Phys. Rev. A 51 (1995) 128 - 35:

Non-numerical determination of the number of bound states in some screened Coulomb potentials

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Abstract

We construct potentials $V^{\{\mathcal{K}\}}(r)$ which support a finite number $\mathcal{K}$ of bound states in such a way that the highest normalizable excitation lies precisely at the threshold energy $E = 0$. We expect that many realistic interactions $V_{(phys)}(r)$ may be bracketed between these forces due to their flexibility and plausible screened Coulombic form. Thus, we propose an estimate of the number N_{BS} of bound states in an arbitrary potential $V_{(phys)}(r)$ via requirements $V^{\{\mathcal{K}_L\}} < V_{(phys)} \leq V^{\{\mathcal{K}_U\}}$ and subsequent inequalities $\mathcal{K}_L > N_{BS} \geq \mathcal{K}_U$. In particular, we get a strict prediction $N_{BS} = \mathcal{K}_U$ whenever the bracketing proves tight enough, with $\mathcal{K}_U \equiv \mathcal{K}_L - 1$.

PACS 03.65.Fd 03.65.Ge 02.70.+d 31.15.+q 71.10.+x

1 Introduction

A difficult choice between simple models (with transparent properties) and realistic descriptions emerges in the different branches of physics. The radial Schroedinger equation

$$\left[-\frac{d^2}{dr^2}+\frac{l(l+1)}{r^2}+V(r)\right]\psi(r)=E\psi(r), \qquad l=0,1,\ldots \tag{1}$$

offers its particular exemplification. The realistic (and complicated) potentials $V(r)$ are currently being replaced by schematic forces not only in nuclear physics (where, after all, the very physical interpretation of $V(r)$ is ambiguous [1]), but also in many atomic and molecular-physics applications of Coulombic superpositions [2]. More recent use of eq. (1) with various tentative $V(r)$'s covers systems as exotic as heavy quarkonia in the non-relativistic limit [3].

In the above range of applications, the practical solution of eq. (1) remains approximative for a majority of the physically relevant potentials $V_{(phys)}(r)$. The character of approximations depends on the particular physical problem in question. Our interest may be paid to the existence (and/or number N_{BS}) of bound states which is, via Levinson theorem, relevant for scattering [4]. For all the "reasonable" $V_{(phys)}(r)$'s, one may recall various specialized techniques of the estimate and/or determination of N_{BS} as listed, e.g., in the review paper [5] or monograph [6].

In an extreme case, one may compare the given $V_{(phys)}(r)$ with its exactly solvable simplification(s). Newton [4] lists the four solvable possibilities: the repulsive core $V(r)\sim r^{-4}$ with $N_{BS}=0$, the harmonic and Coulombic oscillators with $N_{BS}=\infty$ and (the whole family of) square wells with $0\leq N_{BS}\leq\infty$. Whenever a given realistic force $V_{(phys)}(r)$ proves majorized/minorized by a suitable (multiple) square well, we immediately arrive at the most natural (perhaps, semi-numerical) estimate of the number of its bound states.

Recently, for the same purpose of determination of N_{BS}, Chhajlany [7] proposed a majorization of $V_{(phys)}(r)$ by the less common class of forces which were equivalent to the Coulomb or harmonic oscillators. The underlying transformation (called a generalized Schwinger duality and proposed, independently, by Newton [4], p. 443) simplifies the determination of the number of bound states in comparison with the computationally more complicated square-well prescription.

The Chhajlany's class of potentials may be written in the form

$$V_{(Chhaj)}(r) = \frac{c(r)}{r}, \qquad c(r) = -\rho^2\, r^{-j/N} + \sigma^2\, r^{i/N}, \quad i = N-2j, \quad j \in (0, N) \quad (2)$$

where the redundant parameters $N > 1$ and $\rho \neq 0$ represent a scaling of exponents and coordinates, respectively. The variable coupling σ is assumed fixed in such a way that the last (say, $\mathcal{K}$'th) bound state has precisely zero energy,

$$\sigma = \sigma^{\{\mathcal{K}\}} = \frac{\rho}{(1-j/N)(2\mathcal{K}+1)}.$$

The latter feature may be emphasized by an addition of the superscript $\mathcal{K}$ to the forces themselves, $V_{(Chhaj)}(r) = V^{\{\mathcal{K}\}}_{(Chhaj)}(r)$.

Obviously, any interaction $V_{(phys)}(r)$ which is majorized by the Chhajlany's potential,

$$V_{(phys)}(r) < V^{\{\mathcal{K}_U\}}_{(Chhaj)}(r), \quad r \in (0, \infty) \quad (3)$$

possesses $\mathcal{K}_U$ bound states at least [5],

$$N_{BS} \geq \mathcal{K}_U. \quad (4)$$

Vice versa, we may be sure that at least one (namely, threshold) bound state disappears whenever we weaken the attraction,

$$V_{(phys)}(r) > V^{\{\mathcal{K}_L\}}_{(Chhaj)}(r), \quad r \in (0, \infty) \Longrightarrow N_{BS} < \mathcal{K}_L \quad (5)$$

Having this in mind, Chhajlany [7] demonstrated that $N_{BS} = \infty$ for all the attractive screened Coulomb single-term forces $V(r) = -\rho^2 r^{-d}$ with a real exponent $d \in (0, 2)$.

