Singular potentials with quasi-exact Dirac bound states

Miloslav Znojil

Ústav jaderné fyziky AV ČR, 250 68 Řež, Czech Republic

e-mail: znojil@ujf.cas.cz

FAX: (00420) 6857003

Abstract

In a way which establishes a new loose parallel between the non-relativistic and relativistic quantum mechanics we show that and how the exceptional and elementary bound-state solutions may be constructed for the radial Dirac equations with forces which are strongly singular in the origin.

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1 Introduction

Quantum description of the hydrogen atom via a central Coulomb potential remains separable and exactly solvable in non-relativistic picture as well as in the relativistic quantum mechanics [1]. Even within the full-fledged quantum electrodynamics a systematic evaluation of radiation corrections to its energy levels is feasible and fairly straightforward [2]. Everywhere beyond this exceptional system, the mere non-relativistic Schrödinger equation is most frequently employed in the nuclear, atomic and molecular phenomenology. In this way, all the multiparticle wealth of the strong nucleon-nucleon interactions at short distances is being compressed into a non-relativistic two-body potential with a repulsive hard core in the origin [3]. Alternatively, one may choose an elementary power-law form of a short range repulsion for phenomenological purposes,

$$V(r) \approx \omega^2/r^p, \qquad p \geq 2, \quad r \approx 0. \tag{1}$$

In particular, the popular phenomenological Lennard-Jones potentials in atomic physics and quantum chemistry use integer exponents as large as $p = 12$ [4]. The main formal difficulty with similar forces lies in their hindered analytic, perturbative or numerical tractability in the strongly singular regime with $p > 2$ [5]. There exists just one completely solvable model with $p = 4$ [6] but even this one only provides wavefunctions in a fairly involved form of Mathieu special functions [7].

In the non-relativistic setting, the incompletely solvable models and potentials offered a significant methodical as well as practical progress and help. By definition, they just pay attention to a few energy levels and, moreover, they may also admit just a constrained, *ad hoc* restricted variability of their coupling constants. The existence of these extremely useful models has been discovered by A. Hautot more than 25 years ago, during his studies of the polynomially perturbed Coulomb forces [8]. Ten years later there appeared an extension of their analysis to the strongly singular case [9] which attracts a lot of detailed attention up to now [10]. Conveniently, all the partially solvable non-relativistic models are sometimes called quasi-exactly solvable (QES) [11].

In the relativistic context of Dirac equation the wealth of the possible new phenomena (e.g., the existence of antiparticles) is compensated by an understandable shortage of analytic solutions. All the exactly solvable relativistic potentials available in the literature (besides the discontinuous and semi-numerical square wells of course) seem to possess the same weakly singular Coulomb form with $p = 1$ in eq. (1) [12]. Even the recent successful extension of QES method to Dirac equation by Brihaye and Kosinski [13] did not break this rule and remained restricted to the mere polynomial perturbations of the weakly singular Coulomb forces.

Apparently, the possibility of existence of relativistic QES potentials with strong singularities (e.g., with $p = 2, 3, \ldots$ in eq. (1)) would tie a puzzling mathematics with interesting consequences for physics. Indeed, a routine use of a suitable ansatz for relativistic wavefunction fails to provide a QES solution at the very first choice of $p = 2$ in eq. (1). In what follows we intend to clarify the situation, showing in particular that (and why) the general strongly singular QES Dirac constructions become feasible when starting from the next integer exponent $p = 3$.

2 Terminating recurrences

Let us recall the standard form of the radial Dirac equation for a bound state at an energy E, mass M and angular momentum $\ell = 0, 1, \ldots$,

$$\left(\begin{array}{cc} \partial_r - U & M + W - E - V \\ M + W + E + V & \partial_r + U \end{array} \right) \left(\begin{array}{c} f \\ g \end{array} \right) = 0, \qquad r \in (0, \infty). \qquad (2)$$

Besides its vector and scalar potentials $V = V(r, \ell)$ and $W = W(r, \ell)$ it contains a centrifugal term $U = U(r, \ell) = \kappa/r$ such that $\kappa = \pm\sqrt{(\ell+1)(\ell+1+2Q)}$ where Q is a charge of a magnetic monopole. The coulombic choice of the vector and scalar potentials leads to the exact solutions (cf. [12] for more details).

