A simple algebraic approach to coherent states for the Morse oscillator

1992 J. Phys. A: Math. Gen. 25 1671

(http://iopscience.iop.org/0305-4470/25/6/022)

J. Phys. A: Math. Gen. 25 (1992) 1671–1683. Printed in the UK

A simple algebraic approach to coherent states for the Morse oscillator

Ian L Cooper
Department of Chemistry, The University, Newcastle upon Tyne NE1 7RU, UK

Received 4 September 1991

Abstract. Minimum uncertainty coherent states and annihilation operator coherent states for the Morse oscillator are derived and shown to be equivalent. They reduce, in the limit of small anharmonicity constant, or, equivalently, in the limit of large well depth, to the approximate coherent states derived previously from the use of a generalized displacement operator.

1. Introduction

Anharmonic potentials, particularly the Morse potential (Morse 1929), have been used widely to describe chemical bonds, since they take into account both the quasi-harmonic behaviour of the bond in the vicinity of the potential minimum and the ability of the bond to undergo dissociation at high excitation energies. Studies of such anharmonic potential systems are of interest in respect of the interaction of high-frequency radiation with chemical bonds, and, by analogy with the case of harmonic potentials, this requires a knowledge of the so-called coherent states of the anharmonic potential.

Harmonic oscillator coherent states have been widely studied (Louisell 1973) and have the interesting property that they correspond to those states which (i) minimize the uncertainty relation; (ii) are eigenstates of the annihilation operator; and (iii) arise from the operation of a unitary displacement operator to the ground-state wavefunction of the harmonic oscillator. The term coherent reflects the fact that such states evolve coherently in time, remaining localized around the corresponding classical trajectory. (For a recent comprehensive review of coherent states, from the point of view of their topological and algebraic structure, see Zhang *et al* 1990.)

Following a detailed numerical study of the comparison of the response of harmonic and anharmonic potentials to intense electromagnetic radiation (Walker and Preston 1977), considerable interest has been shown in the construction of coherent states for general anharmonic potentials, particularly the Morse potential (Nieto and Simmons 1979a,b, Levine 1982, 1985, Gerry 1986, Kais and Levine 1990). Generalized coherent states for the Morse potential have been generated by two independent procedures. One method, proposed by Nieto and Simmons (1979a), involves a transformation to new position and momentum variables chosen in such a way that the resultant Hamiltonian most closely resembles that for an harmonic oscillator. The coherent states are then obtained by determining those states which minimize the generalized uncertainty relation in the new variables, subject to the constraint that

0305-4470/92/061671+13$04.50

the ground state, itself a minimum uncertainty state, be included in the set. The resultant approximate coherent states remained coherent only in the limit of large well depth.

An alternative approach to the construction of generalized coherent states is associated with irreducible representations of a Lie group which provides a spectrum generating algebra (Perelomov 1972, 1986). Such generalized coherent states for the Morse oscillator have been obtained (Levine 1982, 1985) using an algebraic approach based on a representation of the Morse Hamiltonian in quadratic form using non-commuting operators. The resultant approximate coherent states are also valid in the limit of large well depth. They have been related (Kais and Levine 1990) to those of Nieto and Simmons (1979a), and shown to reduce to the harmonic oscillator coherent states in the appropriate harmonic limit.

It has been demonstrated recently (Cooper 1987) that the Morse oscillator problem can be formulated in a manner similar to that of the harmonic oscillator, through the inclusion of an appropriate anharmonicity constant. The perturbational expansion of the Morse Hamiltonian in powers of the coordinate is known to yield the exact energy eigenvalue spectrum in second order. This result is a consequence of the fact that the square root of the anharmonicity constant serves as a natural perturbational parameter, and the exact bound state eigenvalue spectrum includes this parameter to powers no higher than the second.

The object of the present analysis is to apply this formulation of the Morse Hamiltonian to the determination of Morse oscillator coherent states, where the harmonic limit can be invoked by putting the anharmonicity constant equal to zero. By working with reduced variables, the close connection between the anharmonic and harmonic potentials is emphasized at each stage. Exact coherent states for the Morse oscillator problem are derived, which are not only minimum uncertainty coherent states but are also eigenstates of the annihilation operator for the ground state of the Morse oscillator. The relation between such states and previously determined approximate coherent states is discussed.

