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On exact solutions of the Schrödinger equation

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Abstract. In the one- and three-dimensional Schrödinger equation, a broad class of the regular potentials (rational functions of the rational powers of r) may admit exact bound-state solutions in the generalised harmonic-oscillator elementary form $\psi(r) = r^{\sigma} \times \text{polynomial} \times \exp(-\text{polynomial})$. The necessary and sufficient conditions of this phenomenon are derived in the form of coupled algebraic equations. The methods of their solution and a few examples are discussed. In particular, the well known Coulombic and oscillator solvability and the similar recent results of Singh *et al* and Whitehead *et al* are reproduced as the two simplest special cases.

1. Introduction and summary

Recently, the standard quantum mechanical applications of the radial Schrödinger equation

$$-\frac{\mathrm{d}^2}{\mathrm{d}r^2}\psi(r)+\frac{l(l+1)}{r^2}\psi(r)+V(r)\psi(r)=E\psi(r), \qquad l=0,1,\ldots, \tag{1.1a}$$

were extended even to quark physics where the simple non-relativistic models (1.1a) with $V(r)=c_1r^{\alpha}$, $V(r)=c_1r^{\alpha}+c_2r^{\beta}$, etc exhibit both a reasonable theoretical background and a surprising phenomenological success (cf Quigg and Rosner 1979). We may add the inverse polynomial components to $V(r)$ (Flessas 1981), and apply (1.1a) also as the Klein–Gordon equation for a relativistic particle (Bjorken and Drell 1964) or as the Fokker–Planck equation for a laser (Haken 1970). Finally, the various special cases of the general class of the elementary potentials

$$\begin{aligned} &V(r)=V_1(x)/r^2V_2(x)+V_3(x), \qquad x=x(r)=r^{1/\alpha}, \\ &\alpha=1,2,\ldots, \qquad V_i(x)=\sum_{j=0}^{n_i}c_j^{(i)}x^j, \qquad i=1,2,3, \end{aligned} \tag{1.1b}$$

in (1.1a) may prove to be useful in field theory, e.g. as the nonlinear interaction models in zero dimensions (Kaushal 1979) or in some of its lattice formulations (Fulco and Masperi 1979).

It is well known that the radial Schrödinger equation (1.1) must be solved numerically in general. The complete and non-numerical solution exists in a closed form for a few forces only—Newton (1965) enumerates just the r^{-4}, r^{-1}, r^2 and r^{∞} (square well) potentials. There is also a broad class of the exactly solvable (so-called Bargmann)

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potentials derived from the elementary T-matrices and defined at one fixed l only (Newton 1965). Alternatively, in accord with the simple method mentioned, e.g., by Morse and Feshbach (1953, p 1670), we may start directly from some elementary or special-function bound state ψ and derive the corresponding partially solvable potential $V(r)$ by mere differentiation. In the physical context, such a 'reverted' solution philosophy is not unusual (cf Risken and Vollmer 1967); it may enable one to start off also a perturbative treatment of the 'neighbouring' potentials (Killingbeck 1978, 1980, Aharonov and Au 1979) and it represents a fruitful methodological standpoint in general.

Our present aim is a completion of the latter type of construction as performed recently by Singh *et al* (1978, 1979), Flessas (1979, 1981), Flessas and Das (1980), Magyari (1981), Varma (1981), Whitehead *et al* (1982) and Znojil (1982) for various particular potentials of the class (1.1*b*). In brief, we shall search for all the bound state solutions to (1.1) which have the elementary form

$$\psi(r) = r^{\sigma}\, \mathrm{e}^{-P(r)} Q(r) \tag{1.2a}$$

where P and Q are polynomials of the same type as V_i's in (1.1*b*). We believe that the exact solutions to the general equation (1.1) deserve a systematic description at least in the discrete spectrum case ($E < V(\infty)$), since we may interpret (1.1*b*) with $\alpha = 1$ as a general Padé approximation to an arbitrary regular force $V(r)$.

Before going into details, we may notice that the simple change of variables

$$r^{\omega} = x, \qquad \psi(r) = x^{(1-\omega)/2\omega}\varphi(x), \qquad \omega = 1, 2, \ldots, \tag{1.3}$$

converts the general problem (1.1) written in the modified notation

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{\mathscr{L}(\mathscr{L}+1)}{x^2} + \frac{H}{x^2} + \frac{\sum_{i=1}^{p} (a_i/\omega^2) x^{-2+2i/\omega}}{\sum_{j=0}^{p} \alpha_j x^{2j/\omega}} + \sum_{i=1}^{\omega-1} \frac{g_i}{\omega^2} x^{-2(\omega-i)/\omega} + \sum_{i=\omega+1}^{2q} \frac{g_i}{\omega^2} x^{2(i-\omega)/\omega}\right)\varphi(x)$$

$$= -\frac{g_{\omega}}{\omega^2}\varphi(x), \qquad \mathscr{L} = 0, 1, \ldots, 2q \geqslant \omega;\ g_{2q} > 0, \tag{1.4}$$

to its 'canonical' form

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{l(l+1)}{r^2} + \frac{h}{r^2} + \frac{A(r)}{D(r)} + g_2 r^2 + g_3 r^4 + \ldots + g_{2q} r^{4q-2}\right)\psi(r) = -g_1\psi(r),$$

$$A(r) = \sum_{j=1}^{p} a_j r^{2j-2}, \qquad D(r) = \sum_{j=0}^{p} a_j r^{2j} > 0, \qquad r \geqslant 0, \tag{1.5}$$

