum of two subHamiltonians corresponding to the system motion along two independent Jacoby coordinates:

$$H_1 \equiv h_1 \oplus h_0, \tag{3}$$

where subHamiltonian h_1 defines the NN subsystem motion (including interaction v_1) and subHamiltonian h_0 corresponds to the free motion of the third nucleon relative to the NN subsystem center of mass. Now let's define two sets of momentum bins $[p_{i-1}, p_i]_{i=1}^{M}$ and $[q_{j-1}, q_j]_{j=1}^{N}$ corresponding to the continuum discretizations for subHamiltonians h_1 and h_0. The (two-body) stationary wave-packet bases (WPB) are defined as integrals of the exact continuum wave functions $|\psi_p\rangle$ and $|\psi_{0q}\rangle$ of the subHamiltonians h_1 and h_0 over the respective momentum bins:

$$|z_i\rangle = \frac{1}{\sqrt{b_i}} \int_{p_{i-1}}^{p_i} \mathrm{d}p|\psi_p\rangle, \quad |y_j\rangle = \frac{1}{\sqrt{d_j}} \int_{q_{j-1}}^{p_j} \mathrm{d}q|\psi_{0q}\rangle, \tag{4}$$

where $b_i \equiv p_i - p_{i-1}$ and $d_j \equiv q_j - q_{j-1}$ are bin widths. Now, the three-body WPB states $|S_{ij}\rangle$ are defined just as products of the two-body wave-packet states $|z_i\rangle$ (including the bound state wave function $|z_0\rangle$) and $|y_j\rangle$ along two Jacobi coordinates:

$$|S_{ij}\rangle \equiv |z_i, y_j\rangle. \tag{5}$$

We omit here partial wave indices for the sake of simplicity. The properties of the wave-packet sets $|z_i\rangle$ and $|y_j\rangle$ have been investigated in detail in Refs. [20–23]. In particular, the very useful property of such a packet basis is that the matrices for the projected resolvents of the subHamiltonians $g_1(E) = (E + \mathrm{i}0 - h_1)^{-1}$ and $g_0 = (E + \mathrm{i}0 - h_0)^{-1}$ are diagonal and defined by a simple analytical expression depending only on the spectrum discretization parameters. This property of WPB allows us to construct the f.-d. analytical diagonal representation for the channel resolvent $G_1(E)$, which is a convolution of the two-body resolvents g_1 and g_0.

Indeed, the exact three-body channel resolvent can be written [21] as a sum of two terms, $G_1(E) = G_1^{\mathrm{BC}}(E) + G_2^{\mathrm{CC}}$, where the bound-continuum part has the form

$$G_1^{\mathrm{BC}}(E) = \int_0^{\infty} \mathrm{d}q \frac{|z_0, \psi_{0q}\rangle\langle z_0, \psi_{0q}|}{E + \mathrm{i}0 - \epsilon_0 - \frac{3q^2}{4m}}, \tag{6}$$

and ϵ_0 is the binding energy for the (single) np bound state. The continuum-continuum part takes the form

$$G_1^{\mathrm{CC}}(E) = \int_0^{\infty} \mathrm{d}p \int_0^{\infty} \mathrm{d}q \frac{|\psi_p, \psi_{0q}\rangle\langle\psi_p, \psi_{0q}|}{E + \mathrm{i}0 - \frac{p^2}{m} - \frac{3q^2}{4m}}. \tag{7}$$

Now let's construct a projection of the exact channel resolvent onto the three-body WPB. The following analytical formulas

[2] As far as the present authors are aware, the present work gives the first precise fully L_2 approximated solution for the Faddeev equation above the three-body threshold.