The plan of the paper is as follows. Following a review of the formulation of the Morse oscillator problem in a manner which highlights its relation to the harmonic oscillator problem, section 3 contains a derivation of the Morse coherent states, and relates them to previously determined approximate coherent states for the Morse oscillator. In order to assist comparison between the anharmonic and harmonic systems, an appendix summarizes the relevant results for coherent states of the harmonic oscillator. The paper ends with some concluding remarks.

2. Algebraic formulation of the Morse oscillator problem

The Hamiltonian operator for the one-dimensional Morse oscillator is

$$H_{\mathrm{M}} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + D_{\mathrm{e}}(1 - \mathrm{e}^{-\alpha x})^2 \tag{1}$$

where D_{e} represents the depth of the potential well and α is the range parameter. Transforming to the dimensionless coordinate q defined by

$$q = (m\omega_{\mathrm{e}}/\hbar)^{1/2}x \tag{2}$$

where the vibrational frequency ω_e is defined by

$$\omega_e = (2D_e/m)^{1/2}\alpha \tag{3}$$

we have

$$\frac{H_M}{\hbar\omega_e} = \frac{1}{2}\left(-\frac{d^2}{dq^2} + \frac{1}{2x_e}(1 - e^{-\sqrt{2x_e}q})^2\right) \tag{4}$$

where the anharmonicity constant x_e is defined by

$$x_e = \hbar\omega_e/4D_e. \tag{5}$$

It has been shown (Cooper 1987) that $\sqrt{x_e}$ forms a natural perturbational parameter for the Morse oscillator problem. Note that the harmonic limit is regained as $x_e \to 0$, when H_M reduces to the harmonic oscillator Hamiltonian H_0, given by

$$\frac{H_0}{\hbar\omega_e} = \frac{1}{2}\left(-\frac{d^2}{dq^2} + q^2\right). \tag{6}$$

*In order to relate to the operator (or algebraic) formulation of the simple har-*monic oscillator, we express the Hamiltonian for the Morse oscillator in factorized form through the introduction of appropriate annihilation and creation operators such that (in units of $\hbar\omega_e$)

$$A^\dagger A|v\rangle = \Delta E_{v0}|v\rangle \tag{7}$$

where the energy zero is chosen as the ground vibrational level and the annihilation and creation operators for the Morse oscillator are defined as follows:

$$A = \frac{1}{\sqrt{2}}\left(\frac{d}{dq} + \frac{1}{\sqrt{2x_e}}(1 - e^{-\sqrt{2x_e}q}) - \sqrt{\frac{x_e}{2}}\right) \tag{8}$$

$$A^\dagger = \frac{1}{\sqrt{2}}\left(-\frac{d}{dq} + \frac{1}{\sqrt{2x_e}}(1 - e^{-\sqrt{2x_e}q}) - \sqrt{\frac{x_e}{2}}\right). \tag{9}$$

The annihilation operator A has been chosen so that it annihilates the ground state, namely

$$A|0\rangle \equiv 0. \tag{10}$$

The energy eigenvalues of bound states of the Morse oscillator Hamiltonian (in units of $\hbar\omega_e$) are given by

$$E_v = (v + \tfrac{1}{2}) - (v + \tfrac{1}{2})^2 x_e \tag{11}$$

so that

$$\Delta E_{v0} = E_v - E_0 = v(1 - (v + 1)x_e). \tag{12}$$

It is a straightforward matter to demonstrate that these relations reduce to those for the harmonic oscillator (as summarized in the appendix) in the limit $x_e \to 0$. Note that the energy eigenvalues include the parameter $\sqrt{x_e}$ only as its square, and this is reflected in the perturbational expansion which yields the correct energy eigenvalues at second order (Cooper 1987) in a perturbational expansion using $\sqrt{x_e}$ as perturbational parameter.

The ground-state eigenfunction ψ_0 for the Morse oscillator is obtained by solving equation (10), expressed in the form

$$\left(\frac{d}{dq} - \frac{1}{\sqrt{2x_e}} e^{-\sqrt{2x_e}q} + \frac{1}{\sqrt{2x_e}}(1 - x_e)\right)\psi_0 = 0. \tag{13}$$

Hence

$$\psi_0 = \exp\left(-\frac{1}{2x_e} e^{-\sqrt{2x_e}q}\right) \exp\left(-\frac{1}{\sqrt{2x_e}}(1 - x_e)q\right). \tag{14}$$

In the limit $x_e \to 0$, this reduces (to within a multiplicative constant) to the ground-state wavefunction of the harmonic oscillator, i.e.

$$\psi_0 \xrightarrow{(x_e \to 0)} e^{-q^2/2} \tag{15}$$

Hence the Morse oscillator problem has been formulated algebraically in a manner which closely resembles that of the harmonic oscillator, and to which it reduces in the limit of zero anharmonicity constant. This provides us with a suitable starting point for consideration of coherent states for the Morse oscillator.

