Eigenstates, coherent states, and uncertainty products for the Morse oscillator

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We obtain the exact, normalized, closed-form eigenfunctions for the one-dimensional Morse oscillator, as well as the raising and lowering operators. We next review a new method for obtaining the coherent states for arbitrary potentials, it being based on the classical motion of a particle. We apply this method to the Morse oscillator. After demonstrating that in the appropriate limit our results reduce to those for the harmonic oscillator, we obtain analytic insights into published numerical results on uncertainty products for Morse-oscillator wave packets.

I. INTRODUCTION

In 1929, Morse[1] first introduced the potential[1,2]

$$V(r)=U_0(1-e^{-ar})^2 \tag{1.1}$$

as a useful model for diatomic molecules. For this potential, the Schrödinger equation is only approximately solvable.[3,4] For the one-dimensional analog, however, the problem turns out to be exactly solvable,[5] although to our knowledge exact, normalized eigenfunctions have not been given. The energy levels and wave functions for the $L=0$, three-dimensional case and the one-dimensional case differ because $0\leq r<\infty$, whereas $-\infty < x <\infty$.

Studies of anharmonic potential systems are of current interest as possible models for the interaction of coherent radiation with molecules. In particular, the numerical studies by Walker and Preston[6] of the one-dimensional Morse oscillator produced some interesting results. For example, a forced Morse oscillator diffuses from a near minimum uncertainty-product ground-state wave packet and then evolves back into a near minimum uncertainty state. Standardly, numerical calculations of this sort are done in a harmonic-oscillator basis. However, a clearer view of the situation can result if a more natural basis is used.

In Sec. II of this paper we obtain the exact, normalized, closed-form eigenfunctions for the one-dimensional Morse oscillator, and the raising and lowering operators. Having the natural basis, in Sec. III we review a new method[7] (based on the classical motion of a particle) which yields the coherent states for general potentials. This method is applied to the Morse potential in Sec. IV, to yield in closed form the normalized "approximate" coherent states. (The sense in which these states approximate the true coherent states is explained.) In Sec. V we first demonstrate that all our results reduce to those for the harmonic oscillator in an appropriate limit. Then we use our approximate coherent states to obtain analytical insights into the numerical results of Walker and Preston[6] on uncertainty relations for wave packets in the Morse oscillator.

II. EIGENSTATES

The eigenfunctions for the one-dimensional Morse oscillator are usually written in terms of unnormalized, confluent hypergeometric functions. However, as we now show, they can more conveniently (and in normalized form) be written in terms of associated Laguerre polynomials.

We choose the coordinate system so that the minimum of the potential is at the origin. Then all energies are positive and the harmonic oscillator limit emerges more naturally. The potential is now

$$V(x)=U_0(1-e^{-z})^2, \quad z\equiv ax, \tag{2.1}$$

$$U_0=\lambda^2\mathcal{E}_0, \quad \mathcal{E}_0\equiv\hbar^2a^2/2m\,. \tag{2.2}$$

If we write the eigenenergies as

$$E_n=\mathcal{E}_0\epsilon_n, \tag{2.3}$$

then the Schrödinger equation becomes

$$\left(\frac{d^2}{dz^2}+\epsilon_n-\lambda^2(1-e^{-z})^2\right)\psi_n=0\,. \tag{2.4}$$

The change of variables

$$y=2\lambda e^{-z} \tag{2.5}$$

yields

$$\left(\frac{d^2}{dy^2}+\frac{1}{y}\frac{d}{dy}+\frac{\epsilon_n-\lambda^2}{y^2}+\frac{\lambda}{y}-\frac{1}{4}\right)\psi_n=0\,. \tag{2.6}$$

Extracting the $y\to\infty$ and $y\to 0$ behavior by the substitution

$$\psi_n=e^{-y/2}y^s u_n(y)\,, \tag{2.7}$$

where $s^2=\epsilon_n-\lambda^2$, we obtain

$$\left(y\frac{d^2}{dy^2}+(2s+1-y)\frac{d}{dy}+(\lambda-s-\tfrac{1}{2})\right)u_n(y)=0. \quad (2.8)$$

