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Quantum Scattering Theory in a Discrete Representation

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Abstract. The approach to solving few-body scattering problems in a discrete representation of the stationary wave packets is described briefly. By projecting into the wave-packet basis, all the operators and wave functions are represented with finite matrices and vectors, so that the integral equations of scattering theory are reduced to their matrix analogs. In such a discrete representation, it is easy to construct the matrix analogs for any complicated operators such as total resolvent and also effective interactions between composite particles. Using a special spectral shift function formalism, multichannel scattering problem can be solved in a discrete representation without any scattering equations at all. The approach is illustrated by examples of multichannel and three-body scattering.

1 Introduction

The correct solution for few-body scattering problems has been done, as is well known, many years ago by Faddeev and Yakubovsky [1] which gave rise to an extensive few-body activity worldwide both in theory and experiment. However, when treating realistic interactions, there are some additional problems related to account for internal degrees of freedom of the colliding particles, complex optical interactions of composite particles, correct account of a long-range Coulomb interaction, scattering of particles in resonance states etc., so that a few-body scattering problem with fully realistic interparticle interactions still remains to be a hard numerical task in spite of a great progress in computational facilities. There are few approaches employing the sets of L_2 functions which are adopted for treating the realistic interactions in few-nucleon systems (see the recent review [2]).

Nearly a decade ago, our group in Moscow State University have developed an original approach based on the complete few-body continuum discretization and formulation of the problem in a finite L_2 basis which corresponds to the treatment of a scattering problem in a discrete representation [4–6]. As a result of such a projection one arrives at a fully algebraic scheme for solving the initial problem in which all the operators and wave functions are represented by matrices and vectors, while the scattering equations are reduced to matrix ones. As an appropriate basis set we have taken the stationary wave packets, which have been introduced by Herman Weyl under a title of eigendifferentials [3]. The detailed description of the whole wave-packet approach and the main results attained can be found in our very recent review paper [4]. Here we briefly outline the basic results related to a construction

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of a stationary wave-packet basis in few-body case, solving the realistic $3N$ scattering problem on ordinary PCs using the Graphics Processing Unit (GPU) technique. We present also a short description for the Discrete Spectral Shift formalism which allows to find the multichannel S-matrix without solving scattering equations at all [6]. The latter technique is realized in a discrete representation only and has close relations to the Lüscher finite volume approach, which is well known in the lattice QCD applications [7, 8].

2 Stationary wave-packet basis for solving scattering problems in a discrete representation

Let us consider some two-body Hamiltonian $h = h_0 + v$ where h_0 is a free Hamiltonian (kinetic energy operator) and v is an interaction, and divide the continuous spectrum of h into set of non-overlapping intervals $\{\mathfrak{D}_i \equiv [\mathcal{E}_{i-1}, \mathcal{E}_i]\}_{i=1}^{N}$. The stationary wave packets (WPs) are constructed as integrals of exact scattering wave functions $|\psi_p\rangle$ over such intervals:

$$|z_k\rangle = \frac{1}{\sqrt{B_k}} \int_{\mathfrak{D}_k} f(p)|\psi_p\rangle dp, \quad B_k \equiv \int_{\mathfrak{D}_k} |f(p)|^2 dp, \tag{1}$$

where $p = \sqrt{2mE}$ are relative momenta, m is the reduced mass of the system, B_k and $f(p)$ are normalization factors and weight functions respectively which are interrelated to each other.

The states (1) are well known as the Weyl's eigendifferentials. The integration over energy (or momentum) intervals is just enough to make normalized wave-functions for the continuum. Then the complete system of eigenfunctions for the Hamiltonian h is constructed from its bound states $|\psi_n\rangle$ and eigendifferentials (see the details in ref. [4]). The Hamiltonian matrix h and also the matrix of the resolvent $g(E) = [E + \mathrm{i}0 - h]^{-1}$ for the Hamiltonian h have explicit diagonal forms in a WP representation.

These properties are valid not only for short-range potentials. In fact, one can build the similar wave packets for a Hamiltonian which includes the long-range Coulomb interaction, for example, and then derive an analytical finite-dimensional representation for the Coulomb resolvent [4] as well.

