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Intricate partial waves in nuclear scattering

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Abstract This article is meant as an encomium of the life-span endeavor of Jacques Raynal to relate nuclear scattering density matrices with numerical methods. The mathematical investigations he made involved intricate hypergeometric coupling algebras and transformations. He was among the first to appreciate the general importance of these studies. His efforts over 60 years are most praiseworthy and, for them, Jacques has gained much respect.

1 Introduction and survey

There are many branches in studies of nuclear reactions. Within those, a continuous effort has been to invent new tools with which to better understand regularities in the nuclear realm. Therein, however, pure quantum mechanical states are rather the exception. From the outset, scattering situations require measurement and interpretation of density matrices of the initial and final states involved. The usual approach, the S-matrix formalism, encompassed from the very beginning scattering models and analyses. In that formalism, initial and final states are connected by S-matrices which are deduced from nuclear transition (T) matrices. A common approach to ascertain S-matrices is to solve Schrödinger's or even more advanced wave equations. To do so require sophisticated numerical methods to yield high speed and accurate results. In such developments, Jacques was a pioneer. As a result, today, we are well equipped with his programs to analyze data from very advanced, and often exotic, experiments. So common has this process become, that often its historical development seems to be forgotten. Current generations know much about the benefits of artificial intelligence (AI) and machine learning (ML) [1–3]. Being timely nowadays is often interpreted to mean that sciences, Physics in general, Nuclear Physics and Nuclear Engineering in particular, are completely the province of AI/ML.

After 1950, Nuclear Physics was identified and lauded as an ultimate study for human benefit. Nuclear physics for peace was a paradigm everyone accepted. So universal was that belief that the IAEA, International Atomic Energy Agency, was founded on July 29 1957, as an autonomous specialized agency of the United Nations based in Vienna. The organization's task was to promote the peaceful use of nuclear energy, of cooperation and technology transfer. I remember participating as a scholar at the opening ceremony in the Konzerthaus in Vienna. The international importance of the subject lead, among many other initiatives, to foundation of the Abdus Salam International Center for Theoretical Physics (ICTP); an international research institute for physical and mathematical sciences that operates under a tripartite agreement between the Italian Government, United Nations Educational, Scientific and Cultural Organization, and the IAEA. An important initiative of the ICTP was to foster conferences and courses. The first in which I participated was the ICTP course *Fundamentals in Nuclear Theory*, Trieste 10/3–12/16 1966, IAEA Vienna (1967). On various occasions, Jacques Raynal and other members from CEA-Saclay were listed as speakers at ICTP seminars in Trieste.

This article starts when Jacques Raynal[1] began his professional career at CEA-Saclay S.Ph.Math. in 1959/60, after 1963 S.Ph.Th. During the time when *Jacques* was a student at the elite school l'Ecole Polytechnique, he developed a high degree of proficiency in many topics, which in later years became manifest in his friendly 'Oh' style. My personal contacts with him span the years 1970–2006.

In his (and my) early years, given the importance attached to scientific effort world wide, many students including *Jacques* chose to make their professional life in studies of natural sciences and engineering. Many selected to do so

The article carries the intention: Tribute to Jacques Raynal.

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[1] Hereafter I will abbreviate his name with *Jacques* .

in nuclear physics by working with computers in one way or another. At this time and later, CEA-Saclay acquired the most powerful main frame computing equipment from IBM, CDC and others; the intent to continue to do so persists to this day.

I'm not sure who coined the phrase *computing as a language of physics*. However, it may have been Lew Kowarski, a very remarkable personality associated with CEA-Saclay and CERN, who delivered a grand view lecture at the Seminar Course, ICTP-IAEA Trieste, August 1971, entitled: *The impact of computers on nuclear science* [4,5]. Also, Gordon Moore anticipated an increase of computing power by 2^{30} in 60 years; a change of 10 orders of magnitude. In comparison, the world population grew by a factor 2.5 in that time span. The surge in computing power helped drive productivity in all fields of Physics, nuclear physics especially. At the heart of the nuclear physics 'explosion' were use of the optical models. As a postdoc I counted 150 publications in Phys. Rev. having optical model or optical potential in their titles. Recently, I repeated the search with a wider journal range but the same phrases in the title, it gave significantly more than 15,000 papers.

