J. Phys. A: Math. Gen. 29 (1996) 6443 - 53

Screened Coulomb potential $V(r) = (\alpha + \beta\, r)/(\gamma + \delta\, r)$ in a semi-relativistic Pauli-Schrödinger equation

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Abstract

The well known quasi-exact solvability of Schrödinger equation with Coulomb-like potentials $V(r) = (\alpha + \beta\, r)/(\gamma + \delta\, r)$ is shown to survive a minimally relativistic improvement of the kinetic energy operator $\frac{1}{2m}\hat{p}^2 \to \frac{1}{2m}\hat{p}^2/(1 + \frac{1}{4m^2c^2}\hat{p}^2)$.

1 Introduction

A complete solvability of Schrödinger equation

$$T\,\psi + V\,\psi = E\,\psi \tag{1}$$

with the standard kinetic energy operator $T = \hat{p}^2 \equiv -\triangle$ (units $\hbar = 2\,m = 1$) is a privilege and merit of just a few elementary potentials (e.g., Coulomb $V(\vec{r}) \sim 1/|\vec{r}|$ etc. [1]). Most distortions of these forces require a perturbative or purely numerical treatment [2]. Only after we restrict interaction to a single partial wave, we may significantly extend the class of solvable models, e.g., via supersymmetry [3] or quantum inversion [4]. This inspired a futher weakening of the concept of solvability to a mere finite subset of all the energy levels [5]. The subsequent extensive study of the related partially non-numerical systems (so called "quasi-exact" models as reviewed in the magnificent monograph [6]) is not finished yet [7].

At the higher energies, Schrödinger equation (1) is often being replaced by the Dirac-type equations [8] or, at least, improved by an inclusion of some selected relativistic corrections [9] – one may employ $T = T^{(\mathrm{Pauli})} = \hat{p}^2 - \lambda\hat{p}^4$, $\lambda = 1/c^2$ [10] in the Pauli-type equation (1), etc. As long as the latter choice of T suffers from several formal shortcomings (e.g., spectrum unbounded from below), our older letter [11] recommended a further replacement of $T^{(\mathrm{Pauli})}$ by its alternative representation

$$T = \frac{\hat{p}^2}{1+\lambda\hat{p}^2} = T^{(\mathrm{Pauli})} + O(\lambda^2). \tag{2}$$

Now, we notice that for several phenomenologically interesting interactions exemplified by the screened Coulombic forces

$$V(r) = \frac{\alpha + \beta\,r}{\gamma + \delta\,r} \tag{3}$$

the nonrelativistic quasi-exact (QE) solvability may survive a transition to the relativistic Klein-Gordon equation [12]. In the present paper, we intend to show that a similar "survival" of the QE property of the non-polynomial interaction (3) may also take place in the intermediate-energy regime as described by our modified Pauli equation (1) with the nonperturbative kinetic energy (2).

2 Modified Pauli equation and its bound states

A trivial re-arrangement converts the modified Pauli equation (1) + (2) with an arbitrary phenomenological potential $V(r)$ into a linear differential equation of the second order,

$$\hat{p}^2(1+\lambda w)\psi + w\psi = 0, \qquad w = V - E, \qquad \hat{p}^2 = -\triangle\ .$$

This is our starting point – abbreviation $\chi = (1+\lambda w)\psi$ returns us back to the Schrödinger-type prescription with a nonlinear dependence on the energy. In its radial, ordinary-equation realization

$$-\frac{\mathrm{d}^2}{\mathrm{d}r^2}\chi(r) + \frac{\ell(\ell+1)}{r^2}\chi(r) + W(r,E)\chi(r) = 0, \qquad W = \frac{w}{1+\lambda w}, \tag{4}$$

one has to vary the angular momentum $\ell = 0, 1, \ldots$ (three dimensions, central forces) or distinguish between the two parities $(-1)^{\ell+1}$ with $\ell = -1$ and $\ell = 0$ (one dimension, a symmetric well).

