Postdoc Fellowships for non-EU researchers

Final Report

Name	Bikashkali Midya
Selection	2012
Host institution	Université libre de Bruxelles (ULB)
Supervisor	Prof. Pierre Descouvemont & Prof. Jean-Marc Sparenberg
Period covered by this report	from 01/08/2013 to 31/01/2015
Title	Single- and coupled-channel supersymmetric quantum mechanics and applications to nuclear-physics problems

1. **Objectives of the Fellowship** (1/2 page)

Supersymmetric quantum mechanics is an important algebraic technique in quantum physics, both for the study of bound systems, e.g. atomic nuclei, and for the study of collisions, e.g. nuclear reactions. This technique allows one to generate exactly-solvable models, for which both the bound spectrum and the scattering phase shift possess an analytical expression. It also allows one to solve the scattering inverse problem, i.e. the construction of an interaction potential between two particles from experimental scattering data. This inversion technique relies on the precise determination of the poles of the scattering matrix by directly fitting the sum of arctangent terms (appears as a consequence of supersymmetric transformations) or by the (less used) Taylor series expansion of the effective range function. An extra constraint is necessary, in the first case, to make the poles to lie on the imaginary axis, otherwise complex poles leads to instability e.g. oscillation in the constructed potentials. Whereas, the later method is perfect for the very low energy and fails when the scattering phase-shift data has zero crossing in its energy range.

Extensions of this technique to coupled channels are necessary as soon as the spins and the excitation energies of the interacting particles are taken into account. Including these effects leads to coupled channels with equal thresholds (in the case of spins) or different thresholds (in the case of excitations). These coupled-channel generalizations of the one-channel results turn out to be complicated from the mathematical point of view. Several recent developments show that this method is very promising, in particular for the resolution of the inverse problem, but several difficulties remain regarding its application to coupled channels with threshold differences [D. Baye et al, J.Phys.A 47 (2014) 243001]. A systematic classification of coupled-channel supersymmetric transformations is thus highly required in this context. These general transformations, which differ from each other by the complex or real nature of their factorization energies, as well as by the behaviour at the origin of their factorization solutions, have not been studied systematically yet, in particular for the case of threshold differences. Their extensive study could thus reveal new transformations that might prove able to solve the coupled-channel inverse problem for this case.

In this theoretical project, our main objective is to explore further the single- and coupled-channel nonrelativistic supersymmetric quantum mechanics to resolve some of the issues mentioned above. The precise problems, which are attempted during the project, are given below together with the methodology used.

2. Methodology in a nutshell (1/2 page)

Task A. We develop an optimal inverse scattering method which enables a high precision fit of single-channel experimental elastic scattering data, in the neutral case, and which allows to construct the corresponding exactly-solvable interaction potential. The validity of the technique will be tested by considering several realistic physical problems, in particular the neutron-proton system.

The key ingredients of quantum scattering theory used to complete this task are Padé/Taylor expansions of the effective-range function, and the radial supersymmetric inversion technique. A significant part of the work relies on numerical methods and symbolic calculations, implemented through computer programming using Fortran and Python. These numerical tools are also necessary to implement a systematic comparison between our theoretical developments and experimental data.

Task B. We describe the qualitative behaviour of the central part of the interaction potential for different partial waves in the neutron-proton singlet-spin channels, which reduce to single channels. Thus a search for parity and angular momentum independent central potential is attempted to unify all the partial waves.

Task C. The coupled-channel generalizations of the one-channel results is attempted especially for the different thresholds. Although a single non-conservative supersymmetric transformation already provided interesting results in this direction, it is not sufficient to invert sophisticated scattering matrices. Therefore iterations of such transformations are necessary. We plan to explore these iterations using supersymmetry transformations based on non-diagonal factorization energies, which might eliminate the need for non-conservative transformations.

3. Results (6-8 pages)

So far we are successful in completing the task A mentioned above. Work is in progress for tasks B and C. Complete results of task A and partial results of tasks B, C are given below.

Results for task A (published in Physical Review C 91 (2015) 054004):

A systematic inversion technique is developed to derive an accurate nucleon-nucleon interaction potential from an effective-range function for a given partial wave in the neutral case. To this end, first, the effective-range function is Taylor or Padé expanded, which allows high precision fitting of the experimental scattering phase shifts with a minimal number of parameters on a large energy range. Second, the corresponding poles of the scattering matrix are extracted in the complex wave-number plane. Third, the interaction potential is constructed with supersymmetric transformations of the radial Schrödinger equation.