The bracketing forces (2) form, unfortunately, just a rather special two-component family. In comparison with their (in principle, multi-step) square-well predecessors, these potentials are not rich and flexible enough for any more ambitious practical purposes. This was the main motivation of our present analysis.

In what follows, we are going to show

- how one constructs a partially exactly solvable multi-parametric generalization $V_{(PES)}^{\{\mathcal{K}\}}(r)$ of the above Chhajlany interactions, and
- that, as a consequence, the too rigid and special one-parametric bracketings (5) and (3) may be made much more flexible,

$$V_{(PES)}^{\{\mathcal{K}_L\}}(r) < V_{(phys)}(r) \le V_{(PES)}^{\{\mathcal{K}_U\}}(r), \qquad r \in (0, \infty) \tag{6}$$

  to make the analogous estimates

$$\mathcal{K}_L > N_{BS} \ge \mathcal{K}_U \tag{7}$$

  tighter;

- in particular, we get the exact number of bound states $N_{BS} \equiv \mathcal{K}_U$ from the closest possible sandwich (6) with $\mathcal{K}_U = \mathcal{K}_L - 1$.

The material is split into three parts. Section 2 adds more details to an overall motivation. Section 3 studies and describes such bracketing forces $V_{(PES)}^{\{\mathcal{K}\}}$ which may be assigned the simplest nontrivial wavefunctions at the threshold. This feature corresponds to the first few smallest bound-state capacities $\mathcal{K}$. Section 4 offers an alternative approach, paying attention to the first few simplest nontrivial functional forms of potentials $V_{(PES)}^{\{\mathcal{K}\}}$ themselves. Finally, a summary is provided in Section 5.

2 The generalized Chhajlany potentials $V_{(PES)}^{\{\mathcal{K}\}}(r)$

2.1 A power-law screening

Coulomb force

$$V_C(r) = \frac{e}{r} \tag{8}$$

is an exceptional model in quantum mechanics. It is completely solvable and realistic (say, as a simple picture of hydrogen) and combines the possibility of scattering with the existence of infinitely many bound states at $e < 0$ [4]. In the context of our preceding Section, it represents just the special case of Chhajlany's potential (2) with $N = 1$, $i = 1$, $j = 0$ and $\mathcal{K} \to \infty$.

At large distances, various phenomenological distortions of the oversimplified forces (8) may be represented by their superimposed power-law screenings,

$$V_{C^-}(r) = \sum_{i=1}^{M^-} \frac{f_i}{r}\, r^{-i/N} \tag{9}$$

with some $M^- < N < \infty$ suitable couplings f_i (we shall extend our discussion neither to the strongly repulsive singular cases with $M^- > N$ and $f_{M^-} > 0$ [8] nor to an integral-representation limit $N \to \infty$).

At small distances, the same phenomenological argumentation leads to a short-range-screening alternative

$$V_{C^+}(r) = \sum_{j=1}^{M^+} \frac{g_j}{r}\, r^{+j/N} \tag{10}$$

with $M^+ < N$.

New forces (9) may contain Chhajlany interactions (2) as a special case. Generically, neither (9) nor (10) remains related to any completely solvable interaction. Nevertheless, speaking about physics, their combination is a fairly universal model which is able to distort and/or dominate the standard Coulomb field at both the short and long distances simultaneously. Superpositions $V_{C^+}(r) + V_C(r) + V_{C^-}(r)$ seem suitable as candidates for the above-mentioned non-numerically tractable bracketing forces $V^{\{\mathcal{K}\}}_{(PES)}(r)$.

For the sake of a further simplification of the underlying mathematics (we shall give more details later), we shall put $e \equiv g_0$ and consider

$$V_{(gen)}(r) = \sum_{j=0}^{M^+} \frac{g_j}{r}\, r^{j/N} + \sum_{i=1}^{M^-} \frac{f_i}{r}\, r^{-i/N} \tag{11}$$

at the integer scalings N. Such a formal restriction does not seem too severe in the context of phenomenological applications [3].

In a methodical setting, the latter constraint is welcome. In the purely numerical context, it may facilitate, e.g., the stringent tests of efficiency of new methods for which the long-range character of the forces ($V_{(gen)}(r) \approx g_{M^+}/r^{(N-M^+)/N}$ for $r \gg 1$) is particularly challenging (cf. the use of $M^+ + 1 = N = 2$ in ref. [9]).

Mathematically, the less standard long- and/or short-range behaviour of the class of the distorted Coulomb forces (11) is vital for our purposes. It renders possible a violation of the generic absence of bound states at the threshold energy which may rigorously be proved for all the "more reasonable" potentials [10].

2.2 Bound states at the threshold

The well known Sturm-Liouville oscillation theorem implies that any radial Schrödinger equation (1) with interactions (11) orders the energies of bound states in accordance with the increasing number of the nodal zeros in their wavefunctions [5, 6, 11].

For forces with the property $V(\infty) = 0$ this implies that the existence of a bound state (i.e., of a normalizable wavefunction $\psi(r)$ with $\mathcal{K} - 1$ nodal zeros at $r > 0$) at the threshold (*i.e.*, at the zero energy $E = 0$) is of particular importance. Our knowledge of the number $\mathcal{K}$ trivializes the determination of the total number of bound states which coincides with $\mathcal{K}$. Technically, the absence of the energy term makes the explicit solution of eq. (1)) easier in principle.