Useful special examples of stationary wave packets are free WP states $|x_k\rangle$, which are defined just for the free Hamiltonian h_0. In momentum representation, the free WP states take the form of step-like functions:

$$\langle p|x_k\rangle = \frac{f(p)\theta(p \in \mathfrak{D}_k)}{\sqrt{B_i}}, \quad \theta(p \in \mathfrak{D}_k) = \begin{cases} 1, & p \in \mathfrak{D}_k, \\ 0, & p \notin \mathfrak{D}_k, \end{cases} \tag{2}$$

where θ is the Heavyside-type theta-function. In few-body and multidimensional cases the free WP bases are constructed as direct products of two-body ones, so that the few-body model space can be treated as a multidimensional lattice.

In the discrete representation, the wave packets corresponding to different Hamiltonians (including the Coulomb one) can be approximated very conveniently as superpositions of free WPs by using simple rotation matrices. In contrast, in order to find the scattering wave functions in the initial continuous momentum representation, one needs to solve an integral equation of the Lippmann–Schwinger type[1].

If the few-body Hamiltonian can be written in the form of a direct sum of two-body ones:

$$H_M = h_1 \oplus h_1 \oplus \ldots \oplus h_M, \tag{3}$$

[1] Also the discrete pseudostates of the Hamiltonian h obtained in some finite L_2 basis can be treated as approximations just for the WP states. In our practical calculations, we have employed the harmonic oscillator basis and also the basis of Gaussians and complex Gaussians as well (see [4] and the refs. therein).

the WP basis states for H_M can be constructed straightforwardly as direct products of the two-body ones:

$$|Z_{i_1 i_2 \ldots i_M}\rangle = |z_{i_1}\rangle \otimes |\bar{z}_{i_2}\rangle \otimes \ldots \otimes |\bar{\bar{z}}_{i_M}\rangle, \tag{4}$$

where we use bar marks up the z-function to distinguish states corresponding to different subsystems. In the basis (4), the matrix of the Hamiltonian H_M is diagonal and the matrix of the resolvent $G_M(E) = [E + i0 - H_M]^{-1}$ also has an explicit diagonal form.

When studying scattering in a system of three particles, 1,2 and 3, the useful examples for Hamiltonians of a type (3) are the free Hamiltonian $H_0 = h_{0p} \oplus h_{0q}$ and also the channel Hamiltonian $H_1 = (h_{0p} + v_1) \oplus h_{0q}$ defined for a given Jacobi partition (e.g. {23}1) with momenta (p, q), where h_{0p} and h_{0q} are kinetic energy operators and v_1 is the interaction between particles 2 and 3. Then one can introduce free WP states $|X_{ij}\rangle$ and channel WP states $|Z_{kj}\rangle$ from two-body ones (with account of necessary spin-angular couplings) and also connect the latter with the former by a simple rotation [4] (all the necessary quantum numbers have to be taken into account)[2].

3 GPU-optimization for a practical solution of 3N scattering problem

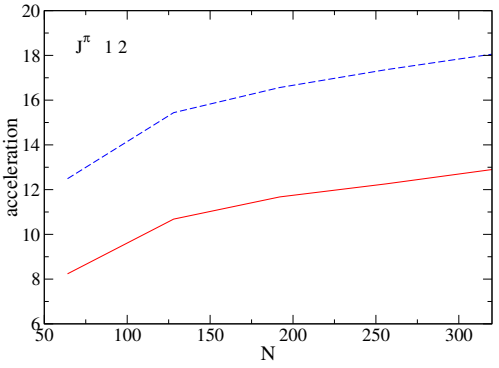

Figure 1. The dependence of the GPU acceleration for the whole solution (solid curve) and the permutation matrix calculation (dashed curve) on the dimension of the basis N (total dimension is N^2) when evaluating the elastic nd scattering amplitude for $J = \frac{1}{2}^+$.

One of the main advantages of the discrete WP approach is that the scattering problem can be solved directly in the basis space corresponding to *the channel Hamiltonian* instead of the three-body free Hamiltonian space. So that, an elastic nd scattering amplitude and a breakup amplitude can be found from the matrix analog of the Faddeev-type equation (in the AGS form) for the transition matrix $\mathbb{U}$ defined in the channel WP basis [4, 5]. The main computational effort in the numerical scheme for solving the nd scattering problem is spent on the calculation of the matrix elements of the particle permutation $\mathbb{P}$ in a channel WP basis. Because all these elements are calculated with the same code and fully independently from each other, the algorithm is very suitable for parallelization and implementation on multiprocessor systems, in particular on a Graphics Prosessing Unit (GPU).

