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1988 J. Phys. A: Math. Gen. 21 875

(http://iopscience.iop.org/0305-4470/21/4/016)

J. Phys. A: Math. Gen. 21 (1988) 875-883. Printed in the UK

SO(2, 1) Lie algebra, the Jacobi matrix and the scattering states of the Morse oscillator

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Received 2 June 1987

Abstract. Previous work exploring the connection between SO(2, 1) Lie algebra and the Jacobi-matrix method for scattering is extended to the Morse potential. Regular and irregular solutions of the three-term recursion associated with the Jacobi matrix are specified by their asymptotic behaviour and closed-form expressions in terms of generalised hypergeometric functions are obtained. This example further illustrates the connection between scattering theory and orthogonal polynomials.

1. Introduction

In the past fifteen years or so, it has emerged that the properties of the continuum states of atoms and molecules can be studied by expanding the wavefunction in a set of square-integrable functions. In the general case, the trick is to recursively generate a basis set in which the Hamiltonian matrix is tridiagonal. The basis set is formally complete, the Hamiltonian matrix is infinite, and its spectrum is continuous over a range of eigenvalues. In practice, the basis set is truncated, the continuous spectrum is discretised and a convergent expansion to the quantity of interest (e.g., a transition-matrix element) is constructed. This method essentially amounts to solving the mathematical 'problem of moments' and it has been used extensively to study photoionisation of molecules (Langhoff 1983). Particular solvable cases, where the Hamiltonian H_0 is tridiagonal in a known complete basis set and the matrix can be diagonalised analytically, assume special importance, not only as illustrations of the method but also as the framework for calculating the scattering states of $H = H_0 + V$, where V is a short-range interaction in the sense that in its matrix representation only a finite submatrix is non-zero. The problem of specifying the scattering states of H by the coefficients of their expansion in the basis set then reduces to that of solving a finite matrix equation. This is the Jacobi-matrix method for scattering (Heller and Yamani 1974, Yamani and Fishman 1975).

A parallel development began with the observation that the bound spectrum of some of the classic problems of quantum mechanics (harmonic oscillator, hydrogen atom, Morse oscillator) can be calculated very elegantly by using the commutation relations of operators. Is it also possible to calculate the scattering phase shift algebraically, at least for some solvable model problems? The answer is in the affirmative

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0305-4470/88/040875+09$02.50

(Alhassid and Wu 1984, Alhassid *et al* 1983, 1984, 1986). The SO(2, 1) Lie algebra, which is also the (bound) spectrum-generating algebra for the problems listed above, plays a central role. It has been discovered that an algebraic determination of the phase shift is possible when the Hamiltonian is a functional of the Casimir invariant of the algebra. (Both Coulomb interaction and Morse potential fall in this category.) The group theoretical analogue of the examination of the asymptotic form of the coordinate-space wavefunction is the contraction of the SO(2, 1) Lie algebra to the Euclidean algebra E_2 of the generators of translations and rotations of the plane. The S matrix is calculated from the corresponding passage from the appropriate representation of the SO(2, 1) Lie algebra to that of E_2.

In fact the Jacobi-matrix method is also intimately connected with the SO(2, 1) Lie algebra (Ojha 1986, 1987). In the two cases considered so far—Coulomb Hamiltonian diagonalised in a Sturmian basis and kinetic energy operator diagonalised in a basis of harmonic oscillator states—it turns out that the basis set constitutes a unitary irreducible representation of the SO(2, 1) Lie algebra and the Hamiltonian is a linear combination of its generators. One thus diagonalises a linear combination of the compact and non-compact generators in a basis in which the compact generator is diagonal. The scattering phaseshift is then extracted from the asymptotic behaviour of the expansion coefficients. These examples illustrate the general connection between scattering theory and polynomials orthogonal on a segment of the real line (Case 1974, Geronimo and Case 1979, 1980).

