PROGRESS IN METHODS TO SOLVE THE FADDEEV AND YAKUBOVSKY DIFFERENTIAL EQUATIONS

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ABSTRACT. We shortly recall the derivation of the Faddeev-Yakubovsky differential equations and point out their main advantages. Then we give a review of the numerical approaches used to solve the bound-state and scattering problems for the three- and four-body systems based on these equations. A particular attention is payed to the latest developments.

1. BRIEF HISTORY

A crucial step in the theory of few-body quantum systems has been done in 1960 when Faddeev introduced his celebrated integral equations [1]. The Faddeev equations became a basis for the three-body scattering theory with short-range interactions. They have also been used through the years in numerical calculations. As for the $N$-body systems with $N > 3$, Faddeev’s idea of an explicit cluster-channel separation was completely elaborated by 1967 when Yakubovsky’s integral equations became available [2]. The Faddeev differential equations, in their $S$-wave two-dimensional version, were first discovered in 1968 by Noyes and Fiedeldey [3]. The Faddeev differential equations in their complete form have been analysed in 1976 by Merkuriev, Gignoux and Laverne [4]. In particular, they found and approved the asymptotic boundary conditions that are needed to be added to the equations in order to find unique physical solutions corresponding to various scattering processes.

It was the great success of the Faddeev differential equations that stimulated Merkuriev to look for a generalization of these equations to few-body systems with arbitrary number of particles. By 1982 he has successfully solved the problem jointly with his then Ph.D. student Sergei Yakovlev [5]. They not only found the “right” differential equations for the Yakubovsky components but also described the boundary-value problems for these equations that correspond to certain scattering processes [6]. In a somewhat more abstract form, the Yakubovsky differential equations can be seen in paper [7] by Benoist-Gueutal and L’Huillier, published also in 1982.

In Section 2 we recall how the Faddeev-Yakubovsky differential equations look like. The best way to do this is simply to derive them. We concentrate only on the algebraic context of the derivation, leaving apart the description of the scattering boundary conditions. In Section 3 we review the numerical approaches used to solve the Faddeev-Yakubovsky differential equations. A particular attention is payed to the latest developments. Finally, in Section 4 we mention some still challenging problems.

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2. **Faddeev and Yakubovsky Differential Equations**

Let $H_0$ be a linear (not necessarily Hermitian) operator on a Hilbert space $\mathcal{H}$, and $V$ another linear operator on $\mathcal{H}$. At the moment we specify neither $H_0$, nor $V$. These operators may be of completely arbitrary nature. Temporarily assuming that both $H_0$ and $V$ are bounded we avoid complications with domains of the operators involved and concentrate mainly on the algebraic part of the Faddeev-Yakubovsky scheme. The only essential assumption is that by some reason the perturbation $V$ is split into the sum $V = V_1 + V_2 + \cdots + V_n$ of $n$ ($2 \leq n < \infty$) terms $V_\alpha$. Surely, one is interested in the perturbed operator $H = H_0 + V$.

Suppose that $z$ is an eigenvalue of $H$ and $\Psi$ the corresponding eigenvector. Assume, in addition, that $z$ does not belong to the spectrum $\sigma(H_0)$ of the unperturbed operator $H_0$. Then $H_0 - z$ is invertible and $(H_0 + V)\Psi = z\Psi$ is equivalent to the Lippmann-Schwinger equation

$$\Psi = -(H_0 - z)^{-1} \sum_{\alpha=1}^{n} V_\alpha \Psi. \quad (1)$$

Introduce the vectors

$$\psi_\alpha = -(H_0 - z)^{-1} V_\alpha \Psi, \quad \alpha = 1, 2, \ldots, n. \quad (2)$$

These vectors are called the Faddeev components of the eigenvector $\Psi$. Obviously, combining (1) and (2) implies $\sum_{\beta=1}^{n} \psi_\beta = \Psi$. Taking this into account, rewrite (2) in the form

$$\psi_\alpha = -(H_0 - z)^{-1} V_\alpha \sum_{\beta=1}^{n} \psi_\beta. \quad (3)$$

Then apply to both sides of (3) the operator $H_0 - z$ and arrive at the equations

$$(H_0 + V_\alpha - z)\psi_\alpha = -V_\alpha \sum_{\beta \neq \alpha}^{n} \psi_\beta. \quad (4)$$

These are just the celebrated Faddeev “differential” equations for the components $\psi_\alpha$ of an eigenvector of $H$. A remark on the spectrum of the associated Faddeev operator can be found in Appendix.

For $z \notin \sigma(H_0 + V_\alpha)$, $\alpha = 1, 2, \ldots, n$, one can invert the operators $H_0 + V_\alpha - z$ and, thus, rewrite (4) in the equivalent form

$$\psi_\alpha = -(H_0 + V_\alpha - z)^{-1} V_\alpha \sum_{\beta \neq \alpha}^{n} \psi_\beta. \quad (5)$$

Equations (5) are known as the Faddeev integral equations.