This is Laguerre's equation, which has polynomial solutions for $\lambda-s-\frac{1}{2}=n=0,\ 1,\ 2,\ldots,$

$$u_n(y)=L_n^{(2\lambda-2n-1)}(y)\ . \quad (2.9)$$

[The general solution of Laguerre's equation (2.8) has unacceptable asymptotic behavior,[8]

$$u(y)\sim[\Gamma(2s+1)/\Gamma(s+\tfrac{1}{2}-\lambda)]e^y y^{-\lambda-s-1/2}$$

as $y\to+\infty$. See Equation 6.13.1 (3) of Erdélyi *et al.*[8]] Thus

$$\psi_n(x)=N(n,\lambda)\,y^{\lambda-1/2-n}e^{-y/2}L_n^{(2\lambda-2n-1)}(y)\,,$$

$$0\le n\le[\lambda-\tfrac{1}{2}] \quad (2.10)$$

$$E_n=\mathcal{E}_0[2\lambda(n+\tfrac{1}{2})-(n+\tfrac{1}{2})^2]>0. \quad (2.11)$$

The normalization constant $N(n,\lambda)$ is determined below.

The above associated Laguerre polynomials are defined by

$$L_n^{(\alpha)}(t)=\sum_{j=0}^{n}\binom{n+\alpha}{n-j}\frac{(-t)^j}{j!}\ . \quad (2.12)$$

This is the standard definition in the mathematical literature, in most books on special functions,[8] and integral tables.[9] The Laguerre polynomials $L_n^{\alpha}(t)$ which often occur in Coulomb wave functions in quantum mechanics texts[10] are different (although related) objects. Up to a phase, they are $L_n^{\alpha}(t)=n!\ L_{n-\alpha}^{(\alpha)}(t)$.

To obtain the normalization, we first prove the result

$$J_{n,\alpha}^{(\beta)}=\int_0^\infty e^{-t}\,t^{\alpha+\beta}[L_n^{(\alpha)}(t)]^2\,dt$$

$$=\frac{\Gamma(\alpha+n+1)}{\Gamma(n+1)}\sum_{k=0}^{n}(-1)^k\,\frac{\Gamma(n-k-\beta)}{\Gamma(-k-\beta)}\,\frac{\Gamma(\alpha+k+1+\beta)}{\Gamma(\alpha+k+1)}\,\frac{1}{\Gamma(k+1)\Gamma(n-k+1)}\ ,\quad \mathrm{Re}(\alpha+\beta+1)>0. \quad (2.13)$$

This is a generalization of known Coulomb integrals[10,11] to noninteger α and β. To show it, write one $L_n^{(\alpha)}(t)$ in the integrand as the power series (2.12) and then use Eq. (7.414.11) of Ref. 9. The normalization constant in Eq. (2.10) is obtained from the special case $J_{n,2\lambda-2n-1}^{(-1)}$:

$$N(n,\lambda)=\left(\frac{a(2\lambda-2n-1)\Gamma(n+1)}{\Gamma(2\lambda-n)}\right)^{1/2}. \quad (2.14)$$

For later use we give the raising and lowering operators:

$$A_n^{\pm}=\frac{1}{2\lambda}\left((\lambda-n-\tfrac{1}{2})e^z\mp e^z\frac{d}{dz}-\frac{\lambda^2}{\lambda-(n+\frac{1}{2})\mp\frac{1}{2}}\right) \quad (2.15)$$

$$=\left(\frac{(\lambda-n-\frac{1}{2})}{y}\pm\frac{d}{dy}-\frac{\lambda}{2[\lambda-(n+\frac{1}{2})\mp\frac{1}{2}]}\right). \quad (2.16)$$

When these are applied to the normalized eigenstates one obtains

$$A_n^{\pm}\psi_n=\frac{(2\lambda-2n-1)}{4\lambda}\,D(n-\tfrac{1}{2}\pm\tfrac{1}{2},\lambda)\,\psi_{n\pm1}\ , \quad (2.17)$$

$$D(n,\lambda)=\frac{4\lambda}{(2\lambda-2n-2)}\left(\frac{(n+1)(2\lambda-n-1)}{(2\lambda-2n-1)(2\lambda-2n-3}\right)^{1/2}. \quad (2.18)$$