In this paper, I extend previous work and explore the connection between SO(2, 1) Lie algebra and the Jacobi-matrix treatment of the scattering states of the Morse oscillator. The specific realisation of the algebra which is required and a basis in which its compact generator is diagonal is introduced in § 2. The free-particle and Morse-oscillator Hamiltonians are then rewritten in terms of the generators of the algebra. The resulting three-term recursion for the free particle is solved in § 3 and that for the Morse oscillator in § 4. The free-particle recursion has been considered before in a different context and its regular solution leads to Pollaczek polynomials. The polynomials arising from the Morse oscillator recursion do not seem to have been studied before and it may be appropriate to call them 'Morse polynomials'. Some remarks concerning the failure of the present treatment to determine the scattering phase shift of the Morse potential algebraically are offered in § 5. A brief description of the standard solution of the Schrödinger equation is given in the appendix.

2. Jacobi-matrix representation of the Hamiltonian

Consider the one-dimensional Hamiltonian

$$H=\frac{1}{2m}p_x^2+V_{\mathrm{M}}(x) \tag{2.1a}$$

where

$$V_{\mathrm{M}}(x)=A\,\mathrm{e}^{-2x}-B\,\mathrm{e}^{-x} \tag{2.1b}$$

is the Morse potential. Transform the independent variable to $z=\mathrm{e}^{-x}$. The resulting Hamiltonian

$$H=-\frac{1}{2m}\left(z^2\frac{\mathrm{d}^2}{\mathrm{d}z^2}+z\frac{\mathrm{d}}{\mathrm{d}z}\right)+Az^2-Bz \tag{2.2}$$

is then Hermitian over the interval $0\leqslant z<\infty$ with weight $1/z$.

Next consider the following realisation of the SO(2, 1) Lie algebra:

$$T_1 = -\frac{1}{2\beta_1} z \frac{d^2}{dz^2} + \frac{\beta_2}{2z} - \frac{\beta_1}{2} z \tag{2.3a}$$

$$T_2 = -iz \frac{d}{dz} \tag{2.3b}$$

$$T_3 = -\frac{1}{2\beta_1} z \frac{d^2}{dz^2} + \frac{\beta_2}{2z} + \frac{\beta_1}{2} z. \tag{2.3c}$$

Here β_1 and β_2 are real parameters subject only to the condition $\beta_1, \beta_2 > 0$. The commutation relations

$$[T_1, T_2] = -iT_3 \qquad [T_2, T_3] = iT_1 \qquad [T_3, T_1] = iT_2 \tag{2.4}$$

are easily verified. The Casimir invariant is just

$$T^2 = T_3^2 - T_1^2 - T_2^2 = \beta_1\beta_2. \tag{2.5}$$

Also note that $T_2 = -p_x$.

The Sturmian basis set,

$$\phi_\nu(z) = \left(\frac{\Gamma(\nu+1)}{\Gamma(\nu+2t+2)}\right)^{1/2} (2\beta_1 z)^{t+1} e^{-\beta_1 z} L_\nu^{2t+1}(2\beta_1 z) \qquad \nu = 0, 1, 2, \ldots, \infty \tag{2.6}$$

where $t(t+1) = \beta_1\beta_2$ and $L_\nu^{2t+1}(2\beta_1 z)$ is a generalised Laguerre polynomial†, constitutes a $\mathscr{D}^+(t)$ representation of the algebra (2.3). (I will occasionally denote the νth basis function by the ket $|t, q = \nu + t + 1\rangle$.) The standard action of the operators T_3 and $T_\pm = T_1 \pm iT_2$ on the basis functions is also easily verified from the properties of generalised Laguerre polynomials:

$$T_3|t, q\rangle = q|t, q\rangle \tag{2.7a}$$

$$T_\pm|t, q\rangle = (q \mp t)^{1/2}(q \pm t \pm 1)^{1/2}|t, q \pm 1\rangle. \tag{2.7b}$$