classified by the two integers $p \geqslant 0$ and $q \geqslant 1$ and by the angular momentum $l \geqslant 0$. Hence, we shall only consider equation (1.5) in what follows. Concerning the backward transformation (1.5)$\rightarrow$(1.1), we would like to emphasise that by (1.3), the regularity of potential in the origin is preserved. We see that $H + \mathscr{L}(\mathscr{L}+1) = -\frac{1}{4} + (h + l(l+1) + \frac{1}{4})/\omega^2 > -\frac{1}{4}$ if and only if $h + l(l+1) > -\frac{1}{4}$. Of course, the solution $\psi(r)$ which is regular or irregular in the origin becomes transformed into the respective

regular or irregular function $\varphi(x)$ and *vice versa*. In (1.3), we must also require that $\omega \leqslant 2q$, in order not to lose the energy term $E = -g_\omega/\omega^2$ in (1.4). For the different ω's, the physical energy is represented by the different constants g_ω, but this cannot change the discrete character of the spectrum. Indeed, $V(x)$ with $\omega < 2q$ remains a confining force due to the positivity of g_{2q}. In the 'exceptional' $\omega = 2q$ cases where $V(\infty) = 0$ and $g_{2q} = -\omega^2 E$, our condition $g_{2q} > 0$ reflects merely the elimination of the continuous part of the spectrum. As an example, we may recall a known equivalence of the harmonic oscillator to the discrete Coulomb states ($p = 0$, $q = 1$, $\omega = 1, 2$).

Our main results may be summarised as follows.

(i) In accord with § 2, the bound states of the generalised harmonic oscillator form (1.2*a*) where $\sigma > \frac{1}{2}$ and P and Q are polynomials in r^2,

$$P(r) = \sum_{i=1}^{q} \beta_i r^{2i}/2i, \qquad Q(r) = \sum_{n=0}^{N} \gamma_n r^{2n},$$
$$q \geqslant 1, \qquad \beta_q > 0, \qquad \gamma_0 \neq 0 \neq \gamma_N, \tag{1.2b}$$

may exist for each p and q in (1.5). The choice of couplings in $V(r)$ must be restricted in a 'self-consistent' way to guarantee the termination (polynomiality) of $Q(r)$. In this way, each 'solvable' differential equation (1.1) may be converted into coupled 'self-consistency' algebraic equations. *Vice versa*, these equations describe completely the class of the 'solvable' V's and their elementary ψ's. For the $p = 0$ subclass of V's, similar equations were derived by Magyari (1981). Besides the trivial $p + q = 1$ case, the elementary subset of solutions ψ for any V is of course always incomplete.

(ii) In the first two non-trivial ($p + q = 2$) cases, the 'solvable' V's were studied and described in detail by Singh *et al* (1978, construction of the $p = 0$, $q = 2$ multiplets of ψ's) and by Whitehead *et al* (1982, properties of the $p = q = 1$ multiplets of Sturmians). For $p + q > 2$, the algebraic self-consistency starts to couple both the ψ and V together. Our most interesting result is an algebraic elimination of the V dependence from the equations (§ 3). From the formal point of view, this resembles the inverse spectral transformation $\psi \to V$ available for the scattering states, and determines all the solvable V's from a complete set of the 'self-consistent' ansatzes for ψ's. From the practical point of view, this nonlinear scheme is well suited for the applications since it is simple for any V and simple ψ's. It also generalises some recent separate $p = 0$, $q > 2$ constructions (Znojil 1982).

(iii) Contrary to the preceding result, the complementary algebraic elimination of ψ is rather formal (§ 4). For the highly excited or complicated ψ's, we therefore recommend employing the original self-consistencies and computing V and ψ simultaneously, by iterated diagonalisation accompanied by the $p + q - 2$ linear constraints. The two forms of such a method are described in detail in §§ 4.1 and 4.2. For $p + q = 2$, they coincide with the algebraic methods of Singh *et al* (1978) and Whitehead *et al* (1982), respectively. The latter method is illustrated on the $q = 1$, $p = 2$ example in § 5.

The present systematic discussion of the exactly solvable Schrödinger equations may extend the class of the simple physical models (particular states in the multiple well or screened Coulomb potentials etc). They may find applications also in laser theory (reconstruction of V, cf Risken and Vollmer 1967), perturbation theory (tests of convergence) and in computation practice (with V represented by a Padé approximant). Sometimes, the infinite-series limit in the polynomials may even inspire the exact and complete analytic solution of the Schrödinger eigenvalue problem (Znojil 1981).

2. Exact solvability of the Schrödinger equation

We shall start by three lemmas which result from an application of the Morse–Feshbach method in the present context.

Lemma 1. If one particular bound state $\psi(r)$ has the form (1.2), the corresponding Schrödinger equation must have the form (1.5) with some $p \leq N$ and with

$$h = (\sigma - \tfrac{1}{2})^2 - (l + \tfrac{1}{2})^2. \tag{2.1}$$

Proof. Let us put

$$\sigma = \tfrac{1}{2} + [(l + \tfrac{1}{2})^2 + h]^{1/2}, \qquad l = 0, 1, \ldots. \tag{2.2}$$

An insertion of (1.2) into (1.1a) gives

$$\begin{aligned} V(r) &= E - l(l+1)r^{-2} + (\psi(r))^{-1}\psi''(r) \\ &= E + hr^{-2} + (P'(r))^2 - 2\sigma r^{-1}P'(r) - P''(r) \\ &\quad + (Q(r))^{-1}[Q''(r) + 2(\sigma r^{-1} - P'(r))Q'(r)], \\ &\quad \psi''(r) = \mathrm{d}^2\psi(r)/\mathrm{d}r^2, \ldots, \end{aligned} \tag{2.3}$$

an inspection of which completes the proof.

Lemma 2. The polynomial $P(r)$ in (1.2b) determines q couplings in the asymptotically dominant part of $V(r)$ and *vice versa*.