The simplifications due to the vanishing energy $E = 0$ do not seem too helpful in general. Hence, denoting all the threshold-state supporting interactions (11) by the curly-bracketed superscript, $V^{\{\mathcal{K}\}}_{(gen)}(r)$, we shall search for their partially solvable subclass $V^{\{\mathcal{K}\}}_{(PES)}(r)$ in what follows.

With a family of generalized Chhajlany potentials $V^{\{\mathcal{K}\}}_{(PES)}(r)$ at our disposal, all the potentials which lie within the semi-open intervals

$$\left(V^{\{\mathcal{K}+1\}}_{(PES)}(r),\, V^{\{\mathcal{K}\}}_{(PES)}(r)\right], \quad r \in (0, \infty) \tag{12}$$

will generate the same number $N_{BS} = \mathcal{K}$ of bound states. This is our basic message; now, let us return to the technicalities.

We shall employ the most direct "brute-force" methods as originally proposed by Hautot [12] and further developed by Singh et al [13] and Magyari [14] (cf. also [15, 16]). The separate $E = 0$ wavefunctions and their "partially exactly solvable"

(PES) "parent" potentials $V_{(PES)}^{\{\mathcal{K}\}}(r)$ will be constructed in two steps as reviewed, e.g., in ref. [17].

When we recall the best known Coulomb and harmonic oscillator examples of solvability, the first step of our construction will just generalize the specification of the exponential in their wavefunctions.

2.2.1 Asymptotics

At zero energy, the radial Schrödinger differential equation (1) + (11) reads

$$\left[-\frac{d^2}{dr^2}+\frac{l(l+1)}{r^2}+V_{(gen)}(r)\right]\psi^{\{\mathcal{K}\}}(r)=0. \tag{13}$$

As long as the small numerically-induced perturbations might destroy our conclusions completely, we must search for its non-numerical solutions. We shall se that at least some of them are very easily constructed.

At large distances, wavefunctions are known to possess an exponential form. The standard WKB or Liouville-Green analysis [18] offers us an explicit "educated PES guess"

$$\psi^{\{\mathcal{K}\}}(r)=e^{-G(r)+O(\ln r)}, \qquad r\gg 1. \tag{14}$$

with, say,

$$G(r)=G_{(PES)}=r\sum_{n=1}^{N-1}\frac{\alpha_n}{1-n/N}\,r^{-n/N}. \tag{15}$$

Its insertion in our zero-energy Schrödinger equation (13) implies that

$$g_{N-1}=0 \tag{16}$$

while

$$\begin{aligned} g_{N-2}&=\alpha_1^2\\ g_{N-3}&=2\alpha_1\alpha_2\\ g_{N-4}&=2\alpha_1\alpha_3+\alpha_2^2\\ \ldots&. \end{aligned} \tag{17}$$

Recurrently, these relations define our PES-compatible couplings g as obtained immediately from our present tentative (and, of course, by far not unique [17]) postulate (15).

The prescription for asymptotic behavior of the potentials compatible with our particular Ansatz (15) reads $V_{(gen)}(r) \approx r^{-2/N}$, $r \gg 1$ for $\alpha_1 \neq 0$ and is unnecessarily restrictive. This may be weakened by a special choice of our free parameters,

$$\alpha_1 = \ldots = \alpha_{T-1} = 0, \quad \alpha_T \neq 0, \quad 1 \leq T \leq N-1. \tag{18}$$

At the small T's, we may re-write our fully general eq. (11) in a modified form compatible with both eqs. (15) and (18),

$$V_{(PES)}(r) = \sum_{j=0}^{M^+} \frac{g_j}{r} r^{j/N} + \sum_{i=1}^{N-1} \frac{f_i}{r} r^{-i/N}, \tag{19}$$

$$M^+ = N - 2T, \quad 1 \leq T \leq T_0 \equiv [N/2], \quad g_{N-2T} \equiv \alpha_T^2 > 0.$$

At the larger $T = T_0 + 1, T_0 + 2, \ldots, N-1$ with many disappearing coefficients α, we get the formula

$$V_{(PES)}(r) = \sum_{i=N^-}^{N-1} \frac{f_i}{r} r^{-i/N}, \tag{20}$$

$$N^- = 2T - N, \quad T_0 < T < N, \quad f_{2T-N} = \alpha_T^2 > 0$$

where the asymptotic PES-compatibility restrictions became more pronounced.

For a given finite superposition of the power-law forces $\sum_{|\delta|<1} h_\delta \, r^\delta$ with rational δ's, we are now prepared to invert equations (17) and re-interpret them as recurrences which define the parameters α in terms of the couplings h. Such a re-construction of $G(r)$ (partial inversion $h \to \alpha$) is easy. The not necessarily minimal common denominator N of all the exponents δ must be chosen in a way compatible with the prescribed explicit asymptotic behaviour of potentials (19) or (20).

