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The algebraic approach to the Morse oscillator

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Abstract. The discrete spectrum for a Morse oscillator is found using an SO(2, 1) algebra. Since this algebra does not prove to be appropriate to compute matrix elements for the oscillator eigenfunctions, we construct a B_1 -type algebra with the aid of an auxiliary angle variable. Matrix elements and recurrence relations are found for several useful operators using this algebra. The limit in which the anharmonicity tends to zero is studied.

1. Introduction

In this paper we present the solution for the bound-state problem of a Morse oscillator in one dimension (Morse 1929) using two different Lie algebras. Many quantummechanical problems have been studied using operator methods (Wybourne 1974), in particular, the harmonic oscillator (Louisell 1973), the Coulomb problem (Englefield 1972, Barut and Kleinert 1967, Bednář 1973) and angular momentum (Edmonds 1957). Little attention, however, has been paid to the Morse potential well, in spite of its practical importance in analysing anharmonic vibrations (Pauling and Wilson 1935, Huffacker 1976), molecular energy transfer (Rapp and Kassal 1969) and atom-surface scattering (Cabrera *et al* 1970). The algebraic approach is proving to be a basic tool in the study of inelastic collisions (Alhassid and Levine 1978). Hence a thorough understanding of the time honoured Morse oscillator in algebraic terms seems appropriate.

Ladder operators for the bound states have been known since the exhaustive work of Infeld and Hull (1951), and some of their properties have been exploited in vibrational problems (Huffacker and Dwivedi 1975). These ladder operators were first obtained with the aid of the factorisation method (Infeld and Hull 1951). They depend explicitly on the vibrational quantum number, so they are well defined as long as they act upon a specified eigenstate.

As a generalisation of the two different types of factorisation (types B and F) (Infeld and Hull 1951), we obtain in this work two different Lie algebras for the Morse oscillator. The first one is a realisation of an SO(2, 1) algebra. It follows from a B-type factorisation. Indeed, the Schrödinger equation for the Morse potential is equivalent (Morse 1929) to the radial equation of the Coulomb problem. This in turn is associated with an SO(2, 1) algebra (Armstrong 1970, 1971, Čížek and Paldus 1977). It is found,

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however, that the ladder operators in this algebra shift the well's depth at *constant* energy (Huffacker and Dwivedi 1975). In other words, two eigenstates of the Morse oscillator correspond to different irreducible representations (IR) of the group SO(2, 1). Therefore, matrix elements between different energy states are awkward to compute in this scheme.

A different approach to the problem consists of introducing an auxiliary variable (Armstrong 1970, 1971, Crubellier and Feneuille 1974, Miller 1968) in order to build an SO(3) algebra or, more properly, a B₁-type algebra (Miller 1968). This approach corresponds to the F-type factorisation (Infeld and Hull 1951). The associated ladder operators shift the vibrational quantum number by one unit. We are then able to compute matrix elements for different bound states. The auxiliary variable can be taken as a dummy angle ranging from 0 to 2π . Alternatively, it may be interpreted as a dilated time (Anderson *et al* 1973) when working in the Schrödinger picture (Chacón *et al* 1976). The time dilation is introduced in order to 'linearise the energy spectrum' (Anderson *et al* 1973). The resulting operators include (partial) derivatives with respect to the dilated time. A similar B₁ algebra can be defined for the hydrogen atom problem. There the ladder operators will have the effect of shifting the angular momentum in the radial equation (Herrick and Sinanoğlu 1972).

Finally, if we let the anharmonicity parameter in the Morse potential go to zero, we recover the harmonic oscillator. In this case, the algebra is contracted into the algebra of the harmonic oscillator as we show below.

In § 2, we define the SO(2, 1) algebra for the Morse potential, following the constructive approach of Čížek and Paldus (1977). Using this algebra, we derive the discrete spectrum, with the aid of its Casimir operator. In § 3, we make use of the auxiliary variable to obtain the B_1 algebra. We then show how the matrix elements for different operators can be calculated. We also discuss the hermiticity properties of the ladder operators in the physical metric. Section 4 shows how the harmonic limit is attained. Finally, in § 5 we present a brief comparison between the two algebras, and point out some further developments.