3. Morse oscillator coherent states

The formulation of the Morse oscillator problem outlined in section 2 may be used to determine coherent states of the Morse oscillator using methods which have been previously applied in the case of the harmonic oscillator (Carruthers and Nieto 1965). Of the three approaches which have been applied in the harmonic oscillator case, namely the construction of states which minimize the uncertainty relation, which are eigenvalues of the annihilation operator and which are generated by action of a unitary displacement operator, only the first two can be applied directly to the Morse oscillator since the final method relies on a form for the displacement operator which is specific to the harmonic oscillator. The results of the present analysis will also be compared with those generated by the group theoretical approach to coherent states (Perelomov 1972, 1986).

3.1. Minimum uncertainty coherent states

Given two Hermitian operators X and P, which obey the relation $[X, P] = \mathrm{i}G$, where $\langle G\rangle \geqslant 0$, states ψ_{cs} which minimize the generalized uncertainty relation

$$(\Delta X)^2(\Delta P)^2/\langle G\rangle^2 \geqslant \tfrac{1}{4}. \tag{16}$$

are solutions of the equation (Nieto and Simmons 1979b)

$$\left(X + \mathrm{i}P\frac{\Delta X}{\Delta P}\right)\psi_{\mathrm{cs}} = \left(\langle X\rangle + \mathrm{i}\langle P\rangle\frac{\Delta X}{\Delta P}\right)\psi_{\mathrm{cs}} \tag{17}$$

where $(\Delta X)^2 = \langle X^2\rangle - \langle X\rangle^2$, etc. The uncertainty relation, equation (16), reduces the number of independent parameters by one, and another may be eliminated by requiring that the ground state be included in the set. The remaining two parameters can then be incorporated into a complex number α.

For the Morse oscillator, it is convenient to choose $X = Q$ and $P = -\mathrm{i}\,\mathrm{d}/\mathrm{d}q$, so that we have

$$\left(Q + \lambda\frac{\mathrm{d}}{\mathrm{d}q}\right)\psi_\alpha = \left(\langle Q\rangle + \lambda\left\langle\frac{\mathrm{d}}{\mathrm{d}q}\right\rangle\right)\psi_\alpha \equiv \sqrt{2}\alpha\psi_\alpha \tag{18}$$

where λ is defined in such a way that the ground state ψ_0 is contained in the set.

The coordinate Q is defined by

$$Q = \frac{1}{\sqrt{2x_{\mathrm{e}}}}\mathrm{e}^{-\sqrt{2x_{\mathrm{e}}}q} + \frac{1}{\sqrt{2x_{\mathrm{e}}}}(1 - x_{\mathrm{e}}) \tag{19}$$

which is, to within a constant, the so-called Morse coordinate $(1 - \mathrm{e}^{-\sqrt{2x_{\mathrm{e}}}q})/\sqrt{2x_{\mathrm{e}}}$.

The solution of equation (18) is

$$\psi_\alpha = \exp\left(-\frac{1}{2x_{\mathrm{e}}\lambda}\mathrm{e}^{-\sqrt{2x_{\mathrm{e}}}q}\right)\exp\left[\frac{q}{\lambda}\left(\sqrt{2}\alpha - \frac{1}{\sqrt{2x_{\mathrm{e}}}}(1 - x_{\mathrm{e}})\right)\right]. \tag{20}$$

For $\lambda = 1$, we have

$$\psi_\alpha = \exp\left[-\frac{1}{2x_{\mathrm{e}}}\mathrm{e}^{-\sqrt{2x_{\mathrm{e}}}q}\right]\exp(\sqrt{2}\alpha q)\exp\left[-\frac{1}{\sqrt{2x_{\mathrm{e}}}}(1 - x_{\mathrm{e}})q\right] \equiv \mathrm{e}^{\sqrt{2}\alpha q}\psi_0 \tag{21}$$

showing that the ground state ψ_0 is included as the special case $\alpha = 0$.

