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Short-range oscillators in a power-series picture

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Abstract. The class of short-range potentials $V^{[M]}(x) = \sum_{m=2}^{M}(f_m + g_m \sinh x)/\cosh^m x$ is considered as an asymptotically vanishing phenomenological alternative to the popular anharmonic long-range $V(x) = \sum_{n=2}^{N} h_n x^n$. We propose a method which parallels the analytic Hill–Taylor description of anharmonic oscillators and represents all the wavefunctions $\psi^{[M]}(x)$ non-numerically, in terms of certain infinite hypergeometric-like series. In this way the well known exact $M = 2$ solution is generalized to any $M > 2$.

1. Introduction

A routine numerical solution of an *asymmetric* Schrödinger bound-state problem on the line $x \in (-\infty, \infty)$ requires a careful verification [1]. One needs non-numerical asymmetric models. For this purpose we may use the shifted harmonic oscillator, Morse's well and the two scarf-shaped hyperbolic forces. All of these models (cf table 1) are listed in the review [2] as possessing the *complete* solution in closed form.

Table 1. Shape-invariant potentials on the line [2].

Model	$V(x)$	$V(-\infty)$	$V(\infty)$	Polynomial $\psi(x)$
Harmonic	$\omega^2(x+b)^2$	∞	∞	Laguerre
Morse	$a\mathrm{e}^{-x} + b\mathrm{e}^{-2x}$	∞	0	Laguerre
Rosen–Morse II	$f/\cosh^2 x + g \tanh x$	$-g$	g	Jacobi
Scarf II	$(f + g \sinh x)/\cosh^2 x$	0	0	Jacobi

There exist *incompletely* solvable polynomials $V(x) = ax + bx^2 + \cdots + zx^N$ [3] and multi-exponentials $V(x) = a\mathrm{e}^{-x} + b\mathrm{e}^{-2x} + \cdots + z\mathrm{e}^{-Nx}$ [4]. They extend the possible tests and further non-numerical applications beyond $N = 2$. In a puzzling contrast, a natural generalization

$$V^{[M]}(x) = \sum_{m=2}^{M} \frac{f_m}{\cosh^m x} + \sinh x \sum_{n=1}^{M} \frac{g_n}{\cosh^n x} \tag{1}$$

of the remaining two items in table 1 is not amenable to a similar elementary treatment [5]. This distracts attention from the hyperbolic oscillators (1) in spite of their obvious phenomenological as well as purely mathematical appeal.

In the present paper we shall return to several formal as well as descriptive parallels between the separate items in table 1. On their basis we shall propose and describe a new semianalytic approach to the 'neglected' family (1).

In section 2 we recall the harmonic and Morse oscillators and their $N > 2$ generalizations as our overall methodical guide. In the language of the well known Lanczos method [6] we underline the key role of simplicity of the repeated action of the Hamiltonian upon a suitable trial state $|0\rangle$. An appropriate choice of this initial ket vector is able to inspire some of the existing non-numerical power-series solutions. In this setting the Lanczos approach is shown to find its natural reincarnations in the well known method of Hill determinants [7] as well as in the symmetric Jost-solution method of [8].

In section 3 we show how the latter two examples pave the way towards equation (1) with any $M \geqslant 2$. Fully parallel to the polynomial case we construct the asymptotically correct bound state solutions which all retain a recurrently defined power-series structure. Via an appropriate D-dimensional partitioning of the basis we preserve their connection to the two remaining exactly solvable hyperbolic $M = 2$ examples of table 1.

Section 4 illustrates the technical details at the first non-trivial $D = 2$. We contemplate there a spatially antisymmetric $M = 2$ exercise (1) using $f_2 = g_1 = 0$. We detail the proof of the pointwise convergence of our 'partitioned hypergeometric' wavefunctions. We show how the symmetry considerations significantly simplify the construction and matching of our wavefunctions near the origin.

Section 5 adds a short summary.

2. The method

2.1. *Wavefunctions in the Lanczos basis*

The Lanczos numerical eigenvalue method [6] works with a set $\{|n\rangle\}$ of the basis ket vectors which are generated via a repeated action of the Hamiltonian H upon an initial vector $|0\rangle$. In a slight generalization of this procedure one has to assume that the action of the full Schrödinger operator $H - z$ upon each ket $|n\rangle$ may be represented as a linear superposition over the same set of the kets [9],

$$(H - z)|n\rangle = |0\rangle \cdot Q_{0,n}(z) + |1\rangle \cdot Q_{1,n}(z) + \cdots. \tag{2}$$

With a matrix of functions $Q_{m,n}(z)$ (cf [10], p 257) we may abbreviate

$$\left[\ (H-z)|0\rangle, (H-z)|1\rangle, \ldots\ \right] \equiv (H-z)\left[\ |0\rangle, |1\rangle, |2\rangle, \ldots\ \right] \equiv (H-z)\,|X\}$$

$$(H-z)\,|X\} = |X\} \cdot Q(z)$$

and solve any linear homogeneous equation $(H - E)|y\rangle = 0$ by the ansatz

$$|y\rangle = \sum_{n=0}^{\infty} |n\rangle h_n \equiv |X\}\,\vec{h}. \tag{3}$$

Provided that the separate Lanczosean kets are linearly independent the resulting identity $|X\}Q(z)\vec{h} = 0$ may be interpreted as a system of conditions

$$Q(E)\vec{h} = 0. \tag{4}$$

The practical applicability of this recipe relies upon several tacit assumptions. Most often one chooses the set $\{|n\rangle\}$ as a common harmonic oscillator basis [11]. It is orthonormal ($\{X|X\} = I$) and complete ($|X\}\{X| = Id$) and we may truncate the linear set (4) to the mere routine matrix diagonalization

$$\sum_{n=0}^{\mathcal{M}} [Q(0) - EI]_{m,n}\, h_n = 0 \qquad m = 0, 1, \ldots, \mathcal{M} \qquad \mathcal{M} \gg 1. \tag{5}$$

This is a textbook variational recipe and its secular equation

$$\det Q(E) = 0 \tag{6}$$

determines the spectrum numerically [12].