2. The discrete spectrum

The Morse potential is defined in terms of two constants, the potential depth D and an inverse distance a:

$$V(u) = D e^{-2au} - 2D e^{-au}.$$
 (2.1)

Here we have chosen the origin u = 0 as the equilibrium distance. The potential tends to zero asymptotically as $U \rightarrow \infty$, so its minimum is V(u = 0) = -D. Throughout this work we shall take equation (2.1) as a one-dimensional potential (Morse 1929, Pauling and Wilson 1935). This implies that the eigenfunctions vanish at $u \rightarrow \pm \infty$.

It is convenient to define a dimensionless distance x = au and to introduce the (inverse) anharmonicity constant K:

$$K = \sqrt{2m_0 D}/\hbar a, \tag{2.2}$$

given in terms of the reduced mass m_0 . The Schrödinger equation for S(x) is then

$$(d^{2}S(x)/dx^{2}) + [\epsilon + K^{2}(2e^{-x} - e^{-2x})]S(x) = 0$$
(2.3)

where ϵ is the dimensionless energy $\epsilon = 2m_0 E/\hbar^2 a^2$. Choosing S(x) as a normalised function, we have that

$$\int_{-\infty}^{\infty} S_n^*(x) S_m(x) \, \mathrm{d}x = \delta_{nm} \tag{2.4}$$

for any bound states n and m.

Equation (2.3) is transformed into a simpler form with a further change of variable and function (Morse 1929):

$$y = K e^{-x} \qquad (\infty > y \ge 0)$$

$$\psi(y) = e^{-x/2} S(x). \qquad (2.5)$$

The equation for $\psi(y)$ is

$$d^{2}\psi(y)/dy^{2} + [(\epsilon + \frac{1}{4})y^{-2} + 2Ky^{-1} - 1]\psi(y) = 0, \qquad (2.6)$$

which can be rewritten as an eigenvalue equation for K (cf Bednář 1973 for the Coulomb case). Introducing the canonical momentum p = -id/dy, we get

$$\frac{1}{2}[yp^2 - (\epsilon + \frac{1}{4})y^{-1} + y]\psi = K\psi.$$
(2.7)

In order to define the proper SO(2, 1) algebra, we first notice that the operators y, yp and yp^2 close under commutation (Čížek and Paldus 1977). Since adding a term proportional to y^{-1} to the latter does not change the commutators, we write

$$W_1 = y$$
 $W_2 = yp$ $W_3 = yp^2 - [(\epsilon + \frac{1}{4})/y].$ (2.8)

The relations

$$[W_1, W_2] = i W_1$$
 $[W_2, W_3] = i W_3$ $[W_1, W_3] = 2 i W_2$ (2.9)

can be obtained directly from the canonical one [y, p] = i.

Comparing (2.8) with the eigenvalue equation (2.7), we define

$$T_3 = \frac{1}{2}(W_1 + W_3) \tag{2.10a}$$

and the corresponding ladder operators are

$$T_{\pm} = \frac{1}{2}(W_3 - W_1) \pm i \ W_2. \tag{2.10b}$$

From (2.8) it indeed follows that $\{T_3, T_+, T_-\}$ form an SO(2, 1) algebra:

$$[T_3, T_{\pm}] = \pm T_{\pm} \qquad [T_+, T_-] = -2T_3. \tag{2.11}$$

We see immediately that the ladder operators T_{\pm} shift the value of $K \rightarrow K \pm 1$ for a given energy ϵ . They change the potential parameters, but not the energy. The corresponding Casimir operator is

$$C^{2} = T_{3}^{2} \mp T_{3} - T_{\pm}T_{\mp} = -\epsilon - \frac{1}{4}.$$
(2.12)