Let us assume now that $V(r, \ell)$ and $W(r, \ell)$ become strongly singular at $r \approx 0$. In principle, this implies large velocities near the origin and makes any non-relativistic considerations subtly inconsistent. Unfortunately, the transition to the relativistic equation (2) introduces a serious unexpected difficulty. In the spirit of ref. [13] we write

$$\left(\begin{array}{c} f(r) \\ g(r) \end{array} \right) = e^{\gamma(r)} \left(\begin{array}{cc} 1 & 1 \\ 1 & -1 \end{array} \right) \left(\begin{array}{c} p(r) \\ q(r) \end{array} \right) \tag{3}$$

with exponent

$$\gamma(r) = a_0\, r^R + a_1\, r^{R-1} + \ldots + a_R\, r^0 + \sigma \ln r + c_T\, r^{-1} + \ldots + c_1\, r^{-T+1} + c_0\, r^{-T}. \tag{4}$$

Its compatibility with the natural requirements of normalizability at $r \approx 0$ and $r \to \infty$ implies that we must use the negative constants $a_0 < 0$ and $c_0 < 0$. At the same time, the differentiation of our exponent leads to a partial change of signs,

$$\gamma'(r) = R\, a_0\, r^{R-1} + \ldots + a_{R-1}\, r^0 + \sigma\, r^{-1} - c_T\, r^{-2} - \ldots - T\, c_0\, r^{-T-1}.$$

In a disappointing contrast to non-relativistic constructions (based on the second-order differential Schrödinger equation) this implies that the insertion of the ansatz (3) in the first-order Dirac system (2) *never* enables us to cancel *both* the dominant components of our relativistic potentials at $r \to 0$ and $r \to \infty$ *simultaneously.*

2.1 The simplest nontrivial example

The first step towards resolution of the above paradox becomes clear when we fix the following form of the sample potentials,

$$M + W(r) = A\, r + B + \frac{\mu}{r} + \frac{D}{r^2} + \frac{C}{r^3}, \qquad V(r) = \frac{F}{r} + \frac{G}{r^2}. \tag{5}$$

For physical reasons (Klein paradox, [1]) we shall demand that $A > 0$, $C > 0$ and $G > 0$. Then, an asymptotic and threshold solution of eq. (2) is elementary and fixes integers $R = 2$ and $T = 2$ as well as the four dominant coefficients in our ansatz (4), $a_0 = -A/2$, $a_1 = -B$, $c_1 = -D$ and $c_0 = -C/2$. With the last, not yet specified coefficient σ in $\gamma(r)$ we re-write our two Dirac differential equations as a system

$$\left(\begin{array}{cc} \partial_r + (\mu - \sigma)/r + 2D/r^2 + 2C/r^3 & E + (F - \kappa)/r + G/r^2 \\ -E - (F + \kappa)/r - G/r^2 & \partial_r - (\mu + \sigma)/r - 2B - 2Ar \end{array} \right) \left(\begin{array}{c} p(r) \\ q(r) \end{array} \right) = 0.$$

It may now be shown solvable by polynomial ansatzs

$$p(r) = \sum_{n=0}^{N} f_{n+1} r^{n+1}, \qquad q(r) = \sum_{n=0}^{N} g_n r^n$$

which contain the $2N+2$ coefficients $\vec{f} = f_1, f_2, \ldots, f_{N+1}$ and $\vec{g} = g_0, g_1, \ldots, g_N$ normalized, say, via $g_0 = 1$. Their insertion makes our differential Dirac equations equivalent to the following 2N+6 algebraic equations

$$(n-1+\mu-\sigma)\, f_{n-1} + 2D\, f_n + 2C\, f_{n+1} + E\, g_{n-2} + (F-\kappa)\, g_{n-1} + G\, g_n = 0, \quad (6)$$

$$-E\, f_{n-1} - (F+\kappa)\, f_n - G\, f_{n+1} - 2A\, g_{n-2} - 2B\, g_{n-1} - (\mu+\sigma-n)\, g_n = 0 \quad (7)$$

where $n = 0, 1, \ldots, N+2$. Obligatorily, these equations have to fix the $2N+3$ physical parameters: Arbitrarily normalized coefficients $\vec{f}$ and $\vec{g}$ of the wavefunction, the remaining free constant σ in the exponent $\gamma(r)$ and the related binding energy E. We see that the system is over-determined and imposes three independent constraints upon available couplings.