2.2.2 Termination

The second step of construction of the generalized Chhajlany potentials (i.e., by definition, of forces which support an elementary threshold bound state) has to pay attention to all the coordinates r. After the above correct selfconsistent specification of the asymptotically dominant couplings and coefficients α_i in $G(r)$, we apply the general Taylor-series method [11] and postulate

$$\psi^{\{\mathcal{K}\}}(r) = e^{-G(r)} \sum_{m=0}^{\infty} c_m \, r^{m/N+l+1}, \quad c_0 \neq 0. \tag{21}$$

This function is explicitly regular (*i.e.*, physical) near the origin. Its insertion converts our differential equation (13) into recurrences which in the simplest $T = 1$ case read

$$B_n c_{n+1} = C_n^{(1)} c_n + C_n^{(2)} c_{n-1} + \ldots + C_n^{(N-1)} c_{n-N+2}, \qquad n = 0, 1, \ldots \tag{22}$$

$$B_n = \frac{1}{N^2}\,(n+1)\,[(2l+1)N + n + 1]$$

$$C_n^{(1)} = f_{N-1} + \frac{\alpha_{N-1}}{N}\,[(2l+1)N + 2n + 1]$$

$$C_n^{(2)} = f_{N-2} + \frac{\alpha_{N-2}}{N}\,[(2l+1)N + 2n] - \alpha_{N-1}^2$$

$$\ldots$$

$$C_n^{(N-1)} = f_1 + \frac{\alpha_1}{N}\,[2lN + 2n + 3] - \sum_{k=2}^{N-1} \alpha_k \alpha_{N+1-k}.$$

Step-by-step, these recurrences define all the Taylor coefficients c_1, c_2, … normalized, say, via a choice of $c_0 \neq 0$. Similarly, we might also proceed at any $T > 1$.

In the way which parallels the standard Taylor-series constructions at $E \neq 0$ [17], we may immediately define the solutions by an explicit formula

$$c_{n+1} = \frac{c_0}{\prod_{k=0}^{n} B_k} \det Q^{[n]} \tag{23}$$

where $n = 0, 1, \ldots$ and all the Hessenberg matrices

$$Q^{[n]} = \left(\begin{array}{cccccc} C_0^{(1)} & -B_0 & & & & \\ C_1^{(2)} & C_1^{(1)} & -B_1 & & & \\ C_2^{(3)} & C_2^{(2)} & C_2^{(1)} & -B_2 & & \\ & & & \ldots & & \\ & & C_n^{(N-1)} & \ldots & C_n^{(2)} & C_n^{(1)} \end{array} \right) \tag{24}$$

remain finite-dimensional.

In the spirit of the standard $E \neq 0$ PES constructions [17], we may demand that our **exact** solutions remain **elementary**, i.e., polynomial,

$$c_L \neq 0, \quad c_{L+1} = c_{L+2} = \ldots = 0. \tag{25}$$

Any choice of the degree L is admissible a priori. The only unanswered question concerns the mutual compatibility of all the termination conditions (25).

The latter question is a difficult one. The rest of our paper will be devoted just to its analysis. We shall proceed constructively: In place of the (presumably, prohibitively difficult) general discussion, we shall provide the reader with a few affirmative answers at a few particular cases.

3 Explicit constructions for the small K's.

In the light of the above explicit determinantal definition (23) of our Taylor coefficients, we may read the termination constraints (25) as a coupled set of nonlinear algebraic conditions imposed, say, on the admissible values of our couplings f_i and/or g_j or coefficients α_j. Alternatively, we may return to recurrences (22) and re-arrange their combination with eq. (25) into a larger linear set of equations with $L+1$ "redundant" unnormalized unknown c_i's,

$$\left(\begin{array}{ccccccc} C_0^{(1)} & -B_0 & & & & & \\ C_1^{(2)} & C_1^{(1)} & -B_1 & & & & \\ & \dots & & & & & \\ C_{N-2}^{(N-1)} & \dots & C_{N-2}^{(2)} & C_{N-2}^{(1)} & -B_{N-2} & & \\ 0 & C_{N-1}^{(N-1)} & \dots & C_{N-1}^{(2)} & C_{N-1}^{(1)} & -B_{N-1} & \\ & \dots & & & & & \\ & & & & 0 & C_{N-3+L}^{(N-1)} & C_{N-3+L}^{(N-2)} \\ & & & & & 0 & C_{N-2+L}^{(N-1)} \end{array} \right) \left(\begin{array}{c} c_0 \\ c_1 \\ \vdots \\ c_L \end{array} \right) = 0. \qquad (26)$$

Whenever $T > 1$, these equations may be further simplified: As long as $\alpha_j = 0$ for all $j \leq T-1$, we get $C_n^{(N-1)} = C_n^{(N-2)} = C_n^{(N-T+1)} = 0$ and the values$C_n^{(N-T)} \neq 0$ will specify the lowest nonzero diagonal in eq. (26). In another formulation, our recurrences will contain precisely $N+1-T$ nonzero terms ($n \leq N+L-T-1$ in eq. (22)), and only the first $N+L-T$ rows in our Hessenberg matrix equation (26) remain nontrivial.

By definition, our physical couplings must remain real. The proof must be given in each particular example separately.