Using (2.12) and the commutation relations (2.11), we can determine the energy spectrum: for any given (negative) energy ϵ , there is a minimum value of K for which such an eigenfunction exists. Calling this value K_0 , and the corresponding eigenfunction ψ_0 , we have that

$$T_3\psi_0 = K_0\psi_0 \qquad T - \psi_0 = 0. \tag{2.13}$$

Since $T_+\psi_K \propto \psi_{K+1}$, the eigenvalues of T_3 are given by $K = K_0 + n$, where $n = 0, 1, 2, \ldots$. From (2.12) and (2.13), we then get

$$(T_3^2 - T_3 - C^2)\psi_0 = [(K_0 - \frac{1}{2})^2 + \epsilon]\psi_0 = 0, \qquad (2.14)$$

which finally yields

$$\epsilon_n = -(K - n - \frac{1}{2})^2 \tag{2.15}$$

in terms of the actual K. For fixed K, $n = 0, 1, 2, ..., (K - \frac{1}{2})$, so that the largest integer in $K + \frac{1}{2}$ gives the number of bound states. If K is smaller than $\frac{1}{2}$, the potential does not support any bound state (Morse 1929).

Although the problem is similar to the hydrogen atom, there is an important difference. In the Coulomb problem, in order to rewrite the equation as an eigenvalue equation for the charge, it is necessary to make a space dilation $r \rightarrow r/n$ which depends on the energy through the quantum number n. This implies different dilations for different eigenstates. For the Morse oscillator, however, the necessary dilation depends only on the potential parameters. It is implicitly introduced in equation (2.5): $e^{-x} \rightarrow K e^{-x}$. In fact, in terms of the variable x, it reduces to a (constant) translation $x \rightarrow x - \ln K$.

3. Auxiliary angle variable and matrix elements

3.1. The B_1 algebra

The solutions to the K eigenvalue equation (2.7) found above form the basis for an IR of the group SO(2, 1). These IR's are labelled by the value of K_0 , and hence by the energy, while their rows determine the actual value of K. Computing matrix elements for different energies would then correspond to choosing two different IR's, rather than two rows of the same IR.

In the present section, we define a new algebra which has the virtue of exchanging these roles. It is based on an F-type factorisation of equation (2.6) (Infeld and Hull 1951). The explicit appearance of the quantum number n in this factorisation (Huffacker and Dwivedi 1975) suggests the introduction of a new variable ϕ (Miller 1968) and the associated momentum:

$$G_0 = -\mathrm{i}\partial/\partial\phi. \tag{3.1}$$

For vibrational states, ϕ ranges from 0 to 2π . Regarding the variable y, it is convenient to introduce an extra K factor:

$$r = K^2 e^{-x}$$
 ($\infty > r \ge 0$). (3.2)

We also define states in the (r, ϕ) space, which are eigenstates of G_0 , as

$$|\mu\rangle = \frac{1}{\sqrt{2\pi}} e^{i\mu\phi} \chi_{\mu}(r).$$
(3.3*a*)

$$\chi_{\mu}(r) = K e^{-x/2} S_{\mu}(x)$$
(3.3b)

is a solution of

$$\frac{\mathrm{d}^{2}\chi_{\mu}(r)}{\mathrm{d}r^{2}} + \left(\frac{2}{r} - \frac{\mu^{2} - \frac{1}{4}}{r^{2}}\right)\chi_{\mu}(r) = K^{-2}\chi_{\mu}(r), \qquad (3.4)$$

which follows directly from (2.6), and we have labelled $\mu = K - n - \frac{1}{2}$, according to (2.15). The functions χ_{μ} are *orthonormal* in the physical metric $r^{-2} dr$:

$$\int_{0}^{\infty} \chi_{\mu}^{*}(r) \chi_{\mu}(r) \frac{\mathrm{d}r}{r^{2}} = \int_{-\infty}^{\infty} S_{\mu}^{*}(x) S_{\nu}(x) \,\mathrm{d}x = \delta_{\mu\nu}.$$
(3.5)

The generalisation of the operator in (3.4) to the (r, ϕ) space is simply

$$\mathscr{L} = \frac{\partial^2}{\partial r^2} + \frac{2}{r} - \frac{G_0^2 - \frac{1}{4}}{r^2},$$
(3.6)

so that

$$\mathscr{L}|\mu\rangle = K^{-2}|\mu\rangle. \tag{3.7}$$

An important point to notice is that the operator \mathcal{L} is *not* self-adjoint in the physical metric defined in (3.5).

