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# 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  $(1/2m)\hat{p}^2 \rightarrow (1/2m)\hat{p}^2/(1 + (1/4m^2c^2)\hat{p}^2)$ .

## 1. Introduction

Complete solvability of the Schrödinger equation

$$T\psi + V\psi = E\psi \quad (1)$$

with the standard kinetic energy operator  $T = \hat{p}^2 \equiv -\Delta$  (units  $\hbar = 2m = 1$ ) 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, may we significantly extend the class of solvable models, e.g., via supersymmetry [3] or quantum inversion [4]. This inspired a further 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 yet finished [7].

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

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

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

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

the non-relativistic 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

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'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 non-perturbative 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 second-order differential equation

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

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

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

one has to vary the angular momentum  $\ell = 0, 1, \dots$  (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), the couplings  $\alpha, \beta, \gamma$  and  $\delta$  enter the Pauli–Schrödinger equation (4) via a special form of the quasi-potential:

$$W(r, E) = \frac{A(E) + B(E)r}{C(E) + D(E)r} \quad (5)$$

$$\begin{pmatrix} A(E) & B(E) \\ C(E) & D(E) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ \lambda & 1 \end{pmatrix} \begin{pmatrix} 1 & -E \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}.$$

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

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

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 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)

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

for

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

then admits the power-series solution

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

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

$$B_m h_{m+1} + A_m h_m + C_m h_{m-1} = 0$$

$$B_m = -(m+1)(m+2\ell+2)C(E)$$

$$A_m = -(m+1)(m+2\ell+2)D(E) + 2(m+\ell+1)\Omega(E)C(E) \quad (7)$$

$$C_m = A(E) - \Omega^2(E)C(E) + 2(m+\ell+1)\Omega(E)D(E) \quad m = 0, 1, \dots$$

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

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

Here, we shall pay attention to the special, terminating solutions only. With  $h_M \neq 0$  and  $h_{M+1} = h_{M+2} = \cdots = 0$  at some  $M < \infty$ , this makes recurrences (7) degenerate to an overdetermined system of  $M + 2$  algebraic equations ( $m = 0, 1, \dots, M + 1$ ) for merely  $M + 1$  arbitrarily normalized coefficients  $h_m$  ( $m = 0, 1, \dots, M$ ). 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 consequence, we may abbreviate  $C_m = 2(m - M - 1)\Omega(E) D(E)$  and equation (8) with  $m = 0, 1, \dots, M - 1$  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

$$\det \begin{pmatrix} A_0 & B_0 & & & & \\ C_1 & A_1 & B_1 & & & \\ & C_2 & A_2 & B_2 & & \\ & & & \dots & & \\ & & & & C_{M-1} & A_{M-1} & B_{M-1} \\ & & & & & C_M & A_M \end{pmatrix} = 0 \tag{10}$$

of a secular equation with non-variational origin. Its matrix elements are real but the whole equation does not possess 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-year-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 the conclusion that calculation 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 ( $\gamma \rightarrow 1$ ) and with a properly shifted energy scale ( $\alpha \rightarrow 0$ ) 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  $\kappa$  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  $\Omega$  themselves.

In the light of equation (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

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

It may be replaced by closed formulae (i.e. the 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  $\Omega$  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.

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

We see that our second constraint (12) defines the shift  $\gamma$  in QE potential (3) as another function of the same optional  $\Omega$ . The numerical value of the shift  $\gamma$  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  $\lambda \rightarrow 0$ , our semi-relativistic  $M = 0$  solution degenerates to its non-relativistic QE partner. The exponent  $\Omega$  coincides with the momentum,  $\Omega \rightarrow \kappa$ . 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 non-standard, non-perturbative insight into the onset and/or overall role of relativistic corrections in the QE context.

At 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  $U_0 = 1(2\ell + 2)$ ,  $U_1 = 2(2\ell + 3)$ ,  $U_2 = 3(2\ell + 4)$ , ..., and  $V_0 = 2(\ell + 1)$ ,



#### 4. The pairs of elementary bound states

In a manner 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. The attraction of such a methodological challenge may be enhanced, in our specific screened Coulomb case, by an immediate physical appeal of the feasibility of a two-level simulation of a radiative (i.e. directly measurable) quantum transition.