In the Fig. 1, the rate of acceleration η (the ratio of ordinary CPU runtime to the GPU-optimized one) for different steps of the whole numerical scheme when calculating $\frac{1}{2}^+$ partial elastic nd amplitude for the Nijmegen I NN potential (with account of 18 spin-angular channels) is given.

It is evident from the Figure, that GPU optimization allows to accelerate the numerical solution nearly 10 times. The details of the procedure can be found in Ref. [5].

The obvious advantage of the above numerical scheme is that the permutation matrix does not depend on the incident energy. So that, when one needs scattering observables at many energies

[2] Also this scheme for the basis construction can be generalized to the charged particle case

(see e.g. the Fig. 2), the entire computation time will not noticeably increase because the most time-consuming part of the code is carried out only once for many energy points. The results of calculation

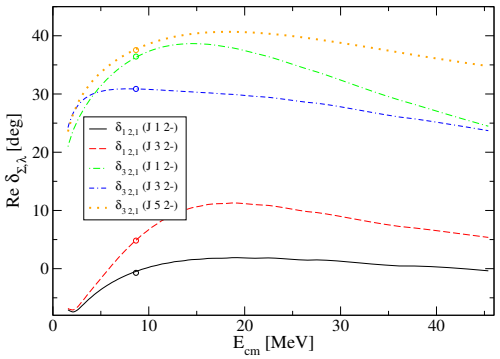

Figure 2. The P-wave partial phase shifts for the elastic *nd* scattering as functions of the neutron incident energy obtained within the wave-packet approach (solid curves) and within the standard Faddeev calculations (circles) [9]. Here Σ, J, π and λ are the total spin, total angular momentum, parity and the neutron orbital momentum respectively.

of elastic *nd* differential cross sections at different neutron incident energies can be found in our papers [4, 5].

4 Discrete spectral shift function formalism

The discrete representation for scattering theory objects opens new possibilities in practical solving scattering problems. Below we briefly report the method based on the spectral shift function formalism, which allows to find multichannel scattering matrix using spectral properties of a free and total Hamiltonian only.

The spectral shift function (SSF) $\xi(E) \equiv \xi(E; h, h_0)$ is an important object in the general spectral theory of perturbations which defines a spectral difference for two Hermitian operators h_0 and $h = h_0 + v$ (e.g., free and total Hamiltonians) both, in discrete and continuous parts of the total spectrum [10, 11]. There are no restrictions that the perturbation v has to be small. It is only assumed that the operator v has a finite trace. The most essential result of the SSF formalism for physical applications is the famous Birman–Krein formula [10], which relates the SSF with the determinant of the scattering operator S: $\det S(E) = \exp(-2\pi i\xi(E))$. In single-channel scattering (e.g. at a fixed angular momentum), this formula implies that the SSF, within a factor $(-\pi)$, is equal directly to a partial phase shift $\delta(E) = -\pi\xi(E)$.

At negative energies, the SSF is a counting function which changes by one unit when crossing each bound state energy [6]. Thus, in conventional scattering theory, the SSF is considered just as some generalized phase shift function. However, the discrete representation for the SSF opens new possibilities in a solution of scattering problems.

To define the SSF in a discretized representation, one has to use a concept of quasi-continuous spectrum introduced by I.M. Lifshits [12] (see also details in ref. [6]). He considers a family of Hermitian operators $\{h_0^{(\alpha)}\}$, where each operator depends on a small parameter α and has a purely discrete spectrum of eigenvalues (EVs) $\{E_j^0(\alpha)\}$ which can be approximated by a single continuous monotonous function $g(u)$:

$$E_j^0(\alpha) = g(j\alpha) + O(\alpha), \quad \text{and} \quad D_j^{(\alpha)} = E_{j+1}^0(\alpha) - E_j^0(\alpha) = \alpha\left[\left.\frac{\mathrm{d}g}{\mathrm{d}u}\right|_{u=j\alpha} + O(\alpha)\right]. \tag{5}$$