The factorisation of the operator \mathscr{L} is achieved using the two operators G_{\pm} (Herrick and Sinanoğlu 1972):

$$G_{\pm} = K e^{\pm i\phi} ((G_0 \pm \frac{1}{2})^2 r^{-1} \mp (G_0 \pm \frac{1}{2})(\partial/\partial r) - 1).$$
(3.8)

Indeed, using the relations

$$e^{\pm i\phi}(G_0 \pm \frac{1}{2}) = (G_0 \mp \frac{1}{2}) e^{\pm i\phi},$$
(3.9)

we obtain

$$G_{\pm}G_{\mp} = K^{2} [1 - (G_{0} \mp \frac{1}{2})^{2} \mathscr{L}].$$
(3.10)

From the equations above we obtain the commutation relations

$$[G_0, G_{\pm}] = \pm G_{\pm} \qquad [G_+, G_-] = 2G_0 I \tag{3.11}$$

which identify $\{G_0, G_+, G_-\}$ as a realisation of a B₁ algebra (Miller 1968). Here I is the identity operator in the space spanned by the kets $|\mu\rangle$, and G_{\pm} are the ladder operators:

$$G_{\pm}|\mu\rangle = G_{\pm} \frac{e^{i\mu\phi}}{\sqrt{2\pi}} \chi_{\mu}(r) = A_{\mu}^{\pm} \frac{e^{i(\mu\pm 1)\phi}}{\sqrt{2\pi}} \chi_{\mu\pm 1}(r) = A_{\mu}^{\pm}|\mu\pm 1\rangle.$$
(3.12)

The constants A^{\pm}_{μ} are chosen so that the kets $|\mu \pm 1\rangle$ remain normalised in the physical metric. They have to be computed taking into account the fact that G_+ , G_- are *not* the adjoint of one another. Indeed, for the metric in (3.5), there is an additional term 2/r when calculating the adjoint of $\partial/\partial r$, which results in

$$(G_{\pm})^{\dagger} = G_{\mp} \mp 2Kr^{-1} e^{\mp i\phi} (G_0 \mp \frac{1}{2})$$
(3.13)

when we take the adjoint of equation (3.8). The term in 1/r above can be re-expressed in terms of the ladder operators as

$$r^{-1} = (G_0^2 - \frac{1}{4})^{-1} + \frac{1}{2}K^{-1}G_0^{-1}[(G_0 + \frac{1}{2})^{-1}e^{-i\phi}G_+ + (G_0 - \frac{1}{2})^{-1}e^{i\phi}G_-].$$
(3.14)

As usual, to calculate the proportionality constants A^{\pm}_{μ} , we evaluate the expectation value of $G_{\pm}G_{\mp}$ in the (r, ϕ) space, so using equations (3.7) and (3.10)–(3.14) we get

$$\langle \mu | G_{\pm} G_{\mp} | \mu \rangle = K^2 - (\mu \mp \frac{1}{2})^2 = |A_{\mu}^{\mp}|^2 (1 \mp \mu^{-1}).$$
(3.15)

The extra $\pm \mu^{-1}$ term can be traced back directly to the extra term in (3.13). It does not appear in the usual angular momentum SO(3) algebra, where J_{\pm} is the adjoint of J_{\pm}