In our particular example (3), couplings α, β, γ and δ enter the Pauli-Schrödinger eq. (4) via a special form of the quasi-potential,

$$W(r,E) = \frac{A(E) + B(E)\,r}{C(E) + D(E)\,r},$$

$$\left(\begin{array}{cc} A(E) & B(E) \\ C(E) & D(E) \end{array}\right) = \left(\begin{array}{cc} 1 & 0 \\ \lambda & 1 \end{array}\right)\left(\begin{array}{cc} 1 & -E \\ 0 & 1 \end{array}\right)\left(\begin{array}{cc} \alpha & \beta \\ \gamma & \delta \end{array}\right). \tag{5}$$

This matrix formula is easily invertible. Under the assumption $D(E) \neq 0$ we have

$$W(r,E) = \frac{B(E)}{D(E)} + O(1/r), \qquad r \gg 1$$

and infer the possible existence of bound states at the real and energy-dependent exponents $\Omega = \Omega(E) = \sqrt{B(E)/D(E)} > 0$ in asymptotics $\chi(r) \approx \exp[-\Omega\, r]$, $r \gg 1$.

At the finite coordinates $r < \infty$, a pole singularity in $w(r,E)$ or $W(r,E)$ must be compensated by a zero in the wavefunction. The properly modified differential equation (4),

$$[-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{\ell(\ell+1)}{r^2}][C(E) + D(E)\,r]\chi_0(r) + [A(E) + B(E)\,r]\chi_0(r) = 0,$$

for

$$\chi_0(r) = \frac{\chi(r)}{C(E) + D(E)\, r} \equiv \frac{\psi(r)}{\gamma + \delta\, r}$$

admits then the power-series solution

$$\chi_0(r) = \mathrm{e}^{-\Omega\, r} \sum_{m=0}^{M} h_m\, r^{m+\ell+1} \qquad M \geq 0 \tag{6}$$

with $h_0 \neq 0$ and, generically, with $M = \infty$. Such an Ansatz leads to the standard recurrences

$$\begin{gathered} B_m\, h_{m+1} + A_m\, h_m + C_m\, h_{m-1} = 0, \\ B_m = -\,(m+1)(m+2\ell+2)C(E), \\ A_m = -\,(m+1)(m+2\ell+2)D(E) + 2\,(m+\ell+1)\Omega(E)\, C(E), \\ C_m = A(E) - \Omega^2(E)\, C(E) + 2\,(m+\ell+1)\Omega(E)\, D(E), \qquad m = 0, 1, \ldots\ . \end{gathered} \tag{7}$$

Their first few rows need not necessarily be treated numerically – we may immediately replace them by the explicit, closed and rigorous determinantal definition of the Taylor coefficients,

$$h_{m+1} = h_0 \frac{(-1)^{m+1}}{B_0 B_1 \ldots B_m} \det \begin{pmatrix} A_0 & B_0 & & & & \\ C_1 & A_1 & B_1 & & & \\ & C_2 & A_2 & B_2 & & \\ & & & \ldots & & \\ & & C_{m-1} & A_{m-1} & B_{m-1} & \\ & & & C_m & A_m & \end{pmatrix}. \tag{8}$$

Here, we shall pay attention to the special, terminating solutions only. With $h_M \neq 0$ and $h_{M+1} = h_{M+2} = \ldots = 0$ at some $M < \infty$, this makes recurrences (7) degenerate to an overdetermined system of $M+2$ algebraic equations ($m = 0, 1, \ldots, M+1$) for mere $M+1$ arbitrarily normalized coefficients h_m ($m = 0, 1, \ldots, M$). Hence, besides the standard secular equation, one must also satisfy an additional condition $C_{M+1}\, h_M = 0$, i.e., $C_{N+1} = 0$ [6]. The latter additional QE-solvability condition implies that the matrix element $A(E)$ ceases to be independent and becomes a prescribed function of M,

$$A(E) = \Omega^2(E)\, C(E) - 2\Omega(E)\, (M+\ell+2) D(E). \tag{9}$$

As a conseqeuence, we may abbreviate $C_m = 2\,(m - M - 1)\Omega(E)\,D(E)$ and equation (8) with $m = 0, 1, \ldots, M-1$ will specify the explicit QE wavefunctions (6) completely. By construction, these wavefunctions remain normalizable at an arbitrary energy, but the last, $m = M$ line of recurrences must still be taken into account. As a formal boundary condition $h_{M+1} = 0$, it fixes the energies at their discrete physical values and may be re-assigned the standard "Hill-determinant" meaning

$$\det \left(\begin{array}{cccccc} A_0 & B_0 & & & & \\ C_1 & A_1 & B_1 & & & \\ & C_2 & A_2 & B_2 & & \\ & & & \ldots & & \\ & & C_{M-1} & A_{M-1} & B_{M-1} \\ & & & C_M & A_M \end{array} \right) = 0 \qquad (10)$$

of a secular equation with non-variational origin. Its matrix elements are real but the whole equation does not posses a symmetric-matrix character. The presence of an imaginary component in its energy roots $E{=}E_j$ cannot be excluded a priori [13].

