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Group-theoretical foundation of the J-matrix theory of scattering

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Abstract. Group-theoretical analysis shows that $SO(2, 1)$ is an underlying dynamical symmetry for all Hamiltonians that are compatible with the Jacobi matrix (J-matrix) formalism. The class of central potentials with this property is obtained including, but not limited to, the oscillator, Coulomb and Morse potentials. The L^2 bases and J-matrix elements for these potentials are found. $SO(2, 1)$-invariant transformation of the solutions of the recursion relation for one potential gives those for another potential in the class. Phase-shift and resonance calculations for a single-channel potential are carried out in the oscillator basis to illustrate the use of our results.

1. Introduction

The Jacobi matrix (J-matrix) theory of scattering exploits the fact that the unperturbed ('reference') Hamiltonian can be diagonalized in a certain complete set of L^2 basis functions. Truncating the short-range perturbing potential in a finite subset of this basis provides the numerical means to obtain scattering information over a continuous range of energies. The L^2 basis set is chosen such that the matrix representation of the reference Hamiltonian is tridiagonal (Jacobi). The importance of this feature becomes apparent when we note that writing the Schrödinger equation for the unperturbed problem in such a basis results in a symmetric three-term recurrence relation for the expansion coefficients of the wavefunction. This produces an intimate association with the theory of orthogonal polynomials and facilitates the use of its powerful mathematical tools. In fact, it makes it possible to diagonalize the reference Hamiltonian analytically, i.e. to obtain a closed-form solution for the associated three-term recursion relation in terms of orthogonal polynomials.

Ojha has shown in a series of papers [1–3] that all reference Hamiltonians previously used in the J-matrix formalism are unified by identifying the underlying $so(2, 1)$ Lie algebra. With this result, he was able to extend the J-matrix formulation in a natural way to include the Morse potential [3]. The regular and irregular solutions of the recursion relations were obtained algebraically.

Casting the J-matrix in this group-theoretical framework and giving a basis-independent treatment of the solution of its unperturbed problem gives the theory a solid foundation and provides for its fundamental setting.

The contribution of our work in this paper can be stated as follows.

(a) As a generalization of Ojha's work, we show that *any* linear self-adjoint operator that spans the space of generators of $so(2, 1)$ Lie algebra can admit an infinite-dimensional tridiagonal matrix representation and, henceforth, fall within the domain of application of the J-matrix theory.

(b) We identify a large class of analytically solvable potentials in the J-matrix formalism and obtain their corresponding bases and J-matrix elements. Besides the familiar Coulomb, oscillator and Morse potentials, this class includes various other potentials at zero energy which may prove to be very useful in some physical applications and at least in limiting cases.

(c) We exploit the $SO(2, 1)$ invariance of the theory and show how to obtain the regular and irregular solutions of the recursion relation and J-matrix elements for any potential in that class by making an $SO(2, 1)$-invariant transformation of the corresponding objects given for one of the other potentials.

(d) All previous work on the J-matrix theory using the oscillator basis, including that of Ojha, was limited to a reference Hamiltonian having the kinetic energy only without the oscillator potential term. In this paper we obtain the analytical solution of the recursion relation for the *generalized* oscillator and illustrate our results in a simple scattering example.

The paper is organized as follows. In section 2 we give a brief overview of the J-matrix theory of scattering [4–7] in which we also define the terminology of the paper. In section 3 we show that by starting from a general statement concerning the basic feature of the J-matrix formalism together with its unitarity requirements we arrive at the underlying symmetry of the theory. In section 4 we account for a large class of analytically solvable potentials in the J-matrix theory having this symmetry and in the appendix we obtain their corresponding bases and J-matrix elements. Finally, in section 5 we show how to exploit the $SO(2, 1)$ invariance of the theory and find the analytical solutions of the recursion relation (i.e. the J-matrix kinematical coefficients T_n and $R_n^{\pm}$) for the oscillator potential. We use these in a simple example in which we calculate the scattering matrix for the single-channel potential $\tilde{V}(r) = 7.5r^2\mathrm{e}^{-r}$ in the oscillator basis.

2. A brief overview of the single-channel J-matrix theory of scattering

Let H be the total Hamiltonian of the system that describes the incident particle(s) and structureless target and let $|\chi\rangle$ be the wavefunction. The time-independent Schrödinger wave equation reads

$$(H - E)|\chi\rangle = 0. \tag{2.1}$$

We write

$$H = H_\infty + V$$

where H_∞ is the free Hamiltonian (i.e. the Hamiltonian of the system when the incident particle is at an infinite separation from the target where $V = 0$). Let us assume that the potential can be written as

$$V = V_0 + \tilde{V} \tag{2.2}$$

where $\tilde{V}$ is short range and V_0 is the analytical part of the potential with the property that when added to H_∞ it gives the reference Hamiltonian

$$H_0 \equiv H_\infty + V_0 \tag{2.3}$$

which admits a tridiagonal matrix representation in a 'proper' L^2 basis $\{|\varphi_n\rangle\}_{n=0}^{\infty}$.

For bound states, one can always expand the wavefunction in this complete basis as

$$|\chi\rangle = \sum_n a_n |\varphi_n\rangle$$

where $|\chi\rangle$ is energy-normalized as $\langle\chi(E)|\chi(E')\rangle = \delta(E - E')$.

In scattering problems, however, this decomposition does not guarantee a solution to the wave equation (2.1). Nevertheless, ignoring the short-range part of the potential (i.e. taking $H = H_0$), we may find an L^2 basis in which the problem is 'solvable' almost everywhere. That is, we can find in this basis a state $|\psi\rangle$ such that the equation

$$\langle\varphi_n| (H_0 - E) |\psi\rangle = 0 \qquad \forall n \tag{2.4}$$

is satisfied outside a dense region of space, Ω^V, around the origin of $\tilde{V}$. Our choice of basis $\{\varphi_n\}$ is limited by the requirement that the matrix representation of the operator $H_0 - E \equiv J$ is tridiagonal or Jacobian. That is,

$$\langle\varphi_n|(H_0 - E)|\varphi_m\rangle = 0 \qquad |n - m| > 1.$$

Expanding $|\psi\rangle$ in this basis, we can write equation (2.4) as

$$\sum_m \langle\varphi_n|(H_0 - E)|\varphi_m\rangle a_m = 0 \qquad \forall n \tag{2.5}$$

or $\sum_m J_{nm} a_m = 0$, where J_{nm} is the tridiagonal matrix representation of $H_0 - E$ in the $\{\varphi_n\}$ basis.

