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LETTER TO THE EDITOR

Multichannel coupling with supersymmetric quantum mechanics and exactly-solvable model for the Feshbach resonance

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Abstract

A new type of supersymmetric transformations of the coupled-channel radial Schrödinger equation is introduced, which do not conserve the vanishing behaviour of solutions at the origin. Contrary to the usual transformations, these 'non-conservative' transformations allow, in the presence of thresholds, the construction of well-behaved potentials with coupled scattering matrices from uncoupled potentials. As an example, an exactly-solvable potential matrix is obtained which provides a very simple model of the Feshbach-resonance phenomenon.

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(Some figures in this article are in colour only in the electronic version)

During the past 20 years, Darboux transformations of the one-dimensional Schrödinger equation, also known as supersymmetric quantum mechanics [1], have evolved into a powerful tool to solve the inverse scattering problem for a given partial wave [2, 3]. Indeed, this formalism allows both the deductive construction from scattering data of a unique interaction potential without bound state [4] and the construction of all potentials, phase-equivalent to that potential but displaying different bound spectra [5]. When the initial potential is zero, the transformed potentials not only fit experimental data with high precision, they are also exactly solvable and have compact analytical expressions [6], a striking feature of the method which reveals its efficiency.

This success seems however restricted to the single-channel case: for coupled channels, supersymmetric transformations were not able up to now to provide a complete solution of the scattering inverse problem, despite the early generalization of their algebraic formalism to coupled equations [7]. Whereas the construction of phase-equivalent potentials has proved to be possible [8], a deductive construction of potentials by inversion of coupled-channel scattering matrices is still missing. In the case of coupled channels with different thresholds, such an inversion even seems impossible, as a matter of principle: applying a supersymmetric transformation to a diagonal (and hence uncoupled) potential matrix may result in a coupled potential matrix [9] but the corresponding scattering matrix will always remain diagonal [10]. This makes it impossible to invert realistic data with coupling, which correspond to non-diagonal scattering matrices, by supersymmetric transformations of simple uncoupled potentials such as the zero potential.

The need for coupled-channel inversion techniques is however strongly growing these days since many problems in physics rely on coupled-channel systems. In nuclear physics for instance, theoretical calculations of hypernuclei [11] require baryon–baryon interactions, which naturally display coupling between channels corresponding to different hyperon–nucleon and hyperon–hyperon states. In the context of experimental Bose–Einstein condensation, atom–atom interactions are monitored with the help of magnetic Feshbach resonances [12], a phenomenon based on the coupling between different spin states displaying distinct thresholds in the presence of an external magnetic field [13].

The purpose of this letter is to prove that the limitations on coupled-channel supersymmetric transformations mentioned in [10] do not hold for a category of transformations not used up to now. These transformations do not conserve the boundary behaviours of solutions of the Schrödinger equation at the origin, which is why we call them 'non-conservative'. Nevertheless, we show below that these transformations lead to physical potentials (i.e., satisfying usual scattering theory assumptions) with well-defined physical solutions. We establish their general properties, compare them with usual transformations and finally apply them in the simplest possible situation: a single transformation of an initial vanishing potential. This leads to a Feshbach-resonance exactly-solvable model.

Using definitions from standard coupled-channel scattering theory [14, 15], we consider a set of N coupled radial Schrödinger equations, which read in reduced units

$$-\psi''(k,r) + V(r)\psi(k,r) = k^2\psi(k,r), \tag{1}$$

where the prime means derivation with respect to the distance r between the two bodies. The potential V is an $N \times N$ real symmetric matrix, supposed to be short ranged and bounded. The complex wave-number diagonal matrix k is defined by its elements $k_i = \sqrt{E - \Delta_i}$, where E is the centre-of-mass energy and $0 = \Delta_1 \leqslant \Delta_2 \leqslant \cdots \leqslant \Delta_N$ are the threshold energies of the N channels. The solution ψ is an $N \times N$ solution matrix made of N solution vectors. As usual in the context of supersymmetric quantum mechanics [7, 16], we do not only consider here *physical* solutions of (1), which are bound for all r and vanish at the origin: we also use *mathematical* solutions as important auxiliary tools to transform potential V.