Our more than ten years old study of the latter problem [11] was motivated by the phenomenological importance of the linearly growing forces and paid attention just to the $\delta = 0$ special case of our present class of potentials (3). As a consequence, we arrived at a conclusion that the calculations of the QE energies may only be performed numerically, due to an exceptional, degenerate form of our first QE-solvability condition (9) at $\delta = 0$. Indeed, after a re-scaling of the couplings ($\gamma \to 1$) and with a properly shifted energy scale ($\alpha \to 0$) it remains energy-independent,

$$2\,(M + \ell + 2)\beta = \lambda^{-3/2}$$

but its right-hand-side value is very large and implies that the QE-compatible dimension M must be also quite large for all the couplings of an immediate physical interest, say, in quarkonium physics ($\beta = O(1)$). As long as the complexity of our secular equation (10) increases with M, one may only generate the QE energies by a suitable numerical algorithm. In what follows, the linearly growing, $\delta = 0$ special cases $V(r) = \alpha + \beta\, r$ of our potential (3) will be omitted as quasi-numerical.

3 QE bound states at $\delta \neq 0$

Let us assume that our $V(r)$ is asymptotically finite, $\delta \neq 0$. As long as, identically,

$$V(r) - E = \frac{\alpha + \beta\, r}{\gamma + \delta\, r} - E = \frac{\beta}{\delta} - E + \frac{\alpha - \beta\gamma/\delta}{\gamma + \delta\, r}$$

we shall re-gauge $\delta = 1$ and shift the energy scale (i.e., fix $\beta = 0$). For the physical reasons, we shall also denote $\alpha = -e^2$ and $E = -\kappa^2$ and assume that e and κ are real, $\alpha < 0$ and $E < 0$ (otherwise, the potential would be repulsive and normalizable bound states would not exist at all). As long as we have $\Omega \equiv \sqrt{\kappa^2/(1+\lambda\,\kappa^2)} < 1/\sqrt{\lambda}$ and, conversely, $\kappa^2 = \Omega^2/(1-\lambda\,\Omega^2)$, binding energies will also be "measured" by the exponents Ω themselves.

In the light of eq. (5) which gives $A(E)\,D(E) - B(E)\,C(E) = \alpha\,\delta - \beta\,\gamma$, our first QE solvability condition (9) appears considerably simplified in the new notation,

$$e^2\,(1 - \lambda\Omega^2)^2 = 2\,(M + \ell + 2)\,\Omega. \qquad (11)$$

It may be replaced by closed formulae (i.e., roots of a biquadratic equation – see Appendix A). In practice, it seems much easier to change our point of view and re-visualise our first QE solvability condition (11) simply as a specification of the unique charge e^2 defined as a function of the exponent Ω or as a function of the input or trial energy E itself, $e^2 = e^2(\Omega)$, $\Omega = \Omega(E)$.

For an illustrative demonstration of existence of at least one QE solution, let us contemplate a trivial case first, with the $M = 0$ representation of the second QE constraint (10). This gives $\gamma = \lambda e^2/D + 1/\Omega$, i.e.,

$$\gamma\Omega = 1 + 2(\ell + 2)\frac{\lambda\Omega^2}{1 - \lambda\Omega^2}, \qquad M = 0. \qquad (12)$$

We see that our second constraint (12) defines the shift γ in QE potential (3) as another function of the same optional Ω. The numerical value of the shift γ remains real. The absence of a singularity of $V(r)$ on the real axis is guaranteed by its positivity, $\gamma \geq 0$. Thus, the whole family of our QE states may be "numbered" by the variable $\Omega \in (0, 1/\sqrt{\lambda})$.

In the limit $\lambda \to 0$, our semi-relativistic $M = 0$ solution degenerates to its non-relativistic QE partner. The exponent Ω coincides with the momentum, $\Omega \to \kappa$. Both these quantities acquire a fixed value $\kappa = e^2/(2\ell + 4)$ at a particular QE-compatible shift $\gamma = (2\ell + 4)/e^2$. Thus, the limiting transition is smooth and our semi-relativistic construction offers a nonstandard, nonperturbative insight into the onset and/or overall role of relativistic corrections in the QE context.