A computer code of this method has been developed using NumPy and SymPy, which facilitates the analysis of experimental data and the study of the qualitative behaviour of the interaction potentials.

We consider a collision between two spinless particles with center of mass energy E = k^2. Each partial wave corresponding to the angular momentum *l*, is characterized by the scattering matrix $S(k) = e^{2i\delta(k)}$. The quantity $\delta(k)$, known as phase-shift, is related to the effective range function defined as $K(k^2) = k^{2l+1} \cot \delta(k) = ik^{2l+1} \frac{S(k)+1}{S(k)-1}$. Since the effective range function is analytic at low energy, it can in general be expanded in Taylor series:

$$K(k^2 \to 0) = -\frac{1}{a} + \frac{r}{2} k^2 - \mathrm{Pr}^3 k^4 + O(k^6)$$

where the scattering length *a*, the effective range *r* and the shape parameter *P* can be seen as a discrete set of parameters characterizing the elastic phase shift at small values of the continuum energy. The effective-range function is actually meromorphic, i.e. it admits poles; it is thus advantageous to replace the above expansion by a Padé approximant of order [M/N] :

$$K(k^2) = \frac{P^{[M]}(k^2)}{Q^{[N]}(k^2)}$$

This equation leads to an expansion of the scattering matrix as a rational function of *k*. Indeed, the scattering matrix can be expressed by

$$S(k) = \frac{K(k^2) + ik^{2l+1}}{K(k^2) - ik^{2l+1}} = \prod_{j=0}^{n-1} \frac{k + i\kappa_j}{k - i\kappa_j},$$

with poles at $k = i\kappa_j$ satisfying

$$P^{[M]}(-\kappa_j^2) - (-1)^{l+1}\kappa_j^{2l+1}Q^{[N]}(-\kappa_j^2) = 0.$$

The above equation shows that these poles depend on the coefficients of the effective-range expansion and satisfy the following properties: (a) Their number $n = \max(2M, 2N + 2l + 1)$, (b) they are either purely imaginary or symmetric with respect to the imaginary axis, which warrants the unitarity of the scattering matrix, (c) when $l>0$, they satisfy the conditions

$$\sum_{j=0}^{n-1} \frac{1}{\kappa_j^{\alpha}} = 0, \alpha = 1,3,..., (2l-1).$$

When parametrizing experimental phase shifts, two approaches are possible to determine the scattering-matrix poles. The first approach consists in finding the minimal orders M and N leading to a satisfactory effective-range function. The poles are then deduced from the above equations. The advantage is that they automatically satisfy properties (c). The drawback of this approach is that these poles can be either imaginary or complex, while complex poles sometimes lead to oscillations in the potentials deduced from supersymmetric quantum mechanics. To avoid such oscillations, it is thus necessary to constrain the poles to stay on the imaginary k−axis. This can be achieved by directly fitting the phase shifts as

$$\delta(k) = -\sum_{j=0}^{n-1} \arctan \frac{k}{\kappa_j}.$$

The drawback is then that the poles have to be constrained by the property (c) for $l > 0$ in order for the effective-range function to be well defined. In the following, both approaches will be used.

The analytical expression of the interaction potential can be constructed using a chain of first order n supersymmetry transformation of the radial Schrödinger equation $H_j\psi = -\psi''(k,r) + V_j(r)\psi(k,r) = k^2\psi(k,r)$ with j =0,1,2,.. and a purely centrifugal initial potential $V_0(r) = l(l+1)/r^2$. Each first order supersymmetry transformation is an algebraic transformation which transform the initial Hamiltonian H_j of the chain to a new Hamiltonian H_{j+1} with a new potential which shares identical spectral characteristics with the old one. In addition each successive transformation of the chain modifies the phase-shift by subtracting an $\arctan(k/\kappa_j)$ term from the phase-shift of the former Hamiltonian. The compact expression of the final potential of the chain can readily be expressed by the following Crum-Krein formula