We derived the $A_n^{\pm}$ by appropriately modifying the Infeld and Hull[12] l raising and lowering operators for their Coulomb eigenfunctions. However, the reader can most easily verify them by applying them to (2.10), and seeing that they reduce to the recurrence relations

$$(n+1)(n+\alpha)L_{n+1}^{(\alpha-2)}(y)=[\alpha(\alpha-1)-y(\alpha+n)]L_n^{(\alpha)}(y)+(\alpha-1)y\left[\frac{d}{dy}L_n^{(\alpha)}(y)\right], \quad (2.19)$$

$$yL_{n-1}^{(\alpha+2)}(y)=-nL_n^{(\alpha)}(y)-(\alpha+1)\left(\frac{d}{dy}L_n^{(\alpha)}(y)\right). \quad (2.20)$$

Equations (2.19) and (2.20) can in turn be obtained independently by combining the standard recurrence relations for the Laguerre polynomials given on p. 241 of Magnus *et al.*[8]

III. GENERAL COHERENT STATES

Elsewhere,[7] we have defined coherent states for general potentials. One first finds those natural variables of the classical bound-state motion which vary sinusoidally in time. Consider the classical Hamiltonian equation,

$$p_c^2/2m+V(x)=E. \quad (3.1)$$

For potentials with one confining region, there exist variables $X_c(x)$ and $P_c=m\dot{X}_c=(mX'(x)\dot{x})$ which are solutions of (3.1) and whose time variations are given by

$$X_c=A(E)\sin[\omega_c(E)t]\,, \quad (3.2)$$

$$P_c=mA(E)\omega_c(E)\cos[\omega_c(E)t]\,. \quad (3.3)$$

$X_c(x)$ is the solution of the equation

$$X_c' = \frac{d}{dx} X_c(x) = \omega_c \left(\frac{m(A^2 - X_c^2)}{2(E - V(x))} \right)^{1/2} . \tag{3.4}$$

Define the quantum operators

$$X = X_c(x) , \tag{3.5}$$

$$P = \tfrac{1}{2}[X_c' p + p X_c'] , \tag{3.6}$$

whose commutator is

$$[X, P] = iG . \tag{3.7}$$

Therefore there is a generalized uncertainty relation for X and P of the form

$$(\Delta X)^2 (\Delta P)^2 \geq \tfrac{1}{4} \langle G \rangle^2 . \tag{3.8}$$

Obtain those states which minimize this uncertainty relation.

It is well known[13] that these states satisfy either of the two equivalent eigenvalue equations

$$\left(\frac{X}{\Delta X} + i \frac{P}{\Delta P} \right) \psi_{CS} = \left(\frac{\langle X \rangle}{\Delta X} + i \frac{\langle P \rangle}{\Delta P} \right) \psi_{CS} , \tag{3.9}$$

$$\left(X + \frac{i \langle G \rangle}{2(\Delta P)^2} P \right) \psi_{CS} = \left(\langle X \rangle + \frac{i \langle G \rangle}{2(\Delta P)^2} \langle P \rangle \right) \psi_{CS} . \tag{3.10}$$

The four parameters $\langle X \rangle$, $\langle X^2 \rangle$, $\langle P \rangle$, and $\langle P^2 \rangle$ which appear here are not independent because of the constraint Eq. (3.8). The coherent states[7] are that two parameter subset of these minimum uncertainty states specified by a certain value of $\Delta X / \Delta P$. This value is chosen such that the ground state belongs to the set of coherent states.

Just as for the harmonic oscillator, one can express[7] the generalized position and momentum operators X and P in terms of raising and lowering operators. However, because energy levels are not in general equally spaced, the raising and lowering operators can be n dependent and $(A_n^+)^\dagger \neq (A_n^-)$. Thus the general representations of the operators X and P are of the more complicated forms

$$X = \tfrac{1}{4} K_1(n) \{ [A_n^- + (A_n^+)^\dagger] + [A_n^+ + (A_n^-)^\dagger] \} , \tag{3.11}$$

$$P = \frac{1}{4i} K_2(n) \{ [A_n^- + (A_n^+)^\dagger] - [A_n^+ + (A_n^-)^\dagger] \} , \tag{3.12}$$

where $K_1(n)$ and $K_2(n)$ are n-dependent c numbers.