At the higher truncations M, a solution of the second QE condition (10) is less obvious. Nevertheless, after an abbreviation $Z \equiv \Omega(E)C(E)/D(E)$ and in terms of the new matrix elements $U_0 = 1(2\ell + 2)$, $U_1 = 2(2\ell + 3)$, $U_2 = 3(2\ell + 4), \ldots$ and $V_0 = 2(\ell + 1)$, $V_1 = 2(\ell + 2)$, $\ldots$, we arrive at a much more transparent equation

$$\det \left(\begin{array}{cccccc} U_0 - V_0 Z & U_0 Z & & & & \\ 2M & U_1 - V_1 Z & U_1 Z & & & \\ & 2M-2 & U_2 - V_2 Z & U_2 Z & & \\ & & & \ldots & & \\ & & 4 & U_{M-1} - V_{M-1} Z & U_{M-1} Z & \\ & & & 2 & U_M - V_M Z & \end{array} \right) = 0. \quad (13)$$

Its roots form the M- and ℓ-dependent $(M + 1)$-plets $Z_j(M, \ell)$, $j = 1, 2, \ldots, M + 1$ which do not depend on the potential,

$$Z_1(0, \ell) = 1, \qquad Z_{1,2}(1, \ell) = \frac{1}{2} \left(3 \mp \sqrt{1 + \frac{4}{\ell + 2}} \right), \qquad \ldots. \quad (14)$$

Having their values at our disposal, we shall be able to return to the original definition $Z = \Omega C/D$ and insert $C(E) = \gamma D(E) - \lambda e^2$ and $D(E) = 1/(1 - \lambda \Omega^2)$ there, giving

$$\gamma \Omega = Z_j(M, \ell) + \lambda e^2 \Omega \, (1 - \lambda \Omega^2). \quad (15)$$

This is our second QE solvability condition: Once we eliminate e^2 by means of eq. (11), such a formula generalizes its $M = 0$ predecessor (12) to an arbitrary M.

The value of Z merely interrelates the energy (represented here by Ω), coupling e^2 and the formal shift of the Coulomb centre γ. Our $M = 0$ conclusions may be extended to an arbitrary M. In addition to our first QE condition (11) which specifies the QE-compatible charge $e^2 \equiv e^2(\Omega)$, our second QE condition (15) may be interpreted as an equation which defines the second QE-compatible and, correctly, non-negative "shift-of-screening" $\gamma = \gamma(\Omega)$ in terms of the same optional variable or "parameter" Ω.

An explicit evaluation of the "auxiliary quantum numbers" Z is easy at the smallest M (cf. its $s-$wave sample in Appendix B). Beyond $M = 3$, Table 1 offers an illustration of their numerical values. Let us underline an interesting empirical observation: All these Z's remain real.

4 The pairs of elementary bound states

In a way underlined in [14] and re-illustrated in [15], there are many (e.g., perturbative or numerical) applications of QE models where a real difficulty in their construction only starts when one needs a multiplet of bound states. Such a methodical challenge may be enhanced, in our specific screened Coulomb case, by an immediate physical appeal of a feasiblity of a two-level simulation of a radiative (i.e., directly measurable) quantum transition.

In the language of sect. 3, the construction of doublet is trivial – a pair of our QE-compatibility equations (subscripted by $J = 1, 2$) must be concatenated. A series of changes of variables is suitable for such a purpose – its thorough description is relegated to Appendix C. In its notation with $L = L_J$ and abbreviation $Y^2 = Y_J^2 = (R_{j_J} + S_{j_J})\ L_J$, two versions of eq. (25) may be converted into the two alternative (and independent) definitions of the QE-doublet-compatible coupling e itself,

$$e^4 = e^4(J) = \frac{1 + Y_J}{Y_J^4}(R_{j_J} + S_{j_J})^2, \quad J = 1, 2. \tag{16}$$

Introducing further a symbol $a_J = R_{j_J}/(R_{j_J} + S_{j_J})$ (with any j_J's from the segment $1, 2, \ldots, M_J + 1$, see Tables 2 and 3 for a numerical sample), the pair of the second QE conditions (29) reads,

$$G = G(J) = \frac{1 - a_J\, Y_J^2}{Y_J^4}(R_{j_J} + S_{j_J})^2, \quad J = 1, 2. \tag{17}$$

As long as the physical "coupling" e^4 and "shift" G must remain state-independent, one arrives at the final, mutually coupled compatibility conditions

$$e^4(1) = e^4(2), \qquad\qquad G(1) = G(2). \tag{18}$$

They are easily convertible into the coupled polynomial equations for the "unknown" Y_1 and Y_2, tractable by the standard Gröbner-basis method [16]. Alternatively, one might also replace eq. (18) by an equivalent pair,

$$e^4(1)/G(1) = e^4(2)/G(2), \qquad\qquad G(1) = G(2) \tag{19}$$

which is reducible to a single equation immediately – the first item is just a quadratic (i.e., solvable) equation in Y_1 or Y_2 while the second item remains a quadratic (i.e., solvable) equation in Y_1^2 or Y_2^2. Nevertheless, an important merit of the former arrangement is that we know the number of the roots in the complex plane at least. This excludes an omission of a solution due to a numerical rounding error.