for the diagonal f.-d. projection of G_1 can then be obtained:

$$\mathbf{G}_1^{\mathrm{BC}} = \sum_j G_{0j}^{\mathrm{BC}} |z_0, y_j\rangle\langle z_0, y_j|,$$
$$\mathbf{G}_1^{\mathrm{CC}} = \sum_{i\neq 0, j} G_{ij}^{\mathrm{CC}} |z_i, y_j\rangle\langle z_i, y_j|, \tag{8}$$

where the matrix elements G_{oj}^{BC} and G_{ij}^{CC} in Eq. (8) are defined as integrals over the respective momentum bins:

$$G_{0j}^{\mathrm{BC}} = \frac{1}{d_j}\int_{q_{j-1}}^{q_j} \frac{\mathrm{d}q}{E + \mathrm{i}0 - \epsilon_0 - \frac{3q^2}{4m}}, \tag{9a}$$

$$G_{ij}^{\mathrm{CC}} = \frac{1}{d_i d_j}\int_{p_{i-1}}^{p_i}\int_{q_{j-1}}^{q_j} \frac{\mathrm{d}p\mathrm{d}q}{E + \mathrm{i}0 - \frac{p^2}{m} - \frac{3q^2}{4m}}. \tag{9b}$$

These matrix elements depend, in general, on the spectrum partition parameters (i.e., p_i and q_j values). However, we found when the wave-packet expansions of the three-body amplitude is convergent the final result turns out to be *independent* of the particular spectral partition parameters. The integrals in Eqs. (9a) and (9b) are analytically tractable, which gives a simple analytical f.-d. representation for the three-body channel resolvent G_1. Such an analytical representation is a main feature of the wave-packet approach because it allows one to drastically simplify the solution of the general three-body scattering problem.

Now the key question arises: how to construct practically the above wave-packet basis. The free packets $|y_n\rangle$ corresponding to the free motion of the third nucleon relative to the NN subsystem c.m. take in the momentum representation the form of simple step-like functions:

$$\langle q|y_j\rangle = \frac{\theta(q - q_{j-1}) - \theta(q - q_j)}{\sqrt{d_j}}, \tag{10}$$

where $\theta(q)$ is the Heaviside function.

The scattering wave packets $|z_i\rangle$ describing the scattering in the NN two-body subsystem can be very well approximated by pseudostates $|\tilde{z}_i\rangle$ obtained from the diagonalization of the subHamiltonian h_1 in some appropriate L_2 basis [20]. In the present work we use for this diagonalization a free wave-packet basis $|x_k\rangle$ corresponding to the free NN motion. Thus, we solve the two-body variational problem directly on the free WPB and as a result obtain a set of variational functions

$$|\tilde{z}_i\rangle = \sum_{k=0}^{M} O_{ik}|x_k\rangle, \qquad i = 0, \ldots, M, \tag{11}$$

the first of which (for the problem in question) is the wave function of the bound state (deuteron) while the others are very good approximations for the exact scattering packets until very large distances.

In Fig. 1 the coordinate-space behavior of some from the first 50 variational functions (including the deuteron) is shown. It is clear that the free-packet basis allows one to approximate the respective scattering wave functions up to a very far asymptotic region (in Fig. 1 the functions $\tilde{z}_i(r)$ are given at $r < 80$ fm, but actually they coincide with exact scattering wave packets up to $r \sim 1000$ fm). This long-range behavior of the basis functions plays a crucial role in the three-body

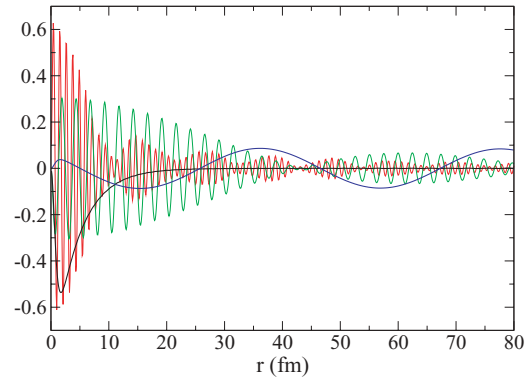

FIG. 1. (Color online) Bound state (solid curve) and several interaction wave packets (different dashed lines) for the MT III potential constructed from the free momentum packets in the coordinate space.