As an aside, *Jacques* was important to me personally by his enabling my contact with many experts. For example, once when in Saclay, *Jacques* introduced me to the eminent scientist, Mme. Henriette Farragi, the random matrix expert, Madan Lal Mehta, the nucleon-nucleon (NN) interaction experts at SATURN, and others.

As part of the survey, I briefly dwell upon inversion topics about which *Jacques* had a most supportive attitude. My interest in inversion theories began when I met Marcel Coz. He was once at the Institute de Physique Nucléaire, D.Ph.Th. in Orsay and later (1967) became a full Professor in theoretical physics at University of Kentucky. He collaborated, and often published, with Christine Coudray from the Institute de Physique Nucléaire in Orsay. They made use of Riemann functions, Marchenko inversion and closely related mathematics, which linked nuclear scattering with inverse problems at fixed angular momentum or fixed energy. Most skillfully, they were able to create generalized translation operators (GTO) and from a key paper entitled *Existence of generalized translation operators from the Agranovitch–Marchenko transformation*. Along with Marcel Coz and Christine Coudray the names, Levitan, Agranovich, Marchenko, Faddeev, Newton, and Sabatier [42–48] are often cited in reports on inversion mathematics and physics. *Jacques* , Marcel Coz, and Christine Coudray, along with many others, are testament to the excellent mathematical education and training in France. After 1976, we in Hamburg widened our view, went to topical conferences and workshops, and made effort in studies of inversion theories and applications. The results are documented in dissertations and associated publications. We tackled quantum inversion theories by Gelfand-Levitan, Marchenko, and Darboux transformations, and numerically solved integral and algebraic equations for inversion of NN data generating NN inversion potentials. For energies, where the S-matrices are unitary, those inversion potentials are real. For non-unitary S-matrices complex two particle optical model inversion potentials were defined. In those studies, we used NN phase-shift data from INS-DAC-Services SAID, George Washington University or from nn-online.org Radbound University Nijmegen [49,50].

Using those inversion potentials, we solved Lippmann-Schwinger or better to say Bethe-Goldstone equations to generate reaction g-matrices which, notably, are energy and medium dependent. They belong to the class of effective complex energy and medium dependent interactions, and which are essential for many fields in nuclear theory [6–12]. Many ancillary studies supported our conjecture that hadron-hadron inversion potentials and/or general complex inversion optical potentials yield appropriate g-matrices as effective interactions that are explicitly energy and target medium dependent. An available optical model parameterization that yields agreement with phase shift data, is readily input into g-matrix calculations. I define them as *two hadron inversion optical potentials*. Andreas Funk [63], and colleagues before him, used primarily data from SAID or from nn-online.org. More on this subject is found in a later section. I have pursued this line of research until my retirement in 2003, after which, unfortunately, the evaluation and updating of inversion optical model potentials has been suspended.

Theoretical and technical aspects of g-matrix calculations are intricate. What is sought are medium and energy dependent effective interactions. The propagator in the defining equations should depend on all particle masses, charges, energies, momenta, angular momenta and spins. In solving such a complicated problem, use of hypergeometric functions could be practical and appropriate, as they have been in investigating three or four quasi-particle systems. *Jacques* was a leading expert in studies using hypergeometric functions.

In the next sections, Sects. 2 and 3, I emphasize aspects of *Jacques* 's work. Directly related with *Jacques* are: Fortran programs widely used for many analyses and in vogue to this day, generalized coupling schemes and relations with hypergeometric functions, generalized 3-j and 6-j symbols, and Moshinsky transformations [6–41]. In Sect. 3, the importance of the exceptional Raynal-Revei coefficients is discussed. Finally, in Sect. 4, more details on inversion and optical model hadron-hadron potentials are given.