The point in introducing this Lie algebra (2.4) is that both the kinetic energy operator and the Morse potential are simple functions of the generators of the algebra

$$H_0 = \frac{1}{2m} p_x^2 = \frac{1}{2m} T_2^2 \tag{2.8a}$$

and

$$V_M(x) = \frac{A}{\beta_1^2}(T_3 - T_1)^2 - \frac{B}{\beta_1}(T_3 - T_1). \tag{2.8b}$$

The task of solving the eigenvalue equation for the free particle

$$\frac{1}{2m} T_2^2|\psi\rangle = E|\psi\rangle \tag{2.9a}$$

or equivalently

$$T_2|\psi\rangle = \pm k|\psi\rangle \tag{2.9b}$$

† As far as possible, I will follow the notation of Abramowitz and Stegun (1970) for all the special functions and orthogonal polynomials.

was accomplished previously in a different context (Ojha 1986) and the results are recapitulated in § 3. For arbitrary values of $\beta_1(>0)$, the Hamiltonian $H = H_0 + V_M$ is quadratic in the raising and lowering operators $T_\pm$. Its matrix representation in the basis of (2.6) is therefore quindiagonal. To obtain a tridiagonal matrix, choose $\beta_1 = (2mA)^{1/2}$. Then the resulting eigenvalue equation

$$[2T_3^2 - T^2 - T_3T_1 - T_1T_3 - \eta(T_3 - T_1) - E]|\psi\rangle = 0 \tag{2.10}$$

is linear in $T_\pm$. On expanding the function $|\psi\rangle$ in the basis set $\{|t, q\rangle,\ q = t+1, t+2, \dots, \infty\}$, one obtains a three-term recursion relation for the expansion coefficients. Appropriate regular and irregular solutions of this recursion are obtained in § 4.

3. States of the free particle

Consider the eigenvalue equation

$$p_x|\psi\rangle = -T_2|\psi\rangle = k|\psi\rangle \tag{3.1a}$$

and expand the wavefunction $|\psi\rangle$ in the basis set $\{|t, \nu+t+1\rangle,\ \nu = 0, 1, 2, \dots, \infty\}$:

$$|\psi\rangle = \sum_{\nu=0}^{\infty} a_\nu |t, \nu+t+1\rangle. \tag{3.1b}$$

It follows from the standard action of T_2 on $|t, \nu+t+1\rangle$ that the expansion coefficients a_ν satisfy the recursion relation

$$[\nu(\nu+2t+1)]^{1/2} a_{\nu-1} + \mathrm{i}2ka_\nu - [(\nu+1)(\nu+2t+2)]^{1/2} a_{\nu+1} = 0. \tag{3.2}$$

There are two linearly independent solutions of the recursion which are given in terms of gamma functions and Gauss hypergeometric functions:

$$a_\nu^{\mathrm{I}}(k) = \frac{[\Gamma(\nu+1)\Gamma(\nu+2t+2)]^{1/2}}{\Gamma(\nu+t+2-\mathrm{i}k)}\, {}_2F_1(t+1-\mathrm{i}k, -t-\mathrm{i}k; \nu+t+2-\mathrm{i}k; \tfrac{1}{2}) \tag{3.3a}$$

and

$$a_\nu^{\mathrm{II}}(k) = \mathrm{e}^{\mathrm{i}\pi\nu} \frac{[\Gamma(\nu+1)\Gamma(\nu+2t+2)]^{1/2}}{\Gamma(\nu+t+2+\mathrm{i}k)}\, {}_2F_1(t+1+\mathrm{i}k, -t+\mathrm{i}k; \nu+t+2+\mathrm{i}k; \tfrac{1}{2}). \tag{3.3b}$$

Asymptotically,

$$a_\nu^{\mathrm{I}}(k) \underset{\nu\to\infty}{\sim} (\nu+t+1)^{-1/2+\mathrm{i}k} \tag{3.4a}$$

and

$$a_\nu^{\mathrm{II}}(k) \underset{\nu\to\infty}{\sim} \mathrm{e}^{i\pi\nu}(\nu+t+1)^{-1/2-\mathrm{i}k}. \tag{3.4b}$$