Omitting the first L rows in eq. (26) (by returning to the explicit "Hill-determinant" c_i's (23)), we may, in principle, determine our generalized PES Chhajlany potentials via a solution of the remaining $N-T$ nonlinear and coupled algebraic equations for some $N-T$ non-independent, "selfconsistent" values among all the PES couplings $f_i^{\{\mathcal{K}\}}$ and $g_j^{\{\mathcal{K}\}}$ and/or parameters $\alpha_j^{\{\mathcal{K}\}}$.

3.1 The emergence of ground states.

The phenomenologically most important information about a potential is carried by a specification of its couplings which guarantee the existence of at least one bound state. In the present language, this corresponds to the construction of a nodeless threshold bound state. Most easily, this may be done via a choice of $L=0$ which fixes $\mathcal{K}=1$ and reduces the whole construction to the following set of equations

$$C_j^{(j+1)}(f_{N-j-1}^{\{\mathcal{K}\}}, \alpha_{N-j-1}^{\{\mathcal{K}\}}) = 0, \qquad j = 0, 1, \ldots, N-T-1.d \tag{27}$$

These implicit definitions of our parameters are absolutely transparent: We may treat the α_i's as independent variables and extract the corresponding $N-1$ dependent couplings

$$\begin{aligned} f_{N-1}^{\{\mathcal{K}\}} &= -\frac{\alpha_{N-1}}{N}\left[(2l+1)N+1\right] \\ f_{N-2}^{\{\mathcal{K}\}} &= -\frac{\alpha_{N-2}}{N}\left[(2l+1)N+2\right] + \alpha_{N-1}^2 \\ &\ldots \\ f_1^{\{\mathcal{K}\}} &= -\frac{\alpha_1}{N}\left[(2l+1)N+N-1\right] + \sum_{k=2}^{N-1} \alpha_k \alpha_{N+1-k} \end{aligned} \tag{28}$$

with $\mathcal{K}=1$ immediately.

3.2 The emergence of the first excited states.

In the case of the higher L's, the basic methodical inspiration may be sought in our partially related PES $E \neq 0$ paper [15]: We shall normalize $c_1 = 1$ and require that $c_0 \equiv -a > 0$ (ground state, $\mathcal{K}=1$) or $c_0 \equiv -a < 0$ (the first excited state, $\mathcal{K}=2$).

With an abbreviation $C_j^{(j+1)}(f_{N-j-1}^{\{\mathcal{K}\}},\, \alpha_{N-j-1}^{\{\mathcal{K}\}}) = \phi_{N-j-1}$, the $L=1$ and, for brevity, $T=1$, our equation

$$\left(\begin{array}{cc} C_0^{(1)} & -B_0 \\ C_1^{(2)} & C_1^{(1)} \\ C_2^{(3)} & C_2^{(2)} \\ \ldots & \\ C_{N-2}^{(N-1)} & C_{N-2}^{(N-2)} \\ 0 & C_{N-1}^{(N-1)} \end{array} \right) \left(\begin{array}{c} c_0 \\ c_1 \end{array} \right) = 0 \tag{29}$$

then reads

$$\left(\begin{array}{cc} \phi_{N-1} & -B_0 \\ \phi_{N-2} & \phi_{N-1} + 2\frac{\alpha_{N-1}}{N} \\ \phi_{N-3} & \phi_{N-2} + 2\frac{\alpha_{N-2}}{N} \\ \ldots & \\ \phi_2 & \phi_3 + 2\frac{\alpha_3}{N} \\ \phi_1 & \phi_2 + 2\frac{\alpha_2}{N} \\ 0 & \phi_1 + 2\frac{\alpha_1}{N} \end{array} \right) \left(\begin{array}{c} -a \\ 1 \end{array} \right) = 0. \tag{30}$$

Step by step, it gives the solutions

$$\begin{array}{c} \phi_1^{\{\mathcal{K}\}} = -2\,\frac{\alpha_1}{N}, \\ \phi_2^{\{\mathcal{K}\}} = -2\,\frac{\alpha_1}{N}\,a - 2\,\frac{\alpha_2}{N}, \\ \phi_3^{\{\mathcal{K}\}} = -2\,\frac{\alpha_1}{N}\,a^2 - 2\,\frac{\alpha_2}{N}\,a - 2\,\frac{\alpha_3}{N}, \\ \ldots . \end{array} \tag{31}$$

In contrast to the preceding subparagraph, there remains one additional row or independent condition

$$\phi_{N-1}^{\{\mathcal{K}\}}(a) = -B_0/a. \tag{32}$$

In the spirit of ref. [15] the latter equation may be interpreted as a single nonlinear algebraic condition which defines the (set of) eligible selfconsistent values of our parameter a. We may notice that the existence of at most one real and positive or negative root $a = a^{\{\mathcal{K}\}}$ may always be guaranteed by an appropriate choice of our independent variables α_i.