Proof. From the comparison of (1.5) with (2.3) at $r^{2q}, r^{2q+2}, \ldots r^{4q-2}$, we get the P dependence of V in the simple form

$$g_{q+m} = \sum_{i=m}^{q} \beta_i \beta_{q+m-i}, \qquad m = 1, 2, \ldots, q. \tag{2.4}$$

An equivalent recurrent prescription

$$\beta_q = g_{2q}^{1/2}, \qquad \beta_{q-n} = \frac{1}{2\beta_q}\left(g_{2q-n} - \sum_{k=1}^{n-1} \beta_{q-k}\beta_{q-n+k}\right), \qquad n = 1, 2, \ldots, q-1, \tag{2.5}$$

specifies the unique V-dependence of P.

Lemma 3. The fixed choice of the minimal p in (1.5) implies that the polynomial $Q(r)$ in (1.2b) must have the factorised form

$$\begin{aligned} &Q(r) = R(r)D(r), \qquad R(r) = \sum_{i=0}^{M} \rho_i r^{2i}, \qquad M = N - p \geqslant 0, \\ &\rho_0 = \gamma_0/\alpha_0 \neq 0, \ldots, \rho_M = \gamma_N/\alpha_p \neq 0. \end{aligned} \tag{1.2c}$$

Proof. The $O(r^{2q-2})$ part of (2.3) reads

$$\begin{aligned} &\frac{A(r)}{D(r)} + B(r) = \frac{2}{Q(r)} \sum_{n=0}^{N-1} (n+1)\gamma_{n+1} r^{2n}\left((2n + 2\sigma + 1) - 2\sum_{i=1}^{q} \beta_i r^{2i}\right), \\ &B(r) = 4 \sum_{j=1}^{q} \delta_j r^{2j-2}, \end{aligned} \tag{2.6}$$

where the definition

$$4\delta_m = g_m + (2m + 2\sigma - 1)\beta_m - \sum_{i=1}^{m-1} \beta_i \beta_{m-i}, \qquad m = 1, 2, \ldots, q, \tag{2.7}$$

reflects the one-to-one correspondence between $B(r)$ in (2.6) and the 'P-independent' polynomial part of $V(r)$. The rest of (2.6) represents the polynomial $A(r)Q(r)$ as a multiple of $D(r)$. By definition, A and D have no non-trivial common divisors, so that we may put $Q = DR$ without loss of generality.

Now, we are prepared to prove

Theorem 1. The radial Schrödinger equation with the rational potential (1.5) admits the exact solution $\psi(r)$ in the elementary form (1.2) if and only if the $M + 2q + 2p + 1$ constants in $V(r)$ and $\psi(r)$ satisfy the $M + q + p$ coupled algebraic relations

$$\sum_{i=\max(0,m-M)}^{\min(m,p+q)} \rho_{m-i}\left(a_i - Z_{mm+1}\alpha_i + 2 \sum_{k=\max(1,i-p)}^{\min(q,i)} [(m-k)\beta_k + \delta_k]\alpha_{i-k}\right) = 0,$$

$$Z_{mm+1} = Z_{mm+1}(\sigma) = m(2m + 2\sigma - 1), \qquad m = 1, 2, \ldots, M + p + q, \tag{2.8}$$

$$a_{p+1} = a_{p+2} = \ldots = \alpha_{p+1} = \ldots = 0.$$

Proof. In accord with the preceding lemmas, we have to define σ by (2.2), β's by (2.5) and δ's by (2.7). Then we may denote $R'' = \mathrm{d}^2R(r)/\mathrm{d}r^2$ etc and rewrite (2.6) in the polynomial form

$$DR'' + 2\left(D' + \frac{\sigma}{r}D - P'D\right)R' + \left(D'' + \frac{2\sigma}{r}D' - 2P'D' - BD - A\right)R = 0 \tag{2.9}$$

or, symbolically, $\Sigma_{m=1}^{M+p+q} s_{m-1} r^{2m-2} = 0$. From the dominant requirement $s_{p+q+M-1} = 0$, we get

$$\delta_q = -(M + p)\beta_q. \tag{2.10}$$

This definition coincides with the $m = M + p + q$ item of (2.8). The remaining items of (2.9) read $s_{m-1} = 0$ and generate the explicit requirements (2.8) for $m = 1, 2, \ldots, M + p + q - 1$.

The theorem is a direct generalisation of Magyari's $p = 0$ result (1981), and equation (2.8) restricts the freedom in our choice of σ or h, α's, a's, β's and δ's or g's and of ρ's. When we assume that the type of the potential (integers p and q) is fixed, the $p + q + 1$ values $\sigma, \alpha_1, \alpha_2, \ldots, \alpha_p$ and $\beta_1, \beta_2, \ldots, \beta_q$ may be treated as independent variables carrying the physical input information about the threshold behaviour of $V(r)$, about its poles (not lying on the real axis!) and about its asymptotic behaviour, respectively. As a consequence, besides the simple explicit definition (2.10) of g_q (a fixed function of $g_{q+1}, g_{q+2}, \ldots, g_{2q}$, to be ignored as trivial), the first $M + p + q - 1$ coupled equations in (2.8) have to determine the values of $\delta_1, \delta_2, \ldots, \delta_{q-1}, a_1, a_2, \ldots, a_p$ and $\rho_1, \rho_2, \ldots, \rho_M$ (ρ_0 is merely an irrelevant normalisation constant). In this way, the solvability requirement (2.8) fixes $R(r)$ in (1.2) and the $O(r^{2p+2q-2})$ part of the polynomial $V(r)D(r)$.

When $h = l = 0$, we may extend our conclusions immediately also to the one-dimensional interpretation of the Schrödinger equation (1.5) with $r \in (-\infty, \infty)$. For

this purpose, it is sufficient to complement the present odd-parity $\sigma = 1$ solutions by the analogous even-parity $\sigma = 0$ series, which would be unphysical (irregular) in the present three-dimensional interpretation of (1.5).