In our two potentials (5) there are seven different couplings at our disposal. Only six of them are independent since we may achieve $A = C$ by a re-scaling of the coordinate r. In addition, we are free to vary the value of the magnetic monopole charge Q in κ and $U(r)$. As a consequence each closed algebraic solution of eqs. (6) and (7) will contain four free parameters. In the other words, the simultaneous existence of *two different* Dirac bound states in the elementary QES form is possible in principle.

In practice, the explicit construction of our QES solution is straightforward. Its two sub-vectors $\vec{f}$ and $\vec{g}$ may be merged to form a single vector. In such an arrangement our equations (6) and (7) form a partitioned non-square matrix problem

$$\left(\begin{array}{cc} \mathcal{A}_1 & \mathcal{A}_2 \\ \mathcal{A}_3 & \mathcal{A}_4 \end{array} \right) \left(\begin{array}{c} \vec{f} \\ \vec{g} \end{array} \right) = 0. \quad (8)$$

At any $N = 0, 1, \ldots$, its first, last and two middle rows determine the ratios of coefficients

$$\frac{f_1}{g_0} = -\frac{G}{2C}, \qquad \frac{g_N}{f_{N+1}} = -\frac{E}{2A}$$

as well as the auxiliary parameter σ and, up to its sign, the energy,

$$\sigma = -\mu + \frac{G^2}{2C}, \qquad E^2 = 2A\left(N + 1 + 2\mu - \frac{G^2}{2C}\right).$$

The consequent backward insertion of these formulae transforms our set of the QES conditions (8) into a mutually coupled algebraic system of $2N+2$ polynomial equations.

At $N=0$ we just have to solve the two coupled equations. This is exceptionally easy. We obtain the unique and positive energy $E=4AC/G>0$ as well as the three transparent constraints upon the variability of couplings. For example, we may treat $C>0$, $G>0$, $A>0$ and any real F (and Q) as freely variable and get the remaining $N=0$ QES three couplings uniquely defined by the formulae

$$\mu=\frac{4AC^2}{G^2}+\frac{G^2}{4C}-\frac{1}{2},\qquad B=\frac{G}{4C}\,(F+\kappa),\qquad D=\frac{C}{G}\,(F-\kappa).$$

This establishes the existence and clarifies the structure of the simplest and consistent QES solution in our strongly singular model (5).

The subsequent excitations with $N>0$ are given by the more lengthy formulae. We recommend symbolic manipulations on a computer for their explicit generation via Gröbner bases [14].

2.2 The more general class of potentials

The reason of solvability of our above particular QES example (5) may be detected as lying in a mutual proportionality of the first and last non-vanishing coefficients in polynomials $p(r)$ and $q(r)$. The same relationship may now be postulated for a broader class of the strongly singular models with $A_0>0$ and $C_0>0$ in the scalar force

$$M+W(r)=A_0\,r^{R-1}+\ldots+A_{R-1}\,r^0++C_T\,r^{-1}+C_{T-1}\,r^{-2}+\ldots+C_0\,r^{-T-1}\qquad(9)$$

when accompanied by the vector potential

$$V(r)=B_0\,r^{P-1}+\ldots+B_{P-1}\,r^0+G_S\,r^{-1}+\ldots+G_0\,r^{-S-1}\qquad(10)$$

with integers $P<R$ and $S<T$. In an immediate generalization of our above construction (3) + (4) we just have to shift the indices in $\vec{g}=g_{-L+1},g_{-L+2},\ldots,g_{K+1}$

and, *mutatis mutandis*, re-write our recurrences as an overdetermined and partitioned matrix equation (8) again.