In the present context, the selfconsistency becomes much simpler when we apply it to another parameter, namely, $\alpha_{N-1}^{\{\mathcal{K}\}}$. In this case, we are left with the same definition of $\phi_{N-1}^{\{\mathcal{K}\}} \equiv \phi_{N-1}^{\{\mathcal{K}\}}(a)$ or

$$f_{N-1}^{\{\mathcal{K}\}} = -2\,\frac{\alpha_1}{N}\,a^{N-2} - 2\,\frac{\alpha_2}{N}\,a^{N-3} - \ldots - 2\,\frac{\alpha_{N-2}}{N}\,a - 2\,\frac{\alpha_{N-1}^{\{\mathcal{K}\}}}{N}[(2l+1)N+2] \qquad (33)$$

with arbirary a. It has to be accompanied by the selfconsistency condition (32) re-interpreted as a linear (!) definition of the parameter

$$\alpha_{N-1}^{\{\mathcal{K}\}} = N\,B_0/(2a) - \alpha_1\,a^{N-2} - \alpha_2\,a^{N-3} - \ldots - \alpha_{N-2}\,a. \qquad (34)$$

We see that the specification of the point of emergence of the first excited state is not complicated. Obviously, in terms of the various admissible sets of independent couplings, the explicit construction of intervals (12) becomes trivial at $\mathcal{K} = 1$.

3.3 Systems with more bound states.

In the next step with $L = 2$, we get

$$\left(\begin{array}{ccc} \phi_{N-1} & -B_0 & 0 \\ \phi_{N-2} & \phi_{N-1} + 2\frac{\alpha_{N-1}}{N} & -B_1 \\ \phi_{N-3} & \phi_{N-2} + 2\frac{\alpha_{N-2}}{N} & \phi_{N-1} + 4\frac{\alpha_{N-1}}{N} \\ & \ldots & \\ \phi_2 & \phi_3 + 2\frac{\alpha_3}{N} & \phi_4 + 4\frac{\alpha_4}{N} \\ \phi_1 & \phi_2 + 2\frac{\alpha_2}{N} & \phi_3 + 4\frac{\alpha_3}{N} \\ 0 & \phi_1 + 2\frac{\alpha_1}{N} & \phi_2 + 4\frac{\alpha_2}{N} \\ 0 & 0 & \phi_1 + 4\frac{\alpha_1}{N} \end{array} \right) \left(\begin{array}{c} ab \\ -a-b \\ 1 \end{array} \right) = 0 \qquad (35)$$

in place of eq. (30). Step by step, we also obtain the following very simple "superposition modification" of the preceding $L = 1$ result (31),

$$\begin{aligned} \phi_1^{\{\mathcal{K}\}} &= -4\,\frac{\alpha_1}{N}, \\ \phi_2^{\{\mathcal{K}\}} &= -2\,\frac{\alpha_1}{N}\,(a+b) - 4\,\frac{\alpha_2}{N}, \qquad (36) \\ \phi_3^{\{\mathcal{K}\}} &= -2\,\frac{\alpha_1}{N}\,(a^2+b^2) - 2\,\frac{\alpha_2}{N}\,(a+b) - 4\,\frac{\alpha_3}{N}, \end{aligned}$$

$$\phi_4^{\{\mathcal{K}\}} = -2\,\frac{\alpha_1}{N}\,(a^3+b^3) - 2\,\frac{\alpha_2}{N}\,(a^2+b^2) - 2\,\frac{\alpha_3}{N}\,(a+b) - 4\,\frac{\alpha_4}{N},$$

$$\ldots .$$

In full analogy, the remaining two rows

$$\begin{array}{l} a\,b\,\phi_{N-1}^{\{\mathcal{K}\}}(a,\,b) = -B_0\,(a+b) \\ a\,b\,\phi_{N-2}^{\{\mathcal{K}\}}(a,\,b) - (a+b)\,\left[\phi_{N-1}^{\{\mathcal{K}\}}(a,\,b) + 2\,\frac{\alpha_{N-1}^{\{\mathcal{K}\}}}{N}\right] = B_1 \end{array} \tag{37}$$

immediately lead to the linear definition of the selfconsistent values of $\alpha_{N-1}^{\{\mathcal{K}\}}$ and $\alpha_{N-2}^{\{\mathcal{K}\}}$,

$$2\,a\,b\,(a-b)^2\alpha_{N-2}^{\{\mathcal{K}\}} = [2\,a\,b\,B_1 - (a+b)^2 B_0]\,N -$$

$$-2\,a\,b\,(a-b)\,[(a^2-b^2)\,\alpha_{N-3} + (a^3-b^3)\,\alpha_{N-4} + \ldots + (a^{N-2}-b^{N-2})\,\alpha_1] \tag{38}$$

$$4\,a\,b\,\alpha_{N-1}^{\{\mathcal{K}\}} = (a+b)\,B_0\,N - 2\,a\,b\,[(a+b)\,\alpha_{N-2}^{\{\mathcal{K}\}} + (a^2+b^2)\,\alpha_{N-3} + \ldots + (a^{N-2}+b^{N-2})\,\alpha_1]. \tag{39}$$

We may conclude that the $L=2$ case does not differ too much from its $L=1$ predecessor. It allows us to study the $\mathcal{K}=2$ sandwichings of potentials in full analogy with their $\mathcal{K}=1$ predecessors. The principle of the further, $L \geq 3$ and $\mathcal{K} \geq 3$ constructions remains similar.

4 The first few simplest potentials.

The use of the computer symbolic manipulations and simplifying assumptions may be recommended in some complicated examples of particular practical interest. First of all, in the way documented, e.g., in ref. [16], the new sources of simplifications may often be found at the smallest denominators N.