Given a specific H_0 and $\{\varphi_n\}$, one can calculate J_{nm} and use it in equation (2.5) to give a three-term recursion relation involving a_n and $a_{n\pm1}$:

$$\begin{aligned} &J_{n,n-1} a_{n-1} + J_{nn} a_n + J_{n,n+1} a_{n+1} = 0 \qquad n \geqslant 1 \\ &J_{00} a_0 + J_{01} a_1 = 0. \end{aligned} \tag{2.6}$$

Typically, H_0 is second order, hence there exist two independent solutions to (2.4). Asymptotically, these two solutions behave like free particles, one of them as $\sin(kr)$ and the other as $\cos(kr)$, where $k = \sqrt{2E}$. Therefore, we need two sets of independent expansion coefficients $\{a_n\}$. Typically, one solution of equation (2.4) is regular everywhere and the other is irregular and blows up at the origin. However, both behave asymptotically in the right way. The regular solution can always be expanded in terms of the basis $\{\varphi_n\}$. We take this solution, which satisfies the recursion relation (2.6), as the regular one that solves (2.5) identically and behaves asymptotically as $\sin(kr)/k$. The other solution is obtained by the requirements that it behaves asymptotically as $\cos(kr)/k$, that it is expandable in terms of $\{\varphi_n\}$ (hence, regular) and that it solves (2.4) only outside the dense subspace Ω^V. This means that outside Ω^V it is equivalent to the irregular solution. We write the two solutions as

$$\begin{aligned} |S\rangle &= \sum_n s_n |\varphi_n\rangle \\ |C\rangle &= \sum_n c_n |\varphi_n\rangle. \end{aligned} \tag{2.7}$$

The set $\{s_n\}$ satisfies the recursion relation (2.6) and

$$\begin{aligned} &\langle\varphi_n|(H_0 - E)|S\rangle = 0 \qquad \forall n \\ &\lim_{r\to\infty} \langle r|S\rangle = \sin(kr) \end{aligned} \tag{2.8}$$

whereas $\{c_n\}$ satisfy the recursion relation (2.6) only for $n \geqslant 1$, while the last relation reads [6]

$$J_{00}c_0 + J_{01}c_1 = k/2s_0. \tag{2.9}$$

Hence

$$\langle\varphi_n|\,(H_0 - E)\,|C\rangle = (k/2s_0)\,\delta_{n0} \qquad \forall n \tag{2.10}$$

and

$$\lim_{r\to\infty}\langle r|C\rangle = \cos(kr). \tag{2.11}$$

Moreover, these coefficients also satisfy the Wronskian-like relation

$$J_{n,n-1}\,(c_n s_{n-1} - c_{n-1}s_n) = k/2 \qquad n \geqslant 1. \tag{2.12}$$

Now it is assumed that $\tilde{V}$ is of short enough range that one can make a good approximation of its matrix representation, in the dense subspace Ω^V, by the first N elements of the basis set $\{|\varphi_n\rangle\}_{n=0}^{N-1}$ for some large enough integer N. That is, the effectiveness of the potential is limited to an 'N-box' as

$$\tilde{V}_{nm} = \begin{cases} \langle\varphi_n|\,\tilde{V}\,|\varphi_m\rangle & n, m \leqslant N-1 \\ 0 & \text{otherwise.} \end{cases} \tag{2.13}$$

This approximation scheme is analogous to that followed in the R-matrix theory of scattering, where it is assumed that the effectiveness of $\tilde{V}$ is limited to a configuration space box ('r-box') of radius R; that is,

$$\tilde{V}(r) = \begin{cases} \tilde{V}(r) & r \leqslant R \\ 0 & \text{otherwise.} \end{cases} \tag{2.14}$$

Finally, we need to solve

$$\langle\varphi_n|\big(H_0 + \tilde{V} - E\big)|\chi\rangle = 0 \qquad \forall n \tag{2.15}$$

where

$$|\chi\rangle = \sum_n b_n|\varphi_n\rangle \qquad b_n \neq a_n.$$

In matrix form equation (2.15) reads

$$\left[\begin{pmatrix} J_{00} & J_{01} & 0 & 0 & & \\ J_{10} & J_{11} & J_{12} & 0 & & \\ 0 & J_{21} & J_{22} & J_{23} & & \\ & & \cdots & \cdots & \cdots & \\ & & & \cdots & \cdots & \cdots \\ & & & & \cdots & \cdots \end{pmatrix} + \begin{pmatrix} \tilde{V}_{00} & \tilde{V}_{01} & \cdots & \tilde{V}_{0,N-1} & 0 & \cdots \\ \tilde{V}_{10} & \tilde{V}_{11} & \cdots & \tilde{V}_{1,N-1} & 0 & \cdots \\ \vdots & \vdots & \cdots & \vdots & \vdots & \cdots \\ \tilde{V}_{N-1,0} & \tilde{V}_{N-1,1} & \cdots & \tilde{V}_{N-1,N-1} & 0 & \cdots \\ 0 & 0 & \cdots & 0 & 0 & \cdots \\ \vdots & \vdots & \cdots & \vdots & \vdots & \cdots \end{pmatrix}\right]\begin{pmatrix} b_0 \\ b_1 \\ \vdots \\ b_{N-1} \\ b_N \\ \vdots \end{pmatrix} = 0.$$

We divide the L^2 Hilbert space into a P-space component (the inner space inside the 'N-box') and a Q-space component (the space outside the 'N-box') and write

$$|\chi\rangle = P|\chi\rangle + Q|\chi\rangle. \tag{2.16}$$

Since the model potential has a vanishing representation in the Q-space, then $Q|\chi\rangle$ exhibits the asymptotic behaviour of the wavefunction, which is a combination of an incoming and an outgoing wave, modified by the S-matrix. Therefore, we can write

$$Q|\chi\rangle = \sum_{n=N}^{\infty} [(c_n - \mathrm{i}s_n) - S(E)(c_n + \mathrm{i}s_n)]\,|\varphi_\mathrm{n}\rangle \tag{2.17}$$

where $S(E)$ is the *exact* S-matrix for the model potential $\tilde{V}$. Finally, equation (2.15) is written as

$$\begin{aligned} &P^\dagger(J+\tilde{V})P|\chi\rangle + P^\dagger JQ|\chi\rangle = 0 \\ &Q^\dagger JP|\chi\rangle + Q^\dagger JQ|\chi\rangle = 0 \end{aligned} \tag{2.18}$$

which couples $P|\chi\rangle$ and $Q|\chi\rangle$ and can now be reduced to an equation for $Q|\chi\rangle$, namely

$$\{(Q^\dagger JQ) - (Q^\dagger JP)[P^\dagger(J+\tilde{V})P]^{-1}(P^\dagger JQ)\}|\chi\rangle = 0. \tag{2.19}$$

If we take the inner product of this null vector with $\langle\bar{\varphi}_N|$, which is an element of the conjugate orthogonal space (i.e. $\langle\bar{\varphi}_n|\varphi_m\rangle = \delta_{nm}$), then we obtain the following closed-form solution for the S-matrix:

$$S(E) = T_{N-1}(E)\frac{1 + g_{N-1,N-1}(E)J_{N-1,N}(E)R_N^-(E)}{1 + g_{N-1,N-1}(E)J_{N-1,N}(E)R_N^+(E)} \tag{2.20}$$

where $g_{n,m}(E) = \langle\bar{\varphi}_n|\,[P^\dagger(J+\tilde{V})P]^{-1}\,|\bar{\varphi}_m\rangle$ is the finite-matrix version of the exact Green function and

$$T_n = \frac{c_n - \mathrm{i}s_n}{c_n + \mathrm{i}s_n} \qquad R_n^\pm = \frac{c_n \pm \mathrm{i}s_n}{c_{n-1} \pm \mathrm{i}s_{n-1}}. \tag{2.21}$$

3. J-matrix formalism and the underlying $SO(2,1)$ symmetry

In this section we show that *any* linear self-adjoint operator which admits a special kind of infinite-dimensional tridiagonal matrix representation must span the space of generators of $so(2,1)$ Lie algebra. Henceforth, operators that are compatible with the J-matrix theory will have this symmetry.