In the language of section 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 variable 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 equation (C2) may be converted into the two alternative (and independent) definitions of the QE-doublet-compatible coupling  $e$  itself:

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

Introducing further a symbol  $a_J = R_{j_j}/(R_{j_j} + S_{j_j})$  (with any  $j_j$ 's from the segment  $1, 2, \dots, M_J + 1$ , see tables 2 and 3 for a numerical sample), the pair of the second QE conditions (C6) reads

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

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

$$e^4(1) = e^4(2) \quad G(1) = G(2). \quad (18)$$

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 equation (18) by an equivalent pair

$$e^4(1)/G(1) = e^4(2)/G(2) \quad G(1) = G(2) \quad (19)$$

which is immediately reducible to a single equation: 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 precludes 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 (14) by taking just the smaller  $Z_1(1, 0)$ . Then, both our alternative equations (18) and (19) fix, numerically, the same values of  $G = 51.945\ 394\ 703\ 4780$  and of the related charge,  $e^4 = 25.770\ 091\ 388\ 6009$ . 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 *successful* numerical identifications of the real QE doublets is displayed in table 3.

**Table 2.** The positivity of differences  $R_j(M, 0)$  in equation (C1) at  $M \leq 7$ .

$M$				
0	3.000 000 000 0			
1	5.366 025 404	3.633 974 596		
2	7.532 088 886 50	6.347 296 355	4.120 614 758	
3	9.628 354 036	8.714 182 496	7.134 410 624	4.523 052 844
4	11.691 484 573 3 4.869 948 467 00	10.943 517 021 0	9.694 583 424	7.800 466 514
5	13.736 165 939 1 8.382 694 785	13.101 850 095 1 5.177 018 224	12.061 679 24	10.540 591 717 0
6	15.769 487 890 0 11.289 650 308	15.218 206 905 2 8.902 917 226 00	14.323 974 748 9 5.453 911 55	13.041 851 375
7	17.795 308 213 3 13.919 145 156	17.307 518 407 5 11.964 972 437 0	16.521 872 721 9 9.375 132 237 00	15.409 028 449 0 5.707 022 38

**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  $a_j = R_{jj}(M_j, \ell)/(2M_j + 2\ell + 4)$ .

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	0.750	0.894	−0.671 846 71	−0.760 523 23	25.770 092	51.945 395
0	1	2	1	0.750	0.942	−0.697 576 90	−0.840 588 35	20.434 620	42.909 415
0	1	4	1	0.750	0.974	−0.718 920 14	−0.917 243 35	16.835 542	36.678 199
0	1	5	1	0.750	0.981	−0.723 924 32	−0.936 801 17	16.083 311	35.359 031
0	1	7	1	0.750	0.989	−0.729 648 37	−0.959 994 12	15.261 404	33.910 198
1	1	2	1	0.750	0.942	−0.821 480 27	−0.872 319 88	14.112 377	31.342 168
1	1	2	3	0.894	0.515	0.482 234 64	0.564 397 82	986.701 65	527.237 04
1	2	2	1	0.606	0.942	−0.303 878 15	−0.345 518 89	2 938.934 4	3 985.747 0
1	2	2	2	0.606	0.793	−0.537 032 31	−0.598 439 10	200.378 69	357.211 72
6	6	7	8	0.556	0.317	0.250 348 58	0.266 381 96	81 487.410	62 898.949

### 5. Summary

We have demonstrated that a certain class of Pauli-type equations (cf equations (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 (namely a screened Coulomb interaction (3) [12]) we constructed these solutions in an explicit form. In spite of our older and discouraging non-Coulombic experience in [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 ( $0 < \lambda \ll 1$ ) kinematic 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  $e^{-\Omega r}$ ), the elementary Taylor coefficients (= ‘Hill’ determinants of dimensions  $\leq M$ ), etc. Also the related QE-solvable potentials  $V(r)$  proved to be specified in an uncomplicated manner: we succeeded in expressing their parameters  $\alpha - \delta$



as elementary functions of the single free variable  $\Omega$ .