A non-variational and less numerical modification of the construction may be based on a more sophisticated choice of the Lanczos basis. Various linear algebraic algorithms of such a type are used to solve various Schrödinger equations in applications [13]. Let us recall two examples as our methodical guide.

2.2. Anharmonic example

Both the above-mentioned multi-exponential and polynomial oscillators prove mutually equivalent after a change of variables [14]. Their 'canonical' [15] representation

$$V(x) = \frac{g_{-1}}{r^2} + g_1 r^2 + g_2 r^4 + g_3 r^6 + \cdots + g_{2N-1} r^{4N-2} \qquad r \in (0, \infty) \tag{7}$$

is easily tractable by the variational algorithms. In the less numerical power-series approaches [16] the harmonic kets are being replaced by the powers $\langle r|n\rangle = \langle r|0^{[HO]}\rangle \cdot r^n$. This leads to an asymmetric matrix $Q(z)$. Its linear algebraic equation (4) often proves solvable as a very simple recurrent specification of the coefficients h_n in equation (3) (cf [17] for more details).

An even more ambitious reduction of Q may be achieved after an anharmonic choice of the initial $|0\rangle$. According to Magyari [3] this assigns a few elementary bound-state solutions to many multi-exponential and polynomial potentials at certain exceptional couplings. At *arbitrary* couplings and energies the same option $|0\rangle$ may provide an extremely compact infinite-dimensional algebraic secular equation (4). For illustration let us consider the famous sextic oscillator example of [18]. With $N = 2$ in equation (7), denoting $g_3 = 16\alpha^2$ and $g_2 = 16\alpha\beta$ and using the WKB-inspired postulate

$$\langle r|n\rangle = r^{n+\ell+1} \mathrm{e}^{-\alpha r^4 - \beta r^2} \qquad \alpha > 0 \tag{8}$$

we obtain the tridiagonal quasi-Hamiltonian

$$Q(E) = \begin{pmatrix} \alpha_0 & \gamma_1 & 0 & 0 & \dots \\ \beta_0 & \alpha_1 & \gamma_2 & 0 & \dots \\ 0 & \beta_1 & \alpha_2 & \gamma_3 & \dots \\ & & \ddots & \ddots & \end{pmatrix}. \tag{9}$$

Its equation (4) may safely be interpreted as an infinite-dimensional limit of the truncated diagonalization (5) provided only that $g_2 > 0$ [19]. The three non-zero diagonals in equation (9) have to be compared with the seven-diagonal structure of the Hamiltonian in the usual orthogonalized harmonic oscillator basis.

For $g_2 \leqslant 0$ and at a special discrete set of the couplings g_1 the infinite-dimensional tridiagonal secular Hill determinant factorizes and the recipe reproduces *a part* of the spectrum correctly [18]. In all the other cases the WKB-compatible Lanczos basis ceases to be adequate. The Hill-determinant recipe (6) loses its relation to the correct asymptotic boundary conditions and the basis (8) must be regularized for certain hidden-symmetry reasons [20]. More diagonals necessarily appear in equation (9). Otherwise, one gets incorrect results from the truncated equation (5) even in its infinite-dimensional limit [21].

Virtually no similar constructions of our short-range hyperbolic oscillators seem to appear in the current literature. Here we intend to explain the difference and develop a new semianalytic approach to equation (1). Our construction will fairly closely parallel the formalism of the Hill-determinant method. In our second preparatory step the appropriately modified choice of the Lanczos basis will be illustrated via the symmetrized Rosen–Morse or scarf model of table 1.

2.3. Pöschl–Teller example

Formula (1) with $M = 2$, attraction $f = -\lambda(\lambda-1)$ *and* vanishing $g = 0$ defines the bell-shaped and spatially symmetric Pöschl–Teller well $V^{(PT)}(x) = f/\cosh^2 x$ [22]. The functional form of the optimal Lanczosean kets is more or less uniquely deduced, very much in the spirit of the 'most ambitious' WKB-like choice in equation (8) above, from the available exact solutions,

$$\langle x|n\rangle = \xi_{n,p,q,\kappa}(x) = \frac{\sinh^{1-q} x}{\cosh^{\kappa+2n+p} x} \in L_2(-\infty,\infty). \tag{10}$$

All these basis states possess the even or odd parity at $q = 1$ or 0, respectively. Within this subsection let us fix $p \equiv 1 - q$. Then, the action of the full Hamiltonian $H^{(PT)} = -\partial_x^2 + V^{(PT)}(x)$ on our symmetrized/antisymmetrized states (10) becomes particularly transparent. For energies $E = -\kappa^2$, it is characterized by the mere two-diagonal matrix

$$Q(E) = \begin{pmatrix} \alpha_0 & 0 & 0 & 0 & \dots \\ \beta_0 & \alpha_1 & 0 & 0 & \dots \\ 0 & \beta_1 & \alpha_2 & 0 & \dots \\ & & \ddots & \ddots & \end{pmatrix} \tag{11}$$

with the vanishing uppermost element $\alpha_0 = 0$. The bound-state solutions (3) of our Schrödinger differential equation read

$$\frac{1}{h_0}\langle x|y\rangle = |0\rangle - |1\rangle \cdot \frac{\beta_0}{\alpha_1} + |2\rangle \cdot \frac{\beta_0\beta_1}{\alpha_1\alpha_2} + \cdots. \tag{12}$$