(Edmonds 1957, Miller 1968). With the usual choice of phase, we finally obtain

$$G_{\pm}|\mu\rangle = A_{\mu}^{\pm}|\mu\pm1\rangle = \left(\frac{\mu}{\mu\pm1}\right)^{1/2} [K^2 - (\mu\pm\frac{1}{2})^2]^{1/2}|\mu\pm1\rangle.$$
(3.16)

3.2. The matrix elements

In order to preserve the orthogonality of $S_{\mu}(x)$, we have introduced the metric $d\phi r^{-2} dr$ for the kets $|\mu\rangle$. Hence, a knowledge of the coefficients A_{μ}^{\pm} allows us to calculate matrix elements for operators expressed in terms of the generators of the algebra. In particular, since r^{-1} is a linear combination of G_{+} and G_{-} , we have a selection rule $\nu = \mu, \mu \pm 1$ for this operator (Huffacker and Dwivedi 1975). Actually, using (3.14), we get

$$(\chi_{\nu}|r^{-1}|\chi_{\mu}) = \langle \nu| e^{i(\nu-\mu)\phi}r^{-1}|\mu\rangle = \frac{4}{4\mu^{2}-1}\delta_{\nu\mu} + \frac{A_{\mu}^{+}}{K\mu(2\mu+1)}\delta_{\nu\mu+1} + \frac{A_{\mu}^{-}}{K\mu(2\mu-1)}\delta_{\nu\mu-1},$$
(3.17)

with A_{μ}^{\pm} given by (3.16), and $\mu = K - n - \frac{1}{2}$ in terms of the number of quanta *n*. By the same token,

$$(\chi_{\nu}|\mathbf{d}/\mathbf{d}\mathbf{r}|\chi_{\mu}) = \frac{4}{4\mu^{2}-1}\delta_{\nu\mu} - \frac{(2\mu-1)A_{\mu}^{+}}{2K\mu(2\mu+1)}\delta_{\nu\mu+1} + \frac{(2\mu+1)A_{\mu}^{-}}{2K\mu(2\mu-1)}\delta_{\nu\mu-1}.$$
(3.18)

Next, we obtain a recurrence relation for the matrix elements of r^{α} in terms of $r^{\alpha+1}$. To this end, we compute the commutator of \mathscr{L} with $r^{\alpha+2}$:

$$[\mathscr{L}, r^{\alpha+2}] = (\alpha+1)(\alpha+2)r^{\alpha} + 2(\alpha+2)r^{\alpha+1}\partial/\partial r.$$
(3.19)

Using now the adjoint of \mathcal{L} ,

$$\mathscr{L}^{\dagger} = \mathscr{L} + 6r^{-2} - 4r^{-1}\partial/\partial r, \qquad (3.20)$$

we calculate the matrix element of the commutator (3.19):

$$(\chi_{\nu}|[\mathscr{L}, r^{\alpha+2}]|\chi_{\mu}) = \langle \nu | e^{i(\nu-\mu)\phi}[\mathscr{L}, r^{\alpha-2}]|\mu\rangle = \langle \nu | e^{i(\nu-\mu)\phi}(\mathscr{L}r^{\alpha+2} - r^{\alpha+2}\mathscr{L})|\mu\rangle.$$
(3.21)

Substituting for $\partial/\partial r$ the expression in terms of G_{\pm} , from their definition (3.8), we finally get the desired recurrence relation:

$$\left(\alpha + \frac{\mu^{2} - \nu^{2}}{\alpha} + 4\mu^{2}\right)(\chi_{\nu}|r^{\alpha}|\chi_{\mu}) = 4(\chi_{\nu}|r^{\alpha+1}|\chi_{\mu}) + \frac{2A_{\mu}^{+}}{K}(\chi_{\nu}|r^{\alpha+1}|\chi_{\mu+1}) + \frac{2A_{\mu}^{-}}{K}(\chi_{\nu}|r^{\alpha+1}|\chi_{\mu-1}).$$
(3.22)

In particular, equation (3.17) follows from the above for $\alpha = -1$.