2 Nucleon-nucleus scattering

Jacques had an important role in this topic. In it he was influenced by the development of the helicity formalism of Jacob and Wick. Maurice René Michel Jacob (28 Mar 1933–May 2007) was a French theoretical particle physicist, he studied physics at l'Ecole Normale Supérieure from 1953 to 1957. During a visit to Brookhaven National Laboratory in 1959, he developed with Gian-Carlo Wick the helicity formalism for relativistic description of scattering of particles with spin and the decay of particles and resonant states. In 1961, he obtained a doctorate on this subject at the University of Paris. His thesis advisers were Professors Francis Perrin and Gian-Carlo Wick. Jacob then moved, as a post-doctoral fellow, to Caltech. He worked in Saclay from 1961 to 1967. Since 1967, he worked at CERN until his retirement in 1998.

In his first years in Saclay, *Jacques* solved a Schrödinger equation with factorization of radial and angular parts, by making use of the helicity formalism. He defined an optical model potential with real Coulomb, complex central and spin-orbit terms components. That optical potential model has now been used in many applications [9–12]. It is central in the widely used DWBA programs of *Jacques* (I do not recall the exact time when and where in Europe, I met *Jacques* and whether he or Richard Schaefer first told me about the development of DWBA70).

There are two theoretical and numerical features of note in the diverse set of DWBA codes (1970-2005, NEA 1209), as well as in all versions of ECIS (1970-2012, NEA 0850). They are the *helicity formalism* and the *Numerov three point integration algorithm* in solving second-order differential equations. A comprehensive and value rating of the Numerov algorithm can be found in the article by Melkanoff et al. [15].

Numerov's method, developed by the astronomer Boris Vasil'evich Numerov, is a numerical method to solve ordinary differential equations of second order in which a first derivative term does not appear. It is also known as Cowell's method. It is a fourth-order linear multi-step method that usually is implicit. It can be made explicit if the differential equation is linear. The helicity formalism, developed by Jacob and Wick, was for use with relativistic descriptions of scattering for particles with spin. For many reasons, this formalism is a must in high energy physics while a conventional formalism of nuclear physics uses the Wigner-Eckart theorem and elements of irreducible tensor algebra.

In *Jacques* 's codes, in which the radial step size is defined as h, the overall accuracy is set as h^4. This was deemed adequate for all practical situations in nuclear reaction calculations. Initially, computers with single precision 32 bits were sufficient to evaluate cross sections and other spin-dependent observables. Later 64 bits structures became standard and *Jacques* converted his programs from Fortran-77 to Fortran-90/95, a useful tool for such conversion is from the pioneering work of M. Metcalf engendering the internet. Today, 128 bits and unlimited multi-precision Fortran is available. In 1990/95 Fortran became restructured and extended versions appeared. The latest version was formed in 2018.

3 Generalized coupling and Raynal-Revai coefficients

In $\mathcal{R}^3$ spherical coordinates, when taken as a polar coordinate system, involve a radius and two angles. In higher dimensions, $\mathcal{R}^d$, $d > 3$, they are called hyperspherical coordinates, which comprise a hyperradius and $d - 1$ hyperangles. In these coordinate systems, the angular momentum and irreducible tensor set re-coupling algebra are practitioners' tools, There are many studies of coupling and re-coupling coefficients [29,31–41] to show that the concepts of angular momentum in quantum physics, Racah-Wigner algebra, and 3-j, 6-j, 9-j, 12-j symbols, all fostered a new calculus that is far beyond that of classical angular momentum. The Clebsch-Gordan coefficients, (3-j symbols), belong to a set of six representations, six 3F2, which suffices for 72 symmetries of the 3-j symbols, while Racah (6-j) coefficients belong to 4F3 and Saalschütz hypergeometric functions.

The news of the development of DWBA70 was a bit of a shock to me. I was totally unaware of it and had developed and written my own Fortran-IV code to analyze inelastic nucleon-nucleus scattering. That code called MEPHISTO was antisymmetrized and flexible with effective NN interactions involving central, two-body spin orbit and tensor terms. This was a collaboration in the time span 1968 to 1970 with Ken Amos, who subsequently joined the University of Melbourne. At this time, Ken was an assistant Professor and I a three year visiting assistant Professor at the Physics department of the University of Georgia in Athens, Ga. In June 1970 I returned to Europe and was briefly with Amand Fässler in Münster, September 1970 to April 1971. Then, in May 1971 to March 1976, I had the chance to work in Jülich, in the newly established Amand Fässler Institut KFA-IKP-Theorie.