The regular solution of the recursion, specified by the condition

$$\bar{S}_{-1}(k) = 0 \tag{3.5a}$$

is given by a linear combination of a_ν^{I} and a_ν^{II} where the coefficient multiplying $a_\nu^{\mathrm{II}}(a_\nu^{\mathrm{I}})$ is $(\nu+1)^{1/2}(\nu+2t+2)^{1/2} a_\nu^{\mathrm{I}}(-a_\nu^{\mathrm{II}})|_{\nu=1}$:

$$\bar{S}_\nu(k) = \frac{[\Gamma(2t+2)]^{1/2}}{2^t}\left(\frac{2^{-\mathrm{i}k}}{\Gamma(t+1-\mathrm{i}k)}\, a_\nu^{\mathrm{II}}(k) + \frac{2\mathrm{i}k}{\Gamma(t+1+\mathrm{i}k)}\, a_\nu^{\mathrm{I}}(k)\right). \tag{3.5b}$$

From standard properties of the gamma function and the Gauss hypergeometric function, it can be shown that

$$\bar{S}_\nu(k) = 2(-1)^\nu\left(\frac{\Gamma(\nu+2t+2)}{\Gamma(2t+2)\Gamma(\nu+1)}\right)^{1/2} {}_2F_1(-\nu, \nu+t+1+\mathrm{i}k; 2t+2; 2). \tag{3.5c}$$

Naturally, this is a polynomial in k. In fact, these are the (normalised) Pollaczek polynomials (Erdelyi 1953, Ojha 1986):

$$P_\nu^{t+1}(k; \pi/2) = \mathrm{e}^{\mathrm{i}\nu\pi/2}\left(\frac{\Gamma(\nu+2t+2)}{\Gamma(2t+2)\Gamma(\nu+1)}\right)^{1/2} {}_2F_1(-\nu, t+1+\mathrm{i}k; 2t+2; 2) \tag{3.6a}$$

which are orthonormal over the interval $-\infty < k < \infty$ with weight

$$W(k; \pi/2) = \frac{2^{2t+2}}{2\pi\Gamma(2t+2)}|\Gamma(t+1+\mathrm{i}k)|^2. \tag{3.6b}$$

Thus

$$\int_{-\infty}^{\infty} \mathrm{d}k[P_\mu^{t+1}(k; \pi/2)]^* W(k; \pi/2) P_\nu^{t+1}(k; \pi/2) = \delta_{\mu\nu}. \tag{3.6c}$$

Obviously, the regular solution in (3.5c), now rewritten as

$$\bar{S}_\nu(k) = 2\,\mathrm{e}^{\mathrm{i}\pi\nu/2} P_\nu^{t+1}(k; \pi/2) \tag{3.7a}$$

is un-normalised but it can be normalised in the sense of

$$\sum_{\nu=0}^{\infty} S_\nu^*(k_1) S_\nu(k_2) = \delta(k_1 - k_2) \tag{3.7b}$$

by multiplying (3.7a) by $\frac{1}{2}(W(k; \pi/2))^{1/2}$. Then the normalised regular solution of the recursion is

$$\begin{aligned} S_\nu(k) &= \frac{2^t}{(2\pi\Gamma(2t+2))^{1/2}}|\Gamma(t+1+\mathrm{i}k)|\bar{S}_\nu(k) \\ &= \mathrm{e}^{\mathrm{i}\pi\nu/2}[W(k; \pi/2)]^{1/2} P_\nu^{t+1}(k; \pi/2). \end{aligned} \tag{3.7c}$$

The normalisation of $S_\nu(k)$ follows from the completeness relation for Pollaczek polynomials:

$$W(k; \pi/2) \sum_{\nu=0}^{\infty} P_\nu^*(k_1; \pi/2) P_\nu(k_2; \pi/2) = \delta(k_1 - k_2). \tag{3.8}$$

Apart from a phase factor, $S_\nu(k)$ is just the coefficient of the νth basis function in the expansion of the plane wave $(2\pi)^{-1/2}\,\mathrm{e}^{\mathrm{i}kx}$. If required, this phase factor may be obtained from the Fourier transform of $\phi_0(x)$.