A formal reason for such (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., equation (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 note such an effective  $M$ -independence of our constructions, which was quite unexpected and, perhaps, may be characteristic of a new role which might be played by non-perturbative kinematic corrections.

A few further formal consequences of the separation of the  $M$  and  $V$  dependence were also extracted. One of them lies in the possibility 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 self-consistent specification of the non-trivial 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.

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

$$\Omega_j^{(M,\ell)}(E) = \frac{e^2}{2(M + \ell + 2)} X_j^2 \quad (\text{A1})$$

we may immediately spot the two complex roots  $\Omega_3$  and  $\Omega_4$  as unphysical and, in the next step, split equation (11) into the pair of relations

$$1 - \eta^2 X_j^4 + (-1)^j X_j = 0 \quad j = 1, 2 \quad \eta^2 = \frac{\lambda e^4}{(2M + 2\ell + 4)^2}. \quad (\text{A2})$$

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

Equation (A2) provides an unambiguous numerical definition of the two physically acceptable (i.e. real and positive) quantities (A1) such that  $0 < X_1^2 < \eta < X_2^2$ . At small  $\eta$ 's

the squares of our new  $\eta$ -dependent roots may be expanded in the power series

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

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

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

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

**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 by their  $\ell = 0$  special cases:

$$\begin{aligned}
 2 - 2Z &= 0 & M &= 0 \\
 12 - 24Z + 8Z^2 &= 0 & M &= 1 \\
 144 - 432Z + 288Z^2 - 48Z^3 &= 0 & M &= 2 \quad (B1) \\
 2880 - 11520Z + 11520Z^2 - 3840Z^3 + 384Z^4 &= 0 & M &= 3 \\
 & & & \vdots
 \end{aligned}$$

Besides their above-mentioned single root  $Z_1(0, 0) = 1$  and the pair  $Z_1(1, 0) = (3 - \sqrt{3})/2 \approx 0.633\ 974\ 5960$  and  $Z_2(1, 0) = (3 + \sqrt{3})/2 \approx 2.366\ 025\ 404$ , one may also easily write down the triplet of roots of the cubic  $M = 2$  equation (B1). It is best represented in trigonometric form:

$$\begin{aligned}
 Z_1(2, 0) &= 2 - 2 \cos \frac{2\pi}{9} \approx 0.467\ 911\ 1135 \\
 Z_2(2, 0) &= 2 - 2 \sin \frac{\pi}{18} \approx 1.652\ 703\ 645 \\
 Z_3(2, 0) &= 2 + 2 \cos \frac{\pi}{9} \approx 3.879\ 385\ 242
 \end{aligned} \quad (B2)$$

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

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

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

An algebraic counterpart of this formula is already less convenient.

### Appendix C. A re-parametrization of the QE formulae

Our simultaneous parametrization of the charge  $e = e(\Omega)$  (equation (11)) and of its QE-compatible shift  $\gamma = \gamma(\Omega)$  (equation (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  $\gamma = \gamma(F, G) = \lambda F \sqrt{G/(1+F)}$ , i.e. from a re-parametrized potential (3)

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

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

$$S = Z_j(M, \ell)/\sqrt{\lambda} \quad R = 2(M + \ell + 2)/\sqrt{\lambda} - Z_j(M, \ell)/\sqrt{\lambda} \quad (C1)$$

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

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

$$K^4 - 2K^2 - \frac{R+S}{e^2}K + 1 = 0 \quad (C2)$$

accompanied by the cubic equation (15),

$$K^3 + (F-1)K - Se^{-2} = 0. \quad (C3)$$

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

Subtraction of equation (C2) from (C3) pre-multiplied by  $K$  eliminates both the fourth and third powers of  $K$  from the resulting new equation

$$(F+1)K^2 + \frac{R}{e^2}K - 1 = 0. \quad (C4)$$

Also subtracting equation (C3) pre-multiplied by  $F+1$  from the new equation (C4) pre-multiplied by  $K$ , we get rid of the third power of  $K$  in the second old equation (C3):

$$RK^2 - e^2F^2K + S(1+F) = 0. \quad (C5)$$

After a slight modification of variables,  $K \rightarrow L = K/e^2$  and  $e \rightarrow G = (1+F)e^4$ , equation (C4), namely