When α gets smaller, all the differences $D_j^{(\alpha)}$ get smaller as well and the quasi-continuous spectrum becomes more and more dense. Thus, in the limit $\alpha \to 0$ one has the limiting operator h_0 with

a continuous spectrum. By adding the perturbation v to $h_0^{(\alpha)}$ operators, one gets a family of total Hamiltonians $h^{(\alpha)}$ with shifted EVs $\{E_j(\alpha)\}$. One or several EVs of the perturbed spectrum may occur to be below the threshold and thus correspond to the bound states of h, while the rest belongs to the quasi-continuous spectrum of this operator. The following relation between perturbed and unperturbed EVs in quasi-continuous spectrum takes place [6, 12]:

$$E_j(\alpha) = E_j^0(\alpha) + D_j^{(\alpha)}\xi_j + o(\alpha), \tag{6}$$

where $D_j^{(\alpha)}$ is defined in Eq. (5) and $\xi_j = \xi(E_j(\alpha))$ is the spectral shift function defined at discrete energy values. The formula (6) is the basic for the Discrete Spectral Shift (DSS) method. It results in a very simple approximate expression for the partial phase shift:

$$\delta(E_j(\alpha)) = -\pi\xi(E_j(\alpha)) \approx -\pi\frac{E_j(\alpha) - E_j^0(\alpha)}{D_j^{(\alpha)}}. \tag{7}$$

This method may be applied for any continuum discretization procedure. For example, when one considers a particle scattering in a box and the box size R increases to infinity ($\alpha \sim \frac{1}{R}$) [6]. Another useful case is the solution of the scattering problem in some finite L_2 basis when the parameter α is decreasing with increasing basis dimension N [6].

In a multichannel case one can evaluate *eigen phase shifts* from the differences of free and total Hamiltonian eigenvalues [6]. Here the discretized spectrum of the multichannel free Hamiltonian has to be degenerated with the multiplicity corresponding to the number of open channels at the current energy. In that case, the spectrum of the total multichannel Hamitonian **h** will consist of series of split levels [6]. Then one can define the different spectral shift functions in the eigenchannel representation (each for a separate eigen channel) and relate them with eigen phases of the multichannel problem. Finally, these eigen phases are defined again from the discrete spectral shifts:

$$\delta^{(\varkappa)}(E_j) \approx -\pi\frac{E_j^{(\varkappa)} - E_j^0}{D_j}, \quad \varkappa = 1, \ldots, d, \tag{8}$$

where $\varkappa$ is the eigenchannel index, E_j^0 is the eigenvalue of the free Hamiltonian $\mathbf{h}_0$ with the multiplicity d and $E_j^{(\varkappa)}$ is the eigenvalue of the total Hamiltonian **h**.

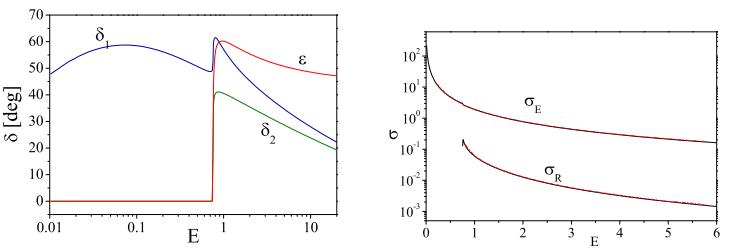

Figure 3. The eigen phases $\delta_{1,2}$, the mixing angle ϵ (left), and the elastic and reaction cross sections (right) found via the DSS method for the two-channel $e - H$ scattering (solid curves). The dash-dotted curves on the right panel reflect results of Ref. [13].

In Fig. 3, our results for the model two-channel $e + H$ scattering problem[3] found in the DSS approach in comparison with the results of Ref. [13] are given[4].

[3]Here we used a coupled-channel potential including $1S - 2S$ excitation of the hydrogen atom. The model parameters of interaction has been taken from Ref. [13].

[4]It is clear that the DSS technique represents the reaction cross section very well in a wide energy region except only one or two energy points just near the threshold of the second channel.

The detailed description of the DSS approach and numerical examples for multichannel scattering can be found in Refs. [6].

5 Summary

We have briefly shown that the discrete WP representation is a very useful tool for solving realistic few-body scattering problems. All details of the approach and the results can be found in the review paper [4].

It should be emphasized here that the discrete spectral shift approach is rather similar to the finite volume approaches and particulary to the Lüscher approach [7, 8]. However, in the DSS, there are no restrictions according to a small values of a perturbation or to low momentum. Also we do not need a special form of a finite volume boundary. Moreover, the discrete SSF approach is based on some fundamental spectral properties of operators and does not depend on the concrete representation. So that, the finite volume relations for partial phase shifts can be considered as some partial realization of the DSS approach. This fact might be important for the multichannel case, because finite volume approaches may use the DSS formalism for this case. The detailed analysis of the above aspects will be published elsewhere.

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