3. Self-consistent construction of an elementary ansatz $\psi(r)$

Assuming that the only uncoupled component (2.10) of (2.8) is satisfied by our choice of g_q, we may rewrite the algebraic self-consistency equations (2.8) in the form

$$(\mathscr{H}\hat{\alpha}\hat{\rho} - \tfrac{1}{2}\hat{a}\hat{\rho} - \hat{\delta}\hat{\alpha}\hat{\rho})\begin{pmatrix} 1 \\ 0 \\ 0 \\ \dots \end{pmatrix} = 0 \tag{3.1}$$

where the matrices

$$\hat{\alpha} = \begin{pmatrix} \alpha_0 & 0 & \dots \\ \alpha_1 & \alpha_0 & 0 \dots \\ & \dots & \\ \alpha_p & \alpha_{p-1} & \dots \\ 0 & \alpha_p & \dots \\ & \dots & \end{pmatrix}, \qquad \hat{\rho} = \begin{pmatrix} \rho_0 & 0 & \dots \\ \rho_1 & \rho_0 & 0 \dots \\ & \dots & \\ \rho_M & \rho_{M-1} & \dots \\ 0 & \rho_M & \dots \\ & \dots & \end{pmatrix},$$

$$\hat{\delta} = \begin{pmatrix} \delta_1 & 0 & \dots \\ \delta_2 & \delta_1 & 0 \dots \\ & \dots & \\ \delta_{q-1} & \delta_{q-2} & \dots \\ 0 & \delta_{q-1} & \dots \\ & \dots & \end{pmatrix}, \qquad \hat{a} = \begin{pmatrix} a_1 & 0 & \dots \\ & \dots & \\ a_p & a_{p-1} & \dots \\ 0 & a_p & \dots \\ & \dots & \end{pmatrix}, \tag{3.2}$$

commute and the more complicated β- and σ-dependent Hessenberg matrix $\mathscr{H}$ reads

$$\mathscr{H} = \frac{1}{2}\begin{pmatrix} 0 & Z_{12} & 0 & \dots \\ 0 & 0 & Z_{23} & 0 \dots \\ & \dots & & \end{pmatrix} + \begin{pmatrix} \beta_1 & 0 & \dots \\ 2\beta_2 & \beta_1 & 0 \dots \\ 3\beta_3 & 2\beta_2 & \beta_1 \dots \\ & \dots & \\ (q-1)\beta_{q-1} & (q-2)\beta_{q-2} & \dots \\ 0 & (q-1)\beta_{q-1} & \dots \\ 0 & 0 & \dots \\ & \dots & \end{pmatrix}$$

$$- \begin{pmatrix} \beta_1 & 0 & \dots \\ 2\beta_2 & 2\beta_1 & 0 \dots \\ 3\beta_3 & 3\beta_2 & 3\beta_1 \dots \\ & \dots & \\ (q-1)\beta_{q-1} & (q-1)\beta_{q-2} & \dots \\ 0 & q\beta_{q-1} & \dots \\ 0 & 0 & \dots \\ & \dots & \end{pmatrix} + \begin{pmatrix} 0 & \dots & \\ 0 & \dots & \\ 0 & \dots & \\ & \dots & \\ 0 & \dots & \\ (M+p)\beta_q & 0 & \dots \\ 0 & (M+p-1)\beta_q & \dots \\ & \dots & \end{pmatrix}. \tag{3.3}$$

Hence, we get

Lemma 4. The mth row of (3.1) is satisfied identically whenever $m \geqslant M+p+q$.

Proof. The band matrix acts on the vector with only the first component different from zero, so that (3.1) is satisfied for $m > M+p+q$. The $m = M+p+q$ item is equivalent to (2.10).

Lemma 5. The first p rows of (3.1) define a's in terms of ρ's and δ's by the formula

$$\begin{pmatrix} a_1 \\ a_2 \\ \cdots \\ a_p \end{pmatrix} = 2I^{(p)}(\hat{\rho}^{-1}\mathcal{H}\hat{\alpha}\hat{\rho} - \hat{\alpha}\hat{\delta}) \begin{pmatrix} 1 \\ 0 \\ \cdots \\ 0 \\ \cdots \end{pmatrix} \tag{3.4}$$

where $I^{(i)}$ denotes an auxiliary i-dimensional unit matrix.

Proof. Since $\rho_0 \neq 0$, we may multiply (3.1) by $\hat{\rho}^{-1}$, which corresponds to an addition of the linear combination of the first $m-1$ rows to the mth one.

Lemma 6. The last $q-1$ non-trivial rows of (3.1) define δ's in terms of ρ's,

$$\begin{pmatrix} \delta_1 \\ \delta_2 \\ \cdots \\ \delta_{q-1} \\ 0 \\ \cdots \end{pmatrix} = \begin{pmatrix} \alpha_p & \alpha_{p-1} & \cdots \\ 0 & \alpha_p & \cdots \\ & \cdots & \\ 0 & \cdots & \\ 0 & \cdots & \\ & \cdots & \end{pmatrix}^{-1} \begin{pmatrix} \rho_M & \rho_{M-1} & \cdots \\ 0 & \rho_M & \cdots \\ & \cdots & \\ 0 & \cdots & \\ 0 & \cdots & \\ & \cdots & \end{pmatrix}^{-1}$$

$$\times \begin{pmatrix} 0 & 1 & 0 & \cdots \\ 0 & 0 & 1 & \cdots \\ & & \cdots & \\ 0 & \cdots & & \\ 0 & \cdots & & \\ & & \cdots & \end{pmatrix}^{M+p} \mathcal{H}\hat{\alpha}\hat{\rho} \begin{pmatrix} 1 \\ 0 \\ \cdots \\ 0 \\ \cdots \\ \cdots \end{pmatrix}. \tag{3.5}$$

Proof. Only the first $M+p$ rows of (3.1) depend on a's. We may eliminate them by the multiplication of (3.1) by the auxiliary infinite matrix $\pi^{(p+M)}$ from the left, where $\pi^{(i)}_{jk} = \delta_{j+i,k}$ (=Kronecker delta here!), $j, k = 1, 2, \ldots$. Since $\alpha_p \neq 0$ and $\rho_M \neq 0$, the upper-triangular matrix $\pi^{(p+M)}\hat{\alpha}\hat{\rho} = \pi^{(p)}\hat{\alpha}\pi^{(M)}\hat{\rho}$ is invertible and the explicit formula (3.5) follows from (3.1).