Since, from equation (8),

$$A \equiv \frac{1}{\sqrt{2}}\left(Q + \frac{\mathrm{d}}{\mathrm{d}q}\right)$$

then, using equation (16) with $\lambda = 1$,

$$A\psi_\alpha = \alpha\psi_\alpha \equiv \frac{1}{\sqrt{2}}\left(\langle Q\rangle + \left\langle\frac{\mathrm{d}}{\mathrm{d}q}\right\rangle\right)\psi_\alpha. \tag{22}$$

Hence the minimum uncertainty coherent states for the Morse oscillator are also eigenstates of the annihilation operator.

We can confirm that these states are indeed minimum uncertainty states by proving that

$$(\Delta Q)^2(\Delta p)^2 = \langle G\rangle^2/4 \tag{23}$$

From the definition of Q, we have

$$[Q,p] = \mathrm{i}\mathrm{e}^{-\sqrt{2x_e}q} \tag{24}$$

so that, in this case,

$$G \equiv \mathrm{e}^{-\sqrt{2x_e}q} = [A, A^\dagger] = 1 - x_e - \sqrt{x_e}(A + A^\dagger). \tag{25}$$

Hence, since $|\alpha\rangle$ is an eigenstate of the operator A with eigenvalue $\alpha/\sqrt{2}$,

$$\langle Q\rangle = \frac{1}{\sqrt{2}}\langle A + A^\dagger\rangle = \frac{1}{\sqrt{2}}(\alpha + \alpha^*) \tag{26}$$

$$\langle p\rangle = \frac{-\mathrm{i}}{\sqrt{2}}\langle A - A^\dagger\rangle = \frac{-\mathrm{i}}{\sqrt{2}}(\alpha - \alpha^*) \tag{27}$$

$$\langle Q^2\rangle = \tfrac{1}{4}(\alpha + \alpha^*) + \tfrac{1}{2}[1 - x_e - \sqrt{x_e/2}(\alpha + \alpha^*)] \tag{28}$$

$$\langle p^2\rangle = \tfrac{1}{4}(\alpha - \alpha^*) - \tfrac{1}{2}[1 - x_e - \sqrt{x_e/2}(\alpha + \alpha^*)]. \tag{29}$$

Then

$$(\Delta Q)^2 \equiv \langle Q^2\rangle - \langle Q\rangle^2 = \tfrac{1}{2}[1 - x_e - \sqrt{x_e/2}(\alpha + \alpha^*)] \tag{30}$$

$$(\Delta p)^2 \equiv \langle p^2\rangle - \langle p\rangle^2 = \tfrac{1}{2}[1 - x_e - \sqrt{x_e/2}(\alpha + \alpha^*)]. \tag{31}$$

Equation (23) is immediately seen to be valid since

$$(\Delta Q)^2(\Delta p)^2 = \tfrac{1}{4}[1 - x_e - \sqrt{x_e/2}(\alpha + \alpha^*)]^2 \equiv \langle G\rangle^2/4 \tag{32}$$

where we have used equation (25) to evaluate G.

3.2. Approximate Morse oscillator coherent states

Approximate coherent states for the Morse oscillator have been generated by Nieto and Simmons (1979a) and by Kais and Levine (1990). The former express the Morse Hamiltonian in terms of transformed position and momentum variables which allow the Morse oscillator to resemble an harmonic oscillator, whereas the latter use the Perelomov (1972, 1986) definition of generalized coherent states within a group theoretical framework. In both cases the results, which are essentially equivalent (Kais and Levine 1990), are valid in the limit of a deep potential well. This corresponds in the present formulation to small values of the anharmonicity constant. These states were constructed in such a way that they would maximize their coherence as a function of time, at least for the low-lying states.

Since the minimum coherent states are given by equation (21), such that

$$\psi_\alpha = \mathrm{e}^{\sqrt{2}\alpha q}\psi_0 \tag{33}$$

we can try to re-express this result in an approximate form which is valid in the limit of small values of the anharmonicity constant.