We can decompose the matrix representation of such an operator into the sum of a diagonal one and two off-diagonals, one above and one below the diagonal. Let us label these three as the representations of the operators L_3, L_+ and L_-, respectively. Clearly, $L_3^\dagger = L_3$ and $L_\pm^\dagger = L_\mp$. Moreover, let us label the basis of this representation, which is obviously discrete, by the integer n as $|n\rangle$. Evidently, the action of these three operators on the basis is as follows:

$$L_3|n\rangle \sim |n\rangle \qquad \text{and} \qquad L_\pm|n\rangle \sim |n \pm 1\rangle.$$

Specifically, for an appropriate choice of functions of n, we write this as

$$L_3|n\rangle = A(n)|n\rangle \qquad L_\pm|n\rangle = B^\pm(n)|n \pm 1\rangle. \tag{3.1}$$

It is required that $A(n)$ be linear in n; that is,

$$A(n) = \alpha n + \alpha_0 \qquad \text{where } \alpha \text{ and } \alpha_0 \text{ are constants.}$$

We also assume that the successive action of the raising operator, L_+, followed by the lowering operator, L_-, on any state $|n\rangle$ is the same as that of the reverse-order modulo action of L_3. This means that $[B^+(n)B^-(n+1) - B^-(n)B^+(n-1)]$ is proportional to $A(n)$. Under these restrictions, we attempt to find the algebra satisfied by the three operators

$$\begin{aligned}\left[L_3, L_\pm\right]|n\rangle &= B^\pm(n)L_3\,|n\pm 1\rangle - A(n)L_\pm|n\rangle \\ &= [A(n\pm 1) - A(n)]\,B^\pm(n)\,|n\pm 1\rangle = \pm\alpha L_\pm|n\rangle \qquad \forall n.\end{aligned} \tag{3.2}$$

Since this is true for all n, we can write the basis-independent algebraic relation

$$\left[L_3, L_\pm\right] = \pm\alpha L_\pm \qquad \alpha \neq 0. \tag{3.3}$$

Moreover, unitarity requires that α is real.

The remaining relation needed to define the algebra is

$$\begin{aligned}\left[L_+, L_-\right]|n\rangle &= B^-(n)L_+\,|n-1\rangle - B^+(n)L_-\,|n+1\rangle \\ &= \left[B^-(n)B^+(n-1) - B^+(n)B^-(n+1)\right]|n\rangle = \beta A(n)|n\rangle = \beta L_3|n\rangle \qquad \forall n\end{aligned}$$

where β is a constant of proportionality. Since this true for all n, we may write

$$[L_+, L_-] = \beta L_3 \qquad \beta \neq 0. \tag{3.4}$$

Furthermore, unitarity requires that β is real.

Next, we perform the following rescaling:

$$L_3 \to \alpha L_3 \qquad L_\pm \to \sqrt{|\alpha\beta|}L_\pm.$$

Thus

$$\left[L_3, L_\pm\right] = \pm L_\pm \qquad \left[L_+, L_-\right] = \eta L_3 \qquad \text{where} \quad \eta = \pm 1. \tag{3.5}$$

Therefore, we end up with two possibilities:

(a) $\eta = +1$, giving the algebra of $so(3) \cong su(2)$
(b) $\eta = -1$, giving the algebra of $so(2,1) \cong su(1,1)$.

The first possibility is compact and has finite-dimensional real representations, while the second is non-compact and can admit only infinite-dimensional real representations. Since our problems of physical interest have infinite spectra, then we must be dealing with the second case and $so(2,1)$ algebra

$$\left[L_3, L_\pm\right] = \pm L_\pm \qquad \left[L_+, L_-\right] = -L_3. \tag{3.6}$$

In terms of the Hermitian operators L_1 and L_2, where $L_\pm = \frac{1}{\sqrt{2}}(L_1 \pm \mathrm{i}L_2)$, this can be written as

$$[L_1, L_2] = -\mathrm{i}L_3 \qquad [L_2, L_3] = \mathrm{i}L_1 \qquad [L_3, L_1] = \mathrm{i}L_2. \tag{3.7}$$

$so(2,1)$ algebra is of rank one and has one Casimir-invariant operator. This operator, which commutes with L_3 and $L_\pm$, is

$$L^2 = L_3^2 - L_+L_- - L_-L_+ = L_3^2 \pm L_3 - 2L_\mp L_\pm. \tag{3.8}$$

Among the four operators L^2, L_3 and $L_\pm$ there is a maximum of two commuting, one of which is L^2. To obtain the discrete representation, we choose the compact operator L_3 to commute with L^2 rather than the non-compact L_1 or L_2. Therefore, L_3 shares the same eigenvectors with L^2. Elements of this representation are labelled with two parameters corresponding to the eigenvalues of L^2 and L_3. In fact, there are three discrete unitary representations of $SO(2, 1)$ [8]. Two of these are bounded, one with a lower bound and the other with an upper bound. The third is not bounded. Physically, we are interested in the one that is bounded from below. It is parametrized by a real constant $\gamma \geqslant -\frac{1}{2}$ and denoted as $D^+(\gamma)$. The action of the operators of the algebra on the basis $|\gamma, n\rangle$ is as follows:

$$
\begin{aligned}
L^2|\gamma, n\rangle &= \gamma(\gamma+1)|\gamma, n\rangle \qquad n = 0, 1, 2, \ldots \\
L_3|\gamma, n\rangle &= (\gamma+n+1)|\gamma, n\rangle \\
L_+|\gamma, n\rangle &= \frac{1}{\sqrt{2}}\sqrt{(n+1)(n+2\gamma+2)}|\gamma, n+1\rangle \\
L_-|\gamma, n\rangle &= \frac{1}{\sqrt{2}}\sqrt{n(n+2\gamma+1)}|\gamma, n-1\rangle
\end{aligned}
\tag{3.9}
$$

giving the functions that were defined in equation (3.1) above with all requirements satisfied

$$
\begin{aligned}
A(n) &= \gamma+n+1 \\
B^+(n) &= \frac{1}{\sqrt{2}}\sqrt{(n+1)(n+2\gamma+2)} \\
B^-(n) &= B^+(n-1) = \frac{1}{\sqrt{2}}\sqrt{n(n+2\gamma+1)}.
\end{aligned}
\tag{3.10}
$$

Realization of the generators of $SO(2, 1)$ in terms of differential operators in one variable, say r, is of great importance since it is intended to solve the physically interesting second-order radial differential equations of the form

$$
\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} + f(r)\right]\phi(r) = 0 \tag{3.11}
$$

where

$$
f(r) = -\frac{l(l+1)}{r^2} - 2V_0(r) + 2E \tag{3.12}
$$

and where E is the energy, l is the angular momentum quantum number and $V_0(r)$ is a real potential function of r that forms part of the reference Hamiltonian.

