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The Faddeev-Merkuriev Differential Equations (MFE) and Multichannel 3-Body Scattering Systems

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Abstract: Numerical implementation of the modified Faddeev Equation (MFE) is presented in some detail. The Faddeev channel wave function displays unique properties of each and every open channel, respectively. In particular, near resonant energies, the structures of the resonances are beautifully displayed, from which, the life-time of the resonances can be determined by simply using the uncertainty principle. The phase shift matrix, or the K-matrix, provides unique information for each and every resonance. This information enables the identification of the physical formation mechanism of the Gailitis resonances. A few of these resonances, previously known as the mysterious shape resonances, have occurred in a number of different collision systems. The Gailitis resonances are actually produced by a quantized Stark-effect within the various collision systems. Since the Stark-effect is a universal phenomenon, the Gailitis resonances are expected to occur in much broader classes of collision systems. We will present the results of a precision calculation using the MFE method in sufficient detail for interested students who wish to explore the mysteries of nature with a powerful theoretical tool.

Keywords: multichannel-quantum scattering theory; Stark-effect; resonance

1. Introduction

The Faddeev-Merkuriev [1,2] or the modified Faddeev Equation (MFE) has existed since 1980. Increasing demands to understand multichannel scattering systems resulted in the first numerical development of MFE in 1992 [3].

In a three-body system with Coulomb interactions, the partial wave expansion of the wave function can be achieved by using bipolar spherical harmonics. These functions are eigenstates of the three-body total angular momentum operator.

The S-state projected MFE used in [3] has been used in a number of numerical tests, from bound-states to low energy scattering systems [4–15]. A number of S-state calculations were carried out using the integral modified Faddeev equation; one of these calculations is represented in Reference [16].

Calculation for differential cross sections needs at least contributions from 9–10 partial waves. A new code capable of calculating all partial waves was developed in 1999 using the bipolar spherical-harmonics expansion [2,17–19], more detail will be presented in Section 2.

In 2002, clear evidences of a new kind of resonance that enhances anti-hydrogen formation in the process of anti-proton + Ps (n = 2) → e + antihydrogen (n ⩽ 2) had been presented in both References [19] and [20].

This evidence became myth, since there was no known resonance in that energy region at that time. It had to wait more than ten years for a supercomputer to solve the mystery.

In Section 3, the complete *K*-matrix and cross section matrix at (near) the three available resonance locations will be presented. The K-matrix, $(tan\ \delta_{ij})$, is simply related to the S-matrix as S = (1 + iK)/(1 − iK). The *K*-matrix is real and symmetric. The *K*-matrix elements and the cross

sections across the resonant energy region will be discussed. Last, but not the least, we consider the role of the resonant wave functions which clearly display the resonant-wave packets formed at the resonant-energies. These wave packets provide the key to unlock the decade-long mystery of Section 2. Section 4, in conclusion, will make suggestions for further numerical improvements to enhance the utility of MFE as a powerful tool to investigate multichannel quantum three-body scattering systems.

2. The Modified Faddeev Equation

The mass-scaled Jacobi vectors $[\vec{x}_\alpha, \vec{y}_\alpha]$ in a general three-body system, with mass m_α and its position vector $\vec{\gamma}_\alpha$, $\alpha = 1, 2, 3$, are defined as:

$$\begin{aligned} \vec{x}_\alpha &= \tau_\alpha \left(\vec{r}_\beta - \vec{r}_\gamma \right) \\ \vec{y}_\alpha &= \mu_\alpha \left(\vec{r}_\alpha - \frac{m_\beta \vec{r}_\beta + m_\gamma \vec{r}_\gamma}{m_\beta + m_\gamma} \right), \\ \tau_\alpha &= \sqrt{2\frac{m_\beta m_\gamma}{m_\beta + m_\gamma}}, \\ \mu_\alpha &= \sqrt{2m_\alpha \left(1 - \frac{m_\alpha}{M}\right)}, \\ M = m_1 + m_2 + m_3 &\text{ and } (\alpha, \beta, \nu) = \text{cyclic } (1,2,3) \end{aligned} \tag{1}$$