In the units $\lambda = 1$ of Appendix C, let us fix, say, $\ell = 0$ and pick up, say, $M = M_1 = 0$, $M = M_2 = 1$. We avoid the $M_2 = 1$ ambiguity in eq. (14) by taking just the smaller $Z_1(1,0)$. Then, both our alternative equations (18) and (19) fix, numerically, the same values of $G = 51.9453947034780$ and of the related charge, $e^4 = 25.7700913886009$. The existence of at least one QE doublet of bound states is proved.

In a more systematic search for the further QE doublets, one may start from any trial quantum numbers (M_1, j_1, M_2, j_2) or their two functions $Z_{j_1}(M_1, \ell)$ and $Z_{j_2}(M_2, \ell)$. We have found no obvious pattern in the existence/non-existence of the real and doublet-compatible QE roots G. For example, our search failed at

$$(M_1, j_1, M_2, j_2) = (0, 1, 1, 2), (0, 1, 2, 2), (0, 1, 2, 3), (0, 1, 3, 1)$$

etc, with the last failure $(M_1, j_1, M_2, j_2) = (6, 7, 7, 8)$ sitting at the very end of our pre-determined range. A complementary sample of a few *succesful* numerical identifications of the real QE doublets is displayed, as a climax of our paper, in its final Table 3.

5 Summary

We have demonstrated that a certain class of Pauli-type equations (cf. (1) – (3)) may parallel its non-relativistic Schrödinger predecessors in possessing a few exceptional elementary (i.e., QE) bound-state solutions. Within a more or less standard physical model (viz., a screened Coulomb interaction (3) [12]) we constructed these solutions in an explicit form. In spite of our older and discouraging non-Coulombic experience made in ref. [11], we picked up the same re-arranged Pauli-Schrödinger differential equation. Our present extension of the class of forces preserved its simplified second-order differential form and, less obviously, did not also violate the applicability of the standard power-series method.

We were able to show that the validity and preservation of the QE solvability smoothly interconnects the non-relativistic ($\lambda = 0$) and semi-relativistic ($0 < \lambda \ll 1$) kinematical regimes. On a more technical level, our construction exhibits several satisfactory features: The elementary form of wavefunctions (polynomials of degree $M + 1$ pre-multiplied by the correct asymptotical factor $\mathrm{e}^{-\Omega r}$), the elementary Taylor coefficients (= "Hill" determinants of dimensions $\leq M$) etc. Also the related QE-solvable potentials $V(r)$ proved specified in an uncomplicated manner – we succeeded in expressing their parameters $\alpha - \delta$ as elementary functions of the single free variable Ω.

A formal reason for such an (unexpected) simplicity lies in the underlying reducibility or "factorization" of the pertinent "boundary condition" $h_{M+1} = 0$ into a universal (i.e., only *implicitly* M-dependent) algebraic formula (cf., e.g., eq. (15)) preceded by another, potential-independent specification of certain auxiliary functions ($\equiv Z_j$) of M. This may be interpreted as a support and encouragement of a future continuation of the semi-relativistic QE constructions: Their complexity need not necessarily grow with M. Here, it was a pleasant surprise to notice such an effective M-independendence of our constructions, quite unexpected and, perhaps, characteristic for a new role which might be played by nonperturbative kinematical corrections.

A few further formal consequences of the separation of the $M-$ and $V-$ dependence were also extracted. One of them lies in the possiblility of the alternative partial linearizations of the underlying algebraic system of equations. This was shown to lead to several “non-equivalent” non-numerical specifications of the separate QE states. In a climax of our paper, we have shown that the same potential $V(r)$ may even generate the two different QE states at once. Unfortunately, the underlying doubly selfconsistent specification of the nontrivial multiplet solutions already ceases to be tractable by elementary means. Non-numerically, we have only reduced it to a problem of determination of certain auxiliary roots of a sixteenth-degree polynomial. A few samples of the resulting rigorous QE doublets were tabulated.

