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Most General Form of Phase-Equivalent Radial Potentials for Arbitrary Modifications of the Bound Spectrum

D. Baye and J.-M. Sparenberg

*Physique Nucléaire Théorique et Physique Mathématique, C.P. 229, Université Libre de Bruxelles, Campus Plaine,
B 1050, Brussels, Belgium
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The most general form for radial potentials with the same phase shifts as a given real potential but arbitrarily different bound spectra is derived with a sequence of supersymmetric factorizations. The wave functions of the phase-equivalent potentials are expressed analytically in terms of the wave functions of the original potential.

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Describing physical problems in terms of a local potential is useful in many branches of physics [1,2]. When these potentials possess bound states, they are not uniquely determined by scattering properties [3,4]. In order to avoid physical ambiguities raised by apparent differences, it is important to dispose of all possible forms for the potentials equivalent to a given potential. In this Letter, we solve this problem for a real potential in the radial equation.

In the radial case, for a given partial wave, phase-equivalent potentials possess the same phase shifts at all energies. They are not allowed to be singular except possibly at the origin. Phase equivalence already imposes qualitative conditions through the Levinson theorem. For nonsingular potentials, the number of bound states cannot change. When the spectrum is fixed, the most general expression for phase-equivalent potentials is available in textbooks [4]. However, even when the number of bound states is conserved, more general types of phase-equivalent potentials exist where the energies of the bound states are modified [5]. In addition, no strict physical rule prevents a potential from being singular at the origin. This opens the way to new classes of phase-equivalent potentials [6] which satisfy a generalized version of the Levinson theorem [7]. This is certainly not an academic problem. In spite of their simplicity, deep real potentials with nonphysical bound states provide very accurate phase shifts in nuclear [8] or atomic [9]

physics. Removing [6] or moving [5] the bound states of these potentials is possible in a way which modifies off-shell properties [10] but not the phase shifts. This raises questions about the nature of the most suitable potential for a given application.

Supersymmetry [11] offers a simple approach to spectrum modifications. Sukumar has classified the different types of supersymmetric transformations [12], but without insisting on phase equivalence. One of us has shown that a pair of supersymmetric factorizations allows removing a bound state without affecting the phase shifts [6]. This solved an old ambiguity problem in $\alpha + \alpha$ scattering. This initial result received several generalizations. Removing and adding bound states were considered in Refs. [13] and [14]. An important step occurred recently with the realization that a condition on supersymmetric factorizations (the “no-node” condition explained below) is not necessary for pairs of transformations [15]. This allows us now not only to consider the most general form of phase equivalence, but also to simplify considerably the analytical treatment. Indeed the following presentation is short and elementary while essentially self-contained.

Let us start with the Hamiltonian

$$H_0 = -\frac{d^2}{dr^2} + V_0(r). \quad (1)$$

The potential V_0 is allowed to be singular at the origin in the following way

$$V_0(r) \underset{r \rightarrow 0}{\approx} \frac{n(n+1)}{r^2}, \tag{2}$$

where n is a non-negative integer. It may contain Coulomb and centrifugal terms. We shall denote as $\varphi_0(r)$ the real solution of the Schrödinger differential equation at some arbitrary energy E , which is bounded at infinity. This solution may represent a physical bound state when E belongs to the bound spectrum of H_0 (in that case, it is assumed to be normalized to unity) or a scattering wave function when E is positive. Physical wave functions of H_0 behave as r^{n+1} near the origin. The function $\varphi_0(r)$ may also represent nonphysical solutions which do not vanish at the origin, when E is negative and does not belong to the bound spectrum. These conventions will also be valid for all the other Hamiltonians encountered in this work (with subscripts different from 0).

We consider some arbitrary negative energy $E^{(1)}$ and the corresponding solution $\varphi_0^{(1)}$ of the Schrödinger equation (1). The initial Hamiltonian H_0 can be factorized [12] as

$$H_0 = A_0^+ A_0^- + E^{(1)}, \tag{3}$$

where the linear differential operators A_0^+ and A_0^- read

$$A_0^+ = (A_0^-)^\dagger = \frac{d}{dr} + \frac{d}{dr} \ln \varphi_0^{(1)}. \tag{4}$$