As long as they are defined by the elementary two-term recurrences (3),

$$\begin{pmatrix} 0 & 0 & 0 & \dots \\ f+(\kappa+p)(\kappa+p+1), & -4(\kappa+1) & 0 & \dots \\ 0 & f+(\kappa+p+2)(\kappa+p+3), & -8(\kappa+2) & \dots \\ \vdots & \ddots & \ddots & \ddots \end{pmatrix} \begin{pmatrix} h_0 \\ h_1 \\ h_2 \\ \vdots \end{pmatrix} = 0 \tag{13}$$

our solution $|y\rangle$ coincides with the Gauss hypergeometric series,

$$\langle x|y\rangle = h_0 \tanh^p x \frac{1}{\cosh^\kappa x}\, {}_2F_1\left(\frac{\kappa+p+\lambda}{2}, \frac{\kappa+p+1-\lambda}{2}; 1+\kappa; \frac{1}{\cosh^2 x}\right). \tag{14}$$

It is defined on a half-axis, say, $x \geqslant 0$. Fortunately, due to the manifest symmetry or antisymmetry of the physical solutions, the necessary analytic continuation across the origin proves equivalent to the termination of this infinite series. The well known Jacobi polynomial solutions are obtained at each physical energy [8].

3. Partitioned expansions

We may conclude that the description of bound states by the infinite series (3) proves easy and efficient not only in the Hill-determinant setting of section 2.2 but also in an alternative Jost-solution spirit of section 2.3. We intend to extend the parallelism far beyond the trivial example of section 2.3.

The action of the kinetic energy $T = -\partial_x^2$ on the basis (10) conserves *both* the independent parity-like parameters p and q. The same conservation law is obeyed by the single-term symmetric potentials $V_s^{(M)}(x) = f/\cosh^M x$ with the even exponents $M = 2K$. The rule is broken by the general Hamiltonians containing superpositions (1) of the symmetric and antisymmetric components $V_s^{(M)}(x)$ and $V_a^{(N)}(x) = g\sinh x/\cosh^N x$, respectively. Nevertheless, the full basis (10) numbered by a composite index $\mu = \mu(n, p, q) = 4n+2p+q \geqslant 1$ (as $\xi_{n,p,q,\kappa}(x) \equiv \langle x|\Xi_\mu\rangle$, $\mu = 1, 2, \ldots$) proves reducible for all the single-term potentials $V_{s,a}^{(N)}(x) = \pm V_{s,a}^{(N)}(-x)$ of a definite parity.

3.1. Symmetric potentials $V(x) = V(-x)$

We may choose the initial Lanczos ket $|0\rangle$ either as the spatially symmetric (and asymptotically correct) element $\langle x|\Xi_{\mu(0,0,1)}\rangle \equiv \cosh^{-\kappa} x$ with $p = 0$ and $q = 1$ *or* as its antisymmetric analogue $\langle x|\Xi_{\mu(0,1,0)}\rangle \equiv \sinh x \cosh^{-\kappa-1} x$ with $p = 1$ and $q = 0$. In both these cases, all the Hamiltonian operators $T + V_s^{(2K)}(x)$ become compatible with recurrences (2) in the two alternative bases

$$|0\rangle, |1\rangle, |2\rangle, \ldots = |\Xi_{\mu(0,0,1)}\rangle, |\Xi_{\mu(1,0,1)}\rangle, |\Xi_{\mu(2,0,1)}\rangle \ldots \equiv |\Xi_1\rangle, |\Xi_5\rangle, |\Xi_9\rangle, \ldots$$

$$|0\rangle, |1\rangle, |2\rangle, \ldots = |\Xi_{\mu(0,1,0)}\rangle, |\Xi_{\mu(1,1,0)}\rangle, |\Xi_{\mu(2,1,0)}\rangle \ldots \equiv |\Xi_2\rangle, |\Xi_6\rangle, |\Xi_{10}\rangle, \ldots$$

with $p = 1 - q = 0$ or 1, respectively. After we abbreviate $a_j = -j(2\kappa + j)$ and $b_j = (\kappa + j)(\kappa + j + 1)$, this enables us to reproduce the two-diagonal Pöschl–Teller realization of $Q = Q^{(p)}$ at $K = 1$,

$$Q^{(0)} = \begin{pmatrix} 0 & 0 & 0 & \ldots \\ f + b_0, & a_2 & 0 & \ldots \\ 0 & f + b_2, & a_4 & \\ \vdots & & \ddots & \ddots \end{pmatrix} \qquad Q^{(1)} = \begin{pmatrix} 0 & 0 & 0 & \ldots \\ f + b_1, & a_2 & 0 & \ldots \\ 0 & f + b_3, & a_4 & \\ \vdots & & \ddots & \ddots \end{pmatrix}.$$

In the 'first unsolvable' case with $K = 2$ the coupling f moves one step down,

$$Q^{(0)} = \left(\begin{array}{c|cc|cc} 0 & 0 & 0 & 0 & \ldots \\ \hline b_0, & a_2 & 0 & 0 & \ldots \\ f & b_2, & a_4 & 0 & \ldots \\ \hline 0 & f & b_4, & a_6 & \\ \vdots & & \ddots & \ddots & \ddots \end{array}\right) \qquad Q^{(1)} = \left(\begin{array}{c|cc|cc} 0 & 0 & 0 & 0 & \ldots \\ \hline b_1, & a_2 & 0 & 0 & \ldots \\ f & b_3, & a_4 & 0 & \ldots \\ \hline 0 & f & b_5, & a_6 & \\ \vdots & & \ddots & \ddots & \ddots \end{array}\right).$$