The most general forms of the three generators L_3 and $L_\pm$, whose linear combination gives the second-order differential operator $\frac{\mathrm{d}^2}{\mathrm{d}r^2} + f(r)$, are

$$
L_3 = \frac{\mathrm{d}^2}{\mathrm{d}r^2} + b_3(r)\frac{\mathrm{d}}{\mathrm{d}r} + a_3(r) \qquad L_\pm = \frac{1}{\sqrt{2}}\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} + b_\pm(r)\frac{\mathrm{d}}{\mathrm{d}r} + a_\pm(r)\right]. \tag{3.13}
$$

Unitarity ($L_\pm^\dagger = L_\mp$, $L_3^\dagger = L_3$) and the fact that in the Hilbert space of $\boldsymbol{L}^2(0, \infty)$ functions

$$
\left(\frac{\overrightarrow{\mathrm{d}}}{\mathrm{d}r}\right)^\dagger = -\left(\frac{\overleftarrow{\mathrm{d}}}{\mathrm{d}r}\right)
$$

give the following:

$$
b_-(r) = -b_+(r) \qquad a_-(r) = a_+(r) - \frac{\mathrm{d}}{\mathrm{d}r}b_+(r) \qquad b_3(r) = 0. \tag{3.14}
$$

Moreover, applying the commutation relations and after some manipulations, we arrive at the following:

$$L_3 = \frac{d^2}{dx^2} + \frac{\mu}{x^2} - \frac{x^2}{16}$$
$$L_\pm = \frac{1}{\sqrt{2}}\left[\frac{d^2}{dx^2} + \frac{\mu}{x^2} + \frac{x^2}{16} \pm \frac{1}{2}\left(x\frac{d}{dx} + \frac{1}{2}\right)\right] \tag{3.15}$$

where $x = r + \kappa$ and μ and κ are real constant parameters.

As a result of this realization, one finds

$$L^2 = -\tfrac{1}{4}\left(\mu + \tfrac{3}{4}\right) \equiv \gamma(\gamma + 1). \tag{3.16}$$

Thus

$$\mu = -4\gamma(\gamma + 1) - \tfrac{3}{4} \qquad \text{and} \qquad \mu \leqslant \tfrac{1}{4}. \tag{3.17}$$

4. Potentials in the $SO(2, 1)$ J-matrix theory and their bases

In this section we set down the Schrödinger equation whose $SO(2, 1)$-invariant transformations form the class of analytically solvable potentials in the J-matrix theory. In the appendix, we consider in detail the following potentials and find their corresponding bases and J-matrix elements.

(a) The three-dimensional (3D) isotropic oscillator potential.
(b) The Coulomb potential.
(c) The S-wave Morse potential.
(d) Various potentials at zero energy.

The *radial* component of the operator

$$J = H_0 - E = -\frac{1}{2}\left[\frac{d^2}{dr^2} + f(r)\right]$$

which is assumed to have the underlying symmetry of the J-matrix theory, can now be expanded as a linear combination of $SO(2, 1)$ generators to

$$J \equiv \sqrt{2}\lambda_+ L_+ + \sqrt{2}\lambda_- L_- + \lambda_3 L_3 + \lambda_0 \tag{4.1}$$

where

$$\lambda_\pm^* = \lambda_\mp \qquad \lambda_3^* = \lambda_3 \qquad \lambda_0^* = \lambda_0.$$

The λ are constant parameters. Using the realization of L_3 and $L_\pm$ obtained in the previous section, we can write this as

$$J = (\lambda_+ + \lambda_- + \lambda_3)\frac{d^2}{dx^2} + \frac{1}{2}(\lambda_+ - \lambda_-)\,x\frac{d}{dx} + (\lambda_+ + \lambda_- + \lambda_3)\frac{\mu}{x^2}$$
$$+ (\lambda_+ + \lambda_- - \lambda_3)\frac{x^2}{16} + \frac{1}{4}(\lambda_+ - \lambda_-) + \lambda_0. \tag{4.2}$$

Therefore

$$\lambda_+ + \lambda_- + \lambda_3 = 1.$$

Moreover, to eliminate the first-order derivative, we require that $\lambda_+ = \lambda_-$, giving

$$J = (1-\lambda_3)\,L_1 + \lambda_3 L_3 + \lambda_0 = \frac{d^2}{dx^2} + \frac{\mu}{x^2} + \frac{1-2\lambda_3}{16}x^2 + \lambda_0. \qquad (4.3)$$

The Schrödinger wave equation $J\psi = 0$ is now written as

$$[(1-\lambda_3)\,L_1 + \lambda_3 L_3 + \lambda_0]\,\psi(x) = \left(\frac{d^2}{dx^2} + \frac{\mu}{x^2} + \frac{1-2\lambda_3}{16}x^2 + \lambda_0\right)\psi(x) = 0. \qquad (4.4)$$

Using only the commutation relations of $so(2,1)$ we can perform a unitary transformation called the 'tilting' transformation:

$$e^{i\theta L_2}(L_3 \pm L_1)e^{-i\theta L_2} = e^{\mp\theta}(L_3 \pm L_1) \qquad (4.5)$$

where θ is a real constant parameter. The Schrödinger equation (4.4) transforms to

$$\left\{\left[1-(2\lambda_3-1)\,e^{2\theta}\right]L_1 + \left[1+(2\lambda_3-1)\,e^{2\theta}\right]L_3 + 2\lambda_0 e^{\theta}\right\}\psi = 0. \qquad (4.6)$$

To obtain the discrete representation, we choose the 'tilting angle' θ such that the coefficient of L_1 vanishes. We should note, however, that the range of possible values of θ is restricted by the value of λ_3 in the problem. For bound states $\lambda_3 > \frac{1}{2}$, while for scattering states (the continuum) $\lambda_3 < \frac{1}{2}$. However, presently we require that

$$\begin{aligned} &(2\lambda_3-1)\,e^{2\theta} = 1 \quad \Rightarrow \quad \lambda_3 > \tfrac{1}{2} \\ &\left(L_3 + \lambda_0 e^{\theta}\right)\psi = 0 \quad \Rightarrow \quad L_3\psi = \pm\frac{\lambda_0}{\sqrt{2\lambda_3-1}}\psi. \end{aligned} \qquad (4.7)$$

Using the spectrum of L_3 in equation (3.9), we can write

$$\frac{\lambda_0}{\sqrt{2\lambda_3-1}} = \pm(\gamma+n+1) \qquad n = 0, 1, 2, \ldots. \qquad (4.8)$$

The two signs correspond to the bounded discrete representations $D^{\pm}(\gamma)$, respectively.

Now, if we define

$$\frac{2\lambda_3-1}{16} \equiv 2\xi^4 \qquad (4.9)$$

then the spectral equation (4.8) gives for $D^+(\gamma)$

$$\lambda_0 = 4\sqrt{2}\xi^2(\gamma+n+1) \qquad (4.10)$$

and the differential equation (4.4) reads (with $\psi_n^\gamma(x) \equiv \langle x|\gamma, n\rangle$)

$$\left[\frac{d^2}{dx^2} - \frac{4\gamma(\gamma+1)+\frac{3}{4}}{x^2} - 2\xi^4x^2 + 4\sqrt{2}\xi^2(\gamma+n+1)\right]\psi_n^\gamma = 0. \qquad (4.11)$$

The normalized solution of this differential equation may be written as [9]

$$\psi_n^\gamma(x) = \sqrt{\frac{2\xi\Gamma(n+1)}{\Gamma(2\gamma+n+2)}}\,(\xi x)^{2\gamma+3/2}\,e^{-\xi^2x^2/2}L_n^{2\gamma+1}(\xi^2x^2) \qquad (4.12)$$

where Γ is the gamma function and $L_n^\nu(x)$ are the Laguerre polynomials.