Another feature of the first meeting with *Jacques* was when he told me about his generalizations of 3-j and 6-j symbols in collaboration with János Révai, and more about use of hypergeometric coordinates. A key was Whipple's work on the symmetries of well–poised 7F6(1) and Saalschütz 4F3(1) series with unit argument applied to study the properties of 6-j symbols generalized to all arguments. For SU2, there are eleven different 4F3(1) series which can be used. Whipple's parameters provide a good description of symmetries and quite simple recurrence relations, valid for any arguments, can be obtained in terms of those parameters. Also, it was found that the transformation from one set of Jacobi coordinates to another for hyperspherical functions is closely related to the Talmi-Moshinsky transformations for two particles in an oscillator well. The corresponding coefficients can be calculated analytically.

4 Inversion and optical model hadron-hadron potentials

This is a précis of our efforts and latest results which are contained in the thesis of Andreas Funk and in its publication in (2001).

Over many years GWU-SAID lists gave many nucleon-nucleon phase shift solutions for low and medium energy regimes, and Arndt et al. have published many details of how those phase shifts are extracted from angular distributions. That SAID database has grown rapidly in the last three decades. While the proton-proton data now extends to 3 GeV, the neutron-proton data are limited to 1.3 GeV. Surprisingly, the solutions from SM97 to WI00 remain very closely the same and are very stable with regard to newly added data. We used the solutions SP00, FA00 and WI00 in calculations, finding results that differ only marginally. So, while most of our ensuing calculations are based upon SP00, the conclusions remain equally valid if other more recent data solutions would be used.

The GWU-SAID solutions [49] are parameterizations of the elastic channel, NN, S-matrices. For various reasons, we did not proceed directly with GWU-SAID rational interpolations. Instead we developed our own scheme for rational function representation of data and combined them with symmetric Padé approximants [8/8] or [10/10] of $exp(2ix)$. This allowed contour integration of the Gel'fand-Levitan-Marchenko integral equations, and thus assure precise radial inversion potentials pertinent for use in

$$\left[-\frac{d^2}{dr^2}+\frac{\ell(\ell+1)}{r^2}+\frac{2\mu}{\hbar^2}V_\ell(r)\right]\psi_\ell(r,k)=k^2\psi_\ell(r,k), \tag{1}$$

where $V_\ell(r)$ is local and energy independent. A simple substitution, and with $k^2=\lambda$, identifies this as a Sturm–Liouville equation,

$$\left[-\frac{d^2}{dx^2}+q(x)\right]y(x)=\lambda y(x). \tag{2}$$

Solving Marchenko, Gel'fand–Levitan integral equations and Darboux transformations all yield principally the same solution and, numerically, they are complementary. In the Marchenko inversion, the input experimental information is the S-matrix, $S_\ell(k)=\exp(2i\delta_\ell(k))$, defining

$$F_\ell(r,t)=-\frac{1}{2\pi}\int_{-\infty}^{+\infty}h_\ell^+(rk)\,[S_\ell(k)-1]\,h_\ell^+(tk)\,dk. \tag{3}$$

which, when used in the Marchenko equation,

$$A_\ell(r,t)+F_\ell(r,t)+\int_r^\infty A_\ell(r,s)F_\ell(s,t)\,ds=0, \tag{4}$$

specifies the translation kernel $A_\ell(r,t)$. The inversion potential of Eq. (1) is a boundary condition for that translational kernel, namely

$$V_\ell(r)=-2\frac{d}{dr}A_\ell(r,r). \tag{5}$$

Gel'fand–Levitan inversion has the same structure but uses Jost-functions which are related to the S-matrix. In the case of coupled channels, an integral equation suggested by Marcel Coz relates the S-matrix with the Jost-matrix.