Partitioning indicated by the auxiliary lines tries to preserve the same two-diagonal pattern as above. At $K = 3$ we have, similarly,

$$Q^{(0)} = \left(\begin{array}{c|ccc|c} 0 & 0 & 0 & 0 & \dots \\ \hline b_0, & a_2 & 0 & 0 & \dots \\ 0 & b_2, & a_4 & 0 & \dots \\ f & 0 & b_4, & a_6 & \\ \hline & \ddots & & \ddots & \ddots \end{array}\right) \qquad Q^{(1)} = \left(\begin{array}{c|ccc|c} 0 & 0 & 0 & 0 & \dots \\ \hline b_1, & a_2 & 0 & 0 & \dots \\ 0 & b_3, & a_4 & 0 & \dots \\ f & 0 & b_5, & a_6 & \\ \hline & \ddots & & \ddots & \ddots \end{array}\right)$$

and so on. The dimension of partitions grows linearly with $M = 2K$ as $D = K$.

The second series of the symmetric potentials $V_s^{(2K+1)}(x) = f/\cosh^{2K+1} x$ with the *odd* powers $M = 2K + 1$ must be investigated separately. It acts on our parity-preserving basis in such a way that the conservation of the quantum number p is broken. The following q-preserving bases must be used,

$$|0\rangle, |1\rangle, |2\rangle, \ldots \equiv |\Xi_2\rangle, |\Xi_4\rangle, |\Xi_6\rangle, |\Xi_8\rangle, \ldots \qquad q = 0$$

$$|0\rangle, |1\rangle, |2\rangle, \ldots \equiv |\Xi_1\rangle, |\Xi_3\rangle, |\Xi_5\rangle, |\Xi_7\rangle, \ldots \qquad q = 1.$$

At $K = 0$ the new lower triangular matrices $Q = Q^{[q]}$ contain just the three non-zero neighbouring diagonals. For preservation of the two-diagonal notation it is sufficient to switch to the $D = 2$ partitioning. Similarly, a three-dimensional partitioning is needed at $K = 1$. With the further increase of K the dimension $D = 2K + 1$ grows more quickly.

3.2. Antisymmetric potentials $V(x) = -V(-x)$

The class of the antisymmetric forces $V_a^{(2L)}(x)$ with $L \geqslant 1$ inter-relates the basis states with different parities q. The value of the index p is conserved,

$$V_a^{(2L)}(x)|\Xi_{\mu(n,p,q)}\rangle = (1-q)g \cdot |\Xi_{\mu(n+L-1,p,1-q)}\rangle + (-1)^{1-q} g \cdot |\Xi_{\mu(n+L,p,1-q)}\rangle.$$

The Hamiltonian $T + V_a^{(2L)}$ acts transitively on the following two reduced Lanczos bases:

$$|0\rangle, |1\rangle, |2\rangle, \ldots \equiv |\Xi_1\rangle; |\Xi_4\rangle, |\Xi_5\rangle; |\Xi_8\rangle, |\Xi_9\rangle; \ldots \qquad p = 0 \qquad (15)$$

$$|0\rangle, |1\rangle, \ldots \equiv |\Xi_2\rangle, |\Xi_3\rangle; |\Xi_6\rangle, |\Xi_7\rangle; |\Xi_{10}\rangle, |\Xi_{11}\rangle; \ldots \qquad p = 1. \qquad (16)$$

Marginally, we may note that at $L = 0$ the structure of the matrix Q ceases to be triangular. This seems closely related to the asymptotic asymmetry of the $g_1 \neq 0$ potentials $V^{[M]}(-\infty) = -g_1 \neq V^{[M]}(\infty) = +g_1$ and to their anomalous non-Jost solvability via a change of variables at $M = 2$ (cf, e.g., [23]). In this subsection we shall assume that $g_1 \equiv 0$, therefore. This constraint is further supported by the observation that at $M = 1$ the monotonic $V_a^{(1)}(x) = g_1 \tanh x$ itself cannot generate any bound states at all. Thus, our study of the antisymmetric models has to start at the exactly solvable $V_a^{(2)}(x) = g \sinh x/\cosh^2 x$ (cf table 1).

This antisymmetric scarf (AS) potential $V_a^{(2)}(x) \equiv V^{[AS]}(x)$ is extremely suitable for methodical purposes. Its significance is connected to the fact that our basis (10) is not tailored precisely to its exact solvability. A $D = 2$ partitioning is needed. In the reduced bases (15) and (16) its recommended boundaries are marked by semicolons. For all the $L = 2, 3, \ldots$ descendants $V_a^{(2L)}(x)$ of the AS example the size D of partitions will grow due to the downward shift of the constant g again.

The action of the last class $V_a^{(2L+1)}(x) = g \sinh x \cosh^{-2L-1} x$ of the simplified single-term potentials on the kets (10) looks irreducible. The impression is wrong. After we introduce a new quantum number $I \equiv 2p + q$ (modulo 4), the basis elements with $I = 0$ and 3 never mix with their $I = 1$ and 2 counterparts. For both the initial choices of $|0\rangle = |\Xi_1\rangle$ and $|0\rangle = |\Xi_2\rangle$ we arrive at the same output,

$$|0\rangle, |1\rangle, |2\rangle, \ldots \equiv |\Xi_{1 \text{ or } 2}\rangle, |\Xi_5\rangle, |\Xi_6\rangle, |\Xi_9\rangle, |\Xi_{10}\rangle, |\Xi_{13}\rangle, \ldots.$$

The difference between the two matrices Q will only lie in their elements.

