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QUANTUM SCATTERING THEORY ON THE MOMENTUM LATTICE

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Here we briefly outline the main results of the Wave-Packet Continuum Discretization method. The formalism uses the complete continuum discretization scheme in terms of the momentum stationary wave-packet basis, which leads to formulation of the scattering problem on a lattice in the momentum space.

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INTRODUCTION

Recently we have developed a new approach to solving few-body scattering problems based on the complete discretization of few-body continuous spectrum [1–6]. We constructed universal formalism which uses the stationary wave packets, i.e., L_2 functions, instead of the exact scattering wave functions. This leads to formulation of the scattering theory on the lattice in the momentum space. In such an approach, finite-dimensional (f.-d.) approximations for basic scattering-theory operators have been obtained and matrix analogs for the scattering equations have been constructed. The approach has recently been tested for the elastic scattering and breakup of a composite projectiles scattered off heavy targets (with neglecting the stripping processes), where a perfect agreement with the conventional Continuum Discretized Coupled Channel (CDCC) method has been found [1]. Further, the method has been successfully applied to the solution of the Faddeev equations for $n - d$ scattering above the three-nucleon breakup threshold [3]. Very recently some new method — the Discrete Spectral Shift (DSS) formalism has been developed on the base of the lattice approach. This approach allows one to find observables for the multichannel scattering problems from the one-fold diagonalization of the Hamiltonian matrix without solution of any scattering equations [5].

The present paper is organized as follows. In Sec. 1 we introduce the generalized stationary wave-packet basis and describe different ways how to extract scattering information from the total Hamiltonian matrix in such a basis. Three-body lattice bases are defined in Sec. 2, where wave-packet scheme for solving general three-body problems is derived. Brief conclusion is given at the end of the paper.

1. TWO-BODY SCATTERING PROBLEM

1.1. The Wave-Packet Lattice Basis. In the discretization procedure, the continuum of the free Hamiltonian h_0 is confined within the maximal value $E_{\max}$ and the interval $[0, E_{\max}]$ is divided into a finite number of nonoverlapping energy bins $[\epsilon_{i-1}, \epsilon_i]_{i=1}^N$ (with $E_0 = 0$ and $E_N = E_{\max}$)*. Each such an energy bin corresponds to the momentum (or wave number) interval $[q_{i-1}, q_i]$ on momentum axis q, where $q = \sqrt{2\mu\epsilon}$ and μ is the reduced mass. The set of *free* stationary wave packets (WPs) is defined as integrals of the plane waves $|\psi_{0q}\rangle$ over the above momentum bins:

$$|x_i\rangle = \frac{1}{\sqrt{B_i}} \int\limits_{q_{i-1}}^{q_i} dq f(q) |\psi_{0q}\rangle, \quad i = 1, \ldots, N, \tag{1}$$

where $f(q)$ is some weight function and B_i are normalization factors. The wave-packet functions (1) form orthonormal set and vanish at infinity in contrast to the initial plane waves. However, these L_2-type functions are not vanishing at very far asymptotic region up to $qr \sim 200$ [3]. Thus, the wave-packet basis is very suitable for the expansion of continuous spectrum wave functions. General properties of WPs have been considered in detail previously [1–6]. The most useful property of the WP basis is the finite-dimensional representation for the resolvent of free Hamiltonian $g_0(E) = [E + i0 - h_0]^{-1} \approx \sum\limits_{i=1}^{N} |x_i\rangle g_i(E) \langle x_i|$, where the corresponding complex-valued eigenvalues $g_i(E)$ (or averaged on the energy ones) have an explicit analytical form [4].

In the few-body case, few-body wave-packet bases are constructed as direct productions of the two-body ones. Simultaneously few-body momentum space becomes a discretized one. Thus, implementation of the WP basis is similar to the formulation of the few-body scattering problem in the multidimensional momentum lattice. That is why we call our wave-packet basis as the lattice one.