The supersymmetric partner H_1 of H_0 is defined as

$$H_1 = A_0^- A_0^+ + E^{(1)} = -\frac{d^2}{dr^2} + V_1(r), \tag{5}$$

with the potential

$$V_1 = V_0 - 2 \frac{d^2}{dr^2} \ln \varphi_0^{(1)}. \tag{6}$$

This Hamiltonian possesses the same bound spectrum as H_0 , with the possible exception of $E^{(1)}$. When $\varphi_0^{(1)}$ is physical, the energy $E^{(1)}$ is ‘‘suppressed’’; otherwise, the bound spectrum remains unchanged [12]. These properties can easily be observed on the wave functions derived below. The potential V_1 is singular at finite distances except when $\varphi_0^{(1)}$ is nodeless, i.e., when $E^{(1)}$ is lower than or equal to the ground-state energy of H_0 . This leads to the no-node condition imposed on supersymmetric transformations [6,12,14].

The solutions corresponding to H_1 are related to those of H_0 by

$$\varphi_1 = (\varphi_0^{(1)})^{-1} \int_r^\infty \varphi_0^{(1)} \varphi_0 dt, \tag{7}$$

as verified directly. For $E \neq E^{(1)}$, (7) can also be proved by starting from the eigensolution $A_0^- \varphi_0$ of H_1 . At this stage, we do not care about normalization. With (7), one can check that the phase shifts are modified. Moreover, for $E = E^{(1)}$, one easily shows that $\varphi_1^{(1)}$ does not vanish at the origin and therefore that the bound state is suppressed when $\varphi_0^{(1)}$ is physical.

Following Ref. [6], we now introduce a second factorization,

$$H_1 = A_1^+ A_1^- + E^{(1)}. \tag{8}$$

The operators A_1^+ and $A_1^- = (A_1^+)^\dagger$ are given by [13]

$$A_1^+ = \frac{d}{dr} + \frac{d}{dr} \ln \left\{ [\varphi_0^{(1)}]^{-1} \left[\beta + \int_r^\infty \varphi_0^{(1)2} dt \right] \right\}, \tag{9}$$

where the real parameter β is defined below. The supersymmetric partner of H_1 is

$$H_2 = A_1^- A_1^+ + E^{(1)} = -\frac{d^2}{dr^2} + V_2(r), \tag{10}$$

with the potential

$$V_2 = V_0 - 2 \frac{d^2}{dr^2} \ln \left(\beta + \int_r^\infty \varphi_0^{(1)2} dt \right). \tag{11}$$

This potential will be phase equivalent to V_0 and have no singularity at finite distances [15], provided that β is defined by

$$\beta = \begin{cases} -1 & \text{(a: } E^{(1)} \text{ physical for } H_0), \\ \alpha & \text{(b: } E^{(1)} \text{ nonphysical for } H_0), \\ \alpha/(1-\alpha) & \text{(c: } E^{(1)} \text{ physical for } H_0), \end{cases} \tag{12}$$

where α is an arbitrary *positive* parameter. The fate of the bound state at energy $E^{(1)}$ differs in cases (a) and (c) according to the value chosen for β . In case (a), the suppressed bound state remains suppressed after the second factorization. In case (b), a new bound state is introduced at energy $E^{(1)}$ and a parameter appears in the potential. In case (c), the second factorization reintroduces a bound state at energy $E^{(1)}$ so that the bound spectrum remains unchanged after the two successive transformations, but a parameter is introduced in the potential. One easily obtains (c) by combining (a) and

(b) [14]. The important point is that V_2 is *not* restricted to cases where $\varphi_0^{(1)}$ is nodeless [5,15].

The corresponding solution at energy E reads

$$\varphi_2 = \mathcal{N}_{\{1\}}^{-1/2} \left\{ \varphi_0 - \varphi_0^{(1)} \left[\beta + \int_r^\infty \varphi_0^{(1)2} dt \right]^{-1} \times \int_r^\infty \varphi_0^{(1)} \varphi_0 dt \right\}, \quad (13)$$

with $\mathcal{N}_{\{1\}} = 1$, except when E is equal to $E^{(1)}$ and the solution φ_2 is physical, where

$$\mathcal{N}_{\{1\}} = \alpha. \quad (14)$$

This is established by introducing (7) in $A_1^- \varphi_1$ and normalizing if necessary. One can also verify that, at energy $E^{(1)}$, $\varphi_2^{(1)}$ is bounded and normalized in cases (b) and (c) while it does not vanish at the origin in case (a). Let us emphasize that (13) is valid at all energies for physical and nonphysical solutions of (10), bounded at infinity. This formula, (11) and (12), summarizes Eqs. (13) to (16), (19) to (22), and (24) to (27) of Ref. [14]. The fact that the phase shifts are not modified is easily seen in (13). Indeed, φ_2 differs from φ_0 by a term which is obviously short ranged.