The formula (3.5) follows also from (3.1) when multiplied by $\pi^{(M)}\hat{\rho}\pi^{(p)}\hat{\rho}^{-1}$. The underlying identity

$$\hat{\rho}\pi^{(i)}\hat{\rho}^{-1} = \pi^{(i)} - \pi^{(i)}\hat{\rho}I^{(i)}(I^{(i)}\hat{\rho}I^{(i)})^{-1}I^{(i)} \tag{3.6}$$

may be verified by partitioning $\hat{\rho}$ into $(i \times i)$-dimensional blocks. Hence, (3.1) becomes

equivalent to the pair of definitions (3.4), (3.5) and to the M nonlinear equations

$$[I^{(M)}\pi^{(p)}-\pi^{(p)}I^{(M)}\hat{\rho}I^{(p)}(I^{(p)}\hat{\rho}I^{(p)})^{-1}I^{(p)}$$
$$-I^{(M)}\hat{\rho}I^{(M)}(\pi^{(M)}\hat{\rho})^{-1}\pi^{(M+p)}]\mathscr{H}\hat{\alpha}\hat{\rho}\begin{pmatrix}1\\0\\\cdots\\0\\\cdots\end{pmatrix}=0. \tag{3.7}$$

We may notice that for $M=0$, the normalisation ρ_0 is arbitrary so that we are left only with the explicit definitions (3.4) and (3.5) of the 'solvable' potential V. For $p=q=1$, this reproduces the first exact solutions found by Flessas (1981). In the general $M\geqslant 0$ case, we may formulate

Theorem 2. Provided that σ, α's in $D(r)$ and β's in $P(r)$ are treated as $1+p+q$ free parameters, the formula (1.2) represents an exact bound-state solution to the radial Schrödinger equation (1.5) if and only if the binding energy and the 'solvable' potential V are explicitly defined by the equations (2.1), (2.4), (2.7), (2.10), (3.4) and (3.5) and the $M+1$ coefficients $\rho_0, \rho_1, \ldots, \rho_M$ satisfy the M nonlinear algebraic equations

$$[I^{(M)}+\pi^{(M)}\hat{\rho}I^{(M)}(\pi^{(M)}\hat{\rho})^{-1}]\pi^{(p)}\mathscr{H}\hat{\alpha}\begin{pmatrix}\rho_0\\\cdots\\\rho_M\end{pmatrix}=\pi^{(p)}I^{(M)}\hat{\rho}I^{(p)}(I^{(p)}\hat{\rho}I^{(p)})^{-1}I^{(p)}\mathscr{H}\hat{\alpha}\begin{pmatrix}\rho_0\\\cdots\\\rho_M\end{pmatrix}. \tag{3.8}$$

Proof. It is sufficient to show that the third term in (3.7) is equivalent to the second term in (3.8), but this follows from the partitioning into $(M\times M)$-dimensional blocks.

With $M=1$ and 2 and $p=0$ (i.e. $\pi^{(p)}=I^{(\infty)}$, $I^{(p)}=0$) the special cases of (3.8) may be found elsewhere (Znojil 1982). The general formula (3.8) is a set of polynomial equations since all the matrices may be considered finite in effect. Moreover, $\pi^{(M)}\hat{\rho}$ and $I^{(p)}\hat{\rho}$ are triangular so that all the algebraic matrix inversions are straightforward (see example in the appendix).

4. The self-consistent specification of $V(r)$

In the preceding section, we have reduced the original implicit specification of the elementary pair of $V(r)$ and $\psi(r)$ to the implicit specification of $\psi(r)$ alone. This procedure loses its merits when $M>p+q$. In such a case, we have to proceed as follows.

First, we write equation (2.8) or (3.1) in the form of an overcomplete system of linear equations for ρ's,

$$\begin{pmatrix}Z_{11} & Z_{12} & 0 & \ldots & 0\\ & \cdots & & & \\ Z_{p+q,1} & Z_{p+q,2} & & \ldots & Z_{MM}Z_{M\,M-1}\\ 0 & Z_{p+q+12} & & \ldots & \\ & \cdots & & & \\ 0 & \ldots & 0 & Z_{p+q+M-1\,M} & Z_{p+q+M-1\,M+1}\end{pmatrix}\begin{pmatrix}\rho_0\\\cdots\\\rho_M\end{pmatrix}=0. \tag{4.1}$$

Here, the finite Hessenberg matrix $Z = \hat{Z} - I^{(p)}\hat{a} = I^{(p+q+M-1)}(2\mathcal{H}\hat{\alpha} - \hat{\alpha}\hat{\delta} - \hat{a})I^{(M+1)}$ has $p+q+1$ diagonals. From the first M rows of (4.1) we obtain the compact determinantal definition

$$\rho_m = \frac{(-1)^m \rho_0}{Z_{12}Z_{23}\ldots Z_{mm+1}} \det \begin{pmatrix} Z_{11} & Z_{12} & 0 & \ldots & 0 \\ & & \cdots & & \\ Z_{m1} & Z_{m2} & \ldots & & Z_{mm} \end{pmatrix}, \qquad m = 1, 2, \ldots, M, \tag{4.2}$$

of ρ's as functions of the couplings.