Since

$$Q = \frac{1}{\sqrt{2x_e}}(1 - x_e - e^{-\sqrt{2x_e}q}) \tag{34}$$

we have

$$q = -\frac{1}{\sqrt{2x_e}} \ln[1 - (\sqrt{2x_e}Q + x_e)] \simeq Q + (x_e/2)^{1/2} \tag{35}$$

in the limit of small x_e. Dropping the constant term, which can be incorporated into the normalization constant, we find

$$\psi_\alpha \simeq e^{\sqrt{2}\alpha Q}\psi_0 = \exp\left[-\frac{1}{2x_e}(1 + 2\sqrt{x_e}\alpha)e^{-\sqrt{2x_e}q}\right] \exp\left[-\frac{1}{\sqrt{2x_e}}(1 - x_e)q\right]. \tag{36}$$

This is to be compared with the approximate result of Nieto and Simmons (1979) and Kais and Levine (1990), in the form

$$\psi_{cs} \simeq e^{-(\lambda-1/2)z} e^{-Ce^{-z}} \tag{37}$$

where C is a complex number, $z \equiv \sqrt{2x_e}q$ and $\lambda \equiv 1/2x_e$. The results are seen to be equivalent with the identification $C = 1 + 2\sqrt{x_e}\alpha$.

Since $Q = (A + A^\dagger)/\sqrt{2}$, it is proposed that a corresponding operator relation, analogous to equation (A11), would be

$$|\alpha\rangle = e^{\alpha(A+A^\dagger)}|0\rangle \tag{38}$$

where the operators and states refer to the Morse oscillator rather than to the harmonic oscillator. However, there is a complication since A and $A^\dagger$ are not only non-commutative, but also the commutators of A and $A^\dagger$ with $[A, A^\dagger]$ are themselves non-commuting. This prevents the use of the Baker–Campbell–Hausdorff (BCH) identity in its usual form.

However, we can derive a related relationship, by exploiting the fact that the sum $(A + A^\dagger)$ does commute with the commutator $[A, A^\dagger]$ (cf equation (25)). We shall use a variant of the proof of the original BCH theorem given in Liouisell.

Let

$$f(\alpha) = e^{\alpha A^\dagger} e^{\alpha A}$$

Then

$$\frac{df}{d\alpha} = (A^\dagger + e^{\alpha A^\dagger} a e^{-\alpha A^\dagger}) f(\alpha)$$

where

$$\begin{aligned} e^{\alpha A^\dagger} A e^{-\alpha A^\dagger} &= A + \alpha[A^\dagger, A] + \alpha^2/2\sqrt{x_e}[A^\dagger, A] + \cdots \\ &= A + g(\alpha)[A^\dagger, A]. \end{aligned}$$

Hence

$$\frac{\mathrm{d}f}{\mathrm{d}\alpha} = (A^\dagger + A) + g(\alpha)[A^\dagger, A].$$

We can integrate this equation since $(A^\dagger + A)$ commutes with $[A^\dagger, A]$, to yield

$$f(\alpha) = \exp(\alpha(A^\dagger + A) + h(\alpha)[A^\dagger, A])$$

where

$$h(\alpha) = \int g(\alpha)\,\mathrm{d}\alpha = \alpha^2/2 + \alpha^3\sqrt{x_e}/6 + \cdots.$$

Since

$$[A^\dagger, A] = -(1 - x_e) + \sqrt{x_e}(A + A^\dagger)$$

we have

$$\mathrm{e}^{(\alpha+\sqrt{x_e}h(\alpha))(A^\dagger+A)} = \mathrm{e}^{h(\alpha)(1-x_e)}\mathrm{e}^{\alpha A^\dagger}\mathrm{e}^{\alpha A}.$$

Hence

$$\mathrm{e}^{(\alpha+\sqrt{x_e}h(\alpha))(A^\dagger+A)}|0\rangle = \mathrm{e}^{h(\alpha)(1-x_e)}\mathrm{e}^{\alpha A^\dagger}|0\rangle. \tag{39}$$

In the harmonic limit, $x_e \to 0$, this gives the corresponding relation

$$\mathrm{e}^{\alpha(a^\dagger+a)}|0\rangle = \mathrm{e}^{\alpha^2/2}\mathrm{e}^{\alpha a^\dagger}\mathrm{e}^{\alpha a}|0\rangle = \mathrm{e}^{\alpha^2/2}\mathrm{e}^{\alpha a^\dagger}|0\rangle \tag{40}$$

which is the harmonic oscillator result, equation (A14). (Note that $A \to a$ and $A^\dagger \to a^\dagger$ in the harmonic limit.)