4.1 Potentials with $N=2$.

At an arbitrary degree of our polynomial threshold wavefunctions L, our Magyari-like equations fix just one unknown coupling f_1 at $N=2$. The real and explicit selfconsistent value of this parameter reads

$$f_1 = f_1(L) = -\frac{\sqrt{g_0}}{2}\,(4l+2L+3). \tag{40}$$

and follows from the last row in eq. (22).

The induced sequence of our PES potentials is very simple – it has the property $L = \mathcal{K}$ and explicit form

$$V(r) = V^{\{L\}}_{(PES)}(r) = \frac{f_1^{\{L\}}}{r^{3/2}} + \frac{g_0}{r}, \quad f_1^{\{L\}} \equiv f_1(L). \tag{41}$$

These forces coincide with the ones constructed by Chhajlany in ref. [7]. Their L-nodal PES wavefunctions are duals to the exactly solvable Coulomb states. As long as the "generalized Schwinger duality" between potentials (8) and (41) is mediated by a change of variables in the underlying differential Schrödinger equations (cf. also ref. [19] or [18] for a few historical remarks) the $N = 2$ case remains trivial.

For illustration purposes, let us notice that for all the potentials of the form (41) with an arbitrary $f_1 \neq f_1^{\{L\}}$, our requirement of sandwiching

$$V^{\{\mathcal{K}+1\}}_{(PES)}(r) < V(r) < V^{\{\mathcal{K}\}}_{(PES)}(r), \qquad r \in (0, \infty) \tag{42}$$

means that

$$f_1 \in (f_1^{\{\mathcal{K}+1\}}, f_1^{\{\mathcal{K}\}}). \tag{43}$$

For all the repulsive Coulomb couplings $g_0 > 0$ (fixed) and attractive (negative) short-range couplings f_1, the number of bound states remains constant in the interval (43).

4.2 Potentials with $N = 3$.

Without any loss of generality, we could have scaled the coordinate r in such a way that $g_0 \to 1$ in eq. (41). Similarly, all the $N = 3$ potentials may be reduced to their respective $T = 1$ and $T = 2$ forms

$$V(r) = \frac{f_2}{r^{5/3}} + \frac{f_1}{r^{4/3}} + \frac{g_0}{r} + \frac{1}{r^{2/3}} \tag{44}$$

and

$$V(r) = \frac{f_2}{r^{5/3}} + \frac{1}{r^{4/3}}. \tag{45}$$

We may skip the latter example as trivial – it represents just another $E = 0$ dual to the Coulomb force. Phenomenologically, it is still worth mentioning: It describes an interesting special PES case of a short-range screening which is significantly weaker than the Coulomb force at large distances.

The former potential combines both the short- and long-range screenings together. It represents one of the simplest models of this type, and it is definitely the simplest nontrivial generalization of the Chhajlany's Coulomb duals. We may re-interpret it as a dual to the unsolvable – sextic – anharmonic oscillators. Its PES property (see below) is in fact inherited from this equivalence and may be traced back to Hautot [12]. Without any recourse to this duality, let us re-describe its (*i.e.*, $N = 3$ and $T = 1$) PES features in the present notation.

First, we derive the trivial $N = 3$ analogue of the $N = 2$ equation (40),

$$f_1 = \frac{1}{4}\, g_0^2 - [2l + 1 + \frac{2}{3}(L + 1)] \tag{46}$$

which has to be accompanied by the single determinantal selfconsistency condition (25),

$$\det Q^{[L]} = 0. \tag{47}$$

At an arbitrary L, the coupling f_2 may be extracted from the latter equation as an eigenvalue.

Due to the tridiagonality of the matrix Q (which is real and may be symmetrized), we get $L + 1$ roots f_2, all of them real. In contrast to the preceding subsection, we only guarantee, by construction, that $\mathcal{K}(L) \le L$ in general.

In the particular $L = 2$ realization of our general scheme, the tridiagonality of equation (47) enables us to re-derive the explicit non-numerical formulas (38) and (39),

$$2\,a\,b\,(a - b)^2 \alpha_1^{\{\mathcal{K}\}} = 3\,[2\,a\,b\,B_1 - (a + b)^2 B_0] \tag{48}$$

$$4\,a\,b\,\alpha_2^{\{\mathcal{K}\}} = 3\,(a + b)\,B_0 - 2\,a\,b\,(a + b)\,\alpha_1^{\{\mathcal{K}\}}. \tag{49}$$

After all the insertions, the final explicit PES formulas follow,

$$\alpha_1^{\{\mathcal{K}\}} = \frac{2}{3}\left(\frac{1}{(a - b)^2} - \frac{3l + 2}{2\,a\,b}\right) > 0 \tag{50}$$

$$\alpha_2^{\{\mathcal{K}\}} = -\frac{a + b}{3}\left(\frac{1}{(a - b)^2} - \frac{3l + 2}{a\,b}\right). \tag{51}$$

4.3 Potentials with $N \geq 4$.

At $N = 4$, the scaling of coordinates "normalizes" the $T = 1$ forces

$$V(r) = \frac{f_3}{r^{7/4}} + \frac{f_2}{r^{3/2}} + \frac{f_1}{r^{5/4}} + \frac{g_0}{r} + \frac{g_1}{r^{3/4}} + \frac{1}{r^{1/2}}. \tag{52}$$

For an independent motivation of interest in these interactions we may remind the reader that in the light of restriction (16), the seemingly $N = 2$ potential

$$V(r) = \frac{f_2}{r^{3/2}} + \frac{g_0}{r} + \frac{1}{r^{1/2}} \tag{53}$$

may be understood as a special case of the full $N = 4$ forces (52).