It is frequently necessary to transform between two sets of Jacobi coordinates. The orthogonal transformation is:

$$\begin{aligned} \begin{pmatrix} \vec{x}_\beta \\ \vec{y}_\beta \end{pmatrix} &= \begin{pmatrix} C_{\beta\alpha} & S_{\beta\alpha} \\ -S_{\beta\alpha} & C_{\beta\alpha} \end{pmatrix} \begin{pmatrix} \vec{x}_\alpha \\ \vec{y}_\alpha \end{pmatrix}, \\ C_{\beta\alpha} &= -\left[\frac{m_\beta m_\alpha}{(M - m_\beta)(M - m_\alpha)} \right]^{\frac{1}{2}}, \\ S_{\beta\alpha} &= (-1)^{\beta - \alpha}\, sgn\,(\alpha - \beta) \left(1 - C_{\beta\alpha}^2\right)^{\frac{1}{2}}, \end{aligned} \tag{2}$$

accordingly, the Coulomb potentials for the pair α is:

$$\begin{aligned} V_\alpha(x_\alpha) &= q_\alpha / x_\alpha \\ q_\alpha &= z_\beta z_\gamma \tau_\alpha \end{aligned} \tag{3}$$

q_α represents the mass-scaled charge, z_β, z_γ are the physical charges (α, β, ν) = cyclic (1, 2, 3).

In a configuration space, the Faddeev equation is a set of three coupled differential equations, one for each pair of Jacobi coordinates. When collision energy is far below the three-body breakup threshold, only two coupled equations are sufficient.

The original Faddeev equations lack mathematical compactness when the particles interact with long-range forces. MFE [1] avoids this problem by carefully splitting the coulomb potentials into a short-range part $V_\alpha^{(S)}$ and a long-range part $V_\alpha^{(l)}$ as follows:

$$\begin{aligned} V_\alpha^{(S)}(x_\alpha, y_\alpha) &= V_\alpha(x_\alpha)\, \zeta_\alpha(x_\alpha, y_\alpha), \\ V_\alpha^{(l)}(x_\alpha, y_\alpha) &= V_\alpha(x_\alpha) \left[1 - \zeta_\alpha(x_\alpha, y_\alpha)\right], \\ \zeta(x, y) &= 2\left\{1 + exp\left[\frac{(x/x_0)^\nu}{y/y_0 + 1}\right]\right\}^{-1} \end{aligned} \tag{4}$$

The function $\zeta_\alpha(x_\alpha, y_\alpha)$ vanishes asymptotically within the three-body sector, where both $x_\alpha, y_\alpha \to \infty$ and approaches one in the two-body cluster region, where $x_\alpha \ll y_\alpha \to \infty$.

The parameters ν, x_0, y_0 must be chosen very carefully, more details are presented in Section 3.

Let $V_3(x_3)$ be repulsive, we can choose $\zeta_3\ (x_3, y_3) \equiv 0$. Such that the MFE is a set of two coupled differential equations. The total wavefunction of the scattering system is $\psi = \sum_{\alpha=1}^{2} \psi_\alpha$, $\alpha = 1, 2$ are the two Faddeev channels.

$$\begin{gathered}\left(-\Delta_{x_\alpha} - \Delta_{y_\alpha} + V_\alpha + \overline{V}_\alpha - E\right) \psi_\alpha \left(\vec{x}_\alpha, \vec{y}_\alpha\right) = -V_\alpha^{(S)} \psi_\beta \left(\vec{x}_\beta, \vec{y}_\beta\right),\ \beta \neq \alpha \\ \overline{V}_\alpha = V_3 + V_\beta^{(l)},\ \alpha,\ \beta = 1,\ 2,\ \ldots\ ,\end{gathered} \tag{5}$$

are the two Faddeev channels.