Now we can attack the general case. Let us consider a set of N *distinct* but otherwise arbitrary negative energies $E^{(i)}$ ($i = 1, \dots, N$). At these energies, we wish to suppress existing bound states, add new bound states, or modify only the potential without removing the state. Since these energies are arbitrary, the order in which they are classified is irrelevant. We consider a succession of N potentials V_{2i} , phase equivalent to V_0 , where some property is modified at energy $E^{(i)}$ [a parameter α_i defined in (12) is also associated to modification i]. With such a chain of potentials, any modification of the bound spectrum can be reached. The behavior of (13) at small r values easily shows that the parameter α_i can modify in an arbitrary way the normalization constant C_i [4] of the bound state at energy $E^{(i)}$ (if it is not suppressed) without affecting the C_j of the other states. Hence, the most general form of phase-equivalent potentials can be obtained. We now derive it.

Following Refs. [14] and [15], a matrix $X_0^{(N)}$ of order N is defined, whose elements read for $i, j = 1, \dots, N$,

$$X_0^{(i,j)} = \beta_i \delta_{ij} + \int_r^\infty \varphi_0^{(i)} \varphi_0^{(j)} dt, \quad (15)$$

where $\varphi_0^{(i)}$ is the solution at energy $E^{(i)}$. The final potential V_{2N} is given by

$$V_{2N} = V_0 - 2 \frac{d^2}{dr^2} \ln \det X_0^{(N)}. \quad (16)$$

Particular cases discussed in Refs. [14] and [15] are unified by this expression. Equation (11) shows that (16) is valid for $N = 1$. We now prove that if (16) is valid for some value $N - 1$, it is still valid for the next value N . Let us apply to potential V_2 a set of modifications at the $N - 1$ energies $E^{(2)}$ to $E^{(N)}$. Then, (16) is applicable and V_{2N} reads

$$V_{2N} = V_2 - 2 \frac{d^2}{dr^2} \ln \det X_2^{(N-1)}. \quad (17)$$

The elements of $X_2^{(N-1)}$ are given by (15) with the subscript 0 replaced by 2 for i, j varying from 2 to N . With (13), a simple integration provides

$$X_2^{(i,j)} = X_0^{(i,j)} - [X_0^{(1,1)}]^{-1} X_0^{(i,1)} X_0^{(1,j)}. \quad (18)$$

With the single determinant property derived in the appendix of Ref. [14], one deduces from (18)

$$\det X_2^{(N-1)} = [X_0^{(1,1)}]^{-1} \det X_0^{(N)}. \quad (19)$$

Combining (17), (11), and (19) proves the validity of (16). Notice that the singularity of V_{2N} at the origin differs from the singularity of V_0 [Eq. (2)], according to the variation of the number of bound states. The condition $n \geq 0$ for V_{2N} limits the possibility of adding bound states to the spectrum of H_0 [5].

A similar treatment provides the solutions, bounded at infinity, of the Schrödinger equation associated with V_{2N} at an arbitrary energy E (positive or negative) as

$$\varphi_{2N} = \mathcal{N}_{\{1, \dots, N\}}^{-1/2} [\det X_0^{(N)}]^{-1} \det Y_0^{(N)}(\varphi_0), \quad (20)$$

where $\mathcal{N}_{\{1, \dots, N\}} = 1$ except when E is equal to one of the $E^{(i)}$ where it is equal to α_i [see (14)]. The elements of matrix $Y_0^{(N)}(\varphi_0)$ of order $N + 1$ are defined by

$$Y_0^{(i,j)} = \begin{cases} X_0^{(i,j)} & (i, j = 1, \dots, N), \\ \varphi_0^{(i)} & (i = 0, \dots, N; j = 0), \\ \int_r^\infty \varphi_0^{(j)} \varphi_0 dt & (i = 0; j = 1, \dots, N), \end{cases} \quad (21)$$

with $\varphi_0^{(0)} \equiv \varphi_0$. The proof of (20) follows exactly the same pattern as the proof of (16). Equation (13) shows that it is valid for $N = 1$. Let us apply (20) to the determination of φ_{2N} as a function of the solutions associated with V_2 :

$$\varphi_{2N} = \mathcal{N}_{\{2, \dots, N\}}^{-1/2} [\det X_2^{(N-1)}]^{-1} \det Y_2^{(N-1)}(\varphi_2). \quad (22)$$