Equation (1) being of second order, its general mathematical solution can be constructed by linear combination, with matrix multiplication on the right-hand side, of two solution matrices made of $2N$ linearly independent vectors. In the following, we use two such pairs of solutions: Jost solution matrices $f(\pm k, r)$, that behave asymptotically as pure exponentials,

$$f(\pm k, r) \underset{r\to\infty}{\sim} \exp(\pm \imath k r), \tag{2}$$

and a pair of solutions made of the regular solution matrix $\varphi(k,r)$, which vanishes at the origin, and solution matrix $\eta(k,r)$, the derivative of which vanishes at the origin. We normalize these as $\varphi'(k,0) = \eta(k,0) = I$, where I is the identity matrix. In terms of Jost solutions, the regular solution reads [15]

$$\varphi(k,r) = \frac{1}{2\imath}[f(k,r)k^{-1}F(-k) - f(-k,r)k^{-1}F(k)], \tag{3}$$

which defines the Jost matrix $F(k)$ as

$$F(k) = f^T(k,0), \tag{4}$$

where T means transposition. This is obtained by calculating, both at the origin and at infinity, the Wronskian $W[\varphi(k,r), f(k,r)] \equiv \varphi^T(k,r)f'(k,r) - \varphi'^T(k,r)f(k,r)$, the value of which is independent of r, taking into account $W[f(-k,r), f(k,r)] = 2\imath k$. The Jost matrix is a key quantity in scattering theory: bound (resp. resonant) states correspond to zeros of its determinant in the upper (resp. lower) k_i planes and the scattering matrix S reads

$$S(k) = k^{-1/2}F(-k)F^{-1}(k)k^{1/2}. \tag{5}$$

For that reason, the following study mostly concentrates on Jost-matrix properties.

To perform a supersymmetric transformation of (1), we follow [7] and first factorize it as

$$[A^+A^- - \kappa^2]\psi(k,r) = k^2\psi(k,r), \tag{6}$$

where $A^\pm = \pm\mathrm{d}/\mathrm{d}r + U(r)$ are mutually adjoint first-order differential operators, defined in terms of the superpotential real symmetric matrix U. Equation (6) is equivalent to (1) when

$$U(r) = \sigma'(r)\sigma^{-1}(r), \tag{7}$$

where $\sigma(r)$ is a mathematical solution matrix of (1) at negative energy $\mathcal{E}$, referred to as the factorization solution. This solution matrix is assumed to be real and invertible for all r; moreover, its self-Wronskian $W(\sigma,\sigma)$ vanishes in order for U to be symmetric. Another important property of (7) is that multiplying the factorization solution on the right by an arbitrary constant regular matrix, which is equivalent to changing the factorization solution, does not affect the superpotential. This strongly reduces the number of possible transformations. Finally, the wave-number diagonal matrix κ is defined by its positive elements $\kappa_i = \sqrt{\Delta_i - \mathcal{E}}$.

We then apply A^- on the left to (6), which leads to a new Schrödinger equation with the potential matrix

$$\tilde{V}(r) = V(r) - 2U'(r) = -V(r) - 2\kappa^2 + 2U^2(r), \tag{8}$$

which satisfies the same regularity and symmetry conditions as V, and with solutions

$$\tilde{\psi}(k,r) = A^-\psi(k,r). \tag{9}$$

The asymptotic behaviour of this relation when ψ is a Jost solution of the initial equation leads to the following expression for the Jost solution of the new equation:

$$\tilde{f}(k,r) = A^-f(k,r)[U(\infty) - \imath k]^{-1}. \tag{10}$$

As will be proved elsewhere, when all thresholds are distinct, $U(\infty)$ is a diagonal matrix with elements $\pm\kappa_i$, the signs depending on the asymptotic behaviour of factorization solution σ. Let us stress that (10) shows that supersymmetric transformations always transform a Jost solution into a Jost solution, up to a multiplicative factor; in particular, when f vanishes at infinity, $\tilde{f}$ vanishes too.