$$GL^2 + RL - 1 = 0 \quad (C6)$$

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

$$(R^2 + GF^2)L = R + (1+F)^2S. \quad (C7)$$

In the final step, a supplementary, independent linear definition of the ‘energy’  $L$  is obtained:

$$[R + (1+F)^2S]L = F^2 - (1+F)^2RS/G \quad (C8)$$

and makes our goal virtually achieved; once we abbreviate  $\Gamma = GF^2/R^2$  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 the  $\Gamma$ 's themselves:

$$(\Gamma + 1)(\Gamma - \sigma) = \left(\frac{1 + \sigma}{F}\right)^2 \Gamma. \quad (C9)$$

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

$$2\Gamma = \left(\frac{\sigma + 1}{F}\right)^2 + \sigma - 1 + (\sigma + 1)\sqrt{\left(\frac{\sigma + 1}{F^2}\right)^2 + 2\left(\frac{\sigma - 1}{F^2}\right) + 1} \quad \sigma = \sigma(F). \quad (C10)$$

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  $E$ :

$$E = -\frac{\Gamma - \sigma}{1 + \sigma + (1 + F)F} \quad (C11)$$

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

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

We may note 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  $\Omega$  did in the formulae of section 3.

## References

- [1] Newton R G 1982 *Scattering Theory of Waves and Particles* (Berlin: Springer) 2nd edn
- [2] Roychoudhury R, Varshni Y P and Sengupta M 1990 *Phys. Rev. A* **42** 184
- [3] Samsonov B F 1995 *J. Phys. A: Math. Gen.* **28** 6989  
Cooper F, Khare A and Sukhatme U 1995 *Phys. Rep.* **251** 267
- [4] Zachariev B N and Suz'ko A A 1990 *Direct and Inverse Problems* (Berlin: Springer)  
Lévai G 1994 *Quantum Inversion Theory and Applications* ed H V von Geramb (Berlin: Springer) p 107
- [5] Haken H 1970 Laser theory *Encyclopedia of Physics* vol XXV/2c (New York: Van Nostrand)  
Hautot A 1972 *Phys. Lett.* **38A** 305  
Singh V, Biswas S N and Datta K 1978 *Phys. Rev. D* **18** 1901  
Flessas G P 1979 *Phys. Lett.* **72A** 289
- [6] Ushveridze A G 1994 *Quasi-exactly Solvable Models in Quantum Mechanics* (Bristol: Institute of Physics Publishing) and references therein
- [7] Gangopadhyaya A, Khare A and Sukhatme U P 1995 *Phys. Lett.* **208A** 261  
Exton H 1995 *J. Phys. A: Math. Gen.* **28** 6739  
Panja N 1995 Algebraic and supersymmetric ... in quantum mechanics *PhD Thesis* unpublished (Calcutta: ISI)
- [8] Vrbik J 1994 *J. Math. Phys.* **35** 2309
- [9] Serot B D and Walecka J D 1986 The relativistic nuclear many-body problem *Advances in Nuclear Physics* vol 16, ed J W Negele and E Vogt (New York: Plenum) p 6
- [10] Messiah A 1961 *Quantum Mechanics II* (Amsterdam: North-Holland) p 947  
Bjorken J D and Drell S D 1964 *Relativistic Quantum Mechanics* (New York: McGraw-Hill) p 177
- [11] Znojil M 1985 *Phys. Lett.* **109A** 251
- [12] Znojil M 1983 *Phys. Lett.* **94A** 120; 1984 *Phys. Lett.* **102A** 289
- [13] Acton F S 1970 *Numerical Methods That Work* (New York: Harper)
- [14] Znojil M and Leach P G L 1992 *J. Math. Phys.* **33** 2785
- [15] Znojil M 1994 *J. Phys. A: Math. Gen.* **27** 7491
- [16] Adams W W and Loustaunau P 1994 *An Introduction to Gröbner Bases* (Providence, RI: American Mathematical Society)
- [17] Gill T and Lindesay J 1993 *Int. J. Theor. Phys.* **32** 2087