For angular momentum conserving interactions, such as Coulomb force, the six-dimensional space of Equation (5) can be reduced to a two-dimensional equation using the partial wave decomposition via the bipolar representation of the wave functions $\psi_\alpha \left(\vec{x}_\alpha, \vec{y}_\alpha\right)$

$$\psi_\alpha \left(\vec{x}_\alpha, \vec{y}_\alpha\right) = \frac{1}{x_\alpha y_\alpha} \sum_{L=0}^{\infty} \sum_{M=-L}^{L} \sum_{\vec{l}+\vec{\lambda}} \psi_{\alpha l\lambda}^{L}\left(x_\alpha, y_\alpha\right) Y_{l\lambda}^{LM}\left(\hat{x}_\alpha, \hat{y}_\alpha\right)\ \alpha = 1, 2 \tag{6}$$

The two-dimensional L – partial wave projected coupled differential equations can be found in References [17] and [2]. Thus, Equation (5) will be solved one partial wave at a time. The total wave function, Equation (6), can be represented very well with nine partial waves for the calculations carried out in References [17–19].

3. Numerical Method

The method is designed to represent the two dimensional (x_α, y_α) and $\alpha = 1, 2$, coupled differential equations as accurately as possible with available computer resources.

A Quintic-Hermite polynomial spline and collocation procedure is adopted for $x_\alpha, y_\alpha\ (\alpha = 1, 2)$ coordinates. An explicit form of the splines can be found in References [12,21].

The continuous variables x or y are replaced by discrete grids called natural knots, for example:

$$[y_i] = \{y_0 = 0,\ y_1, y_2,\ \ldots\ldots\ y_n = y_{max}\} \tag{7}$$

The quintic spline basis $\varphi_{im}\ (y)$, $m = 0,\ 1,\ 2$ are fifth degree Hermite polynomials. They are constructed to be non-zero only on two adjacent intervals $[y_{i-1}, y_i] \cup [y_i, y_{i+1}]$ and have continuous values, first and second derivatives at the knot i. Namely they satisfy the conditions at y_i:

$$\partial_y^{m'} \varphi_{im}\left(y_i\right) = \delta_{mm'}\ , m,\ m' = 0,\ 1,\ 2 \tag{8}$$

at y_0 and y_{max} only the splines that satisfy the boundary conditions can be used.

It must be emphasized that knots do not have to be uniformly distributed. Although a uniform grid for y coordinate works very well, the knots for the x-coordinate must be chosen to accurately reproduce the wave functions and binding energies of all the two-body bound states involved in the scattering system, which are anything but uniform.

Each interval provides three collocation coordinates according to the Gaussian rule. These simple procedures reduce the differential equations into matrix equations, details in Section 4 of Reference [17]. The total angular momentum L partial wave projected coupled differential equation [17] can be represented very accurately, even for very large y_{max}. Although earlier calculation [17] for y_{max} was limited by computer resources, asymptotic dipole coupling was introduced. In Section 3 of Reference [17], that part is no longer necessary with present (and future), powerful super computers.

The proper choice of the parameters in Equation (4) is essential to obtain accurate results. A certain amount of numerical experimentation is necessary. It is observed that:

a $\nu = 2.1$ for both Faddeev channels produced the most stable solutions.

b Both x_0, y_0 depend on the respective Faddeev channels. Since x_0 is proportional to the size of the two-body bound states and y_0 is related to the cutoff parameters, y_{max}.

At the present time, fine tuning of x_0. and y_0 to produce a symmetric K-matrix $\left(tan\,\delta_{ij}\right)$ is necessary. For example, some details of a calculation [22] that solved a set of N = 488,808 coupled linear equations are presented below.