The matrix Z has a shape symmetric with respect to the simultaneous reordering of the rows and columns. As a consequence, the last M rows of (4.1) imply

$$\rho_{M-m} = \frac{(-1)^m \rho_M}{Z_{KM}Z_{K-1\,M-1}\ldots Z_{K-m+1\,M-m+1}} \det \begin{pmatrix} Z_{K-m+1\,M-m+2} & \ldots & Z_{K-m+1\,M+1} \\ & \cdots & \\ 0 \quad \ldots \quad 0 & Z_{KM} & Z_{KM+1} \end{pmatrix}$$
$$K = M + p + q - 1, \qquad m = 1, 2, \ldots, M. \tag{4.3}$$

The explicit V-dependence of ψ ((4.2) or (4.3)) is a formal counterpart to the explicit definitions (3.4) and (3.5) of $V = V(\psi)$. Unfortunately, an insertion of (4.2) or (4.3) into (4.1) does not simplify the general result of

Theorem 3. The radial Schrödinger equation (1.5) has an elementary solution (1.2) if and only if g_q is defined by (2.10) and the couplings $a_1, a_2, \ldots, a_p$ and $g_1, g_2, \ldots, g_{q-1}$ satisfy the $p+q-1$ coupled algebraic equations

$$\det Z^{(i)} = 0, \qquad i = 1, 2, \ldots, p+q-1, \tag{4.4}$$

where $\{Z^{(i)}\}$ denotes any set of the $p+q-1$ independent $[(M+1)\times(M+1)]$-dimensional submatrices of Z.

Proof. This is trivial—equations (4.4) are the standard solvability conditions for equation (4.1).

Theorem 3 may be illustrated on the $p=0$, $q=2$ example of Singh *et al* (1978) where the only unknown parameter δ_1 corresponds to the physical energy and lies on the main diagonal of the tridiagonal matrix $Z^{(1)}$ which may be symmetrised. Hence, there always exists a multiplet of the polynomial eigenstates ψ provided that the underlying sextic anharmonic potential $V(r) = g_2 r^2 + g_3 r^4 + g_4 r^6$ satisfies the only self-consistency requirement (2.10), i.e.

$$g_2 = g_3^2/4g_4 - (4M + 2\sigma + 3)\sqrt{g_4}. \tag{4.5}$$

4.1. The constrained diagonalisation

For $p+q>2$, the determinantal equations (4.4) are coupled and must therefore be treated by purely numerical methods. Of course, the convergence and even the existence of a solution are difficult to prove. Let us describe here one of the most natural computational schemes based on a combination of the algebraic results of §§ 3 and 4 which still preserves the formally linear character of the coupled equations.

The main idea is simple—we preserve, say, the first $p-1$ rows of (3.4) or (4.1),

$$\begin{pmatrix} a_1 \\ a_2 \\ \dots \\ a_{p-1} \end{pmatrix} = \begin{pmatrix} \rho_0 & 0 & \dots & \\ \rho_1 & \rho_0 & 0 & \dots \\ & \dots & & \\ \rho_{p-2} & \dots & & \rho_0 \end{pmatrix}^{-1} \begin{pmatrix} \tilde{Z}_{11} & \tilde{Z}_{12} & 0 & \dots & 0 \\ \tilde{Z}_{21} & \tilde{Z}_{22} & \tilde{Z}_{23} & 0 & \dots 0 \\ & \dots & & & \\ \tilde{Z}_{p-1\,1} & \dots & & \tilde{Z}_{p-1\,M+1} & \end{pmatrix} \begin{pmatrix} \rho_0 \\ \rho_1 \\ \dots \\ \rho_M \end{pmatrix} \tag{4.6}$$

and the last $q-1$ rows of (4.1) in the form of (3.5), i.e.

$$\begin{aligned} \delta_{q-1} &= -(M+p)\beta_{q-1} + (\alpha_{p-1}/\alpha_p + \rho_{M-1}/\rho_M)\beta_q, \\ \delta_{q-2} &= -(M+p)\beta_{q-2} + (\alpha_{p-1}/\alpha_p + \rho_{M-1}/\rho_M)\beta_{q-1} \\ &\quad + [2\alpha_{p-2}/\alpha_p + 2\rho_{M-2}/\rho_M - (\alpha_{p-1}/\alpha_p)^2 - (\rho_{M-1}/\rho_M)^2]\beta_q, \\ &\quad \dots \end{aligned} \tag{4.7}$$

Then, the rest of (4.1) reads

$$\begin{pmatrix} \tilde{Z}_{p1} & Z_{p2} & \dots & Z_{p\,M+1} \\ Z_{p+1,1} & \tilde{Z}_{p+1,2} & Z_{p+1,3} \dots & Z_{p+1\,M+1} \\ & & \dots & \\ Z_{p-M\,1} & Z_{p+M\,2} & \dots Z_{p+M\,M} & \tilde{Z}_{p+M\,M+1} \end{pmatrix} \begin{pmatrix} \rho_0 \\ \rho_1 \\ \dots \\ \rho_M \end{pmatrix} = a_p \begin{pmatrix} \rho_0 \\ \rho_1 \\ \dots \\ \rho_M \end{pmatrix} \tag{4.8}$$

and specifies the last unknown coupling in a self-consistent way as an eigenvalue a_p (zero of $\det Z^{(p)}$—cf (4.4)).

In practical computations, we have to start, e.g., from an initial (trial) set of couplings $a_1, \dots, a_{p-1}$ and $\delta_1, \dots, \delta_{q-1}$ and define the left-hand side in (4.8). If the real eigenvalue a_p does not exist, we have to try another initialisation. From the corresponding eigenvector $(\rho_0, \dots, \rho_M)^{\mathrm{T}}$ and (4.6), (4.7), we then get a new trial set. If the iteration converges, we obtain the solution.