The Faddeev equations (4) turn into truly differential equations if $H_0$ is a differential operator as this happens in the case of few-body problems with pairwise interactions, studied in coordinate representation. In this case $H_0$ is simply the kinetic energy operator in the center-of-mass frame and $V_\alpha$’s stand for the two-body potentials.

In the three-body case the Faddeev equations (4) or (5) represent simultaneously the first and the last step in the Faddeev-Yakubovsky approach. This reflects the fact that with sufficiently rapidly decreasing and smooth potentials $V_\alpha$, $\alpha = 1, 2, 3$, the four times iterated Faddeev integral equations (5) are Fredholm and even compact (unlike the Lippman-Schwinger equation (1) that remains non-Fredholm after any number of iterations, even for the complex energies $z$).
Now we turn to the four-body case. It is convenient to depict the four-body system by an icon like $\text{囲み}$ where the dots denote the particles and the connecting line segments are associated with both the particle pairs and respective two-body interactions. There are $n = 6$ different pairs (and potentials $V_\alpha$) that are numbered by $\alpha = 1, 2, \ldots, 6$.

It turns out [2] that the four-body Faddeev integral equations (5) are not Fredholm even for complex $z$. This can be understood already from the fact that in the four-body coordinate space $\mathbb{R}^9$ the supports of any two finite non-zero two-body potentials $V_\alpha$ and $V_\beta$, $\beta \neq \alpha$, have an unbounded cylindrical intersection.

Yakubovsky’s recipe to tackle the four-body problem consists in the following. First, introduce the two-cluster partitions: $\text{囲み} \text{囲み} \text{囲み} \text{囲み} \text{囲み} \text{囲み}$. Number them by the Roman letter $a$ (or $b, c$ etc.). Then say that a pair $\alpha$ belongs to a partition $a$ and write $\alpha \subset a$ if the two-body subsystem $\alpha$ belongs to one of the clusters in the partition $a$. For example, $\text{囲み} \subset \text{囲み}$ while $\text{囲み} \subset \text{囲み} \text{囲み} \text{囲み} \text{囲み}$. In such a case the sequence $a\alpha$ is called the chain of (consecutive) partitions. It is assumed that the partition $\alpha$ consists of one two-particle cluster formed by the pair $\alpha$ and two one-particle clusters obtained from the partition $a$ by breaking the corresponding “bonds”. It is easy to see that there are 18 different chains of partitions: 12 due to $3 + 1$ and 6 due $2 + 2$ starting partitions.

Using the four-body Faddeev integral equations (5) introduce the following new vectors, called the Yakubovsky components (of the eigenvector $\Psi$):

$$\psi\alpha = -(H_0 + V_\alpha - z)^{-1}V_\alpha \sum_{(\beta \neq \alpha) \subset a} \psi_\beta. \quad (6)$$

Then apply to both parts of (6) the operator $H_0 + V_\alpha - z$ and obtain

$$(H_0 + V_\alpha - z)\psi\alpha = -V_\alpha \sum_{(\beta \neq \alpha) \subset a} \psi_\beta = -V_\alpha \sum_{(\beta \neq \alpha) \subset a} \sum_{b \supset \beta} \psi_\beta \quad (7)$$

taking into account that $\sum_{b \supset \beta} \psi_\beta = \psi_\beta$. Further, by applying some combinatorics one arrives at the identity

$$\sum_{(\beta \neq \alpha) \subset a} \sum_{b \supset \beta} \psi_\beta = \sum_{b \subset \alpha} \sum_{(\beta \neq \alpha) \subset a} \psi_\beta$$

and then from (7) it follows that

$$(H_0 + V_\alpha - z)\psi\alpha + V_\alpha \sum_{(\beta \neq \alpha) \subset a} \psi_\alpha = -V_\alpha \sum_{b \neq a} \sum_{(\beta \neq \alpha) \subset a} \psi_\beta. \quad (8)$$

These 18 equations for the 18 unknowns $\psi\alpha$ are just the desired Yakubovsky differential equations.
The table above demonstrates the remarkable structure of the $18 \times 18$ block operator matrix associated with the Yakubovsky equations $\{8\}$. The icons of three-cluster partitions depict the indices $\alpha$ of the potentials $V_{\alpha}$ in the non-zero entries of the matrix.