In the appendix we consider coordinate transformations of equation (4.4) that preserve the Schrödinger-like property (i.e. the first-order derivative terms vanish) and leave the form of the function $f(r)$ invariant. These point transformations have been considered extensively in the literature: in studying ‘shifting operators between Hilbert spaces’ [10], ‘rescaling in path integration’ [11], ‘shape-invariant potentials’ [12], ..., etc. Besides the familiar Coulomb, oscillator and Morse potentials, we find that this class includes various other potentials at the limit of zero energy. The general transformation is considered formally in the appendix.

The realization we have obtained in the previous section for the generators L_3 and $L_\pm$ in terms of differential operators in one variable was intended to solve the second-order radial differential equation $(H_0 - E)\phi = 0$ (equation (3.11)). The same differential equation can be cast in another form which is suitable for tackling other problems. For example, when studying the $SO(4,2)$ symmetry of Kepler's problem, the differential equation is rewritten as $r(H_0 - E)\phi = 0$. The *radial* component of this equation is

$$\left[r\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{\mathrm{d}}{\mathrm{d}r} + q(r)\right]\phi(r) = 0 \qquad (4.13)$$

where $q(r) = -\frac{\sigma^2/4}{r} - 2rV_0(r) + 2rE$ and σ is a constant parameter. In Kepler's problem $V_0(r) \sim r^{-1}$ and one finds an invariant subgroup which is the direct product $SO(2,1) \otimes SO(2,1)$.

The appropriate forms of the three generators L_3 and $L_\pm$ whose linear combination gives the second-order differential operator in equation (4.13) and, at the same time, satisfy the $so(2,1)$ subalgebra are

$$\begin{aligned} L_3 &= x\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{\mathrm{d}}{\mathrm{d}x} - \frac{\sigma^2/4}{x} - \frac{x}{4} \\ L_\pm &= \frac{1}{\sqrt{2}}\left[x\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{\mathrm{d}}{\mathrm{d}x} - \frac{\sigma^2/4}{x} + \frac{x}{4} \pm \left(x\frac{\mathrm{d}}{\mathrm{d}x} + \frac{1}{2}\right)\right]. \end{aligned} \qquad (4.14)$$

This realization gives the following value of the Casimir invariant:

$$L^2 = \frac{\sigma^2 - 1}{4} \equiv \gamma(\gamma + 1). \qquad (4.15)$$

Thus

$$\gamma = -\frac{1}{2} + \frac{|\sigma|}{2}.$$

Following a similar treatment to that carried out at the beginning of this section, one finds that the linear combination of these generators, which gives the operator $rJ \equiv r(H_0 - E)$ in equation (4.13), is

$$(1-\lambda_3)\,L_1 + \lambda_3 L_3 + \lambda_0 = x\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{\mathrm{d}}{\mathrm{d}x} - \frac{\sigma^2/4}{x} + \frac{1-2\lambda_3}{4}x + \lambda_0 \qquad (4.16)$$

where the parameters λ_0 and λ_3 are related by the spectral equation (4.8).

Ojha [2] investigated the Coulomb problem in parabolic coordinates in the context of the J-matrix method. He obtained the differential equation

$$[(1-\lambda_3)(L_1 \oplus L_1) + \lambda_3 (L_3 \oplus L_3) + \lambda_0]\,\psi = 0 \qquad (4.17)$$

in which the generators are written as a direct sum in the subalgebra $so(2,1) \oplus so(2,1)$, which is realized in terms of the differential operators given in (4.14) with the variable x being replaced by either one of the two parabolic coordinates $r \pm \hat{z}\cdot\vec{r}$. The equation is separable in the two coordinates, which means that the basis of the representation is the direct product of the functions given in equation (A.10) of the appendix with the parameter l being replaced by $\frac{|\sigma|-1}{2}$. The analytical solution of the recursion relation was also obtained in [2].

5. Phase-shift and resonance calculations

We illustrate the use of our results in a simple example of a single-channel oscillator potential scattering in the presence of a short-range perturbing potential $\tilde{V}(r) = 7.5r^2\mathrm{e}^{-r}$ and calculate the scattering matrix and obtain resonance information.

To calculate the scattering matrix (equation (2.20)), we need to find the J-matrix kinematical coefficients $T_{N-1}(E)$ and $R_N^{\pm}(E)$, i.e. the regular and irregular solutions of the recursion relation. Previous work on the J-matrix using the oscillator basis was limited to the reference Hamiltonian H_0 having the kinetic energy only without the oscillator potential term [1, 4, 6, 13]. However, using the findings in this paper, we can take the results obtained in an earlier work on the complete reference Hamiltonian with the Coulomb potential [6] and apply to it the $SO(2,1)$-invariant transformation to obtain the corresponding kinematical coefficients in the oscillator basis. In a significant paper by Yamani and Abdelmonem [13], these coefficients, in the Laguerre basis, were studied extensively and calculated recursively in a continued-fraction scheme using the initial ones which were written as

$$R_1^{\pm}(E) = \frac{\sqrt{2l+2}}{l+2\mp \mathrm{i}t}\mathrm{e}^{\mp\mathrm{i}\theta}\frac{{}_2F_1\left(-l\mp\mathrm{i}t, 2, l+3\mp\mathrm{i}t; \mathrm{e}^{\mp 2\mathrm{i}\theta}\right)}{{}_2F_1\left(-l\mp\mathrm{i}t, 1, l+2\mp\mathrm{i}t; \mathrm{e}^{\mp 2\mathrm{i}\theta}\right)} \tag{5.1}$$

$$T_0(E) = \frac{l+1-\mathrm{i}t}{l+1+\mathrm{i}t}\mathrm{e}^{2\mathrm{i}\theta}\frac{{}_2F_1\left(-l+\mathrm{i}t, 1, l+2+\mathrm{i}t; \mathrm{e}^{+2\mathrm{i}\theta}\right)}{{}_2F_1\left(-l-\mathrm{i}t, 1, l+2-\mathrm{i}t; \mathrm{e}^{-2\mathrm{i}\theta}\right)} \tag{5.2}$$

where

$$t = -Z/\sqrt{2E} \qquad \text{and} \qquad \theta = \cos^{-1}\left(\frac{E-\xi^2/8}{E+\xi^2/8}\right). \tag{5.3}$$

Now, we perform the following $SO(2,1)$-invariant transformations, which are obtained from the appendix, to calculate the corresponding coefficients in the oscillator basis:

$$\begin{aligned} &\lambda_0 = -8Z \to 2E \\ &\frac{1-2\lambda_3}{16} = 8E \to \tau^2 \\ &\gamma = l \to l/2 - 1/4 \\ &\xi \to \xi^2. \end{aligned} \tag{5.4}$$