The asymptotic behaviour of $S_\nu(k)$ is obtained from (3.4), (3.5b) and (3.7c):

$$S_\nu(k) \underset{\nu\to\infty}{\sim} \left(\frac{2}{\pi}\right)^{1/2} \frac{1}{(\nu+t+1)^{1/2}}\,\mathrm{e}^{\mathrm{i}\pi\nu/2} \cos\{\tfrac{1}{2}\pi\nu - k\ln[2(\nu+t+1)] + \arg\Gamma(t+1+\mathrm{i}k)\}. \tag{3.9}$$

The required linearly independent solutions of the eigenvalue equation

$$\frac{1}{2m}p_x^2|\psi\rangle = \frac{1}{2m}T_2^2|\psi\rangle = E|\psi\rangle$$

are $S_\nu(\pm k)$. The phase shift due to a short-range interaction $V(x)$ can be calculated along the lines of Heller and Yamani (1974) with a slight modifications acknowledging the fact that the matrix representation of the kinetic energy operator in the basis of (2.6) is block tridiagonal where each block is a diagonal 2×2 matrix.

4. Scattering states of the Morse oscillator

Expansion of the wavefunction in the eigenvalue equation (2.10) as

$$|\psi\rangle = \sum_{\nu=0}^{\infty} b_\nu |t, \nu+t+1\rangle \tag{4.1a}$$

leads to the following three-term recursion for expansion coefficients:

$$(\nu+t+\tfrac{1}{2}-\tfrac{1}{2}\eta)[\nu(\nu+2t+1)]^{1/2}b_{\nu-1}+[k^2+t(t+1)+\eta(\nu+t+1)-2(\nu+t+1)^2]b_\nu \\ +(\nu+t+\tfrac{3}{2}-\tfrac{1}{2}\eta)[(\nu+1)(\nu+1)(\nu+2t+2)]^{1/2}b_{\nu+1}=0. \tag{4.1b}$$

This recursion has been considered previously by Broad (1982). He made the further assumption that $t=\frac{1}{2}\eta-\frac{1}{2}-\bar{N}$ where $\bar{N}$ is the largest integer less than $\frac{1}{2}+\frac{1}{2}\eta$. This separates the first $\bar{N}\times\bar{N}$ block corresponding to the bound spectrum of the oscillator from the remaining infinite matrix. The solutions of (4.1b) for $\nu\geqslant\bar{N}$ then represent the scattering states.

This assumption is unnecessarily restrictive and I do not make it here. The solutions obtained in the rest of this section are therefore more general and contain the one given by Broad.

It can be verified from (4.4) of Bailey (1954) that the following functions containing the generalised hypergeometric functions ${}_3F_2(a, b, c; d, e; 1)$ do indeed satisfy the recursion (4.1b):

$$b_\nu^{\rm I}(k)=\frac{[\Gamma(\nu+1)\Gamma(\nu+2t+2)]^{1/2}}{\Gamma(\nu+t+2+ik)}\,{}_3F_2\left[\begin{matrix}-t+ik,\ t+1+ik,\ \frac{1}{2}\eta+\frac{1}{2}+ik; \\ 1+i2k,\ \nu+t+2+ik;\end{matrix}\ 1\right] \tag{4.2a}$$