scattering, especially above the breakup threshold, because it provides a proper overlapping between basis functions in different Jacoby coordinate sets. It should be mentioned that in our previous calculations [21] we used a Gaussian basis to approximate the interaction packets in the whole space and so the wrong long-range behavior of the basis functions did not allow us to obtain well converged results above the breakup threshold (while for the smaller energies the Gaussian approximation worked quite well).[3]

In addition, the momentum lattice basis is very convenient to find the matrix elements of the permutation operator P. Using approximation (11) for the scattering packets $|z_i\rangle$, these matrix elements can be expressed in the form

$$P_{ij,i'j'} = \langle z_i y_j|P|z_{i'} y_{j'}\rangle \approx \sum_{kk'} O_{ik} O^*_{i'k'} P^0_{kj,k'j'}, \tag{12}$$

where $P^0_{kj,k'j'} \equiv \langle x_k y_j|P|x_{k'} y_{j'}\rangle$ is the permutation matrix element taken on the two-dimensional free wave packets (for a two-dimensional lattice) and the O_{ik} are the superposition coefficients given in Eq. (11). Using further hyperspherical momentum coordinates, the calculation of $P^0_{kj,k'j'}$ can be reduced to a one-dimensional numerical integration over hypermomentum $p^2 + q^2$. The technique of this calculation will be given in detail elsewhere. It should be stressed here that this is one of the key points for the whole of our approach. In fact, to solve two-dimensional Faddeev equations by conventional methods [4] one needs (because of the appearance of the permutation operator P in the integral kernel) to use very time-consuming two- and three-dimensional interpolations (many thousands or even millions of such interpolations) at each iteration step to find the solution in the initial Jacoby

[3] It should be noted the free packet basis (i.e., the step-like functions in the momentum space) is, of course, not optimal for calculation of bound states. For example, in our case only 20 Gaussian functions are necessary to obtain $E_b = -2.225$ MeV for the deuteron binding energy and ca. 100 step-like functions are required to reach the same precise bound energy value. However, very good approximation of scattering wave functions in two-body subsystems is the decisive factor here.

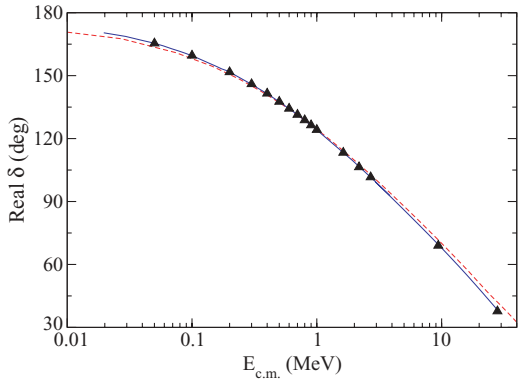

FIG. 2. (Color online) The energy dependence of the real phase shift for S-wave quartet nd scattering calculated by means of the momentum-packet discretized Faddeev equation at different dimensions $M \times N$ of the lattice basis: 100×100 (dashed curve), 200×200 (solid curve). Results of the direct Faddeev equation solution from Refs. [7] and [8] are marked as ▲.

set from the "rotated" (by the permutation P) Jacoby sets. So, such numerous multidimensional interpolations at each iteration step take a big portion of computational time in practical solutions of three-body integral equations. When solving the four-body Yakubovsky equations, the dimension and the number of interpolations at each iteration step get even higher. Thus, the present wave-packet approach allows one to avoid completely such multidimensional interpolations and to simplify enormously the solution process.

After solving the matrix equation, Eq. (2), the on-shell elastic amplitude $A_{\rm el}(E)$ in wave-packet approximation can be found as a diagonal (on-shell) matrix element of the X matrix [which is a solution of the matrix equation (2)]:

$$A_{\rm el}(E) \approx \frac{2m}{3q_0} \frac{X_{0n_0,0n_0}}{d_{n_0}}, \tag{13}$$

where index n_0 denotes the singular q bin to which the on-shell momentum $q_0 = \sqrt{\frac{4}{3}m(E-\epsilon_0)}$ belongs: $q_0 \in (q_{n_0-1}, q_{n_0})$. It should be stressed here that the breakup amplitude can be found from the same matrix $\mathbf{X}$ but using its nondiagonal matrix elements. Thus, to find both the elastic and breakup amplitudes one needs to solve one linear equation, only for single