Applying this transformation to T_0 and $R_1^{\pm}$ above, we obtain the following *generalized* oscillator coefficients:

$$R_1^{\pm}(E) = \frac{\sqrt{l+\frac{3}{2}}}{\frac{1}{2}l+\frac{7}{4}\mp\mathrm{i}\hat{t}}\mathrm{e}^{\mp\mathrm{i}\hat{\theta}}\frac{{}_2F_1\left(-\frac{1}{2}l+\frac{1}{4}\mp\mathrm{i}\hat{t}, 2, \frac{1}{2}l+\frac{11}{4}\mp\mathrm{i}\hat{t}; \mathrm{e}^{\mp 2\mathrm{i}\hat{\theta}}\right)}{{}_2F_1\left(-\frac{1}{2}l+\frac{1}{4}\mp\mathrm{i}\hat{t}, 1, \frac{1}{2}l+\frac{7}{4}\mp\mathrm{i}\hat{t}; \mathrm{e}^{\mp 2\mathrm{i}\hat{\theta}}\right)} \tag{5.5}$$

$$T_0(E) = \frac{\frac{1}{2}l+\frac{3}{4}-\mathrm{i}\hat{t}}{\frac{1}{2}l+\frac{3}{4}+\mathrm{i}\hat{t}}\mathrm{e}^{2\mathrm{i}\hat{\theta}}\frac{{}_2F_1\left(-\frac{1}{2}l+\frac{1}{4}+\mathrm{i}\hat{t}, 1, \frac{1}{2}l+\frac{7}{4}+\mathrm{i}\hat{t}; \mathrm{e}^{+2\mathrm{i}\hat{\theta}}\right)}{{}_2F_1\left(-\frac{1}{2}l+\frac{1}{4}-\mathrm{i}\hat{t}, 1, \frac{1}{2}l+\frac{7}{4}-\mathrm{i}\hat{t}; \mathrm{e}^{-2\mathrm{i}\hat{\theta}}\right)} \tag{5.6}$$

where

$$\hat{t} = E/2\tau \qquad \text{and} \qquad \hat{\theta} = \cos^{-1}\left(\frac{\tau^2-\xi^4}{\tau^2+\xi^4}\right). \tag{5.7}$$

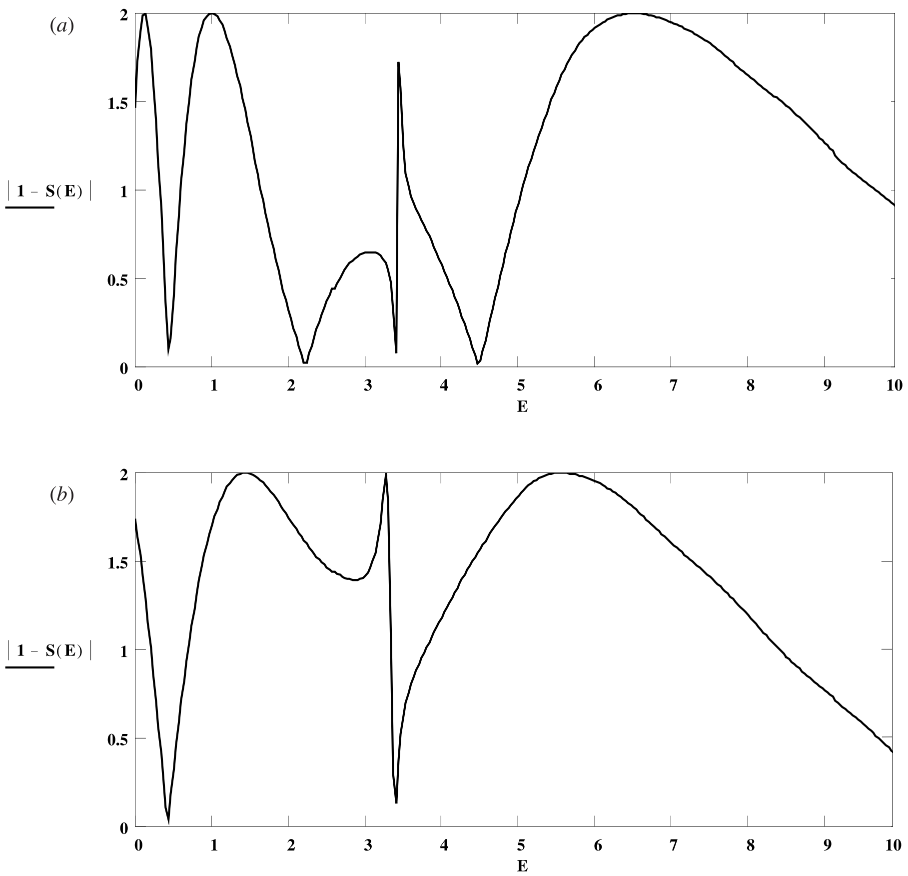

Figure 1. A plot of $|1 - S(E)|$ for the oscillator potential perturbed by the short-range potential $\tilde{V}(r) = 7.5r^2\mathrm{e}^{-r}$ for the following two cases whose parameters are: (*a*) $N = 50$, $\tau = 0.2$, $l = 0$ and $\xi = 1.5$; (*b*) $N = 50$, $\tau = 0.5$, $l = 0$ and $\xi = 2.0$

To find the remainder of the coefficients in terms of these, we use the recursion relation (2.6) which gives

$$R_{n+1}^{\pm} = -\frac{1}{J_{n,n+1}}\left(J_{n,n} + \frac{J_{n,n-1}}{R_n^{\pm}}\right) \qquad \text{and} \qquad T_n = T_{n-1}\frac{R_n^-}{R_n^+} \qquad n \geqslant 1. \tag{5.8}$$

To complete the calculation of the S-matrix, we need the 'J-matrix hooks' $J_{N-1,N}(E)$ which have already been found in equation (A.5) of the appendix. We should make note of the fact that we can also obtain the J-matrix elements for the oscillator potential, aside from an overall normalization constant, by applying the same transformation in (5.4) to the corresponding J-matrix elements for the Coulomb potential in equation (A.11). The Green function matrix element $g_{N-1,N-1}(E)$, which is also needed in the calculation of the S-matrix, can be written as

$$g_{N-1,N-1}(E) = \sum_{\mu=0}^{N-1} \frac{\Lambda_{N-1,\mu}^2}{\varepsilon_\mu - E} \tag{5.9}$$

where $\{\varepsilon_\mu\}_{\mu=0}^{N-1}$ are the eigenvalues of the $N \times N$ matrix $H_0 + \tilde{V}$ in the oscillator basis and $\{\Lambda_{\nu,\mu}\}_{\mu,\nu=0}^{N-1}$ are the corresponding normalized eigenvectors. The matrix elements of H_0 can be

Table 1. The resonance energy, ϵ_r, for the single-channel oscillator potential in the presence of a short-range perturbing potential $\tilde{V}(r) = 7.5r^2e^{-r}$. The results are shown for increasing dimension N and for two values of the oscillator strength parameter τ and basis scale parameter ξ.

τ, ξ	N	ϵ_r
0.2, 1.5	20	3.4050
	30	3.4080
	40	3.4091
	50	3.4096
	60	3.4099
	70	3.4100
	80	3.4101
0.5, 2.0	20	3.129
	30	3.224
	40	3.237
	50	3.242
	60	3.245
	70	3.246
	80	3.247

obtained from equation (A.5) in the appendix by taking $E = 0$, while the elements $\tilde{V}_{nm}$ of the potential matrix may be calculated using Gauss quadrature as outlined in [14]. Figure 1(a) is a plot of $|1 - S(E)|$ for the potential mentioned above with the following parameters: $N = 50$, $\tau = 0.2$, $l = 0$ and $\xi = 1.5$. Figure 1(b) is the same except for $\tau = 0.5$ and $\xi = 2.0$. Table 1 shows resonance calculation results for increasing dimension N and for two values of the oscillator strength parameter τ.