and

$$b_\nu^{\rm II}(k)=b_\nu^{\rm I}(-k). \tag{4.2b}$$

The standard series expansion of the generalised hypergeometric function ${}_3F_2(a, b, c; d, e; 1)$ which appears in (4.2) converges because $\mathrm{Re}(d+e-a-b-c)>0$ (Bailey 1935). It follows that asymptotically (as $\nu\to\infty$), both the generalised hypergeometric functions tend to their limiting value of 1 and the correction is of order $(1/\nu)$. The asymptotic behaviour of $b_\nu^{\rm I}(k)$ and $b_\nu^{\rm II}(k)$ is then determined by the ratio of gamma functions:

$$b_\nu^{\rm I}(k) \underset{\nu\to\infty}{\sim} (\nu+t+1)^{-1/2-ik} \tag{4.3a}$$

$$b_\nu^{\rm II}(k) \underset{\nu\to\infty}{\sim} (\nu+t+1)^{-1/2+ik} \tag{4.3b}$$

The un-normalised regular solution of the recursion is given by the following linear combination of $b_\nu^{\mathrm{I}}(k)$ and $b_\nu^{\mathrm{II}}(k)$:

$$\bar{S}_\nu(k) = (\Gamma(2t+2))^{1/2}\Gamma(t+\tfrac{3}{2}-\tfrac{1}{2}\eta)\left(\frac{\Gamma(1+\mathrm{i}2k)}{\Gamma(\frac{1}{2}-\frac{1}{2}\eta+\mathrm{i}k)(\Gamma(t+1+\mathrm{i}k))^2}\,b_\nu^{\mathrm{II}}(k) - \frac{\Gamma(1-\mathrm{i}2k)}{\Gamma(\frac{1}{2}-\frac{1}{2}\eta-\mathrm{i}k)(\Gamma(t+1-\mathrm{i}k))^2}\,b_\nu^{\mathrm{I}}(k)\right). \tag{4.4}$$

This can be brought into the form of a polynomial in k^2 by using the transformation for ${}_3F_2(a, b, c; d, e; 1)$ given in equation (2) § 3.2 of Bailey (1935) and the standard properties of gamma functions. Thus

$$\bar{S}_\nu(k) = \mathrm{i}2k\left(\frac{\Gamma(\nu+2t+2)}{\Gamma(2t+2)\Gamma(\nu+1)}\right)^{1/2} {}_3F_2\left[\begin{matrix} -\nu,\ t+1+\mathrm{i}k,\ t+1-\mathrm{i}k; \\ t-\frac{1}{2}\eta+\frac{3}{2},\ 2t+2; \end{matrix}\ 1\right]. \tag{4.5}$$

This system of polynomials does not seem to have been studied before. Although it is possible to calculate their weight distribution from the defining recursion relation, I thought it more expedient to calculate it directly from the overlap integral of the normalised coordinate-space wavefunction $\psi(x)$ and the basis functions $\phi_0(x)$. The normalised solution of the recursion is

$$\begin{aligned} S_\nu(k) &= \frac{1}{\mathrm{i}2k}\,\frac{1}{(2\pi\Gamma(2t+1))^{1/2}}\,\frac{|\Gamma(\frac{1}{2}-\frac{1}{2}\eta+\mathrm{i}k)|}{|\Gamma(\mathrm{i}2k)|}\,\frac{|\Gamma(t+1+\mathrm{i}k)|^2}{\Gamma(t+\frac{3}{2}-\frac{1}{2}\eta)}\,\bar{S}_\nu(k) \\ &= \left\{\frac{1}{(2\pi\Gamma(2t+2))^{1/2}}\,\frac{|\Gamma(\frac{1}{2}-\frac{1}{2}\eta+\mathrm{i}k)|}{|\Gamma(\mathrm{i}2k)|}\,\frac{|\Gamma(t+1+\mathrm{i}k)|^2}{\Gamma(t+\frac{3}{2}-\frac{1}{2}\eta)}\right\} \\ &\quad\times\left\{\left(\frac{\Gamma(\nu+2t+2)}{\Gamma(2t+2)\Gamma(\nu+1)}\right)^{1/2} {}_3F_2\left[\begin{matrix} -\nu,\ t+1+\mathrm{i}k,\ t+1-\mathrm{i}k; \\ t-\frac{1}{2}\eta+\frac{3}{2},\ 2t+2; \end{matrix}\ 1\right]\right\}. \end{aligned} \tag{4.6}$$