$$V_n(r) = \frac{l(l+1)}{r^2} - 2\frac{d^2}{dr^2}\ln W[u_0, u_1,..., u_{n-1}],$$

where u_j are the solutions of the initial Schrödinger equation $-u_j'' + l(l+1)r^{-2}u_j = -\kappa_j^2 u_j$. When u_j is associated to a pole which lies in the upper (lower) half k−plane and is regular at the origin and exponentially increasing at infinity (respectively singular at the origin and exponentially decreasing at infinity), it is characterized as the left- (respectively right-) regular solutions. Each supersymmetry transformation corresponding to these solutions is responsible for the increment (decrement) of the potential singularity at the origin by one unit. Since V0 has a repulsive core of the form *l(l+1)/r²*,the singularity strength of the final potential is therefore equal to l plus the difference of the number of left-regular minus right-regular transformations. Thus the aforementioned two types of factorization solutions are the key ingredients to build a potential with singularity at the origin.

For the *l=0* partial wave, the solutions of the Hamiltonian H_0 are given by $u_j = \sinh \kappa_j r$, or $\exp \kappa_j r$. The first (second) solution corresponds to the left- (right-) regular transformation if $\mathrm{Re}(\kappa_j) > 0$ (respectively <0). On the other hand, for *l > 0*, the solutions u_j of the purely centrifugal potential can be obtained by applying *l* zero-energy transformations on the above mentioned *l = 0* left and right regular solutions.

As an illustration, the method is applied to the experimental phase shifts of the neutron-proton elastic scattering in the *S*- and *D*-wave channels on the [0 − 350] MeV laboratory energy interval. First, let us revisit the *l = 0* results, for which no conditions on the poles apply. Hence, the simplest method is based on the direct fit of the phase shifts with the sum of arctangent. In Ref. [Phys. Rev. C 55 (1997) 2175], a five-pole fit of the data was found satisfactory but two poles were complex, which led to a small oscillation in the potential. This default was fixed in Ref. [Phys. Rev. C 66 (2002) 034001], where a satisfactory fit with six poles was found by constraining them to lie on imaginary axis. The quality of this fit, by the poles κ = −0.0401,−0.7540, 0.6152, 2.0424, 4.1650, 4.6 fm⁻¹, can be seen on figure 1. The corresponding effective-range function is associated with the following [3/2] expansion

$$K_S(k^2) = \frac{.0422 + 1.3793\,k^2 + 2.0105\,k^4 - .058\,k^6}{1 + 1.5986\,k^2 - .06164\,k^4}$$

which is shown in figure 1. On the other hand, a 3-term Taylor expansion of the effective-range function $K_S(k^2) = .04219 + 1.3038\,k^2 + .06883\,k^4$ with scattering length a= -23.7 fm, effective range r= 2.608 fm and with 4 poles -.0401, -4.6917, .8365, 3.8953 fm⁻¹, is able to fit the phase shifts up to 30 MeV lab energy only. This shows the interest of using a Padé expansion rather than a Taylor expansion. Moreover, the order of the Padé expansion appropriately resembles the correct high energy behavior of the phase shifts (which is −π, as can be checked immediately). The corresponding interaction potential can be written in two equivalent forms:

$$V_S = -2\frac{d^2}{dr^2}\ln W[e^{-\kappa_0 r}, e^{-\kappa_0 r}, \sinh(\kappa_2 r), \sinh(\kappa_3 r), \sinh(\kappa_4 r), \sinh(\kappa_5 r)]$$

$$= -2\frac{d^2}{dr^2}\ln W[\cosh(\kappa_2 r + \alpha_{02} + \alpha_{21}), \sinh(\kappa_3 r + \alpha_{03} + \alpha_{13}), \sinh(\kappa_4 r + \alpha_{04} + \alpha_{14}), \sinh(\kappa_5 r + \alpha_{05} + \alpha_{15})]$$

with $\alpha_{ij} = \arctan(\kappa_i / \kappa_j)$. The potential is represented on figure 3; it displays both a correct one-pion-exchange asymptotic behaviour and a repulsive core at the origin, like standard nucleon-nucleon potentials.