The situation is very different for the behaviour at the origin: when applied to a regular solution of the initial equation, (9) does not systematically lead to a regular solution of the new equation, which leads to the distinction between two types of transformations. We call 'conservative' transformations those that transform a regular solution of the initial equation into a regular solution of the new equation: $\tilde{\varphi}(k,r) \propto A^-\varphi(k,r)$. Most transformations used up to now in the literature [7, 8] belong to this category; in particular, they transform physical solutions into physical solutions, at least for $E \neq \mathcal{E}$. Using (3) and (4), these transformations can be shown to lead to simple modifications of the Jost matrix, similar to the single-channel case [4, 17],

$$\tilde{F}(k) = [\mp U(\infty) - \imath k]^{\pm 1}F(k). \tag{11}$$

In this equation, the upper (resp. lower) signs correspond to σ diverging (resp. vanishing) at the origin, two cases which will be considered in detail elsewhere. For vanishing $\sigma(0)$, (11), combined with (5), leads for instance to the scattering-matrix modification by supersymmetric transformations obtained in [7].

For one-channel elastic scattering, (11) is most useful in the context of inverse scattering problem: such transformations can easily be iterated, which leads to a Padé approximant of the Jost matrix of arbitrary order, used to fit experimental scattering data [3]. In the coupled-channel case with distinct thresholds, however, this Jost-matrix modification is very restrictive: since both k and $U(\infty)$ are diagonal matrices, an initial decoupled potential always transforms into a potential with a decoupled Jost matrix, and hence a decoupled scattering matrix, as found in [10]. Consequently, these transformations are not able to fit data corresponding to non-diagonal scattering matrices.

In the present work, we consider a new category of supersymmetric transformations: those for which the factorization solution is a finite regular matrix at the origin. In this case, the value of the superpotential at the origin, $U(0)$, is also finite and can be fixed arbitrarily. This can be shown by expressing σ as a linear combination of φ and η satisfying (7),

$$\sigma(r) = \eta(\imath\kappa, r) + \varphi(\imath\kappa, r)U(0), \tag{12}$$

where the assumption $\sigma(0) = I$ does not reduce the generality of the superpotential. Applying (9) to a regular solution of the initial equation leads in this case to a solution of the new equation which does not vanish at the origin. This type of supersymmetric transformations hence break boundary conditions (this can also happen for usual transformations, but only for $E = \mathcal{E}$; here, the boundary condition is broken for *any* energy E). We propose to call them 'non-conservative'. Similar transformations have already been used in [18] but for the very particular case of zero factorization energy in the single-channel case. Since the new potential (8) satisfies standard scattering theory assumptions, its regular solution, Jost matrix and scattering matrix are well-defined. Using (4) and (10), one gets its Jost matrix

$$\tilde{F}(k) = [U(\infty) - \imath k]^{-1}[F(k)U(0) - f'^{T}(k, 0)]. \tag{13}$$

This relation is clearly more complicated than for conservative transformations, with the drawback that its iteration might be difficult. However, it presents the enormous advantage that even when the initial potential is uncoupled, which means its Jost solution and matrix are diagonal, the transformed Jost matrix becomes coupled by choosing a non-diagonal $U(0)$. This new type of supersymmetric transformation thus seems to solve the main drawback of supersymmetric quantum mechanics for coupled-channel systems with distinct thresholds stressed in [10].

Let us now illustrate these findings by applying the above formalism to an initial vanishing potential $V = 0$, for which $F(k) = S(k) = I$. The most general factorization solution matrix for a non-conservative transformation can be written in two equivalent ways,

$$\sigma(r) = \cosh(\kappa r) + \sinh(\kappa r)\kappa^{-1}U(0) = \exp(\kappa r)C + \exp(-\kappa r)D. \tag{14}$$

For N channels, the transformed potential, as obtained from (7)–(8), depends on $\kappa_1, \ldots, \kappa_N$ (or equivalently on $N - 1$ thresholds and one factorization energy) and on $N(N + 1)/2$ arbitrary parameters appearing in $U(0)$. It is exactly solvable and is equivalent to the potential derived by Cox [19, 20] in his $q = 1$ case. However, the present derivation not only leads to a much simpler analytical expression for the potential (compare (4.7) of [19] to (7) and (8)) but also subsumes it: the restriction $\det A \neq 0$ of [19], which is equivalent to $\det C \neq 0$ in (14), does not apply here.