Using the finite-dimensional WP analog for the free resolvent, one can derive easily a matrix scheme for WP solution of the Lippmann–Schwinger equation for the total Hamiltonian $h = h_0 + v$, where v is the short-range interaction potential [2, 4].

It is also possible to construct f.-d. representations for the scattering operators using pseudostate WP formalism based on the diagonalization procedure for the total Hamiltonian matrix in free WP basis. After this procedure one gets the set of eigenenergies $\{E_i\}_{i=1}^N$ and corresponding eigenfunctions $\{|z_i\rangle_{i=1}^N\} \in L_2$.

*We assume that the value $E_{\max}$ is sufficiently large to provide a proper solution of the discussed problem.

Some part of the eigenfunctions with $i \leqslant N_b$ approximates the bound states of the system (if they exist), while the rest $(N - N_b)$ of the eigenfunctions can be considered as discretized (normalized) analogs of the scattering wave functions of the Hamiltonian — the so-called pseudostates. It has been shown, that such states approximate *scattering wave packets* of the total Hamiltonian h. The properties of the scattering WPs are absolutely the same as those of the free WPs. The full set of bound states of h and scattering WP states $\{|z_i\rangle\}_{i=1}^{N}$ form a basis in a Hilbert space. This basis can be used to construct f.-d. representation for the total resolvent.

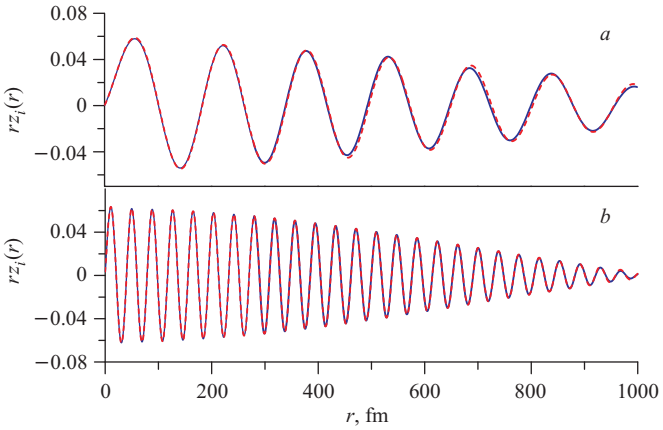

Fig. 1. Comparison of exact Coulomb wave packets (solid curves) and Coulomb pseudostates obtained in the lattice basis (dashed curves) at two different energies $E = 0.07$ MeV (*a*) and $E = 11.3$ MeV (*b*) of the Coulomb pp Hamiltonian

The correspondence between pseudostates and scattering WPs assists also in a case of the long-range Coulomb interaction. In Fig. 1, we compare Coulomb scattering wave packets, corresponding to the pp interaction, constructed by the diagonalization of Coulomb Hamiltonian on the free WP basis with those obtained from exact Coulomb regular scattering wave functions by formula (1). It is clear from the figure that pseudostates are indistinguishable from the exact Coulomb WPs.

1.2. Discrete Spectral Shift Formalism. There is another possibility of extracting scattering information directly from the diagonalization procedure for the Hamiltonian matrix in the lattice basis via the novel Discrete Spectral Shift (DSS) formalism [5].

It has been shown in our recent paper [5], that local differences of the total discretized spectrum of h_0 caused by the switching on the perturbation v, i.e., $h_0 \to h = h_0 + v$, are related to the spectral shift function (SSF) $\xi(E)$. This

function has been introduced in the rigorous mathematical quantum scattering theory [7, 8] and in a single-channel case, it is equal to a partial phase shift: $\delta(E) = -\pi\xi(E)$ within a factor $(-\pi)$. It has been shown [5, 9] that the discrete analog of the SSF, defined for the discretized spectrum of the free Hamiltonian h_0, can be found from the simple formula:

$$\xi_i = \frac{E_i - E_i^0}{D_i}, \quad i = N_b + 1, \ldots, N, \tag{2}$$

where D_i are bin widths. Thus, by making use of the explicit interrelation between SSF and phase shifts, one gets discrete approximation for phase shift as a function of energy:

$$\delta(E_i^0) = -\pi\frac{E_i - E_i^0}{D_i}, \quad i = N_b + 1, \ldots, N. \tag{3}$$

This equation allows one to find, besides eigenenergies and eigenfunctions of bound states, also partial phase shifts in a very broad energy range.