For neutron-proton elastic scattering experimental phase shifts in the 1D2 channel, the 3-term Taylor effective-range expansion is sufficient to fit the data with high precision, as shown on figure 2. The corresponding parameters read : a = 0.88762 fm, r = 15.33061 fm, P = −0.00246 and the corresponding poles of the scattering matrix are κ = −0.4294,−0.8827,−8.7653, 0.7750, 0.4376 fm^{-1}. Remarkably, all these poles lie on the imaginary axis of the complex wave-number plane, whereas this constraint was not imposed to them. The sum of five arctangents corresponding to these five poles is plotted in figure 2, which confirms the excellent quality of the fit with the experimental data. However, since the condition $M-N = l+1$ is not satisfied, the high energy behaviour of the phase shift tends to π/2.

The compact expressions of the corresponding effective potential can be obtained analogously to S-wave potential, where right regular transformation functions and left regular solutions are associated with negative poles and positive poles, respectively and read

$$u_j(r) = \left(1+\frac{3}{\kappa_j r}+\frac{3}{\kappa_j^2 r^2}\right)e^{-\kappa_j r},\ j=0,1,2$$

$$u_j(r) = \frac{3}{\kappa_j r}\cosh(\kappa_j r)-\left(1+\frac{3}{\kappa_j^2 r^2}\right)\sinh(\kappa_j r),\ j=3,4$$

In figure 3, we have plotted this potential, together with the corresponding central potential after extracting the centrifugal term. Clearly the central potential is a deep potential with attractive singular core. Contrary to the S-wave potential, this potential belongs to the family of deep potentials, as proposed by the Moscow group [Phys. Rev. C 59 (1999) 3021)]. This is due to the fact that the D-wave phase shifts are positive. This also supports the results of Ref. [Europhys. Lett. 59 (2002) 507], where a parity-independent deep potential was obtained from S- and P-wave phase-shift inversion, with the inclusion of Pauli forbidden states. A question raised at that time was the incompatibility of this potential with the D- and F-waves, hence the interest of directly inverting phase shifts for these waves. Let us stress that because of the centrifugal term the D-wave potential obtained here is only constrained by data above 0.7 fm. Even above this radius the S-wave potential is deeper than the D-wave one. Hence, adding a forbidden bound state to the S-wave potential will probably not allow to fit the D-wave simultaneously. A similar conclusion was drawn in Ref. [Nucl. Phys. A 242 (1975) 141], which can be accounted by allowing explicit non-locality or by allowing a quadratic dependence on angular momentum $\boldsymbol{L}$ in the potential.

Below, we present some results pictorially.

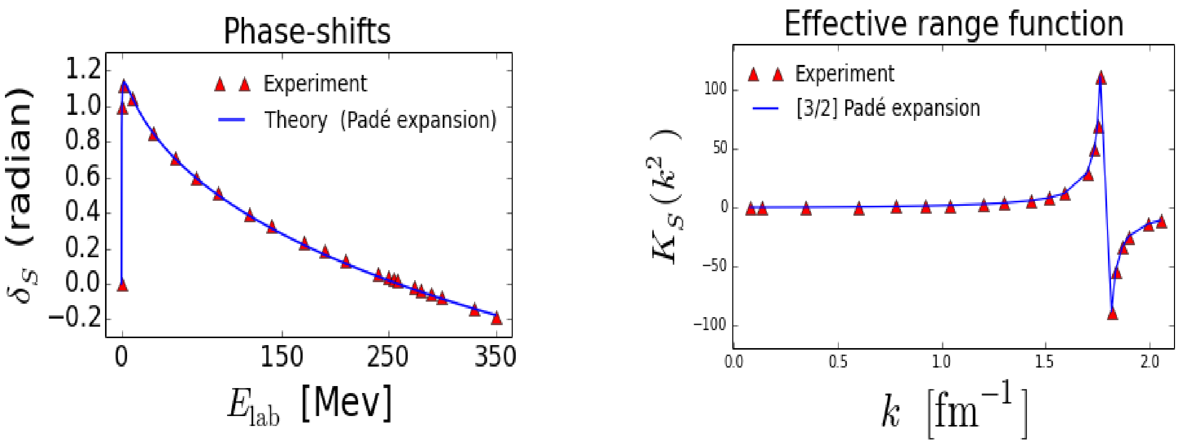

Fig 1. First figure represents the high quality fit of the experimental phase-shifts for the neutron-proton S partial wave in the singlet case. Second figure corresponds to the Effective range function.