We may conclude that, in the light of the well know difficulty of making quantum mechanics at least approximatively compatible with relativistic kinematics [17, 9], our present nonperturbative semi-relativistic QE constructions are encouraging. In contrast to ref. [11], no nonrelativistic singularity of the type $M \to \infty$ has been detected. Along with the smooth $\lambda \to 0$ behaviour of our new QE states, also the challenging problem of multiplets proved manageable. At the same time, the well known role of certain dynamical-like Lie structures in the QE context (cf., e.g., review [14] with further references) stays unclear in the new kinematical domain. Still, we may express a belief that a broader class of applications of the QE solvability (viz., numerical tests, perturbatived interpolations as well as straight phenomenology [6]) may be expected to survive an introduction of a minimal relativity into quantum mechanics.

Appendix A.

The first QE condition as a biquadratic equation

At the given quantum numbers M and ℓ, equation (11) assigns at most four different (though, in general, complex) "energy candidates" $\Omega = \Omega_j$, $j = 1, 2, 3, 4$ to the coupling e^2. Re-scaling, for simplicity,

$$\Omega_j^{(M,\ell)}(E) = \frac{e^2}{2(M+\ell+2)} X_j^2 \tag{20}$$

we may immediately spot the two complex roots Ω_3 and Ω_4 as unphysical and, in the next step, split eq. (11) into the pair of relations

$$1 - \eta^2 X_j^4 + (-1)^j X_j = 0, \quad j = 1, 2, \quad \eta^2 = \frac{\lambda e^4}{(2M + 2\ell + 4)^2}. \tag{21}$$

They may be understood as a single equation on the whole real axis, with the two real roots $X_1 < 0 < X_2$.

Equation (21) provides an unambiguous numerical definition of the two physically acceptable (i.e., real and positive) quantities (20) such that $0 < X_1^2 < \eta < X_2^2$. At the small η's the squares of our new η-dependent roots may be expanded in the power series,

$$X_1^2 = 1 - 2\eta^2 + 9\eta^4 - 52\eta^6 + \ldots,$$

$$X_2^2 = \eta^{-4/3} + 2\eta^{-2/3}/3 - 1/3 + 28\eta^{2/3}/81 - \ldots$$

where, of course, $\eta = \eta(e, M, \ell)$. Simultaneously, at the large variables η we may put $g = g_{1,2} = \pm 1/\sqrt{\eta}$ and derive the asymptotic series

$$X_{1,2}^2 = g^2 + g^3/2 - g^5/64 + g^6/128 - 9g^7/4096 + \mathrm{O}(g^8).$$

Appendix B.

Auxiliary parameters in the second QE solvability constraint: An s-wave example

The compact polynomial structure of the Hill-determinant conditions (13) may be illustrated on their $\ell = 0$ special cases,

$$\begin{array}{c} 2 - 2\,Z = 0, \qquad M = 0 \\ 12 - 24\,Z + 8\,Z^2 = 0, \qquad M = 1 \\ 144 - 432\,Z + 288\,Z^2 - 48\,Z^3 = 0, \qquad M = 2 \\ 2880 - 11520\,Z + 11520\,Z^2 - 3840\,Z^3 + 384\,Z^4 = 0, \qquad M = 3 \\ \ldots . \end{array} \tag{22}$$

Besides their above-mentioned single root $Z_1(0,0) = 1$ and the pair $Z_1(1,0) = \left(3 - \sqrt{3}\right)/2 \approx 0.6339745960$ and $Z_2(1,0) = \left(3 + \sqrt{3}\right)/2 \approx 2.366025404$, one may also write down, easily, the triplet of roots of the cubic $M = 2$ equation (22). It is best represented in a trigonometric form,

$$Z_1(2,0) = 2 - 2\cos\frac{2\,\pi}{9} \approx 0.4679111135, \quad Z_2(2,0) = 2 - 2\sin\frac{\pi}{18} \approx 1.652703645,$$
$$Z_3(2,0) = 2 + 2\cos\frac{\pi}{9} \approx 3.879385242, \tag{23}$$

although the more usual Cardano formulae also remain reasonably transparent, giving $Z_3(2,0) = 2 + 2^{-1/3}\sqrt[3]{1 + \mathrm{i}\sqrt{3}} + 2^{1/3}/\sqrt[3]{1 + \mathrm{i}\sqrt{3}}$, etc.