In the case $\det C \neq 0$, one has $U(\infty) = \kappa$, as shown by (7) and (14). According to (13), the Jost matrix of the new potential then reads

$$\tilde{F}(k) = (\kappa - \imath k)^{-1} [U(0) - \imath k]. \tag{15}$$

For $N = 2$ channels for instance, the potential depends on five real parameters

$$\kappa = \begin{pmatrix} \kappa_1 & 0 \\ 0 & \kappa_2 \end{pmatrix}, \qquad U(0) = \begin{pmatrix} \alpha_1 & \beta \\ \beta & \alpha_2 \end{pmatrix} \tag{16}$$

and (15) is equivalent to (5.1) of [19].

As stressed above, our formalism is also valid for rank $C = 1$. For $\alpha_2 \neq -\kappa_2$, one has in this case $U(\infty) = \mathrm{diag}(-\kappa_1, \kappa_2)$, which leads to the Jost matrix

$$\tilde{F}(k) = \begin{pmatrix} \frac{k_1+\imath\alpha_1}{k_1-\imath\kappa_1} & \frac{\imath\beta}{k_1-\imath\kappa_1} \\ \frac{\imath\beta}{k_2+\imath\kappa_2} & \frac{k_2+\imath\alpha_2}{k_2+\imath\kappa_2} \end{pmatrix}. \tag{17}$$

This new result cannot be obtained from Cox' formula. Moreover, for $\det C = \det D = 0$, which is equivalent to the particular choice of parameters

$$\alpha_{1,2} = \pm\sqrt{(\kappa_1\kappa_2 - \beta^2)(\kappa_1/\kappa_2)^{\pm 1}} \qquad (\kappa_1\kappa_2 > \beta^2 > 0), \tag{18}$$

further simplifications occur. First, one gets explicitly

$$U(r) = \frac{1}{\cosh y} \begin{pmatrix} -\kappa_1 \sinh y & \sqrt{\kappa_1\kappa_2} \\ \sqrt{\kappa_1\kappa_2} & \kappa_2 \sinh y \end{pmatrix} \tag{19}$$

with $y = (\kappa_2 - \kappa_1)r - \mathrm{arccosh}\sqrt{\kappa_1\kappa_2/\beta^2}$, and hence

$$\tilde{V} = \frac{2(\kappa_2 - \kappa_1)}{\cosh^2 y} \begin{pmatrix} \kappa_1 & \sqrt{\kappa_1\kappa_2}\sinh y \\ \sqrt{\kappa_1\kappa_2}\sinh y & -\kappa_2 \end{pmatrix} \tag{20}$$

where the diagonal term $\tilde{V}_{11}$ (resp. $\tilde{V}_{22}$) is positive (resp. negative). Second, the determinant of the Jost matrix (17) has two analytical zeros: one at $k_{1\mathrm{R}} = \sqrt{\kappa_2/\kappa_1}\beta - \imath\alpha_1, k_{2\mathrm{R}} = -\sqrt{\kappa_1/\kappa_2}\beta - \imath\alpha_2$, the other one at $-k_{1\mathrm{R}}^*, -k_{2\mathrm{R}}^*$. Since these zeros lie in the lower-half k_1 and in the upper-half k_2 complex planes, they correspond to a resonance in channel 1, only visible below threshold $\Delta = \kappa_2^2 - \kappa_1^2$. The three remaining parameters κ_1, κ_2 and β can be expressed in terms of this resonance energy E_R and width Γ, as defined by $k_{1\mathrm{R}}^2 \equiv E_\mathrm{R} - \imath\Gamma/2$. They read

$$\begin{aligned} 2\kappa_{1,2}^2 &= \sqrt{E_\mathrm{R}^2 + \Gamma^2/4 + \sqrt{(E_\mathrm{R} - \Delta)^2 + \Gamma^2/4} \mp \Delta}, \\ 4\beta^4 &= \left(E_\mathrm{R} + \sqrt{E_\mathrm{R}^2 + \Gamma^2/4}\right)\left(E_\mathrm{R} - \Delta + \sqrt{(E_\mathrm{R} - \Delta)^2 + \Gamma^2/4}\right) \end{aligned} \tag{21}$$

and can be replaced in potential (20), which solves a schematic two-channel inverse problem with one resonance.