The S-partial wave $e^+ + H$ scattering system has six-open channels, they are:

$$\begin{array}{c} e^+ + H\ (n = 1) \\ e^+ + H\ (n = 2,\ l = 0) \\ e^+ + H\ (n = 2,\ l = 1) \\ p + Ps\ (n = 1) \\ p + Ps\ (n = 2,\ l = 0) \\ p + Ps\ (n = 2,\ l = 1) \end{array} \tag{9}$$

The first three channels belong to Faddeev channel one, the last three channels, 4, 5, and 6, belong to Faddeev channel two. The two Faddeev channels have different parameter sets and grids for x, y coordinates. They are listed in Table 1:

Table 1. Faddeev channel parameters [22], lengths in Bohr Radius.

Faddeev Channel α	x_0	y_0	ν	y_{max}	x_{max}
One	7.0	50.0	2.1	500.0	57.5
Two	10.0	100.0	2.1	1000.0	81.0

The calculation [22] was carried out using much finer energy grids than that used in Reference [19]. Such that the first three resonances in channel 5 and 6 are clearly resolved in Figure 3 of Reference [22], and $K_{55} = tan\,(\delta_{55})$, $K_{66} = tan\,(\delta_{66})$ are plotted in Figure 1 of Reference [22]. The singularities of the first two resonances are clearly displayed. They are distinctly different from that of Fesbach resonances. Reference [22] concluded that the physical mechanism for these resonances are Stark-effects. Tables 2–5 display the K-matrix and cross section matrix near the three resonant energies from Reference [22] at E_1, E_2, E_3; $\varepsilon_1, \varepsilon_2, \varepsilon_3$. These energies are measured from channel 1 and channel 6, respectively, the unit is Ry.

Table 2. Properties of the first resonance.

E_1 = 0.8748; ε_1 = 0.34432 $\times$ 10^{-3}					
Cross Section Matrix					
0.9998E−01	0.3191E−02	0.1913E−02	0.8951E−02	0.1399E−03	0.1611E−03
0.2230E−01	0.1046E+02	0.6338E+01	0.3918E+00	0.4924E+00	0.5676E+00
0.1336E−01	0.6338E+01	0.1258E+02	0.2602E+00	0.3274E+00	0.3774E+00
0.1044E−01	0.6538E−01	0.4343E−01	0.5063E+01	0.4397E−02	0.5068E−02
0.1778E+00	0.8958E+02	0.5957E+02	0.4794E+01	0.4710E+04	0.7676E+02
0.2048E+00	0.1032E+03	0.6866E+02	0.5524E+01	0.7676E+02	0.8756E+03
***K*-Matrix**					
−0.8299E−01	0.1070E+00	−0.4787E+00	0.1557E+01	−0.1148E+00	−0.6303E−01
0.1070E+00	0.8278E+00	−0.2225E+01	0.3038E+01	−0.3513E+00	−0.1929E+00
−0.4721E+00	−0.2229E+01	0.3336E+01	−0.9990E+01	0.1563E+01	0.8580E+00
0.1547E+01	0.3074E+01	−0.1004E+02	0.3559E+02	−0.2703E+01	−0.1484E+01
−0.1154E+00	−0.3560E+00	0.1563E+01	−0.2682E+01	0.2990E+01	0.5194E+00
−0.6331E−01	−0.1955E+00	0.8581E+00	−0.1472E+01	0.5193E+00	−0.3098E+00

Table 3. Properties of the second resonance.