In terms of the angle φ such that $\tan 3\varphi = \sqrt{5/3}$, an unexpectedly and unusually compact representation of the auxiliary Z's remains also available at $M = 3$ and all the subscripts $j = 1, 2, 3, 4$,

$$2 \times Z_j(3,0) = 5 + (-1)^{entier[(j+4)/2]} 5^{1/4} \sqrt{\sqrt{5} - \sqrt{8}\cos(\varphi + \pi/6)}$$
$$+(-1)^{entier[(j+1)/2]} 5^{1/4} \sqrt{\sqrt{8}\sin(\varphi + \pi/3) + \sqrt{5}} + (-1)^j 5^{1/4} \sqrt{\sqrt{5} - \sqrt{8}\sin\varphi}.$$

An algebraic counterpart of this formula is already less comfortable.

Appendix C.

A re-parametrization of the QE formulae

Our simultaneous parametrization of the charge $e = e(\Omega)$ (eq. (11)) and of its QE-compatible shift $\gamma = \gamma(\Omega)$ (eq. (15)) uses an input specification of the energy $E \in (-\infty, 0)$ or of the exponent $\Omega = \Omega(E) \in (0, 1/\sqrt{\lambda})$. Such a parametrization is not unique: An alternative QE construction may start from a re-defined coupling $e^2 = e^2(F,G) = \sqrt{G/(1+F)}$ and shift $\gamma = \gamma = \gamma(F,G) = \lambda\, F\, \sqrt{G/(1+F)}$, i.e., from a re-parametrized potential (3),

$$V(r) = -[\lambda\, F + (\sqrt{(1+F)/G})\, r]^{-1}.$$

In a preparatory step, let us introduce the further auxiliary constants

$$S = Z_j(M,\ell)/\sqrt{\lambda}, \qquad R = 2\,(M+\ell+2)/\sqrt{\lambda} - Z_j(M,\ell)/\sqrt{\lambda} \tag{24}$$

and re-emphasize their potential-independent character. Each of them carries the information contained in, and extracted from, eq. (13). The value of R (or S) may be used in place of the triplet of integers j, M and ℓ, as a unique characteristics of a selected QE bound state. The positivity, an unexpected property of these "quasi-quantum" numbers is empirically documented in Tables 1 and 2. Their range may be extended up to certain $M_{max} > 7$ if necessary – our hypothesis is that $M_{max} = \infty$.

A core of our further effort will lie in the elimination of the energy variables, re-scaled as $E \to K = \sqrt{\lambda}\Omega$. The set of the pertaining QE conditions consists of the biquadratic eq. (11),

$$K^4 - 2\,K^2 - \frac{R+S}{e^2}\,K + 1 = 0 \tag{25}$$

accompanied by the cubic eq. (15),

$$K^3 + (F-1)\,K - S\,e^{-2} = 0. \tag{26}$$

We may notice that λ, the measure of smallness of relativistic corrections, is only present here via R, S and F. For convenience, we shall work in units $\lambda = 1$.

The subtraction of eq. (25) from eq. (26) pre-multiplied by K eliminates both the fourth and third powers of K from the resulting new equation

$$(F+1)\,K^2 + \frac{R}{e^2}\,K - 1 = 0. \tag{27}$$

Subtracting also eq. (26) pre-multiplied by $F+1$ from the new eq. (27) pre-multiplied by K, we get rid of the third power of K in the second old equation (26),

$$R\,K^2 - e^2F^2K + S\,(1+F) = 0. \tag{28}$$

After a slight modification of variables, $K \to L = K/e^2$ and $e \to G = (1+F)\,e^4$, equation (27), namely,

$$G\,L^2 + R\,L - 1 = 0 \tag{29}$$

becomes complemented, via an analogous subtraction procedure, by the linear relation

$$(R^2 + G\,F^2)\,L = R + (1+F)^2\,S. \tag{30}$$

In the final step, a supplementary, independent linear definition of the "energy" L is obtained,

$$[R + (1+F)^2\,S]\,L = F^2 - (1+F)^2\,R\,S/G \tag{31}$$

and makes our goal virtually achieved; once we abbreviate $\Gamma = G\,F^2/R^2$ and introduce another positive auxiliary function $\sigma = \sigma(F) = (1+F)^2S/R$, an easy elimination of L results in the single QE-compatibility condition formulated as a restriction imposed upon Γ's themselves,

$$(\Gamma+1)\,(\Gamma-\sigma) = \left(\frac{1+\sigma}{F}\right)^2\Gamma. \tag{32}$$