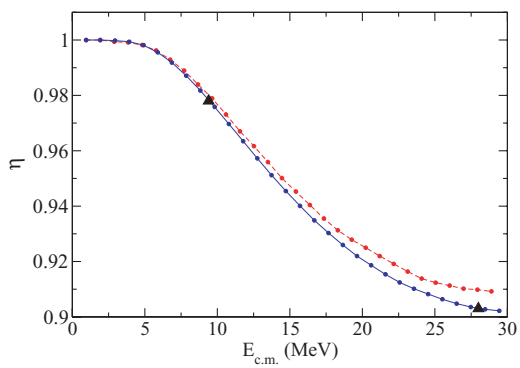

FIG. 3. (Color online) The same as in Fig. 2 but for the inelasticity parameter η.

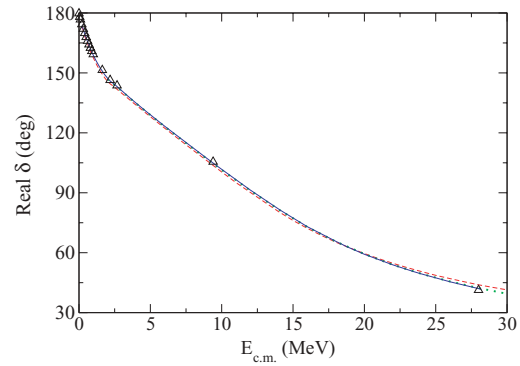

FIG. 4. (Color online) The energy dependence of the real phase shift for the S-wave doublet nd scattering calculated by means of the momentum-packet discretized Faddeev equation at different dimensions $M \times N$ of the lattice basis: $(50+50) \times 50$ (dashed curve), $(80+80) \times 80$ (dotted curve), and $(100+100) \times 100$ (solid curve). Results of the direct Faddeev equation solution from Refs. [7] and [8] are marked as △.

column $X_{mn,0n_0}$, rather than to do a full matrix inversion in Eq. (2).

III. NUMERICAL RESULTS

To illustrate the accuracy and effectiveness of the proposed wave-packet technique we calculated the real phase shifts and inelasticity parameters for the three-body elastic nd scattering in the quartet and doublet S-wave channels with the model Malfliet-Tjon NN potential MT-III. In the case of doublet scattering one has a system of two matrix equations instead of one matrix equation (2) where two amplitudes correspond to two possible spin states (triplet and singlet) in the NN subsystem.

The results of these calculations are shown in Figs. 2 and 3 for the spin-quartet channel, in Figs. 4 and 5 for the spin-doublet channel, and in Table I.

To check the accuracy of the method we have compared carefully our results with the previous benchmark calculation results from Ref. [7] (below the deuteron breakup threshold) and Refs. [8] and [26] (above the deuteron breakup threshold).

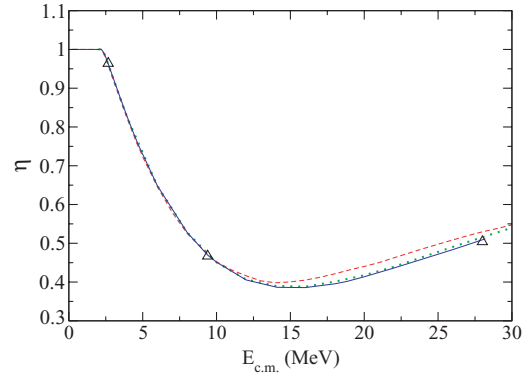

FIG. 5. (Color online) The same as in Fig. 4 but for the inelasticity parameter η.

TABLE I. The convergence the *nd* scattering results for MT III potential obtained from the momentum-packet discretized Faddeev equations when increasing the basis dimension $N \times N$ in comparison with results of exact benchmark Faddeev calculations [26] (Bochum and LA/Iowa).