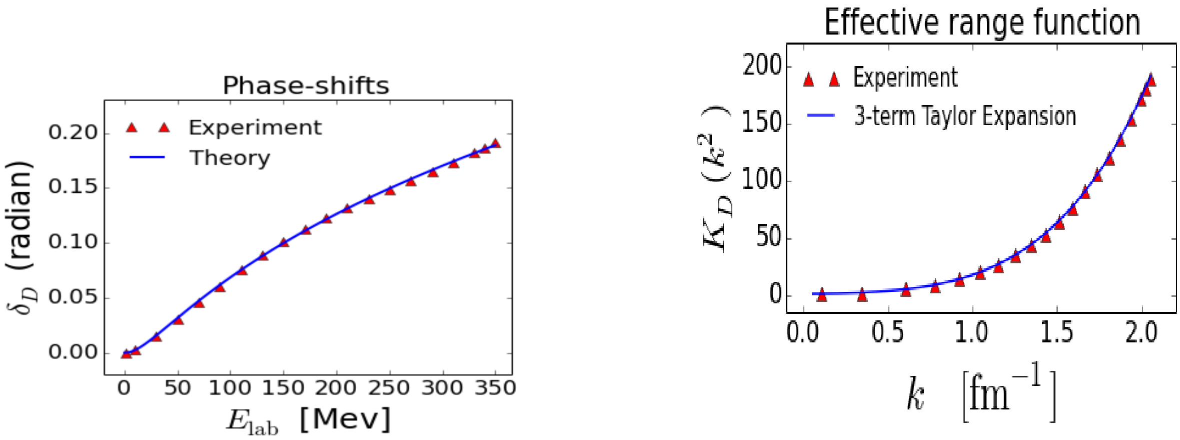

Fig 2. Same as figure 1, but for the singlet D-partial wave.

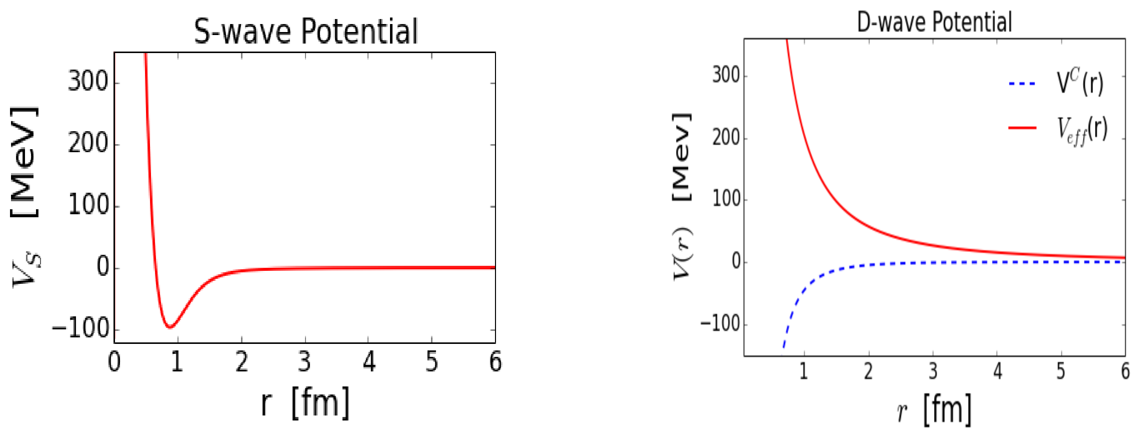

Fig 3 : Neutron-proton inversion potentials for the singlet S- and D-waves (central and effective potentials).

Summing up, the method developed here can be considered as an optimal inversion technique for a given partial wave in the neutral case: it provides a minimal parametrization of the scattering phase shifts in terms of either scattering-matrix poles or effective-range Padé expansion, together with an analytical expression for the corresponding potential. The whole algorithm can readily be summarized by a short computer code. The only difficulty of the method is that the scattering-matrix poles sometimes become complex when the effective-range function is used as starting point for the inversion, which might lead to oscillating potentials. A direct fit of the poles should then be performed, with the double constraint of staying on the imaginary axis (except for possible resonances) and of satisfying a well-defined effective-range expansion for $l > 0$. For the singlet neutron-proton case in the *S* and *D* waves, the obtained poles and potentials are satisfactory. The S-wave potential is shallow while the *D*-wave potential is deep, which opens the way to a new discussion of the deep/shallow ambiguity in this case. Further developments of the method might include the link between different partial waves, the comparison between the neutral and charged cases, generalization to the coupled-channel case, and application to elastic collisions in atomic physics.