The requirement of positivity makes the root $\Gamma = \Gamma(F)$ unique,

$$2\,\Gamma = \left(\frac{\sigma+1}{F}\right)^2 + \sigma - 1 + (\sigma+1)\sqrt{\left(\frac{\sigma+1}{F^2}\right)^2 + 2\,\left(\frac{\sigma-1}{F^2}\right) + 1}, \qquad \sigma = \sigma(F). \tag{33}$$

It even satisfies a slightly stronger inequality $\Gamma > \sigma > 0$ and specifies the correct QE coupling $e^4 = \Gamma R^2/(1+F)F^2$ as well as the related bound-state energy E,

$$E = -\frac{\Gamma - \sigma}{1 + \sigma + (1+F)\,F} \tag{34}$$

i.e., $E = -(1 - RL)/(F + RL)$, with the slightly simpler subexpression

$$R\,L = \sigma(F) + 1 + \frac{F^2\sigma(F)}{\sigma(F)+1} + \sqrt{(\sigma(F) + 1 + F^2)^2 - 4\,F^2}.$$

We may notice that the energy E is defined as a closed function of the parameter F so that, in section 4, the “shift” $F = \gamma/(\lambda e^2)$ may play the same role as the exponent Ω did in the formulae of sect. 3.

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Table 1. Numerical roots $Z_j(M, 0)$ of Hill determinants (13) at $M \leq 7$.

M				
0	1.0000000000			
1	0.6339745960	2.366025404		
2	0.4679111135	1.652703645	3.879385242	
3	0.3716459640	1.285817504	2.865589376	5.476947156
4	0.3085154266	1.056482979	2.305416576	4.199533486
	7.130051533			
5	0.2638340609	0.8981499048	1.938320760	3.459408283
	5.617305215	8.822981776		
6	0.2305121099	0.7817930948	1.676025251	2.958148625
	4.710349692	7.097082774	10.54608845	
7	0.2046917866	0.6924815924	1.478127278	2.590971551
	4.080854844	6.035027563	8.624867763	12.29297762

Table 2. The positivity of differences $R_j(M,0)$ in eq. (24) at $M \leq 7$.

M				
0	3.0000000000			
1	5.366025404	3.633974596		
2	7.53208888650	6.347296355	4.120614758	
3	9.628354036	8.714182496	7.134410624	4.523052844
4	11.6914845733	10.9435170210	9.694583424	7.800466514
	4.86994846700			
5	13.7361659391	13.1018500951	12.06167924	10.5405917170
	8.382694785	5.177018224		
6	15.7694878900	15.2182069052	14.3239747489	13.041851375
	11.289650308	8.90291722600	5.45391155	
7	17.7953082133	17.3075184075	16.5218727219	15.4090284490
	13.919145156	11.9649724370	9.37513223700	5.70702238

Table 3. A sample of the semi-relativistic QE bound-state doublets, supported by the screened Coulomb potential (3) at $\ell = 0$, energies $Y_J = \sqrt{2\,(M_J + \ell + 2)\,L_J(E_J)}$ and auxiliary quantum numbers $a_J = R_{j_J}(M_J, \ell)/(2\,M_J + 2\,\ell + 4)$.

quantum numbers						energies		couplings	
M_1	j_1	M_2	j_2	a_1	a_2	Y_1	Y_2	e^4	$G(\gamma)$
0	1	1	1	.750	.894	$-.67184671$	$-.76052323$	25.770092	51.945395
0	1	2	1	.750	.942	$-.69757690$	$-.84058835$	20.434620	42.909415
0	1	4	1	.750	.974	$-.71892014$	$-.91724335$	16.835542	36.678199
0	1	5	1	.750	.981	$-.72392432$	$-.93680117$	16.083311	35.359031
0	1	7	1	.750	.989	$-.72964837$	$-.95999412$	15.261404	33.910198
1	1	2	1	.750	.942	$-.82148027$	$-.87231988$	14.112377	31.342168
1	1	2	3	.894	.515	.48223464	.56439782	986.70165	527.23704
1	2	2	1	.606	.942	$-.30387815$	$-.34551889$	2938.9344	3985.7470
1	2	2	2	.606	.793	$-.53703231$	$-.59843910$	200.37869	357.21172
6	6	7	8	.556	.317	.25034858	.26638196	81487.410	62898.949