3. NUMERICAL APPROACHES, IDEAS AND TRICKS

Compared to the Schrödinger equation, the main numerical advantage of the Faddeev-Yakubovsky differential equations is that the asymptotical boundary conditions for their physical solutions imposed at infinitely large distances are much simpler than those for the total wave function, and they can be much easier incorporated into the numerical scheme, especially in the case of scattering processes. Compared to the Faddeev-Yakubovsky integral equations, it is much easier to tackle the local two-body potentials. Typically, with such potentials the matrices of the discretized differential equations have a band structure unlike in the case of the integral ones.

If particles are identical, the number of the essentially different Faddeev-Yakubovsky components reduces. The components corresponding to different indices may be obtained from each other by a simple unitary transformation. For example, the Yakubovsky equations $\{8\}$ for four identical bosons reduce to a system of only two equations $\{8\}$.

The next step is to reduce the dimension of the equations by making a partial-wave decomposition. Since the total angular momentum $L$ is a conserving quantity, projections onto the reducing subspaces associated with a fixed value of $L$ keep the emerging equations exact. At this stage the three Eulerian angles fixing the particles plane turn out to be separated and the dimension of the Faddeev equations reduces to 3. This is a modern development to stop at this stage and solve the three-dimensional Faddeev equations. Such an approach was first developed in $\{9\}$. It is especially well suited to the case where two-body interactions depend only on the distance between particles. The three-dimensional Faddeev differential equations were first solved numerically in $\{10\}$. 
But historically, the first were the two-dimensional partial-wave (integro-) differential Faddeev equations where, for a fixed value of $L$, another variable, the angle between Jacobian vectors, was eliminated [11]. Further reduction, already to a one-dimensional form, consists in performing the hyperspherical adiabatic expansions (see, e.g., [12]).

As for the discretization of the equations with respect to the spatial variables, the finite-difference approximation was initially used [11]. Starting from [13], for this purpose various spline approximations are often employed. An interesting trick with a tensor factorization of the left-hand sides of the discretized Faddeev equations has been suggested in [14]. The factorization trick works very well within iterative approaches (see [15], [16]).

Four-body calculations based on the Yakubovsky differential equations are still rather scarce. Recent examples of such calculations can be found in [17, 18].

Latest developments in approaches to solving the Faddeev-Yakubovsky differential equations are related to the case where the interaction potentials have an extremely strong repulsive component at small distances between particles (like, e.g., in atom-atom potentials). One of the options to tackle such potentials is in approximating the repulsive part by a hard core. A generalization of the three-body Faddeev differential equations to the hard-core interactions has been done yet in 1983 by Merkuriev and the present author [19]. Differential Yakubovsky equations for this model were derived in [20]. According to [19, 20], the effect of hard cores is reproduced by imposing two-sided boundary conditions on the Faddeev-Yakubovsky components at $x_\alpha = c_\alpha$, $\alpha = 1, 2, \ldots, n$, where $x_\alpha$ denotes the distance between particles of the pair $\alpha$ and $c_\alpha$ the sum of their core radii. In the three-body case these conditions are quite natural: $\sum_{\beta=1}^{3} \psi_\beta |_{x_\alpha = c_\alpha} = 0$, $\alpha = 1, 2, 3$, while in the four-body one they are more nontrivial:

$$\left(\psi_{a\alpha} + \sum_{\beta < a} \psi_{a\beta} + \sum_{b \neq a} \sum_{(\beta \neq \alpha) < a} \psi_{b\beta}\right) |_{x_\alpha = c_\alpha} = 0 \quad \text{for any chain } a\alpha. \quad (9)$$

It is assumed that $V_\alpha = 0$ for $x_\alpha < c_\alpha$ and that equations (4) and (8) are considered on the respective whole coordinate space $\mathbb{R}^6$ or $\mathbb{R}^9$, except the hypercylinders $x_\alpha = c_\alpha$ where the hard-core boundary conditions are imposed. Thus, when a potential with a strong repulsive core is replaced by the hard-core model, one approximates inside the core domains only the kinetic energy operator $H_0$ instead of the sum of $H_0$ and the huge repulsive term. In this way a much better numerical approximation is achieved.

In recent years this approach was extensively used to calculate binding energies, resonances, and scattering observables for the systems of three helium atoms (see papers [21, 22] and references therein). In 2006 the Yakubovsky differential equations (8) with the hard-core boundary conditions (7) were employed for the first time and with a big success by Lazauskas and Carbonell [23] to calculate properties of the four-atomic $^4\text{He}_4$ system. They have also performed $^4\text{He}_3$ calculations with the hard-core Faddeev differential equations.

Another (purely numerical) approach to tackle the two-body potentials with extremely strong repulsion at small distances has been developed by Roudnev and Yakovlev. A quite detail description of this approach is given in [15].