In comparison with the preceding $N = 3$ examples, the representation of the new $V(r)$'s in terms of the single (or double) square roots of the coordinate seems natural and, in a way, represents a possible "next-to-Coulombic" coordinate-dependence [9]. The flexibility of their shape is very high, in spite of quite a small N. This may simplify the sandwiching of the general forces $V_{(phys)}$.

In a reversal of physical considerations, some of the couplings may be omitted if redundant, provided only that this omission does not violate the underlying PES solvability conditions. The resulting potential models might exemplify the systems tractable by the nonstandard perturbative series (so called δ-expansions [20]) which use exponents (or, more precisely, their deviations from the "solvable" values -2, 0 or 2 [21]) as the "small" expansion parameters.

Mathematically, the PES analysis at $N = 4$ will start from the trivial condition of the type (40) and (46) which, implicitly, reads

$$C^{(N-1)}_{N+L-2} = 0 \tag{54}$$

for $T = 1$. It has to be complemented by some $N-2$ coupled polynomial (determinantal) conditions. Their complexity increases quickly with the growing N. Additional assumptions leading to their simplification may prove vital for their nonnumerical solvability. More details may be found in ref. [16].

In the purely formal context, the $N \geq 4$ solutions are rarely routine. Unexpectedly, they imply that unless we add a further nonzero component (e.g., $f_1 \neq 0$) to our present $N = 2$-like potentials (53), we get no real PES solutions at all. At the same time, an analysis of the respective $T = 2$ and $T = 3$ descendants of our general potential (52),

$$V(r) = \frac{f_3}{r^{7/4}} + \frac{f_2}{r^{3/2}} + \frac{f_1}{r^{5/4}} + \frac{1}{r} \tag{55}$$

and

$$V(r) = \frac{f_3}{r^{7/4}} + \frac{1}{r^{3/2}} \tag{56}$$

may be omitted as trivial, "dual" to their simpler predecessors. To the latter, Coulomb-equivalent case, we may add the same physically oriented comment as to eq. (45) above. The former, unsolvable example exhibits asymptotically sub-Coulombic behaviour. Perhaps, similar forces might simulate the Lennard-Jones-type interactions [8] in some applications, but conjectures of this type would already go too far beyond the scope of the present paper.

5 Summary

Non-numerical determination of the number $\mathcal{K}$ of bound states in some screened Coulomb potentials was presented. The majorizing and minorizing (or mixed – sandwiching) use of these (here called generalized Chhajlany) potentials was proposed. As a number-of-state determination, the technique is applicable to a broad class of phenomenological potentials.

In the technically detailed discussion, we considered all the forces of the form $\sum_\delta h_\delta \, r^\delta$ which were at most weakly singular in the origin and disappeared in infinity. We came to the conclusion that the problem of the explicit non-numerical determination of their number of bound states $\mathcal{K}$ remains very easily tractable for the two large subclasses of interactions.

The first tractable subclass was specified as supporting not too many (symbolically, $L + 1$) bound states. The second subclass was characterized by the functional simplicity of the bracketing PES potentials: Exponents δ were assumed given as some very simple fractions ($\delta = integer/N$ with a small denominator N). In both these cases, the values of the PES coupling constants were shown obtainable as roots of certain coupled algebraic Magyari-type equations.

Mathematically, the main difficulty was found in a (generally, missing) guarantee of existence of the real solutions. In contrast to the recent and very popular $E \neq 0$ and $N_{BS} = \infty$ constructions of the partial exact solutions within confining potential wells, we have shown that in the present case, the underlying algebraic Magyari-type equations often admit a linearization. After a suitable choice of independent variables, the present PES constructions seem simpler in comparison with confining cases.

Another source of simplifications has been found in a possible disappearance of some auxiliary parameters (characterized, e.g., by an integer T). In the overall structural analogies of our $E = 0$ PES solutions to their confining dual predecessors, the concept of the Schwinger duality proved useful far "beyond the realm of the known exact solutions": There, in accord with the Chhajlany's sceptical remark, its use seemed "out of the question" [7].

In a numerical setting, an important role may be played by an immanent unstability of bound states $\psi^{\{\mathcal{K}\}}(r)$ at threshold. In some "sufficiently regular" cases, one might still hope to follow the present scheme and, in accord with the recommendation of one of the referees, try to construct the "selfconsistent" bracketing wavefunctions with $\mathcal{K} < \infty$ for any suitable class of potentials.

In particular, the numerically oriented approach of this type might represent a viable alternative to the present algebraic treatment of the very complicated potentials and/or of the very large $\mathcal{K}$'s. Any reliable alternative numerical solution[22] could then serve our "node-counting" purposes equally well.

In an opposite, purely analytic context, a natural continuation of our present study may be sought in an exploration of resonances. Unfortunately, the state of our understanding of the structure of solutions of the screened Coulomb forces in the analytically continued variables (cf., e.g., [23]) seems rather restricted and technically discouraging.

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