Equations (18) and (13), and a simple integral also involving (13), lead to

$$Y_2^{(i,j)}(\varphi_2) = \mathcal{N}_{\{1\}}^{-1/2} \{ Y_0^{(i,j)}(\varphi_0) - [X_0^{(1,1)}]^{-1} \times Y_0^{(i,1)}(\varphi_0) Y_0^{(1,j)}(\varphi_0) \} \quad (23)$$

for $i, j = 2, \dots, N$. Hence, one has

$$\det Y_2^{(N-1)}(\varphi_2) = \mathcal{N}_{\{1\}}^{-1/2} [X_0^{(1,1)}]^{-1} \det Y_0^{(N)}(\varphi_0) \quad (24)$$

which, with (19) and (22), proves (20). When $E = E^{(i)}$, φ_0 is equal to the corresponding $\varphi_0^{(i)}$, and $\det Y_0^{(N)}(\varphi_0^{(i)})$ can be reduced to the determinant of a $N \times N$ matrix by subtracting row i from the similar row 0. One obtains a generalized version of Eqs. (43) and (64) in Ref. [14] or of Eqs. (19) and (22) in Ref. [15].

The potential V_{2N} can be recast in a form similar to those encountered in the paper of Abraham and Moses [16]. These authors address the same problem but on the line. They derive equivalent local potentials from integral kernels obtained by solving equations of the Gelfand-Levitan type. Abraham and Moses propose an algorithm to solve their integral equation but do not provide an explicit solution. Equation (16) can be rewritten as in Ref. [16],

$$V_{2N} = V_0 + 2 \frac{d}{dr} K(r, r), \quad (25)$$

and Eq. (20) can be expanded in a form where the same kernel appears, as

$$\varphi_{2N} = \mathcal{N}_{\{1, \dots, N\}}^{-1/2} \left\{ \varphi_0 - \int_r^\infty K(r, t) \varphi_0(t) dt \right\}. \quad (26)$$

In these expressions, the kernel K is defined explicitly as

$$K(r, t) = -[\det X_0^{(N)}(r)]^{-1} \det Z_0^{(N)}(r, t), \quad (27)$$

where the elements of the $(N+1) \times (N+1)$ matrix $Z_0^{(N)}$ are given by

$$Z_0^{(i,j)} = \begin{cases} X_0^{(i,j)}(r) & (i, j = 1, \dots, N), \\ \varphi_0^{(i)}(r) & (i = 1, \dots, N; j = 0), \\ \varphi_0^{(j)}(r) & (i = 0; j = 1, \dots, N), \\ 0 & (i = j = 0). \end{cases} \quad (28)$$

With the determinant property (25) of Ref. [15], one easily shows that this kernel is a solution of the integral equation, similar to the equation of Abraham and Moses for the line problem,

$$K(r, t) = \Omega(r, t) - \int_r^\infty K(r, u) \Omega(u, t) du, \quad (29)$$

with

$$\Omega(r, t) = \sum_{i=1}^N \beta_i^{-1} \varphi_0^{(i)}(r) \varphi_0^{(i)}(t). \quad (30)$$

An alternative expression for K involving initial and final states reads

$$K(r, t) = \sum_{i=1}^N \beta_i^{-1} \alpha_i^{1/2} \varphi_{2N}^{(i)}(r) \varphi_0^{(i)}(t). \quad (31)$$

The factor $\alpha_i^{1/2}$ arises from the normalization convention adopted here. The present expressions generalize those of Refs. [5] and [15] in several respects: all forms of phase equivalence are now included and (26) is valid for both physical and nonphysical solutions.

In summary, the most general form of phase-equivalent potentials for arbitrary bound spectra is obtained in closed form with simple calculations. The expressions are valid for a class of potentials without singularities except at the origin, including possible Coulomb and centrifugal terms. We not only generalize and unify earlier works, but also significantly simplify the presentation and the proofs. The main origin of the simplification is the disappearance of the no-node condition for pairs of supersymmetric factorizations [15]. The expressions are established here for the radial problem, but a similar treatment of the line problem is possible and is in progress.

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