The expression in the first set of parenthesis { } is the square root of the weight for the polynomials and the expression in the second set of parenthesis is the (normalised) polynomial subject to the condition $P_{-1}(k^2)=0$, $P_0(k^2)=1$. The asymptotic form of $S_\nu(k)$ is then obtained from (4.3), (4.4) and (4.6):

$$\begin{aligned} S_\nu(k) \underset{\nu\to\infty}{\sim} \left(\frac{2}{\pi}\right)^{1/2} \frac{1}{(\nu+t+1)^{1/2}} &\sin[k\ln(\nu+t+1)+\arg\Gamma(1+\mathrm{i}2k) \\ &-\arg\Gamma(\tfrac{1}{2}-\tfrac{1}{2}\eta+\mathrm{i}k)-2\arg\Gamma(t+1+\mathrm{i}k)]. \end{aligned} \tag{4.7}$$

The irregular solution of the recursion is defined to equal asymptotically the amplitude of the regular solution and to lead it in phase by $\pi/2$. This is accomplished by changing the $-$ sign in (4.4) to $+$. After the transformation mentioned following (4.4) and multiplication by the scale factor given in the first line of (4.6), I obtain the following expression for the normalised irregular solution of the recursion, $C_\nu(k)$:

$$\begin{aligned} C_\nu(k) &+ \mathrm{i}\,\frac{\cos[\pi(t+\frac{1}{2}+\frac{1}{2}\eta)] - \cos[\pi(t+\frac{3}{2}-\frac{1}{2}\eta)]\cosh(2\pi k)}{\sinh(2\pi k)\sin[\pi(t+\frac{3}{2}-\frac{1}{2}\eta)]}\,S_\nu(k) \\ &= \frac{1}{\mathrm{i}2k}\,\frac{1}{(2\pi\Gamma(2t+2))^{1/2}} \end{aligned}$$

$$\times\frac{\Gamma(\frac{1}{2}-\frac{1}{2}\eta+t)|\Gamma(1+\mathrm{i}2k)|}{|\Gamma(\frac{1}{2}-\frac{1}{2}\eta+\mathrm{i}k)|}\left(\frac{\Gamma(\nu+1)\Gamma(\nu+2t+2)}{\Gamma(2t+2)\Gamma(\nu+t-\frac{1}{2}\eta+\frac{3}{2})}\right)^{1/2}$$
$$\times{}_3F_2\left[\begin{matrix}\frac{1}{2}+\frac{1}{2}\eta-\mathrm{i}k,\frac{1}{2}+\frac{1}{2}\eta+\mathrm{i}k,-\nu-t+\frac{1}{2}\eta-\frac{1}{2};\\ -t+\frac{1}{2}\eta+\frac{1}{2},\ t+\frac{1}{2}\eta+\frac{3}{2};\end{matrix}\ 1\right]. \tag{4.8}$$

Asymptotically,

$$C_\nu(k)\underset{\nu\to\infty}{\sim}\left(\frac{2}{\pi}\right)^{1/2}\frac{1}{(\nu+t+1)^{1/2}}\cos[k\ln(\nu+t+1)+\arg\Gamma(1+\mathrm{i}2k)$$
$$-\arg\Gamma(\tfrac{1}{2}-\tfrac{1}{2}\eta+\mathrm{i}k)-2\arg\Gamma(t+1+\mathrm{i}k)]. \tag{4.9}$$

These two solutions form a base pair in terms of which scattering from an additional short-range interaction can be considered.