3.3. Asymmetric Lanczos kets

Asymmetric oscillators (1) admit a non-conservation of parity by each Lanczos element $|n\rangle$ separately. The functions

$$\langle x|n\rangle = \xi_{n,p,q,a,\kappa}(x) = \frac{\sinh^{1-q} x}{\cosh^{\kappa+2n+p} x} e^{a \arctan(\sinh x)} \in L_2(-\infty, \infty) \tag{17}$$

generalize their $a = 0$ predecessors (10) and represent a very good new candidate since, due to the presence of a new parameter a, the number of the new terms in equation (2) may be lowered, for any potential (1), more efficiently. First of all, this implies that we may admit the non-zero g_1 again. Via a suitable choice of the value of a we shall be able to reproduce *all* the 'missing' (namely Rosen Morse and scarf) terminating solutions of [2] or table 1.

At $a \neq 0$ also the action of an arbitrary hyperbolic Hamiltonian remains transparent and elementary in the purely kinetic limit,

$$\frac{\xi''_{n,p,q,a,\kappa}(x)}{\xi_{n,p,q,a,\kappa}(x)} = (\sigma + q - 1)^2 + \frac{a^2 - \sigma(\sigma+1) - (2\sigma+1)a \sinh x}{\cosh^2 x} + (q-1)\frac{q - 2a \sinh x}{\sinh^2 x}.$$

Here, $\sigma = \sigma(n, p) = \kappa + 2n + p$ and the prime denotes the differentiation with respect to x. The action of the purely kinetic Hamiltonian $T = -\partial_x^2$ on our innovated kets $\langle x|\Xi_\mu\rangle \equiv \xi_{n,p,q,a,\kappa}(x)$ may employ the multi-indices $\mu(n, p, q) = 4n + 2p + q$ again,

$$\begin{aligned} T|\Xi_{\mu(n,p,0)}\rangle &= -(\sigma-1)^2|\Xi_{\mu(n,p,0)}\rangle + (2\sigma-1)a|\Xi_{\mu(n,p,1)}\rangle \\ &\quad +(\sigma^2+\sigma-a^2)|\Xi_{\mu(n+1,p,0)}\rangle - (2\sigma+1)a|\Xi_{\mu(n+1,p,1)}\rangle \\ T|\Xi_{\mu(n,p,1)}\rangle &= -\sigma^2|\Xi_{\mu(n,p,1)}\rangle + (2\sigma+1)a|\Xi_{\mu(n+1,p,0)}\rangle + (\sigma^2+\sigma-a^2)|\Xi_{\mu(n+1,p,1)}\rangle. \end{aligned}$$

The kinetic matrix elements of Q depend on σ and a and all of them increase with n. Due to the presence of the new parameter a the kinetic operator T inter-twines the states (17) with different parities $q = 0, 1$. The states with different $p = 0, 1$ stay decoupled.

3.4. Partitioned hypergeometric-like series

Our present proposal may be summarized as an application of expansions (3) to potentials (1) inspired by the analogies between the Pöschl–Teller and harmonic oscillators. The feasibility of our construction stems from the fact that the action of the present class of Hamiltonians on the suitable Lanczos kets may be characterized by the lower triangular matrices $Q(z)$. Their partitioning brings us back to the two-diagonal pattern of equation (11) and replaces its scalars α_j and β_j by the respective two-dimensional submatrices A_j and B_j,

$$Q = \begin{pmatrix} A_0 & 0 & 0 & 0 & \ldots \\ B_0 & A_1 & 0 & 0 & \ldots \\ 0 & B_1 & A_2 & 0 & \ldots \\ & & \ddots & \ddots & \end{pmatrix}. \tag{18}$$

In both the respective $a = 0$ and $a \neq 0$ bases (10) and (17) the D-plets of kets $(|m+1\rangle, |m+2\rangle, \ldots, |m+D\rangle)$ with $m = m(n) = nD - d_0$ and with any d_0 may be denoted as $||n\rangle\rangle$. In such an abbreviated notation our linear system (4) implies the recurrence relations

$$F_n \equiv \begin{pmatrix} h_{m(n)+1} \\ \ldots \\ h_{m(n)+D} \end{pmatrix} = -(A_n)^{-1} B_{n-1} F_{n-1} \qquad n = 1, 2, \ldots \tag{19}$$

which define the D-dimensional vectors of coefficients in terms of finite products of certain $D \times D$-dimensional matrices. In place of $d_0 = 1$ in a consequently D-dimensional 'democratic' partitioning we may use the shift $d_0 = D$. Both these options appear in our AS example where we recommended $d_0 = D - p$. The latter one is globally preferable as it leaves the uppermost element of Q vanishing, $A_0 = 0$. The initial array F_0 degenerates to the mere scalar norm then.

At any d_0 the formal solution (3) of the Schrödinger equation $(H - E)|y\rangle = 0$ may be rewritten in the form of the double or partitioned sum,

$$|y\rangle = \sum_{n=0}^{\infty} \sum_{j=1}^{D} ||n\rangle\rangle_j \, [F_n]_j = \sum_{n=0}^{\infty} ||n\rangle\rangle \cdot F_n. \tag{20}$$

In a slightly vague sense it looks like an immediate hypergeometric-like generalization of equation (14). Equation (19) defines all of its coefficients in closed form. They depend on the 'measure of asymmetry' a and on the unknown energy $E = -\kappa^2$.

4. Example

Our recipe strongly resembles the Hill-determinant method which proves useful in many (e.g. perturbative [24]) applications. In the majority of similar applications one must analyse, first of all, the convergence of infinite series (3) or (20). In the x-representation their pointwise convergence is basically controlled by the asymptotics of the coefficients. They are dominated by the purely kinetic terms which are asymptotically increasing. All the characteristics of the potential itself (e.g. parity mixing) will play, necessarily, a secondary role.