We now consider the effect of the annihilation operator A for the Morse oscillator on the approximate coherent state defined by equation (36). Since

$$\frac{\mathrm{d}}{\mathrm{d}q}\psi_{cs} = -Q\psi_{cs} + \alpha \mathrm{e}^{-\sqrt{2x_e}q}\psi_{cs} \tag{41}$$

and

$$\mathrm{e}^{-\sqrt{2x_e}q} = [A, A^\dagger] \equiv 1 - x_e - \sqrt{x_e}(A + A^\dagger)$$

then

$$[A + \alpha\sqrt{x_e}(A + A^\dagger)]\psi_{cs} = \alpha(1 - x_e)\psi_{cs}. \tag{42}$$

The *approximate* coherent state is only an eigenstate of the annihilation operator A when $\alpha = 0$ and in the harmonic limit when $x_e \to 0$.

The approximate coherent state was defined in such a way that it would retain its coherence in time as far as possible, whereas this is not the case with the minimum uncertainty coherent states. It is worth noting, however, that these latter states, defined by equation (33), do reduce to the harmonic oscillator coherent states, defined by equation (A10), in the limit $x_e \to 0$, when the ground state of the Morse oscillator reduces to that of the harmonic oscillator. These harmonic oscillator coherent states do retain their coherence as a function of time, so the minimum uncertainty coherent states for the Morse oscillator should retain to some extent their coherence in time, particularly for low-lying states in the limit of large well depth.

3.3. Displacement operator coherent states

As noted by Nieto and Simmons (1979b), displacement operator coherent states are not necessarily the same as minimum uncertainty coherent states in the case of general potentials. The displacement operator $D(\alpha)$ given by

$$D(\alpha) = \mathrm{e}^{\alpha a^\dagger - \alpha^* a} \tag{43}$$

is appropriate for the harmonic oscillator, where, as shown in the appendix,

$$|\alpha\rangle = D(\alpha)|0\rangle$$

in the harmonic case.

In the Morse oscillator case, we are still free to consider the effect of the operator $D(\alpha)$ on $|0\rangle$, but, since

$$[\alpha A^\dagger - \alpha^* A, [A, A^\dagger]] \neq 0$$

we cannot determine its effect by use of the simple operator treatment discussed earlier. However, we note that if α is chosen to be purely imaginary, then

$$D(\alpha) \equiv \mathrm{e}^{\alpha(A^\dagger + A)} \tag{44}$$

which is precisely the operator relation proposed earlier for approximate coherent states.

In these approximate coherent state formulae, we need to operate with powers of $A^\dagger$ on the ground state of the Morse oscillator. It is a simple matter to show that

$$A^\dagger|0\rangle = \sqrt{2}Q|0\rangle \tag{45}$$

whereas, in the harmonic limit,

$$a^\dagger|0\rangle = \sqrt{2}q|0\rangle$$

which corresponds to the first excited vibrational state of the harmonic oscillator, in accord with the harmonic oscillator relation $a^\dagger|0\rangle = |1\rangle$. Note that the effect of $A^\dagger$ on ψ_0 is to produce a function which is *not* an eigenstate of the Morse oscillator, although it correctly reduces to an eigenstate of the harmonic oscillator in the limit $x_\mathrm{e} \to 0$.

Using the methods of supersymmetric quantum mechanics, it can be shown (Cooper, in preparation) that the set of ground states of the Morse potential and its various supersymmetric partner potentials are eigenstates of the annihilation operator corresponding to real eigenvalues such that

$$A|0(n)\rangle = n\sqrt{2x_\mathrm{e}}|0(n)\rangle \tag{46}$$

where

$$|0(n)\rangle = \mathrm{e}^{n\sqrt{2x_\mathrm{e}}q}|0\rangle \tag{47}$$

corresponds to the ground state of the nth shifted Morse potential.

These partner potentials each have the same energy spectrum except that there is one less bound state as one progresses along the series. The effect of the operator $A^\dagger$ on any ground state is to generate the first excited state of a shifted Morse potential with an additional bound state, there being no change in energy.

3.4. Linearly forced Morse oscillator

The linearly forced harmonic oscillator provided an early illustration of the use of the coherent state concept (Carruthers and Nieto 1965). The linearly forced Morse oscillator has been the subject of considerable interest, both numerically (Walker and Preston 1977) and analytically (Nieto and Simmons 1979a, Levine 1982,1985).