6. Conclusion and summary of results

In this paper we have shown that any linear self-adjoint operator that spans the space of generators of the $so(2, 1)$ Lie algebra falls in the domain of applications of the J-matrix theory. We have identified a large class of analytically solvable potentials in the J-matrix formalism and obtained their corresponding bases and J-matrix elements. This class includes the Coulomb, oscillator and Morse potentials, in addition to various other potentials at the limit of zero energy. We have demonstrated how to obtain the regular and irregular solutions of the recursion relation and J-matrix elements for any of these potentials by making an $SO(2, 1)$-invariant transformations of the corresponding objects given for another potential in the same class. We have obtained the analytical solution of the recursion relation for the generalized oscillator, where the reference Hamiltonian includes not only the kinetic energy term but also the oscillator potential term. A one-channel scattering example was given to illustrate the utility of these results.

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Appendix

In this appendix we consider coordinate transformations of equation (4.4) that preserve the Schrödinger-like property (i.e. the first-order derivative terms vanish) and leave the form of the function $f(r)$, as given by equation (3.12), invariant. We also obtain the basis functions and J-matrix elements for some of the potentials found by this transformation.

A.1. The 3D isotropic oscillator potential

If we consider the identity transformation $r = x$ and $\phi = \psi$, then we obtain

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} + f(r)\right]\phi(r) = \left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} + f(r(x))\right]\psi(x) = 0.$$

This equation is equivalent to (4.4) if we write

$$f(r) = \frac{\mu}{x^2} + \frac{1-2\lambda_3}{16}x^2 + \lambda_0 = -\frac{4\gamma(\gamma+1)+\frac{3}{4}}{r^2} + \frac{1-2\lambda_3}{16}r^2 + \lambda_0. \tag{A.1}$$

Comparing this with $f(r) = -\frac{l(l+1)}{r^2} - 2V_0(r) + 2E$, we obtain

$$V_0(r) = -\frac{1}{2}\left(\frac{1-2\lambda_3}{16}\right)r^2 \equiv -\frac{1}{2}\tau^2 r^2 \tag{A.2}$$

$$\gamma = \tfrac{1}{2}l - \tfrac{1}{4} \qquad \text{and} \qquad \lambda_0 = 2E. \tag{A.3}$$

Using the transformation and the value of γ we can write the basis function as

$$\phi_n^l(r) = \sqrt{\frac{2\xi\Gamma(n+1)}{\Gamma\left(l+n+\frac{3}{2}\right)}}(\xi r)^{l+1}\mathrm{e}^{-\xi^2r^2/2}L_n^{l+1/2}(\xi^2r^2). \tag{A.4}$$

In this basis, the elements of the symmetric tridiagonal matrix $J = H_0 - E$ are

$$\begin{aligned} J_{n,n} &= \frac{\xi^2}{2}\left(1-\frac{\tau^2}{\xi^4}\right)(l+2n+3/2) - E \\ J_{n,n+1} &= \frac{\xi^2}{2}\left(1+\frac{\tau^2}{\xi^4}\right)\sqrt{(n+1)(l+n+3/2)} \end{aligned} \qquad n = 0, 1, 2, \ldots. \tag{A.5}$$

The conjugate orthogonal space is spanned by $\{\bar{\phi}_n^l\}$, where

$$\bar{\phi}_n^l(r) = \phi_n^l(r) \qquad \text{and} \qquad \langle\bar{\phi}_n^l|\phi_{n'}^{l'}\rangle = \delta_{ll'}\delta_{nn'}. \tag{A.6}$$

A.2. The Coulomb potential

The transformation $r = x^2$ and $\phi = \sqrt{x}\psi$ gives

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} + f(r)\right]\phi(r) = \frac{\sqrt{x}}{4x^2}\left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{\frac{3}{4}}{x^2} + 4x^2 f(r(x))\right]\psi(x) = 0.$$

This equation is equivalent to (4.4) if we write

$$4x^2 f(r(x)) = \frac{\mu+\frac{3}{4}}{x^2} + \frac{1-2\lambda_3}{16}x^2 + \lambda_0.$$

Thus

$$f(r) = \frac{\mu + \frac{3}{4}}{4x^4} + \frac{1 - 2\lambda_3}{4 \times 16} + \frac{\lambda_0}{4x^2} = -\frac{\gamma(\gamma+1)}{r^2} + \frac{1 - 2\lambda_3}{4 \times 16} + \frac{\lambda_0/4}{r}. \tag{A.7}$$

Comparing this with $f(r)$ in equation (3.12) we obtain

$$V_0(r) = \frac{-\lambda_0/8}{r} \equiv \frac{Z}{r} \tag{A.8}$$

$$\gamma = l \qquad \text{and} \qquad 1 - 2\lambda_3 = 8 \times 16E. \tag{A.9}$$

Using the transformation and $\gamma = l$ we can write the basis function as

$$\phi_n^l(r) = \sqrt{\frac{\xi\Gamma(n+1)}{\Gamma(2l+n+2)}}\,(\xi r)^{l+1}\,\mathrm{e}^{-\xi r/2} L_n^{2l+1}(\xi r) \tag{A.10}$$

where we have redefined $\xi^2 \to \xi$.

In this basis

$$\begin{aligned} J_{n,n} &= \xi Z - 2\left(E - \frac{\xi^2}{8}\right)(l+n+1) \\ J_{n,n+1} &= \left(E + \frac{\xi^2}{8}\right)\sqrt{(n+1)(2l+n+2)} \end{aligned} \qquad n = 0, 1, 2, \ldots. \tag{A.11}$$

The conjugate orthogonal space is spanned by $\{\bar{\phi}_n^l\}$, where

$$\bar{\phi}_n^l(r) = \frac{1}{\xi r}\phi_n^l(r) \qquad \text{and} \qquad \langle \bar{\phi}_n^l | \phi_{n'}^{l'} \rangle = \delta_{ll'}\delta_{nn'}. \tag{A.12}$$

A.3. The S-wave Morse potential

The transformation $r = -\zeta \ln x$ and $\phi = \frac{1}{\sqrt{x}}\psi$, where ζ is a real positive constant, gives

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} + f(r)\right]\phi = \frac{x^2}{\zeta^2\sqrt{x}}\left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{\frac{1}{4}}{x^2} + \frac{\zeta^2}{x^2} f(r(x))\right]\psi = 0.$$

This equation is equivalent to (4.4) if we write

$$\frac{\zeta^2}{x^2} f(r(x)) = \frac{\mu - \frac{1}{4}}{x^2} + \frac{1 - 2\lambda_3}{16}x^2 + \lambda_0.$$

Thus

$$\begin{aligned} f(r) &= \frac{\mu - \frac{1}{4}}{\zeta^2} + \frac{1 - 2\lambda_3}{16\zeta^2}x^4 + \frac{\lambda_0}{\zeta^2}x^2 \\ &= -\frac{1 + 4\gamma(\gamma+1)}{\zeta^2} + \frac{1 - 2\lambda_3}{16\zeta^2}\mathrm{e}^{-4r/\zeta} + \frac{\lambda_0}{\zeta^2}\mathrm{e}^{-2r/\zeta}. \end{aligned} \tag{A.13}$$