The first non-trivial asymmetric potential $V^{[AS]}(x)$ seems best suited for a more explicit illustration of this role. Its coefficients $h_j = h_j^{(q)}(p)$ in both the $p = 0$ and 1 solutions (3) are easily derived from the respective recurrences. Choosing the simplest $a = 0$ and using the same abbreviations a_j and b_j as above we have

$$Q^{(0)} = \left(\begin{array}{c|cc|cc|cc|c} 0 & & & & & & & \\ \hline g & a_1 & & & & & & \\ b_0 & g & a_2 & & & & & \\ \hline 0 & b_2 & g & a_3 & & & & \\ & -g & b_2 & g & a_4 & & & \\ \hline & & 0 & b_4 & g & a_5 & & \\ & & & -g & b_4 & g & a_6 & \\ \hline & & & & \ddots & \ddots & \ddots & \ddots \end{array} \right) \tag{21}$$

$$
Q^{(1)} = \left(\begin{array}{cc|cc|cc|c}
0 & & & & & & \\
g & a_1 & & & & & \\
\hline
b_1 & g & a_2 & & & & \\
-g & b_1 & g & a_3 & & & \\
\hline
 & 0 & b_3 & g & a_4 & & \\
 & & -g & b_3 & g & a_5 & \\
\hline
 & & & \ddots & \ddots & \ddots & \ddots
\end{array} \right). \tag{22}
$$

The contribution of the coupling g is clearly separated from the growing and energy-dependent kinetic terms.

After a return to the general $a \neq 0$ we just have to modify the values of the matrix elements accordingly. We may preserve the reduction of bases (15) and (16) as well as their $D = 2$ partitioning. It is obvious that the exact Jacobi polynomial solutions may be reproduced in our $D = 2$ language. It is an instructive exercise to show how this reproduction proceeds. Firstly, the variability of the parameter a and of the energy or momentum κ enables us to achieve a complete disappearance of the 2×2 submatrix $B_K = 0$ at an arbitrary optional K. The resulting series (20) then strictly terminates and reproduces the known Gauss hypergeometric solution. Its termination just reflects the factorization of the secular determinant.

Let us underline that the simpler, 'termination-incompatible' basis (10) with $a = 0$ is an analogue of the non-WKB bases in section 2.2. Hence, we may fix $a = 0$ and recall the same AS model also as one of the simplest illustrative examples of a general non-terminating solution.

4.1. AS oscillator in the $a = 0$ representation

The AS solutions (3) may be split into two separate sums with well defined parity,

$$
|Y^{[AS]}\rangle = |Y^{[AS]}(p)\rangle = |Y^{(\text{even})}(p)\rangle + |Y^{(\text{odd})}(p)\rangle. \tag{23}
$$

The first few terms in the even partial sums with $q = 1$,

$$
\begin{aligned}
|Y^{(\text{even})}(0)\rangle &= |\Xi_1\rangle \cdot h_0^{(1)}(0) + |\Xi_5\rangle \cdot h_2^{(1)}(0) + |\Xi_9\rangle \cdot h_4^{(1)}(0) + \cdots \\
|Y^{(\text{even})}(1)\rangle &= |\Xi_3\rangle \cdot h_1^{(1)}(1) + |\Xi_7\rangle \cdot h_3^{(1)}(1) + |\Xi_{11}\rangle \cdot h_5^{(1)}(1) + \cdots
\end{aligned} \tag{24}
$$

as well as their odd, $q = 0$ counterparts

$$
\begin{aligned}
|Y^{(\text{odd})}(0)\rangle &= |\Xi_4\rangle \cdot h_1^{(0)}(0) + |\Xi_8\rangle \cdot h_3^{(0)}(0) + |\Xi_{12}\rangle \cdot h_5^{(0)}(0) + \cdots \\
|Y^{(\text{odd})}(1)\rangle &= |\Xi_2\rangle \cdot h_0^{(0)}(1) + |\Xi_6\rangle \cdot h_2^{(0)}(1) + |\Xi_{10}\rangle \cdot h_4^{(0)}(1) + \cdots
\end{aligned} \tag{25}
$$

are easily computed in the recurrent manner,

$$
\begin{array}{llll}
h_0^{(1)}(0) = 1 & h_1^{(0)}(0) = -g/a_1 & h_2^{(1)}(0) = -b_0/a_2 + g^2/(a_1 a_2) & \ldots \\
h_0^{(0)}(1) = 1 & h_1^{(1)}(1) = -g/a_1 & h_2^{(0)}(1) = -b_1/a_2 + g^2/(a_1 a_2) & \ldots.
\end{array} \tag{26}
$$

A compact general determinantal formula for these coefficients also exists [15]. It would enable us to rewrite equation (23), i.e.

$$
|Y^{[AS]}(p)\rangle = \sum_{j=0}^{\infty} |\Xi_{\mu(j,p,1)}\rangle \cdot h_{2j+p}^{(1)}(p) + \sum_{j=0}^{\infty} |\Xi_{\mu(j+1-p,p,0)}\rangle \cdot h_{2j+1-p}^{(0)}(p) \tag{27}
$$

in the explicit form if needed. Here, we prefer the recurrent generation of the doublets of coefficients

$$F_{n+1-p} = F_{n+1-p}(p) = \begin{pmatrix} h^{(0)}_{2n+1-p}(p) \\ h^{(1)}_{2n+2-p}(p) \end{pmatrix} \qquad p = 0 \text{ or } 1 \qquad n = 0, 1, \ldots$$

as a matrix product,

$$F_j(p) = \left[-A_j(p)\right]^{-1} B_j(p) F_{j-1}(p) \qquad j = 1, 2, \ldots. \tag{28}$$