In terms of the integers P, R, S and T we may now repeat the story with the pair-wise matching of the uppermost elements in $\mathcal{A}_{1,2}$ and $\mathcal{A}_{3,4}$ and infer the conditions $T = S + L$ and $S = L$. This means that we must have $T = 2S$. Similarly, the bottom's matchings imply that $N = P + K$ and $P + N = R + K$, giving the second scalar $\leftrightarrow$ vector compatibility constraint $R = 2P$. As a net result, all our four, $(M_j + 1) \cdot (N_j + 1)-$dimensional sub-matrices $\mathcal{A}_j$ with $M_j \geq N_j$ acquire the same multi-diagonal structure. Due to their shape and construction, their upper as well as lower triangular parts are completely vanishing, $(\mathcal{A}_j)_{mm+1} = (\mathcal{A}_j)_{mm+2} = \ldots = (\mathcal{A}_j)_{M_j-m,N_j-m-1} = (\mathcal{A}_j)_{M_j-m,N_j-m-2} = \ldots = 0$ for $m = 0, 1, \ldots$. The numbers $M_j - N_j + 1$ of non-vanishing diagonals are equal to $T + 1$ for $j = 1$, to $P + S + 1$ for $j = 2$ and 3 and to $R + 1$ for $j = 4$. As long as $K \geq \min(P, S)$, the whole system (8) is formed by $M_1 + M_3 + 2 = 3S + 3P + 2K + 2$ equations in general.

Step by step we may discuss the special cases. At the weak Coulomb singularity $S = 0$ and linear confinement $P = 1$ our construction remains applicable and returns us back to the regular potentials and to the five, seven, ... equations of ref. [13] at the respective degrees $K = 0, 1, \ldots$ of our polynomials. Next, our first singular $S = P = 1$ example (5) leads to the six, eight, ... equations at the respective integers $K = -1, 0, 1, \ldots$. This is to be compared with the minimum of eight equations in the regular Coulomb plus cubic case with $S = 0$ and $P = 2$. The minimum of nine equations corresponds to the two strongly singular QES models,

$$M + W(r) = A_0\, r^3 + \ldots + \frac{C_0}{r^3}, \qquad V(r) = B_0 r + \ldots + \frac{G_0}{r^2} \tag{11}$$

and

$$M + W(r) = A_0\, r + \ldots + \frac{C_0}{r^5}, \qquad V(r) = B_0 + \frac{G_2}{r} + \ldots + \frac{G_0}{r^3} \tag{12}$$

where $S = 1$ and $P = 2$ and $S = 2$ and $P = 1$, respectively. Ten equations are then encountered for the subsequent $S = P = 2$ superposition of eqs. (11) and (12), etc.

3 Summary

We have seen that the QES features of the polynomial + Coulomb Dirac equations as formulated in ref. [13] survive a transition to singular forces with $p > 1$. The core of their QES property still lies in the termination of recurrences. In a way which *partially* parallels the nonrelativistic case this termination fixes some admissible values of a few selected couplings. The explicit QES constraints upon couplings have the form of coupled polynomial algebraic equations and we have demonstrated that they admit straightforward (though not always easy) solutions.

We have to emphasize that a seemingly natural transition from non-relativistic to relativistic QES solvability is mathematically nontrivial. The main reason for that lies in a global difference between the non-relativistic and relativistic quantum mechanics itself. One has to recollect [11] that the radial Schrödinger equation itself is extremely "friendly" to QES considerations. In fact, it immediately defines any potential in terms of any of its bound state wavefunctions, $V(r) = E - \ell(\ell+1)/r^2 + \Psi''(r)/\Psi(r)$. Mathematically, the non-relativistic QES "inverse bound-state problem" only becomes mathematically interesting in the presence of constraints or during the search for multiplets (cf., e.g., ref. [15] for more details). In contrast to that, the second-order re-formulation of our relativistic Dirac equation (say, via elimination of $g(r)$ in the present notation) already contains the explicit first and second derivatives of its potentials. The parallels break down and the relativistic "inversion" $\Psi(r) \to V(r)$ becomes at least as difficult as the "direct" solution $V(r) \to \Psi(r)$.

For our present strongly singular class of models (9) and (10) we may only summarize that their relativistic QES tractability is, unexpectedly, quite comfortable and flexible. An overall structure of our final implicit algebraic definitions of the QES constrained couplings is different from, but, after all, not too much formally dissimilar to, its non-relativistic predecessors [9, 10, 11].

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