The coherent states of the harmonic oscillator remain coherent for unperturbed and linearly perturbed motion, the latter effect arising from the fact that the Hamiltonian, although quadratic in the annihilation and creation operators, forms a closed set with them and the identity operator. This does not occur in the case of the Morse oscillator, even though the Hamiltonian retains its quadratic form. Higher terms arise in the operation of the Hamiltonian on the annihilation and creation operators. In consequence, dephasing will occur from the initially coherent ground state of the Morse oscillator. This effect has been demonstrated most effectively in the numerical studies of Walker and Preston (1977).

4. Concluding remarks

We have demonstated that coherent states for the Morse oscillator may be obtained by a simple algebraic procedure which is based on an extension of the well known approach used in the case of the harmonic oscillator and is based on a formulation of the Morse oscillator problem which involves the explicit introduction of an anharmonicity constant into the Hamiltonian. The resultant states represent both minimum uncertainty coherent states and annihilation operator coherent states, where the annihilation operator is chosen to annihilate the ground state of the Morse oscillator. In the limit of small anharmonicity parameter (or, equivalently, in the limit of large well depth), the Morse oscillator coherent states have been shown to reduce to the approximate coherent states constructed independently via a generalized displacement operator associated with an appropriate invariance group. However, only in this limit of large well depth do the Morse oscillator minimum uncertainty coherent states retain approximate coherence as a function of time.

Appendix. Harmonic oscillator coherent states

Here, we shall summarize the main results concerning coherent states for the harmonic oscillator (see, for example, Nieto and Simmons (1979b)) to assist comparison with the corresponding relations for the anharmonic Morse oscillator. The harmonic oscillator eigenvalue problem may be expressed in dimensionless variables in the form

$$\left[\frac{1}{2}\left(-\frac{\mathrm{d}^2}{\mathrm{d}q^2}+q^2\right)-\frac{1}{2}\right]\psi_n = n\psi_n \tag{A1}$$

where $n = 0, 1, 2, \ldots$. This may be written equivalently as the operator equation

$$a^\dagger a|n\rangle = n|n\rangle \tag{A2}$$

where the annihilation (a) and creation ($a^\dagger$) operators are defined by

$$a = \frac{1}{\sqrt{2}}\left(\frac{\mathrm{d}}{\mathrm{d}q} + q\right) \tag{A3}$$

$$a^\dagger = \frac{1}{\sqrt{2}}\left(-\frac{\mathrm{d}}{\mathrm{d}q} + q\right) \tag{A4}$$

such that

$$[a, a^\dagger] = 1. \tag{A5}$$

Since the operator a annihilates the ground state $|0\rangle$, the ground-state wavefunction ψ_0 satisfies the relation

$$\left(\frac{\mathrm{d}}{\mathrm{d}q} + q\right)\psi_0 = 0 \tag{A6}$$

so that

$$\psi_0 = \mathrm{e}^{-(1/2)q^2} \tag{A7}$$

to within a constant of normalization.

Coherent states, which approximate the motion of a classical particle, and so are localized, may be defined in a number of ways, all of which are equivalent in the case of the harmonic oscillator.

A.1. Annihilation operator coherent states

Eigenstates of the annihilation operator a are

$$a|\alpha\rangle = \alpha|\alpha\rangle \tag{A8}$$

so that

$$\frac{1}{\sqrt{2}}\left(\frac{\mathrm{d}}{\mathrm{d}q} + q\right)\psi_\alpha = \alpha\psi_\alpha. \tag{A9}$$

The solution of this equation can be written in the form

$$\psi_\alpha = \mathrm{e}^{\sqrt{2}\alpha q}\mathrm{e}^{-(1/2)q^2} \equiv \mathrm{e}^{\sqrt{2}\alpha q}\psi_0. \tag{A10}$$

This result suggests the operational definition

$$|\alpha\rangle = \mathrm{e}^{\alpha(a+a^\dagger)}|0\rangle \tag{A11}$$

since

$$q = \frac{1}{\sqrt{2}}(a + a^\dagger). \tag{A12}$$

Using the well known BCH identity (Louisell, 1973),

$$e^{A+B} = e^{B}e^{A}e^{\frac{1}{2}[A,B]} \tag{A13}$$

for two Hermitian operators A and B, each of which commute with the commutator $[A, B]$, we have

$$|\alpha\rangle = e^{\alpha a^{\dagger}}e^{\alpha a}e^{(\alpha^{2}/2)[a,a^{\dagger}]}|0\rangle = e^{\alpha^{2}/2}e^{\alpha a^{\dagger}}|0\rangle \tag{A14}$$

where we have used the fact that $a|0\rangle \equiv 0$.