Comparing this with $f(r)$ in (3.12) we obtain

$$V_0(r) = \frac{2\lambda_3 - 1}{32\zeta^2}\mathrm{e}^{-4r/\zeta} - \frac{\lambda_0}{2\zeta^2}\mathrm{e}^{-2r/\zeta} \equiv -\frac{1}{2}A\mathrm{e}^{-4r/\zeta} + B\mathrm{e}^{-2r/\zeta} \tag{A.14}$$

$$1 + 4\gamma(\gamma+1) = -2\zeta^2 E \qquad \text{and} \qquad l = 0 \quad (S\text{-wave}). \tag{A.15}$$

Using the transformation we can write the basis as

$$\phi_n(r) = \sqrt{\frac{2\Gamma(n+1)}{\zeta\Gamma(2\gamma+n+2)}}\left(\xi e^{-r/\zeta}\right)^{2\gamma+1}\exp\left(-\frac{1}{2}\xi^2 e^{-2r/\zeta}\right)L_n^{2\gamma+1}\left(\xi^2 e^{-2r/\zeta}\right). \tag{A.16}$$

This basis gives

$$\begin{aligned} J_{n,n} &= \left(\frac{1}{\zeta^2} - \frac{A}{\xi^4}\right)(\gamma+n+1) + \frac{B}{\xi^2} \\ J_{n,n+1} &= \frac{1}{2}\left(\frac{1}{\zeta^2} + \frac{A}{\xi^4}\right)\sqrt{(n+1)(2\gamma+n+2)} \end{aligned} \qquad n = 0, 1, 2, \ldots. \tag{A.17}$$

The basis functions for the conjugate orthogonal space are

$$\bar{\phi}_n(r) = \xi^2 e^{-2r/\zeta}\phi_n(r) \qquad \text{and} \qquad \langle\bar{\phi}_n|\phi_{n'}\rangle = \delta_{nn'}. \tag{A.18}$$

A.4. Zero-energy cases

The following are other cases that have been calculated:

A.4.1. If we let $r = e^x$, $\phi = e^{x/2}\psi$ then we find

$$\begin{aligned} f(r) &= -\frac{l(l+1)}{r^2} - 2\left[a\frac{(\ln r)^2}{r^2} + b\frac{(\ln r)^{-2}}{r^2}\right] \\ \Rightarrow E &= 0 \qquad \text{and} \qquad V_0(r) = a\frac{(\ln r)^2}{r^2} + b\frac{(\ln r)^{-2}}{r^2}. \end{aligned} \tag{A.19}$$

A.4.2. If we let $r = e^{x^2}$, $\phi = \sqrt{x}e^{x^2/2}\psi$ then we find

$$\begin{aligned} f(r) &= -\frac{l(l+1)}{r^2} - 2\left[a\frac{(\ln r)^{-1}}{r^2} + b\frac{(\ln r)^{-2}}{r^2}\right] \\ \Rightarrow E &= 0 \qquad \text{and} \qquad V_0(r) = a\frac{(\ln r)^{-1}}{r^2} + b\frac{(\ln r)^{-2}}{r^2}. \end{aligned} \tag{A.20}$$

A.4.3. If we let $r = x^{2\,m+1}$, $\phi = x^m\psi$, where $m > -\frac{1}{2}$ and $m \neq 0, \pm\frac{1}{2}$, then we will obtain $\gamma = (m+\frac{1}{2})l + \frac{m-\frac{1}{2}}{2}$ and find

$$\begin{aligned} f(r) &= -\frac{l(l+1)}{r^2} - 2\left[a \times r^{-2\left(\frac{m-1/2}{m+1/2}\right)} + b \times r^{-2\left(\frac{m}{m+1/2}\right)}\right] \\ \Rightarrow E &= 0 \qquad \text{and} \qquad V_0(r) = a \times r^{-2\left(\frac{m-1/2}{m+1/2}\right)} + b \times r^{-2\left(\frac{m}{m+1/2}\right)}. \end{aligned} \tag{A.21}$$

The basis functions in this case are

$$\begin{aligned} \phi_n^l(r) = &\sqrt{\frac{\Gamma(n+1)}{(m+\frac{1}{2})\Gamma\left[(m+\frac{1}{2})(2l+1)+n+1\right]}}\,\xi^{m+1/2}\left(\xi^2 r^{1/(m+1/2)}\right)^{(m+1/2)(l+1)} \\ &\times \exp\left[-\tfrac{1}{2}\xi^2 r^{1/(m+1/2)}\right]L_n^{(m+1/2)(2l+1)}\left(\xi^2 r^{1/(m+1/2)}\right). \end{aligned} \tag{A.22}$$

The conjugate orthogonal space is spanned by

$$\bar{\phi}_n^l(r) = \left[\xi^2 r^{1/(m+1/2)}\right]^{-2m}\phi_n^l(r) \qquad \text{where} \quad \langle\bar{\phi}_n^l|\phi_{n'}^{l'}\rangle = \delta_{ll'}\delta_{nn'}. \tag{A.23}$$

An interesting special case is when $m = \frac{3}{2}$ where the potential takes the form $V_0(r) = \frac{Z}{r} + \frac{b}{r^{3/2}}$ and the corresponding basis functions are

$$\phi_n^l(r) = \sqrt{\frac{\xi\Gamma(n+1)}{2\Gamma(4l+n+3)}}\,(\xi r)^{l+1}\,\mathrm{e}^{-\sqrt{\xi r}/2}L_n^{4l+2}\left(\sqrt{\xi r}\right) \qquad \text{(A.24)}$$

where, in this special case, we have redefined $\xi \to \xi^{1/4}$.

The transformation in this zero-energy case has been studied in the literature [15] in the context of an N-dimensional Schrödinger equation for a general central potential without the constraint of $SO(2, 1)$ invariance.

A.5. The general case

We perform the transformation

$$r = g(x) \qquad \phi(r) = h(x)\psi(x) \qquad \text{(A.25)}$$

and require that this transformation preserves the Schrödinger-like property of the differential equation

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} + f(r)\right]\phi(r) = 0.$$

That is, the first-order derivative terms vanish. This constraint requires that

$$h(x) = \sqrt{\frac{\mathrm{d}}{\mathrm{d}x}g(x)}. \qquad \text{(A.26)}$$

Then the differential equation reads

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} + f(r)\right]\phi(r) = \left(g'\right)^{-3/2}\left\{\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{2}\left[\frac{g'''}{g'} - \frac{3}{2}\left(\frac{g''}{g'}\right)^2\right] + \left(g'\right)^2 f(g)\right\}\psi = 0$$

where the prime symbol denotes $\frac{\mathrm{d}}{\mathrm{d}x}$. This equation is equivalent to (4.4) if we write

$$f(g(x(r))) = (g')^{-2}\left[\frac{\mu}{x^2} + \frac{1-2\lambda_3}{16}x^2 + \lambda_0 - \frac{1}{2}\frac{g'''}{g'} + \frac{3}{4}\left(\frac{g''}{g'}\right)^2\right]. \qquad \text{(A.27)}$$

One can verify all of the cases worked out above. The admissible class of transformations, $g(x)$, are those that produce $f(r)$ in the form given in equation (3.12). An exhaustive study of such transformations has not been carried out in this paper.

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