In our partitioned notation with $D = 2$ the solution $|y\rangle$ may be presented as a two-dimensional hypergeometric series since its matrix coefficients remain surprisingly elementary,

$$\left[-A_j(p)\right]^{-1} = \begin{pmatrix} 1 & 0 \\ 0 & 1/a_{2j+p} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ g & 1 \end{pmatrix} \begin{pmatrix} 1/a_{2j+p-1} & 0 \\ 0 & 1 \end{pmatrix}.$$

As long as $0 > a_1 > a_2 > \cdots$ at any $\kappa > 0$, all our vectors of coefficients are well defined and unique. Their initialization is provided by the 'model space' equation $A_0(p)F_0(p) = 0$ which depends on p. At $p = 0$, we have the vanishing scalar $A_0(0) \equiv 0$, while the exceptional singlet $F_0(0) = h^{(1)}_0(0)$ (conveniently put equal to one) is the norm. In the parallel two-dimensional initialization at $p = 1$, the first component $h^{(0)}_0(1) = 1$ of $F_0(1)$ is the norm. The second component must be recalculated, $h^{(1)}_0(1) = gh^{(0)}_0(1)/(2\kappa + 1)$.

We are ready to prove the convergence. Its decisive simplification occurs in the $j \gg 1$ asymptotic domain. The upper and lower components of equation (28) decouple there in a p-independent manner,

$$\left[F_j(p)\right]_q \left[\equiv h^{(q)}_{2j+p+q-1}(p)\right] = \left[1 + \frac{1-4q}{2j} + \mathcal{O}\left(\frac{1}{j^2}\right)\right] \left[F_{j-1}(p)\right]_q \qquad q = 0 \text{ or } 1. \tag{29}$$

For both our infinite series (27) the proof is easy at $x \neq 0$. As long as $\cosh x > 1$ for all the non-zero and real coordinates x, the ordinary geometric criterion together with the estimate (29) implies that our series (27) are convergent absolutely, i.e. for all the (complex) couplings g and energies $-\kappa^2$. The same geometric argument extends the validity of our conclusion to all the complex coordinates $x + \mathrm{i}y$ which lie outside of a wiggly bounded domain such that $|\cosh(x + \mathrm{i}y)| = \sqrt{\sinh^2 x + \cos^2 y} \leqslant 1$ or, in a cruder approximation, out of the fairly narrow strip with $|x| \leqslant \ln(1 + \sqrt{2})$ at least.

On the real axis, an indeterminate behaviour of the type $0 \times \infty$ emerges at the point $x = 0$. This follows from equation (29) and from the slightly more sophisticated Raabe criterion. Strictly speaking, this forces us to work on a punctured domain of $x \in (-\infty, 0) \bigcup (0, \infty)$ in principle. As a consequence, logarithmic derivatives of our left and right Jost solutions have to be matched at the origin. This task is to be fulfilled numerically. Let us outline its two steps.

4.2. Generalized parity

Since our $D = 2$ hypergeometric AS series $\langle x|Y^{[AS]}(p)\rangle \equiv \varphi^{(p)}(g, x, \kappa)$ (27) satisfy the differential Schrödinger equation on a punctured domain $(-\infty, 0) \bigcup (0, \infty)$ only, we necessarily have to match them at the origin. In the Pöschl–Teller example of section 2.3 where the non-matrix Gauss solutions also developed a certain discontinuity at the origin at a general unphysical energy E, the point has easily been settled after an account of parity. As long as our potentials lose their spatial symmetry in general, the parity is broken and a matching of the two sub-intervals $(-\infty, 0) \bigcup (0, \infty)$ becomes non-trivial.

We have to employ a broader invariance of our model(s) with respect to the product $\hat{P}$ of parity $\mathcal{P}$ with the reflections of couplings $g_j \to -g_j$. The operator (such that $\hat{P}^2 = 1$) commutes with our Hamiltonian(s), $H = \hat{P}H\hat{P}$. Each physical bound state $\psi(x)$ may be assigned an even or odd $\hat{P}$-parity, $\hat{P}\psi(x) = \pm\psi(x)$.

In a way resembling the parity-breaking systems with $\mathcal{PT}$ invariance [25] the assignment of the $\hat{P}$-parity to our AS states $\chi(g, x)$ depends on their normalization,

$$\{\hat{P}\chi(g,x) = \pm\chi(g,x)\} \quad \Longrightarrow \quad \{\hat{P}[g\cdot\chi(g,x)] = \mp[g\cdot\chi(g,x)]\}.$$

Fortunately, our AS coefficients $h_n^{(q)}(p) = h_n^{(q)}(p,g)$ are explicitly defined by the triangularized Hamiltonians (21) and (22) and we immediately notice that

$$h_j^{(q)}(p,-g) = (-1)^{p+q+1}h_j^{(q)}(p,g).$$

Both our AS hypergeometric-like series $\varphi^{(p)}(g,x,\kappa) = \langle x|Y^{[AS]}(p)\rangle$ (27) behave as eigenstates of our double-parity operator $\hat{P}$,

$$\hat{P}\varphi^{(p)}(g,x,\kappa) = \varphi^{(p)}(-g,-x,\kappa) = (-1)^p\varphi^{(p)}(g,x,\kappa).$$

With a pair of some constants $\mathcal{M} \neq \mathcal{M}(g)$ and $\mathcal{N} \neq \mathcal{N}(g)$ we may postulate that the bound states read

$$\psi^{[AS]}(x) = \mathcal{M}\varphi^{(0)}(g,x,\kappa) + g\cdot\mathcal{N}\varphi^{(1)}(g,x,\kappa) \qquad x \neq 0. \tag{30}$$

The same (conventionally, even) $\hat{P}$-parity may be assigned to all our physical solutions since their energy spectrum is non-degenerate.