4. The harmonic limit

We now turn our attention to the case in which the Morse potential admits many bound states, and approaches a harmonic oscillator potential. Expanding (2.1) in powers of au, we get

$$W(u) \equiv D + V(u) = Da^{2}(u^{2} - au^{3} + \cdots).$$
(4.1)

Letting $a \to 0$ and $D \to \infty$, but keeping the force constant $k_e = 2Da^2$ finite, the (inverse) anharmonicity parameter $K \to \infty$, the number of bound states increases, and we get the harmonic limit $W = \frac{1}{2}k_eu^2$.

We now want to study the contraction of the algebra $\{G_0, G_+, G_-\}$ in this limit. For any finite value of the number of quanta *n*, we have that $\mu \rightarrow K$, and hence

$$G_0|\mu\rangle = \mu|\mu\rangle \to K|\mu\rangle, \tag{4.2}$$

so that G_0 becomes the identity operator times K. On the other hand, expanding the exponential in (3.2), we get for G_{\pm}

$$G_{\pm} \rightarrow \sqrt{2K} e^{\pm i\phi} \frac{1}{\sqrt{2}} \left(\pm \frac{1}{a\sqrt{K}} \frac{\partial}{\partial u} + a\sqrt{K}u \right)$$
(4.3)

where $a\sqrt{K} = \sqrt{m_0\omega/\hbar}$ remains finite in the harmonic limit. Hence the algebra $\{G_0, G_+, G_-\}$ contracts into $\{K. I, \sqrt{2K}A, \sqrt{2K}A^\dagger\}$, where

$$[A, A^{\dagger}] = I. \tag{4.4}$$

This commutation relation is the limit of (3.11a), and the operators A^{\dagger} and A are the usual harmonic creation and annihilation operators. In this limit A and A^{\dagger} become the adjoint of one another, as they should, while (3.16) reduces to

$$A|n\rangle = \sqrt{n}|n-1\rangle \qquad A^{\dagger}|n\rangle = \sqrt{n+1}|n+1\rangle.$$
(4.5)

The factor $\left[\mu/(\mu \pm 1)\right]^{1/2}$ in (3.16) tends to one in this limit, since $\mu \to \infty$ for any finite *n*.

5. Discussion

The SO(2, 1) algebra found in § 2 seems more appropriate for obtaining the discrete spectrum of the Morse oscillator. The spectrum is obtained by solving for the energy in terms of the anharmonicity parameter K. This in turn is the eigenvalue of the operator T_3 in the algebra. To be able to calculate matrix elements between different energy eigenfunctions, it is necessary to introduce an additional variable and define tensor operators (Armstrong 1970). These tensors are not irreducible, but are indecomposable in this case (Chacón *et al* 1976). The matrix elements can thus be expressed in terms of the Wigner coefficients for the SO(2, 1) group (Holman and Biedenharn 1966).

The alternative route, followed in this paper, is to find an appropriate algebra whose ladder operators shift the value of the energy itself, rather than the potential parameters. The resulting Lie algebra is a realisation of a B₁ algebra. The generators of this algebra do not present the usual adjointness properties of an SO(3) algebra when using the scalar product with physical meaning for the Morse oscillator. This, however, is not a real shortcoming for the computation of matrix elements for operators which are expressible in terms of the generators. This is done in a straightforward way without the need to define tensor operators.

These matrix elements can be used in perturbation expansions in which the Morse vibrational states are used as a starting point. These are utilised in spectroscopic problems for diatomic molecules (Huffacker 1976). In the case of dynamic problems involving the Morse oscillator, such as the problem of vibrational energy transfer for simple molecules (Rapp and Kassal 1969), or collinear reactive collisions (Hofacker and Levine 1971), a better approximation is usually required. Algebraic methods like

the ones developed in this paper allow for the evaluation of the corresponding transition probabilities (Levine and Wulfman 1979) in a non-perturbative fashion. Further work along these lines will be reported elsewhere.

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