5. Concluding remarks

One would imagine that a comparison of the asymptotic form of $S_\nu(k)$ in (4.7) with the asymptotic form of the free-particle wavefunctions (with wavevectors $\pm k$) in (3.9) would give the phase shift for scattering from the Morse potential. This is not the case. The reason for this seems to be the long-range nature of the Morse potential. (Recall that $V_{\mathrm{M}}(x)$ is unbounded as $x\to-\infty$.) Mathematically, it is reflected in the fact that the non-zero matrix elements of $V_{\mathrm{M}}(x)$ in the basis (2.6) are of the same order as the matrix elements of kinetic energy for all basis functions. In fact, exact cancellation of the matrix elements $\langle\nu|V_{\mathrm{M}}(x)|\nu\pm2\rangle$ with the corresponding matrix elements of kinetic energy $\langle\nu|(2m)^{-1}p_x^2|\nu\pm2\rangle$ when $\beta_1=(2mA)^{1/2}$ was necessary to obtain a Jacobi-matrix (tridiagonal) representation of the Hamiltonian. Alternatively, the free-particle recursion (3.2) is not a limiting case of the Morse oscillator recursion (4.1*b*).

Nevertheless, the regular and irregular solutions of the Morse oscillator and free particle recursions obtained in this article provide the necessary framework for calculating the phase shift for scattering from additional short-range interactions and may be useful in practical calculation of atom-atom scattering. The characteristic polynomials associated with the Morse oscillator (4.6) do not seem to have been studied previously. It is perhaps appropriate to call them 'Morse polynomials'.

Appendix

The Schrödinger equation

$$\left(-\frac{1}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+A\,\mathrm{e}^{-2x}-B\,\mathrm{e}^{-x}-E\right)\psi(x)=0 \tag{A1}$$

is essentially Whittaker's equation (Abramowitz and Stegun 1970) in the variable $z_1=(8mA)^{1/2}\,\mathrm{e}^{-x}$. The solutions

$$\psi_\pm(x)=\mathrm{e}^{-z_1/2}z_1^{\mp\mathrm{i}k}\,{}_1F_1(\tfrac{1}{2}\mp\mathrm{i}k-\tfrac{1}{2}\eta;\,1\mp\mathrm{i}2k;\,z_1) \tag{A2a}$$

represent plane waves at infinity, i.e.

$$\psi_\pm(x)\underset{x\to\infty}{\sim}(8mA)^{\mp\mathrm{i}k/2}\,\mathrm{e}^{\pm\mathrm{i}kx}. \tag{A2b}$$

Here $k=(2mE)^{1/2}$ and $\eta=(2mB^2/A)^{1/2}$. Another solution

$$\psi(x)=z_1^{-1/2}W_{\eta/2,\mathrm{i}k}(z_1)=\mathrm{e}^{-z_1/2}z_1^{\mathrm{i}k}U(\tfrac{1}{2}+\mathrm{i}k-\tfrac{1}{2}\eta;\,1+\mathrm{i}2k;\,z_1) \tag{A3a}$$

satisfies the boundary condition

$$\lim_{x\to\infty}\psi(x)=0. \tag{A3b}$$

Its alternative representation as a linear combination of $\psi_\pm(x)$,

$$\psi(x)=\frac{\Gamma(-\mathrm{i}2k)}{\Gamma(\frac{1}{2}-\mathrm{i}k-\frac{1}{2}\eta)}\psi_-(x)+\frac{\Gamma(\mathrm{i}2k)}{\Gamma(\frac{1}{2}+\mathrm{i}k-\frac{1}{2}\eta)}\psi_+(x) \tag{A4}$$

determines its asymptotic form as $x\to\infty$ and hence the reflection amplitude

$$R(k)=(8mA)^{-\mathrm{i}k}\frac{\Gamma(\mathrm{i}2k)\Gamma(\frac{1}{2}-\mathrm{i}k-\frac{1}{2}\eta)}{\Gamma(-\mathrm{i}2k)\Gamma(\frac{1}{2}+\mathrm{i}k-\frac{1}{2}\eta)}. \tag{A5}$$

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