As an example, we may recall the $p=q=1$ potential $V(r) = r^2 + \lambda r^2/(1+gr^2)$ as considered by Mitra (1978), Kaushal (1979) and solved in the present spirit by Flessas (1981), Whitehead *et al* (1982) and Varma (1981). To preserve their notation, let us put $\sigma = 0$ or 1, $a_1 = -\lambda/2g$ and $\alpha_1 = g$. Then, the energy is fixed by (2.10), there are no restrictions (4.6) and (4.7), and equation (4.8) has the simple form

$$0 = \begin{pmatrix} g+2M+2-a_1 & 1 & 0 & & \dots & 0 \\ 2gM & 6g+2M-a_1 & 6 & 0 & \dots & 0 \\ 0 & 2g(M-1) & & & \dots & 0 \\ & & \dots & & & \\ 0 & \dots & 0 & 2g & (M+1)(2M+1)g+2-a_1 & \end{pmatrix} \begin{pmatrix} \rho_0 \\ \rho_1 \\ \rho_2 \\ \dots \\ \rho_M \end{pmatrix}. \tag{4.9}$$

It permits an easy symmetrisation of the matrix $Z^{(1)}$ and defines therefore the $M+1$ real and non-zero eigenvalues $a_1 = -\lambda/2g$. In contrast to Singh's oscillator, they correspond to different potentials. Due to the factorisation $D \times R$ of Q, the present form of the result is slightly simpler than the original one as given by Whitehead *et al* (1982) where also the existence and positivity of a_1's was first proved.

4.2. Transition to the harmonic-oscillator basis

Being inspired by Whitehead *et al* (1982) and by their alternative treatment of equation

(4.9), we may notice that the ansatz (1.2) has the form

$$\psi(r) = \exp\left[-\left(\frac{\beta_q}{2q}r^{2q} + \ldots + \frac{\beta_2}{4}r^4\right)\right] \sum_{n=0}^{N} y_n \langle r|n\rangle \tag{4.10}$$

where $\langle r|n\rangle$ denotes a normalised eigenstate of the harmonic oscillator,

$$\begin{aligned} &H_0|n\rangle = \varepsilon_n|n\rangle, \qquad \varepsilon_n = \beta_1(4n + 2\sigma + 1), \qquad n = 0, 1, \ldots, \\ &H_0 = -\mathrm{d}^2/\mathrm{d}r^2 + l(l+1)/r^2 + h/r^2 + \beta_1^2 r^2. \end{aligned} \tag{4.11}$$

When we insert (4.10) into (1.5) and employ the orthonormality of $\langle r|n\rangle$'s we may repeat all the formal manipulations of the preceding paragraphs. Unfortunately, the resulting formulae become more complicated whenever $q \geqslant 2$.

For the particular choice of $q = 1$ in $V(r)$, the transition (4.10) to the oscillator basis deserves special attention since the exponential factor in (4.10) (responsible for some complications (asymmetry) of the resulting equations) is equal to one. In the next section, we shall therefore illustrate the typical features of the $q = 1$ oscillators on the first non-trivial $p = 2$ example. The generalisation to any $p > 2$ is straightforward.

5. Fractionally perturbed harmonic oscillators—the $p = 2$ example

Let us assume that $q = 1$ and $p = 2$ in (1.5). With the ansatz (4.10), we may write this equation in the form

$$\left(H_0 + \frac{a_1 + a_2 r^2}{1 + \alpha_1 r^2 + \alpha_2 r^4}\right) \sum_{n=0}^{N} |n\rangle y_n = E \sum_{n=0}^{N} |n\rangle y_n \tag{5.1}$$

where $y_N \neq 0$ and $N \geqslant 2$ in the light of lemma 3.

With respect to the regularity of $D(r)$ and orthonormality of the basis, we obtain from (5.1)

$$\begin{aligned} &\sum_{m=0}^{N} [\langle n|(1 + \alpha_1 r^2 + \alpha_2 r^4)|m\rangle(\varepsilon_m - E) + \langle n|(a_1 + a_2 r^2)|m\rangle] y_m = 0, \\ &n = 0, 1, \ldots, N_T. \end{aligned} \tag{5.2}$$

We must put $N_T = N + 2$ since $\langle m|r^2|n\rangle$ and $\langle m|r^4|n\rangle$, $m, n = 0, 1, \ldots$ may be treated as the infinite three- and five-diagonal matrices T and T^2, respectively. Since $y_{N+1} = y_{N+2} = \ldots = 0$, we may replace T by its truncated $(M_T + 1)$-dimensional form with $M_T \geqslant N + 2$. If necessary, this T may be diagonalised by an orthogonal matrix U such that $(UTU^{\mathrm{T}})_{jk} = r_j^2 \delta_{j,k}$, $j, k = 0, 1, \ldots, M_T$.

The last row of the overcomplete system (5.2) with $n = N + 2$ gives

$$E = \varepsilon_N \tag{5.3}$$

which reproduces simply our previous result (2.10). Similarly, we obtain the relations

$$w_{11} y_N + w_{12} y_{N-1} = 0, \qquad w_{21} y_N + w_{22} y_{N-1} + w_{23} y_{N-2} = 0, \tag{5.4}$$

with $w_{11} = a_2 T_{N+1\,N}$, $w_{12} = (\varepsilon_{N-1} - \varepsilon_N)\alpha_2 (T^2)_{N+1\,N-1}$, $w_{21} = a_1 + a_2 T_{NN}$, $w_{22} = a_2 T_{N\,N-1} + (\varepsilon_{N-1} - \varepsilon_N)(\alpha_1 T_{N\,N-1} + \alpha_2 (T^2)_{N\,N-1})$, and $w_{23} = (\varepsilon_{N-2} - \varepsilon_N)\alpha_2 (T^2)_{N\,N-2}$, from the $n = N + 1$ and $n = N$ items of (5.2). Since w_{12} and w_{23} are non-zero (negative),

we may rewrite (5.4) in the form

$$y_{N-1} = -\frac{w_{11}}{w_{12}} y_N, \qquad y_{N-2} = \frac{1}{w_{12} w_{23}} \det \begin{pmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{pmatrix} y_N. \tag{5.5}$$

When we choose y_N as an arbitrary normalisation and introduce the new y_N-independent N-dimensional vector $z_i = g_{ii} y_i$, $i = 0, 1, \ldots, N-1$ (g is the N-dimensional positive diagonal matrix such that $g_{ii}^2 = \varepsilon_N - \varepsilon_i$), then the equations (5.5) fix the normalisation of z and specify the ratio of the components z_{N-1}/z_{N-2} of this new vector.