4.3. Match in the origin

A return to the ordinary spatial parity $\mathcal{P}$ enables us to distinguish between the cosine-like (i.e. spatially even) and sine-like (i.e. spatially odd) components of our generalized hypergeometric functions (27),

$$c(x,\kappa) = \tfrac{1}{2}[\varphi^{(0)}(g,x,\kappa) + \varphi^{(0)}(g,-x,\kappa)]$$

$$\tilde{s}(x,\kappa) = \tfrac{1}{2}[\varphi^{(0)}(g,x,\kappa) - \varphi^{(0)}(g,-x,\kappa)]$$

$$\tilde{c}(x,\kappa) = \tfrac{1}{2}[\varphi^{(1)}(g,x,\kappa) + \varphi^{(1)}(g,-x,\kappa)]$$

$$s(x,\kappa) = \tfrac{1}{2}[\varphi^{(1)}(g,x,\kappa) - \varphi^{(1)}(g,-x,\kappa)].$$

The tildes $\tilde{}$ marking the asymptotical subdominance are not too relevant since we dwell in a vicinity of the origin where $x = \pm\varepsilon \approx 0$. Wavefunctions must be continuous there,

$$\lim_{\varepsilon\to 0^+}\psi^{[AS]}_{(\text{physical})}(\varepsilon) = \lim_{\varepsilon\to 0^+}\psi^{[AS]}_{(\text{physical})}(-\varepsilon).$$

The even, cosine-like components of our solutions satisfy such a requirement identically. In the light of equation (30) we are left with a reduced continuity condition

$$\mathcal{M}\tilde{s}(\varepsilon,\kappa) + g\cdot\mathcal{N}s(\varepsilon,\kappa) = 0 \qquad \varepsilon \to 0. \tag{31}$$

In the same manner, the continuity of derivatives is required. In the uppercase notation with abbreviations

$$S(x,\kappa) = \tfrac{1}{2}[\partial_x\varphi^{(0)}(g,x,\kappa) + \partial_x\varphi^{(0)}(g,-x,\kappa)]$$

$$\tilde{C}(x,\kappa) = \tfrac{1}{2}[\partial_x\varphi^{(0)}(g,x,\kappa) - \partial_x\varphi^{(0)}(g,-x,\kappa)]$$

$$\tilde{S}(x,\kappa) = \tfrac{1}{2}[\partial_x\varphi^{(1)}(g,x,\kappa) + \partial_x\varphi^{(1)}(g,-x,\kappa)]$$

$$C(x,\kappa) = \tfrac{1}{2}[\partial_x\varphi^{(1)}(g,x,\kappa) - \partial_x\varphi^{(1)}(g,-x,\kappa)]$$

this leads to the second reduced matching condition

$$\mathcal{M}S(\varepsilon,\kappa) + g\cdot\mathcal{N}\tilde{S}(\varepsilon,\kappa) = 0 \qquad \varepsilon\to 0. \tag{32}$$

In the limit $\varepsilon \to 0$ a root $\kappa(\varepsilon)$ of the two-dimensional secular equation

$$\det\begin{pmatrix} \tilde{s}(\varepsilon,\kappa) & s(\varepsilon,\kappa) \\ S(\varepsilon,\kappa) & \tilde{S}(\varepsilon,\kappa)\end{pmatrix} = 0$$

will determine the physical energy. Matrix elements of this secular equation are convergent series in $t = \cosh^{-2}\varepsilon < 1$,

$$\tilde{s}(\varepsilon,\kappa) = \sum_{n=1}^{\infty} h_n^{(0)}(0,g)t^n \qquad s(\varepsilon,\kappa) = \sum_{n=0}^{\infty} h_n^{(0)}(1,g)t^n$$

$$S(\varepsilon,\kappa) = \sum_{n=0}^{\infty}(\kappa+2n)h_n^{(1)}(0,g)t^n \qquad \tilde{S}(\varepsilon,\kappa) = \sum_{n=0}^{\infty}(\kappa+2n+1)h_n^{(1)}(1,g)t^n.$$

Norms $h_0^{(1)}(0,g) = h_0^{(0)}(1,g) = 1$ are fixed and the higher coefficients carry the κ dependence. An analogy with the spatially symmetric Pöschl–Teller example of section 2.3 is fully restored.

5. Summary

We described a new approach to the Schrödinger bound-state problem with any Rosen–Morse-like multi-term potential (1). For all these forces we have shown how:

- the ordinary differential Schrödinger equation for the wavefunctions $\psi(x)$ may be reduced to a linear homogeneous algebraic problem $Q(E)\vec{h} = 0$;
- an 'inspired' choice of the Lanczos-like (i.e. Hamiltonian-dependent) basis makes the related infinite-dimensional secular determinant vanish identically, det $Q(E) = 0$;
- the very special (namely lower-triangular) structure of our quasi-Hamiltonian matrices $Q(E)$ reduces the construction of the separate Taylor-like coefficients h_n in our wavefunctions $\psi(x)$ to the mere (partitioned) two-term recurrences.

On a characteristic AS example we have illustrated that:

- all our solutions $\psi(x)$ are convergent and may be understood as a certain generalization of the Gauss hypergeometric series (which further degenerates to the Jacobi polynomials at the physical energies in the solvable cases);
- a certain generalized parity symmetry of our forces enables us to determine Jost solutions which are compatible with *both* our asymptotic boundary conditions;
- via our final two-by-two condition (31) + (32), the values of the remaining two free parameters (namely energy and p-mixing) in our Jost solutions may (and have to) be tuned to their necessary continuity and smoothness at the origin.

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