When $E_\mathrm{R} < \Delta$, this resonance is a Feshbach resonance, for which the model constitutes a good pedagogical example: when $\Gamma = 0$, all elements of $\tilde{V}$ vanish, except for $\tilde{V}_{22}$ which has then a bound state at energy E_R. This corresponds to a zero of the Jost-matrix determinant at $k_{1\mathrm{R}} = \sqrt{E_\mathrm{R}}, k_{2\mathrm{R}} = \imath\sqrt{\Delta - E_\mathrm{R}}$. When $\Gamma > 0$, coupling turns this bound state into a resonance by moving the zero off the axes, counter-clockwise for k_2 and clockwise for k_1. For instance, for $\Delta = 10$, $E_\mathrm{R} = 7$ and $\Gamma = 1$, one gets the potential plotted in figure 1, which is well behaved despite a slower asymptotic decrease of the off-diagonal terms than of the diagonal ones. The corresponding scattering matrix, as defined by its eigenphases and mixing parameter [15, 20], is represented in figure 2, where the Feshbach resonance can be seen on δ_1. Crossing threshold, which corresponds to going from positive imaginary k_2 to positive real k_2, produces an interesting cusp effect in δ_1 [15], for which the present model

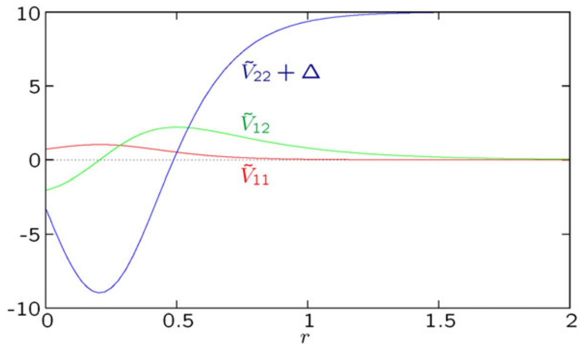

Figure 1. Two-channel potential matrix (20) as defined by parameters (21) for the threshold energy $\Delta = 10$, Feshbach-resonance energy $E_R = 7$ and width $\Gamma = 1$.

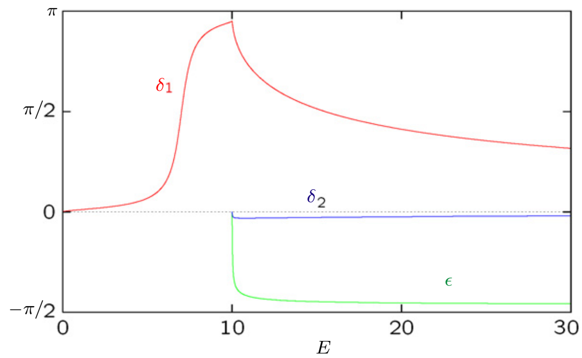

Figure 2. Eigenphases δ_1, δ_2 and mixing parameter ϵ of the scattering matrix corresponding to the potential of figure 1, as defined by (5), (17), (18) and (21).

also constitutes an analytical example. The case $E_R > \Delta$, though allowed, is less interesting from the physical point of view: when $\Gamma = 0$, coupling does not disappear and the zero of the Jost-matrix determinant lies at $k_{1R} = \sqrt{E_R}$, $k_{2R} = -\sqrt{E_R - \Delta}$, with no strong impact on the physical region $k_1 > \sqrt{\Delta}$, $k_2 > 0$.

In conclusion, we have introduced a new type of supersymmetric transformations which are able to transform an uncoupled potential into a potential with a non-diagonal scattering matrix for non-vanishing thresholds (see the non-trivial behaviour of ϵ in figure 2). The simplest possible application of this formalism leads to an exactly-solvable, two-channel s-wave potential with one resonance which, for particular choices of parameters, provides a textbook example of the Feshbach-resonance phenomenon, with compact analytical expression both for the potential and its Jost matrix. This is a promising first step for coupled-channel inversion, the purpose of which is to construct interaction potentials that fit thresholds, bound states and resonant states measured experimentally. Future research will extend this result to higher partial waves and to iteration of transformations in order to get a more flexible potential fitting several states simultaneously. In particular, it is possible to combine one non-conservative transformation with an arbitrary number of usual conservative transformations. This might be sufficient to get a supersymmetric-quantum-mechanics inversion technique as efficient in the coupled-channel case as it is in the single-channel case [3].

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