4. CHALLENGES

For years the Faddeev-Yakubovsky differential equations showed their high suitability and efficiency when one solves the three- and four-body problems, particularly the scattering ones. Recent advances are related to solving the problems with hard-core (or practically
hard-core) interactions. Still challenging, however, is the numerical solving of the scattering problems that involve triple collisions. Also many questions remain unanswered in the case of few-body scattering problems with Coulomb interactions, especially with the attractive ones.

APPENDIX: ON THE SPECTRUM OF THE FADDEEV OPERATOR

Faddeev equations \( H_F \) represent the spectral problem for the \( n \times n \) block operator matrix

\[
H_F = \begin{pmatrix}
H_0 + V_1 & V_1 & \cdots & V_1 \\
V_2 & H_0 + V_2 & \cdots & V_2 \\
\vdots & \vdots & \ddots & \vdots \\
V_n & V_n & \cdots & H_0 + V_n
\end{pmatrix}
\]

considered as an operator on the Hilbert space \( \tilde{\mathcal{H}} = \mathcal{H} \oplus \mathcal{H} \oplus \cdots \oplus \mathcal{H} \). The matrix \( H_F \) is called the Faddeev operator associated with a Hamiltonian of the form \( H = H_0 + V_1 + V_2 + \cdots + V_n \).

The passage from \( H \) to \( H_F \) adds to \( \sigma(H) \) some auxiliary spectrum. But this auxiliary spectrum is nothing but that of \( H_0 \). More precisely, \( \sigma(H_F) = \sigma(H) \cup \sigma(H_0) \) (for a proof see, e.g., [24]). The spectrum \( \sigma(H_0) \) is usually called the spurious spectrum of the Faddeev operator, although it is quite not "dangerous", since it is assumed that one knows everything about the unperturbed Hamiltonian \( H_0 \).

REFERENCES

[1] Faddeev, L. D.: Zh. Eksp. Teor. Fiz. 39, 1459 (1960)
[2] Yakubovsky, O. A.: Sov. J. Nucl. Phys. 5, 937 (1967)
[3] Noyes, H. P., Fiedeldey, H.: In: Three-Particle Scattering in Quantum Mechanics (Proc. Texas A&M Conference), p. 195. N.Y.: Benjamin 1968
[4] Merkuriev, S. P., Gignoux, C., Laverne, A.: Ann. Phys. 99, 30 (1976)
[5] Merkuriev, S. P., Yakovlev, S. L.: Dokl. Akad. Nauk SSSR 262, 591 (1982)
[6] Merkuriev, S. P., Yakovlev, S. L.: Theor. Math. Phys. 56, 673 (1983)
[7] Benoist-Gueutal P., L’Huillier, M.: J. Math. Phys. 23, 1832 (1982)
[8] Merkuriev, S. P., Yakovlev, S. L., Gignoux, C.: Nucl. Phys. A 311, 125 (1984)
[9] Kostrykin, V. V., Kvitsinsky, A. A., Merkuriev, S. P.: Few-Body Syst. 6, 97 (1989)
[10] Hu, C.-Y., Kvitsinsky, A. A., Merkuriev, S. P.: Phys. Rev. A 45, 2723 (1992)
[11] Laverne, A., Gignoux, C.: Nucl. Phys. A 203, 597 (1973)
[12] Nielsen, E., Fedorov, D. V., Jensen, A. S.: J. Phys. B 31, 4085 (1998)
[13] Friar, J. L., Gibson, B. F., Payne, G. L., Chen C. R.: Phys. Rev. C 30, 1121 (1984)
[14] Schellingerhout, N. W., Kok, L. P., Bosveld, G. D.: Phys. Rev. A 40, 5568 (1989)
[15] Roudnev, V. A., Yakovlev, S. L., Sofianos, S. A.: Few-Body Syst. 37 (2005), 179
[16] Roudnev, V.: Chem. Phys. Lett. 367, 95 (2003)
[17] Yakovlev, S. L., Filikhin I. N., Roudnev, V. A., Vlahovic, B.: J. Phys. B 35, 501 (2002)
[18] Lazauskas R., Carbonell, J.: Few Body Syst. 34, 105 (2004)
[19] Merkuriev, S. P., Motovilov, A. K.: Lett. Math. Phys. 7, 497 (1983)
[20] Merkuriev, S. P., Motovilov, A. K., Yakovlev, S. L.: Theor. Math. Phys. 94, 306 (1993)
[21] Motovilov A. K., Sandhas, W., Sofianos, S. A., Kolganova, E. A.: Eur. Phys. J. D 13, 33 (2001) arXiv: physics/9910016
[22] Kolganova, E. A., Motovilov A. K., Sandhas, W.: Nucl. Phys. A 790, 752c (2007) arXiv: 0707.2210.
[23] Lazauskas R., Carbonell, J.: Phys. Rev. A 73, 062717 (2006)
[24] Yakovlev, S. L.: Theor. Math. Phys. 107, 835 (1996)