Partial results for task B :

Supersymmetric quantum mechanics is applied to the determination of a family of deep neutron-proton S-wave interaction potentials which are phase-equivalent to the shallow potential. Deep potentials are obtained by two ways : first by changing a left-regular transformation (used for constructing shallow potential) to a transformation which is singular at both boundaries, and second by adding a pair of phase equivalent transformation. In the later case, we have used confluent supersymmetric algorithm to find the phase-equivalent transformations and corresponding potential in closed analytical form. These transformations introduce one (respectively two) free parameters in the potential providing more flexibility in choosing the potential shape without affecting the phase-shifts. Moreover, the resulting potential contains an (unphysical) Pauli forbidden bound state, the bound state energy of which can be tuned at will. The obtained deep potential has also been used to fit the experimental phase-shifts for other partial waves. The detailed investigation, in case of D-wave, shows that it is impossible to fit the data for both partial waves simultaneously. However, when the parameters are so chosen that the S-wave potential becomes singular at finite distance (and fails to keep intact the phase-equivalent property), the corresponding D-wave effective potential reproduces accurate phase-shifts (as shown in figures 4(b), 4(c)). Further study towards this direction is in progress.

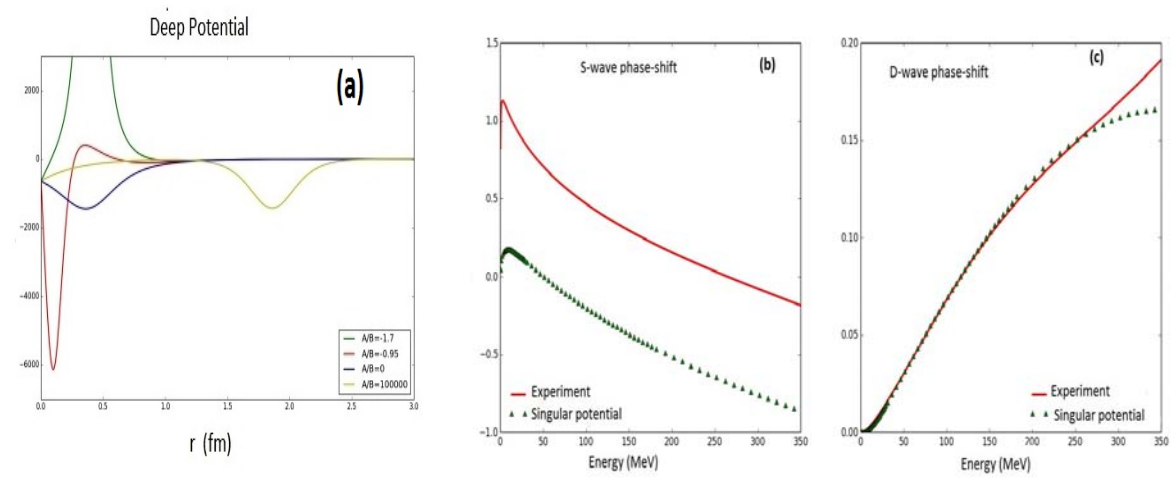

Fig 4 : (a) Deep neutron-proton S-wave phase equivalent potentials for some chosen values of the parameters. (b) and (c) S- and D-wave phase shifts corresponding to the singular potential.

Partial results for task C :

We consider an old problem of coupled-channel supersymmetric quantum mechanics which states that it is impossible to construct non-trivial coupling between channels using conservative transformation. To this end, a coupled-channel non-conservative supersymmetry transformation, of zero initial potential matrix, was proposed [D. Baye et al, J.Phys.A 47 (2014) 243001]. We have shown that this non-conservative transformation can be formulated in terms of a pair of conservative transformations, provided a purely exponential transformation is used which relies on a non-diagonal factorization energy matrix. This allows to understand, in a simpler way, the behaviour of the corresponding scattering matrix (which is difficult to determine for the non-conservative transformation). We have also shown that these purely exponential transformations can be iterated and then the transformation consisting of hyperbolic functions can be used to obtain the desired nondiagonal potential matrix. Further work is in progress in this direction, in particular to establish compact analytical expression for the constructed potentials and for their scattering matrix, and to compare them with existing coupled-channel potentials.