Leaving aside the constant term which can be incorporated into the normalization factor, we have

$$|\alpha\rangle = e^{\alpha(a+a^{\dagger})}|0\rangle \sim e^{\alpha a^{\dagger}}|0\rangle. \tag{A15}$$

In order to determine the normalization factor, we use the relation

$$a^{\dagger}|n\rangle = \sqrt{(n+1)}|n+1\rangle \tag{A16}$$

and expand the exponential to give

$$\begin{aligned} e^{\alpha a^{\dagger}}|0\rangle &= \left(|0\rangle + \alpha|1\rangle + \frac{\alpha^{2}}{\sqrt{2}}|2\rangle + \cdots\right) \\ &= \sum_{n=0}^{\infty} \frac{\alpha^{n}}{\sqrt{n!}}|n\rangle. \end{aligned} \tag{A18}$$

Since the eigenstates are orthonormal, we have

$$\langle\alpha|\alpha\rangle = \sum_{n=0}^{\infty} \frac{(\alpha\alpha^{*})^{n}}{n!} \equiv e^{|\alpha|^{2}} \tag{A19}$$

so that normalized coherent states are given by

$$|\alpha\rangle = e^{-|\alpha|^{2}/2}e^{\alpha a^{\dagger}}|0\rangle \tag{A20}$$

A.2. Displacement operator coherent states

These states are defined by the operation of the unitary displacement operator

$$D(\alpha) = e^{\alpha a^{\dagger} - \alpha^{*}a} \tag{A21}$$

on the ground state $|0\rangle$, where the operator is chosen so that

$$D^{\dagger}(\alpha)aD(\alpha) = a + \alpha. \tag{A22}$$

Note that this particular form of D is specific to the harmonic oscillator problem (Nieto and Simmons 1979b). Then

$$D(\alpha)|0\rangle = e^{\alpha a^{\dagger} - \alpha^{*}a}|0\rangle = e^{-|\alpha|^{2}/2}e^{\alpha a^{\dagger}}|0\rangle \tag{A23}$$

as given in equation (A20).

A.3. Minimum uncertainty coherent states

For $X = q$ and $P = -\mathrm{i}\,\mathrm{d}/\mathrm{d}q$, we have

$$\left(q + \lambda \frac{\mathrm{d}}{\mathrm{d}q}\right) \psi_{\mathrm{cs}} = \sqrt{2}\psi_{\mathrm{cs}} \tag{A24}$$

with solution

$$\psi_{\mathrm{cs}} = \mathrm{e}^{-q^2/2\lambda} \mathrm{e}^{\sqrt{2}\alpha q/\lambda} \tag{A25}$$

The ground state is included if $\lambda = 1$, when equation (A24) becomes

$$\left(\frac{\mathrm{d}}{\mathrm{d}q} + q\right) \psi_{\mathrm{cs}} = \sqrt{2}\alpha\psi_{\mathrm{cs}} \tag{A26}$$

which corresponds to the eigenvalue relation $a|\alpha\rangle = \alpha|\alpha\rangle$ in A.2.

References

Carruthers P and Nieto M M 1965 *Am. J. Phys.* **33** 537
Cooper I L 1987 *Chem. Phys.* **112** 67
Gerry G C 1986 *Phys. Rev.* A **33** 2207
Kais S and Levine R D 1990 *Phys. Rev.* A **41** 2301
Levine R D 1982 *Chem. Phys. Lett.* **95** 87
—— 1985 *J. Phys. Chem.* **89** 2122
Louisell W H 1973 *Quantum Statistical Properties of Radiation* (New York: Wiley)
Morse P M 1929 *Phys. Rev.* **34** 1929
Nieto M M and Simmons L M Jr 1979 *Phys. Rev.* A **19** 438
—— 1979 *Phys. Rev.* D **20** 1321
Perelomov A 1972 *Commun. Math. Phys.* **26** 222
—— 1986 *Generalized Coherent States* (Berlin: Springer)
Walker R B and Preston R K 1977 *J. Chem. Phys.* **67** 2017
Zhang W-M, Feng D H and Gilmore R 1990 *Rev. Mod. Phys.* **62** 867