An introduction of the new vector z is motivated by its appearance in the rest of (5.2), which may be given the form

$$\sum_{m=0}^{N-1} \left(g \frac{1 + \alpha_1 T + \alpha_2 T^2}{\cos\varphi + \sin\varphi T} g \right)_{mn}, \qquad z_n = \lambda z_n, \qquad \tan\varphi = a_2/a_1, \qquad \lambda = (a_1^2 + a_2^2)^{1/2}, \tag{5.6}$$

provided that

$$\det(a_1 + a_2 T) = \lambda^{M_T + 1} \prod_{i=0}^{M_T} (\cos\varphi + r_i^2 \sin\varphi) \neq 0. \tag{5.7}$$

Fortunately, the latter condition is easy to satisfy since we may distinguish two cases:

(i) $a_1 = a_2 = \lambda = 0$. Then, obviously, equation (5.2) admits only the harmonic-oscillator solution $y_i = y_N \delta_{iN}$, $i \leq N$. This may be omitted here as trivial ($p \neq 2$).

(ii) $a_1 = \lambda \cos\varphi$, $a_2 = \lambda \sin\varphi$ with some $\lambda > 0$. It may happen that $\cos\varphi + r_i^2 \sin\varphi = 0$ for some $i \leq M_T$. Then, in some vicinity of φ, it is sufficient to remove this random zero of (5.7) by the change of the auxiliary cut-off M_T.

Due to the symmetry of the left-hand-side matrix in (5.6), its diagonalisation is standard and gives always some real eigenvalues $\lambda^{(i)}(\varphi)$, $i = 1, 2, \ldots, N$ and the corresponding orthogonal eigenvectors $z_j^{(i)}(\varphi)$, $j = 0, \ldots, N-1$; $i = 1, 2, \ldots, N$, as functions of the parameter φ. For each i, this parameter has to be fixed by the requirements (5.5), i.e. by the transcendental equation

$$z_{N-1}^{(i)}(\varphi) \det \begin{pmatrix} w_{11}(\varphi, i) & w_{12} \\ w_{21}(\varphi, i) & w_{22}(\varphi, i) \end{pmatrix} = -\frac{g_{N-1}}{g_{N-2}} w_{11}(\varphi, i) w_{23} z_{N-2}^{(i)}(\varphi) \tag{5.8}$$

which has to be solved numerically. Thus, the problem of existence of the elementary V and ψ is reduced to the geometric proof of the real intersection of the two curves. Contrary to the original diagonalisation (4.8), we obtain here also the $p = 1$ subset of solutions.

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Appendix

The function $R(r) = \Sigma_{n=0}^{M} p_n r^{2n}$ determines the zeros $\sqrt{A_i}$ of $\psi(r) \sim R(r) = \rho_M \Pi_{i=1}^{M} (r^2 - A_i)$. In the nth excited state $\psi(r)$, n of the A_i's are positive. When we

express ρ's in terms of the new variables A_i, $\rho_{M-1}/\rho_M = t_1 = -A_1 - A_2 - \ldots - A_M, \ldots \rho_0/\rho_M = t_M = (-1)^M A_1 A_2 \ldots A_M$, the physical interpretation of $\psi(r)$ becomes easier. At the same time, the inversion of the upper-triangular matrix $\pi^{(M)}\hat{\rho}$ in (3.8) is also simplified, since the evaluation of determinants may be replaced by the decomposition formula

$$\begin{pmatrix} 1 & t_1 & t_2 & \ldots & t_M & 0 & \ldots \\ 0 & 1 & t_1 & \ldots & t_{M-1} & t_M & 0 \quad \ldots \\ & & & \ldots & & & \end{pmatrix} = \begin{pmatrix} 1 & -A_1 & 0 & \ldots \\ 0 & 1 & -A_1 & 0 \\ & & \ldots & \end{pmatrix}$$

$$\times \ldots \times \begin{pmatrix} 1 & -A_M & 0 & \ldots \\ 0 & 1 & -A_M & 0 \quad \ldots \\ & & \ldots & \end{pmatrix}$$

which implies the compact result

$$\begin{pmatrix} 1 & t_1 & \ldots & t_M & 0 & \ldots \\ 0 & 1 & t_1 & \ldots & t_M & 0 \quad \ldots \\ & & & \ldots & & \end{pmatrix}^{-1}$$

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$$= \begin{pmatrix} 1 & A_1 & A_1^2 & A_1^3 & \ldots \\ 0 & 1 & A_1 & A_1^2 & \ldots \\ & & \ldots & & \end{pmatrix} \times \ldots \times \begin{pmatrix} 1 & A_M & A_M^2 & \ldots \\ 0 & 1 & A_M & \ldots \\ & & \ldots & \end{pmatrix}$$

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$$= \begin{pmatrix} 1 & \xi_1 & \xi_2 & \ldots \\ 0 & 1 & \xi_1 & \ldots \\ & & \ldots & \end{pmatrix},$$

$$\xi_m = \sum_{i=1}^{M} A_i^{M+m} / \Pi_{j=1, j\neq i}^{M} (A_i - A_j).$$

A similar technique of inversion may be used also in the $I^{(p)}\hat{\rho}I^{(p)}$ term in (3.8) or for $\pi^{(p)}\hat{\alpha}$ in (3.5).

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