4. Perspectives for future collaboration between units (1 page)

Some works of the project are still ongoing, in particular regarding deep neutron-proton potentials with compact analytical expression and coupled-channel supersymmetric transformations in the case of threshold difference. Below is the brief description of the on-going work.

One of the main objective of this project is to investigate if a single central potential can be used for all partial waves. To do this, we are analysing the multiple forms of the S-wave potential based on the six supersymmetric transformations including a pair of phase equivalent transformations and compare these forms with the D-wave deep potential obtained through five scattering matrix poles. Specifically we are investigating more closely a shallow potential as well as two families of deep potentials. The shallow potential presenting a repulsive core is commonly accepted as a more physical form of the potential while deep potentials include unphysical states which are meant to take into account effects of the Pauli principle, while remaining purely attractive. The shallow potential is uniquely defined and we find that the unification of several waves is impossible. On the other hand, there is a family of deep potentials depending on one parameter, which are obtained by switching from a regular to a singular transformation. This allows for more flexibility in finding a right potential form for multiple partial waves. However, this deep potential cannot offer a good enough fit of S and D partial waves phase shifts for a single value of the parameter. Another flexibility is obtained by adding a pair of transformations which add a bound state and conserve the phase shifts. But, as with the previous deep potential, both waves phase shifts cannot be fitted simultaneously and the phase-equivalent character of the potential is broken by the appearance of a singularity near the origin. The reason behind this phenomenon is not yet clear and warrants further inquiries.

Regarding coupled-channel transformations, the work started in the case of threshold differences between channels will be continued. In particular, the iteration of purely-exponential transformations with non-diagonal factorization energies will be systematically treated in order to establish a complete inversion scheme for this case.

Precise plans for further collaborations on other topics have not been made yet, due to a new postdoc position with new research associated, but mutual information about new research results will be exchanged regularly, which could lead to other joint projects in the future.

5. Valorisation/Diffusion (including Publications, Conferences, Seminars, Missions abroad...)

[1] Bikashkali Midya, Jérémie Evrard, Sylvain Abramowicz, Óscar Leonardo Ramírez Suárez, Jean-Marc Sparenberg, **Supersymmetric inversion of effective-range expansions**, published in **Physical Review C 91, 054004 (2015).**

[2] Bikashkali Midya and Jean-Marc Sparenberg, **Deep nucleon-nucleon potential from supersymmetric inverse scattering,** under preparation.

[3] Bikashkali Midya and Jean-Marc Sparenberg, **Coupled-channel supersymmetric transformation with non-diagonal factorization energy**, under preparation.

Paper [1] has been presented in the meeting of Belgian Research Initiative on eXotic nuclei for atomic, nuclear and astrophysics studies (BriX) network which was held on November 26, 2014 in Mol, Belgium.

6. Skills/Added value transferred to home institution abroad (1/2 page)

During his stay at ULB, Dr. Midya has learned quantum scattering theory, inverse problem, coupled channels supersymmetry transformations, as well as become familiar to several physical problems of nuclear physics and nuclear astrophysics studied at the Nuclear Physics and Quantum Physics research unit in the framework of the BriX network. He also got the opportunity to meet and exchange ideas with the experimentalists involved in these studies, thus extending his views from purely theoretical considerations. He has acquired knowledge on several numerical techniques and developed efficient computer codes for constructing nucleon-nucleon interactions and determining phase-shifts. High-level language like Python has been used for this purpose.

The post-doctoral position in the BriX network has thus been highly profitable to Dr. Midya, as it has brought him into contact with new physical applications of supersymmetric quantum mechanics e.g. quantum scattering problems. It has also given new perspectives on international research and brought him into contact with renowned specialists of supersymmetric quantum mechanics.

These new skills have participated in the development of Dr. Midya's CV, which led him to get a new postdoc position at the Institute of Science and Technology (IST), Austria. The Belspo postdoctoral position can thus be seen as a kick-off of Dr. Midya's international career, which should in turn allow him to get a permanent position back in India.