The DSS method is fully applicable to a broad class of interactions, even for complex-valued interaction potentials. In this case, one uses a real wave-packet basis, however, the total non-Hermitian Hamiltonian eigenvalues will be complex-valued. So, the phase shifts derived from these complex eigenvalues will be also complex. As a good illustration of the applicability of the above new technique we find the complex phase shifts for the neutron scattering off a nuclear target

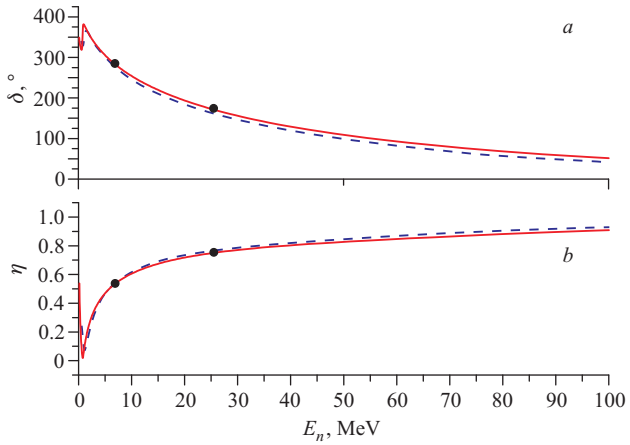

Fig. 2. Real parts of S-wave phase shifts δ (a) and inelasticity parameters η (b) for neutron–nucleus scattering obtained via DSS formalism in a lattice basis with dimensions $N = 100$ (dashed line) and $N = 200$ (solid line). Black circles denote the accurate phase shifts found with local phase-shift-equivalent potentials at neutron energies $E_n = 7$ and 26 MeV

when the $n-A$ interaction has the form of *a complex nonlocal* potential of the Perey and Buck type. The complex S-wave phase shift $\delta_0(E)$ calculated from the complex-valued eigenenergies $\{E_i\}$ as a function of energy together with those found from the direct numerical integration of the Schrödinger equation at two energies (for the local phase-equivalent potentials) are displayed in Fig. 2. The potential parameters are taken the same as in [4].

In [5] we have introduced generalization of DSS formalism to the multichannel case.

2. THREE-BODY SCATTERING PROBLEM

To solve the general three-body scattering problem for particles 1, 2 and 3, interacting via pair short-range potentials v_a $(a=1,2,3)$, it is convenient to use three Jacobi coordinate sets corresponding to three channel Hamiltonians H_a $(a=1,2,3)$ which define asymptotic motions in the system. The respective wave-packet basis should be constructed independently for each Jacobi set [4]. The channel Hamiltonian H_a has the form of the direct sum $H_a \equiv h_a \oplus h_0^a$, where sub-Hamiltonian h_a defines the interaction in the $\{bc\}$-subsystem (i.e., including the potential v_a) and the sub-Hamiltonian h_0^a corresponds to the free relative motion of this subsystem (its center of mass) and the spectator particle a. So, one has to introduce the WP bases $\{|z_i\rangle\}_{i=1}^K$ and $\{|x_j\rangle\}_{j=1}^N$ for two-body sub-Hamiltonians h_a and h_0^a. The three-body wave packets (3WP) are defined just as products of two type wave-packet states for the above two sub-Hamiltonians (whose angular parts are combined to the total angular momentum value): $|Z_S^{(a)}\rangle \equiv |z_i, x_j\rangle$, where $S = i, j, \ldots$ is the multiindex including bin numbers, partial wave values, etc. The properties of the 3WP constructed in this way are the same as properties of the two-body wave packets. We constructed [4] an analytical f.-d. approximation for each three-body channel resolvent $G_a(E) \equiv [E + i0 - H_a]^{-1}$ in its 3WP basis. This representation is the basic feature for the wave-packet approach since it allows one to simplify solution of the general three-body scattering problem drastically.