E_2 = 0.87465; ε_2 = 0.19436 $\times$ 10^{-3}					
Cross Section Matrix					
0.9996E−01	0.3311E−02	0.1907E−02	0.8921E−02	0.1300E−03	0.1630E−03
0.2315E−01	0.1030E+02	0.6402E+01	0.4000E+00	0.4559E+00	0.5709E+00
0.1334E−01	0.6402E+01	0.1255E+02	0.2693E+00	0.3031E+00	0.3795E+00
0.1040E−01	0.6670E−01	0.4490E−01	0.5060E+01	0.4054E−02	0.5080E−02
0.2927E+00	0.1468E+03	0.9755E+02	0.7826E+01	0.8987E+04	0.8021E+02
0.3669E+00	0.1838E+03	0.1222E+03	0.9807E+01	0.8021E+02	0.5349E+03
***K*-Matrix**					
−0.8962E−01	0.8594E−01	−0.3864E+00	0.1402E+01	0.1345E+00	−0.2820E−01
0.8617E−01	0.7618E+00	−0.1940E+01	0.2553E+01	0.4102E+00	−0.8601E−01
−0.3795E+00	−0.1941E+01	0.2073E+01	−0.7834E+01	−0.1825E+01	0.3827E+00
0.1390E+01	0.2578E+01	−0.7863E+01	0.3194E+02	0.3164E+01	−0.6638E+00
0.1352E+00	0.4161E+00	−0.1826E+01	0.3140E+01	−0.3236E+01	−0.4327E+00
−0.2840E−01	−0.8727E−01	0.3829E+00	−0.6592E+00	−0.4327E+00	0.2335E+00

Table 4. Properties of the third resonance.

E_3 = 0.87454; ε_3 = 0.84344 $\times$ 10^{-4}					
Cross Section Matrix					
0.1000E+00	0.2972E−02	0.1740E−02	0.8890E−02	0.2387E−03	0.2853E−03
0.2080E−011	0.9661E+01	0.5677E+01	0.3444E+00	0.8368E+00	0.1003E+01
0.1218E−01	0.5677E+01	0.1343E+02	0.2337E+00	0.5565E+00	0.6669E+00
0.1037E−01	0.5740E−01	0.3895E−01	0.5077E−01	0.7496E−02	0.8967E−02
0.1238E+01	0.6201E+03	0.4124E+03	0.3334E+02	0.1025E+04	0.2340E+03
0.1480E+01	0.7433E+03	0.4942E+03	0.3988E+02	0.2340E+03	0.1989E+05
***K*-Matrix**					
−0.6261E−01	0.1684E+00	−0.7479E+00	0.2029E+01	0.3930E−01	−0.4449E+00
0.1678E+00	0.1011E+01	−0.3037E+01	0.4451E+01	0.1193E+00	−0.1352E+01
−0.7426E+00	−0.3053E+01	0.6953E+01	−0.1628E+02	−0.5306E+00	0.6011E+01
0.2026E+01	0.4518E+01	−0.1637E+02	0.4669E+02	0.9248E+00	−0.1047E+02
0.3956E−01	0.1212E+00	−0.5312E+00	0.9195E+00	−0.1623E+00	0.2459E+00
−0.4471E+00	−0.1373E+01	0.6016E+01	−0.1040E+02	0.2460E+00	0.7620E+01

Table 5. Partition of the matrices.

Ch \ Ch	1	2	3	4	5	6
1	$e^+ + H\,(n) \rightarrow e^+ + H\,(n')$			$e^+ + H\,(n) \rightarrow p + Ps\,(n')$		
2	$n = 1,\ 2,\ 3$			$n = 1,\ 2,\ 3$		
3	$n' = 1,\ 2,\ 3$			$n' = 4,\ 5,\ 6$		
4	$p + Ps\,(n) \rightarrow e^+ + H\,(n')$			$p + Ps\,(n) \rightarrow p + Ps\,(n')$		
5	$n = 4,\ 5,\ 6$			$n = 4,\ 5,\ 6$		
6	$n' = 1,\ 2,\ 3$			$n' = 4,\ 5,\ 6$		

Tables 2–5 show that:

a All *K*matrices are symmetric with an error less than 2%.

b All cross sections are small except that in resonant channels 5 and 6 that include all Hydrogen (antihydrogen) formation cross sections.

The total hydrogen formation cross sections from *S*-partial wave at the resonances are in Table 6:

Table 6. In units of πa_0^2 .