	Doublet				Quartet			
$E_{\text{c.m.}}$	9.4 MeV		28 MeV		9.4 MeV		28 MeV	
N	Re(δ), deg	η	Re(δ), deg	η	Re(δ), deg	η	Re(δ), deg	η
64	104.30	0.4740	43.88	0.5235	70.89	0.9984	42.19	0.9199
96	104.82	0.4715	42.28	0.5130	70.15	0.9864	39.70	0.9174
128	105.05	0.4690	41.98	0.5075	69.85	0.9823	38.95	0.9086
192	105.25	0.4683	41.73	0.5039	69.55	0.9797	38.43	0.9045
256	105.33	0.4672	41.63	0.5032	69.40	0.9790	38.21	0.9034
Fully converged[a]	105.54	0.4649	41.37	0.5020	68.94	0.9788	37.65	0.9029
Bochum	105.50	0.4649	41.37	0.5022	68.96	0.9782	37.71	0.9033
LA/Iowa	105.48	0.4648	41.34	0.5024	68.95	0.9782	37.71	0.9033

[a]The values obtained by means of extrapolation $N \to \infty$.

The exact parameters of the NN potential are taken from Ref. [8].

As can be seen from Figs. 2 to 5 the wave-packet discretization technique for the three-body continuum works successfully for the general three-body scattering problem both below and above breakup threshold. A more detailed comparison with the results of benchmark calculations for the same scattering energies is presented in Table I, where we compare our results with those found by two groups, viz., the Bochum and Los-Alamos/Iowa groups [26], which employed completely different approaches. From Table I, it can be seen that with the present wave-packet approach one can reach, in general, the numerical accuracy similar to accurate benchmark results [26] in the calculation of three-body observables for both doublet and quartet channels.

Thus, for the first time we have solved the three-body scattering problem above the breakup threshold using only f.-d. approximation of the L_2-type for the Faddeev kernel. The use of the momentum-lattice basis allowed us to achieve a good convergence and accuracy this way. It worth to noting here that all calculations above the three-body breakup threshold were carried out with a standard personal computer.

IV. CONCLUSION

Let's briefly outline here the most important points of this study. For the first time the three-body scattering problem in the Faddeev framework above the breakup threshold has been successfully solved in the three-body L_2-basis representation using the lattice approximation scheme (which is the technique of three-body continuum discretization). The success and advantages of the lattice approach are related to the following distinctive features.

(i) Due to matrix representation for the pairwise potentials there is no difference between the local and the nonlocal type of the interaction and therefore the approach is applicable for any complicated interactions, in particular, for modern NN interactions based on effective Lagrangians and chiral perturbation theory.

(ii) The explicit analytical f.-d. approximation for the three-body channel resolvent G_1 allows to reduce the initial integral Faddeev equation to the matrix one that can be solved directly on the real energy axis.

(iii) The scattering wave packets (corresponding to the NN interaction) can be approximated by pseudostates of the two-body NN subHamiltonian matrix in the free wave-packet basis, which allows one to avoid completely calculation of the off-shell two-body t matrix and obtain explicitly matrix elements of the permutation operator P that include overlapping between wave-packet basis states of the different three-body channel Hamiltonians.

(iv) This convenient closed form for the matrix elements of the permutation operator P in the WPB also makes it possible to avoid completely very time-consuming multidimensional interpolations of the iterated kernels that usually assist in conventional techniques of the Faddeev equation numerical integration in the momentum space.

(v) The very long-range type of wave-packet functions (nonvanishing at distances $\sim$1000 fm) allow one to approximate properly the overlapping between basis states in different Jacoby coordinate sets. This leads to the proper asymptotic behavior of the solutions along different Jacoby coordinates, which could not be provided by means of conventionally used short-range type L_2 bases.

In addition, this long-range behavior of the wave-packet basis functions looks also very promising for the proper incorporation of the long-range Coulomb interaction in the treatment of few-nucleon scattering with charged particles. Our further investigations are aimed at this purpose.

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