By the wave-packet projection of the Faddeev equations, one gets the following f.-d. equations for the Faddeev components of the «packetized» wave function:

$$|\hat{\psi}^{(a)}\rangle = |Z_{S_0}^{(1)}\rangle \delta_{a1} + \mathfrak{G}_a \mathfrak{v}_a \sum_{b \neq a} |\hat{\psi}^{(b)}\rangle, \quad a = 1,2,3, \tag{4}$$

where $|Z_{S_0}^{(1)}\rangle$ is the 3WP state corresponding to the initial state $|\Phi_{01}\rangle$, while $\mathfrak{G}_a$ and $\mathfrak{v}_a$ are wave-packet representations for the channel resolvent and pair interaction. One of the main advantages of the momentum-lattice scheme here is that the transformation between components in different Jacobi sets can be

expressed by a f.-d. matrix of the «permutation operator» [3] with elements $P^{ab}_{S,S'} \equiv \langle Z^{(a)}_S | Z^{(b)}_{S'} \rangle$ in contrast to the direct solving of the Faddeev equations in the momentum space, where time-consuming multidimensional interpolations for scattering solution should be taken in different Jacobi coordinates required in each step of the iteration.

As illustration of the effectiveness for the above lattice technique, we calculated the real phase shifts and inelasticity parameters for the three-body elastic $n-d$ scattering in the quartet and doublet S-wave channels with model Malfliet–Tjon NN potential [3]. The results of these calculations are shown in Fig. 3 for the spin-quartet channel.

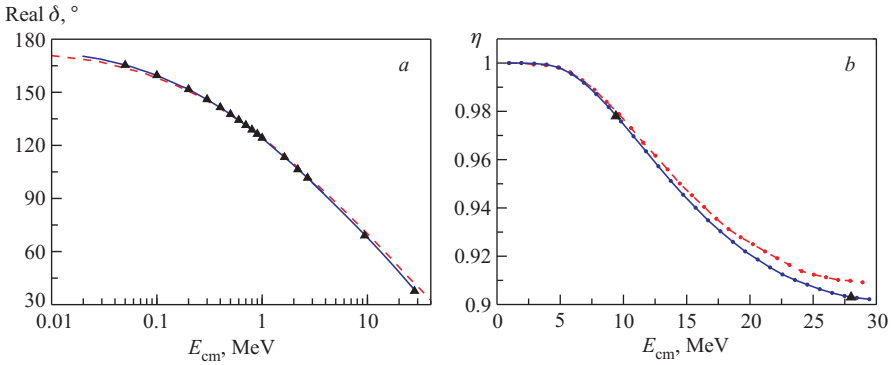

Fig. 3. The energy dependence of the real phase shift and inelasticity parameters for S-wave quartet $n-d$ scattering calculated by means of momentum-packet discretized Faddeev equation at different dimensions $M \times N$ of the lattice basis: 100×100 (dashed curve), 200×200 (solid curve). Results of the direct Faddeev equation solution from [10] are marked as ▲

Thus, at the first time we have solved the three-body scattering problem above the breakup threshold using f.-d. approximation of the L_2 type for the Faddeev kernel.

CONCLUSION

We have demonstrated here that the formulation of the quantum scattering problems in terms of a wave-packet lattice basis is a very convenient language of discretization and an effective tool for practical solutions. Along with the main results explained in this paper, the wave-packet approach has a wide field of application: very economical solving of coupled-channel problems for atomic, molecular and nuclear physics cases [1], construction of effective optical potentials of composite particle interaction [6], etc.

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