In all practical applications rational functions are very appropriate to fit data within the unitary range, 0–300 MeV, with a simple extrapolation $1/k$ towards infinity. For the range $0.3 < T_{Lab} < 3$ GeV we add an auxiliary complex energy dependent potential to explain that non-unitary regime. Initially, a local energy dependent auxiliary potential (Gaussian) served the purpose. In 2001, Andreas Funk replaced that local Gaussian by a set of symmetric separable Gaussian's. It is useful to use the Feshbach projection operator theory of optical potentials to discuss the process that was followed. In the Feshbach formulation, projection operators P and Q where $(P+Q)=1$, are conjectured. The operator P is chosen to project into the unitary reference space, while inelastic and reaction channels are associated with Q space. Using this, Andreas Funk distinguished three Hamiltonians, the *reference* Hamiltonian H_0, a projected Hamiltonian H_{PP}, and a full optical model Hamiltonian $\mathcal{H}$. With $H_0 := T+V_0$, the interaction V_0 is the unitary inversion potential. Using this he obtained solutions $\psi_0 := \psi_0^+(\mathbf{r},\mathbf{k},E)$ of H_0 from which a unitary reference S-matrix, $PH_0P = H_{PP}$, is defined. The Q space is simplified by assuming it can be spanned by a minimum of states. Ultimately one or two harmonic oscillator functions with strengths, λ_{ij}, sufficed. Underlying resonances influence the values of those strengths. Thus, the full optical model Hamiltonian comprises the reference Hamiltonian H_0 and the optical model potential

$$\mathcal{V}=\sum_{ij}|r,i>\lambda_{ij}<r',j|, \tag{6}$$

$$\mathcal{H}:=T+V_0+\mathcal{V}(\lambda_{ij},r,r';lsj,E). \tag{7}$$

This Hamiltonian, $\mathcal{H}$, has regular solutions

$$\Psi^+ := \Psi^+(r,k,lsj,E),$$

whose asymptotic boundary conditions match the *experimental* elastic channel optical model potential S-matrix. The reference potential $V_0(r,lsj)$ and separable potential form factors were fixed, again by using $1s$ and/or $2s$ harmonic oscillator functions. The energy dependent strengths λ_{ij} are uniquely determined with coordinate space reference potential Greens functions, the unitary $S_0(k)$ and full non-unitary $S(k)$.

I note here a few applications using inversion and inversion optical model potentials. In 1996, Hugo Arellano, Francisco Brieva, Mathias Sander and I used NN inversion potentials in calculations of (p,Ca) and (p,Pb) scattering cross sections taken at 500 MeV incident energy. A microscopic optical model for nucleon-nucleus scattering was used. While the NN inversion potentials implied alternative off-shell properties, when compared with those of meson theoretical models. The results of proton-nucleus elastic scattering in the 500 MeV region showed that otherwise often purported off-shell contributions are misleading. Better fits to data require, at the outset, accurate on-shell potentials, such as is assured with the generalized inversion potentials. A similar result was found by Martin Jetter from analyses of Bremsstrahlung data.

Hugo Arellano and I (2005) used KN phase shifts to obtain Gel'fand-Levitan-Marchenko reference inversion potentials for those elementary systems. Those potentials were supplemented with a short range complex separable term in such a way that the corresponding unitary and non-unitary KN S-matrices were reproduced exactly. In the first lower momentum range the KN real inversion potential (reference potential) enabled standard calculation of all on- and off-shell contributions for the t-matrices. In the second higher momentum range the KN complex optical model potentials were used for the t-matrices and to determine the full-folding KA optical model potentials. The beam momenta covered the range 400-1000 MeV/c. The full folding optical model potentials gave agreement with elastic scattering data of KA for ^{6}Li, ^{12}C, ^{28}Si and ^{40}Ca. As this study included cases in which the elementary interaction implied a unitary S-matrix and the KA optical potential many body inelasticities and reactions from the target alone. At higher momenta the KN potential contains elementary complex reactions with a non-unitary S-matrix and KA reactions are supplemented by many-body effects from the target nucleus. The study implied and confirmed nicely the transition from a unitary to a no-unitary KN elementary interaction in KA reaction cross sections. The elementary and many-body reaction routes don't interfere but simply add. The result was expected and the confirmation welcomed.

I am confident about the use of inversion mathematics and elementary phase shift data to investigate successfully certain topics in nuclear scattering. It is an effective data driven approach. As well as I wish Jacques Raynal to be remembered for his remarkable achievements, I hope our inversion approach, that he so kindly supported, will find others of like mind.

Conclusion

Jacques, merci.

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