σ_{ε_1}	σ_{ε_2}	σ_{ε_3}
321.51	551.13	2272.82

c. Comparison with 2002 calculation [19].
Reference [19] calculated a total of nine partial waves for a number of energies. The one that is closest to E_1 is at 0.8749 Ry. According to Reference [19], the total hydrogen formation cross sections, including all nine partial waves, is 1670.02 πa_0^2. The contribution from the *S*-partial wave is 219.25 πa_0^2. The calculation from Reference [19] used the first generation of super computers, named Blue Horizon. The recent *S*-partial wave cross section at 0.8749 Ry is 276.77 πa_0^2. This calculation was carried out on a much more improved super computer, named Ranger. There is a significant increase in *S*-partial wave cross section. Accordingly, the total hydrogen formation cross section from the first resonance alone could be over 2000 πa_0^2.

4. Conclusions

The numerical procedure described is suitable for accurate, in-depth calculation of multichannel quantum three-body scattering systems below three-body break-up energy. The calculation of Hu and Caballero [22] indicates that there are decades of hard work that remain, just to understand the quantum three-body scattering systems.

a For the $e^+ + H$ system, Reference [22] revealed only three *S*-state resonances above the Ps $(n = 2)$ formation threshold. They are named Gailitis resonances due to their unique formation mechanism. The y_{max} should be doubled to ~2000 a_0 to test the fine structure energy limit. Near the fine structure energy, the Coulomb degeneracy of the target atom is removed. Without the degeneracy, the incoming charged particle can not induce a first order electric dipole moment in the target atom [23]. Such Gailitis resonances are supported by a higher order Stark effect.

b Higher angular momentum Gailitis resonances must be investigated thoroughly. Reference [19] calculated nine partial wave cross sections near the first resonance, discussed in Section 3. About 70% of the contribution to the total cross comes from that of *P* and *D* partial waves.

c The MFE is able to provide wave amplitudes for each and every one of all the open channels. A simple three dimensional plot at a constant angle between $\vec{x}$ and $\vec{y}$ reveals important physics. For example [22], the structure of the wave amplitude along the *x*-axis reveals the bound states characteristics. Normally, along the *y* axis, one finds that the de Broglie wave structure, with the appropriate wave length, belongs to the channel plotted. If resonance exists in some channel or channels, wave packets appear along the *y*-axis. For the resonances listed in Tables 2–4 $y_1 = 296.8\ a_0$, $y_2 = 702.4\ a_0$, and $y_3 = 1306\ a_0$. In this case, the physical "size" of the resonances are too large. In other cases [24], the energy widths are too wide. It will be a challenging task to find them using traditional methods, which are designed for the more compact portion of the Feshbach resonances. It is clear that the life-time of the wave packet formed along the *y* axis is the same as the life-time of the resonance. The width of the wave packet, Δy, can be measured directly from the graph. The minimum uncertainty principle provides as good an estimate of the energy width as any other method. In Hu and Papp [24], the width of all 2nd order Stark-effect induced Gailitis resonances are obtained by searching the poles in the complex energy plane using the integral equation version of MFE. In addition, the positions of the wave packets y_m, m is the quantum number of Gailitis resonances, which provided information to uncover the physical mechanism and Stark effect for Gailitis resonances. However, both Gailitis resonances, found above a threshold, and Feshbach resonances, found below a threshold, are induced by

the same Coulomb field of the incoming charged particle. That is consistent with the Levinson theorem. Clearly, larger calculations capable of locating all resonances are necessary for both Feshbach and Gailitis resonances.

d For the case investigated in Reference [22], the width of the wave packets measured from the plots can be approximated by the de Broglie wave length. Whether that can be generalized to high partial wave resonances must be determined with further calculations.

In general, for each series of resonances, width = constant $\times$ λ_m, $m = 1, 2, 3 \ldots$ this is the case in $e + Ps$ $(n = 1)$ where the constant is less than one [24].

Finally, Reference [22] revealed only the "tip of the iceberg" of the properties of the recently named Gailitis resonances, they appeared as threshold cross sections oscillations in Reference [25]. All tools are ready for in-depth investigation of this intricate phenomenon. The mechanism for its formation is universal; however, only the three-body multichannel calculations are able to provide the complete properties of these resonances at the present time.

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