In all of the examples treated previously[7] X_c was independent of the classical constant of the motion E. As Eq. (3.4) demonstrates, this is not generally true. If $X_c = X_c(x, E)$, to obtain the appropriate quantum operator X one must make the replacement $E \to H$, possibly allowing for a zero-point energy, and symmetrize. The Morse potential provides an example of this situation.

IV. MORSE-OSCILLATOR COHERENT STATES

A. Natural variables of the Morse oscillator

For the classical Morse oscillator potential of Eq. (2.1), the solutions are[14]

$$X_c(x, E) = e^{ax} - U_0/(U_0 - E) = A \sin \omega_c t , \tag{4.1}$$

$$P_c = m \dot{x} a e^{ax} = m \omega_c A \cos \omega_c t , \tag{4.2}$$

$$A = (U_0 E)^{1/2} / (U_0 - E) , \tag{4.3}$$

$$\omega_c = [2a^2 (U_0 - E)/m]^{1/2} , \tag{4.4}$$

with classical equations of motion

$$\dot{X}_c = P_c / m , \tag{4.5}$$

$$\dot{P}_c = -m \omega_c^2 X_c = -a^2 (U_0 - E) X_c . \tag{4.6}$$

The correct quantum operators are

$$X = e^z - \frac{U_0}{U_0 - H - \mathcal{E}_0/4} , \tag{4.7}$$

$$P = \frac{\hbar a^2}{2i} \left(e^z \frac{d}{dz} + \frac{d}{dz} e^z \right) . \tag{4.8}$$

In Eq. (4.7) we have inserted the zero-point energy $\mathcal{E}_0/4$. That this is correct can be seen by inserting the operators $A_n^\pm$ of Eq. (2.15) in Eqs. (3.11) and (3.12), with $K_1(n) = 2\lambda/(\lambda - n - \frac{1}{2})$ and $K_2(n) = 2\lambda \hbar a^2$. One obtains Eq. (4.7) for X [with H replaced by E_n of Eq. (2.11)], and Eq. (4.8) for P.

The quantum equations of motion are

$$\dot{X} = (-i/\hbar)[X, H] = P/m , \tag{4.9}$$

$$\dot{P} = (-i/\hbar)[P, H] = -a^2 (\{X, U_0 - H\} + \{e^z, -\mathcal{E}_0/4\}) , \tag{4.10}$$

which are the analogs of the classical equations of motion (4.5) and (4.6). The time-dependent operators $X(t)$ and $P(t)$ can also be calculated exactly. The results are

$$\begin{aligned} X(t) &= e^{iHt/\hbar} X e^{-iHt/\hbar} \\ &= X e^{-i\omega_0 t} \left[\cos \omega_H t + \frac{i}{2} \left(\frac{\mathcal{E}_0}{U_0 - H} \right)^{1/2} \sin \omega_H t \right] \\ &\quad + (P/\hbar a^2) e^{-i\omega_0 t} \left(\frac{\mathcal{E}_0}{U_0 - H} \right)^{1/2} \sin \omega_H t , \end{aligned} \tag{4.11}$$

$$\begin{aligned} P(t) &= P e^{-i\omega_0 t} \left[\cos \omega_H t - \frac{i}{2} \left(\frac{\mathcal{E}_0}{U_0 - H} \right)^{1/2} \sin \omega_H t \right] \\ &\quad - (\hbar a^2 X) e^{-i\omega_0 t} \left(\frac{U_0 - H - \mathcal{E}_0/4}{\mathcal{E}_0} \right) \left(\frac{\mathcal{E}_0}{U_0 - H} \right)^{1/2} \sin \omega_H t , \end{aligned} \tag{4.12}$$

where the zero-point angular velocity ω_0 and the quantum operator angular velocity ω_H (the analog to the classical ω_c) are

$$\omega_0 = \mathcal{E}_0/\hbar\,, \tag{4.13a}$$

$$\omega_H = \frac{2\mathcal{E}_0}{\hbar}\left(\frac{U_0 - H}{\mathcal{E}_0}\right)^{1/2} = \left(\frac{2a^2}{m}(U_0 - H)\right)^{1/2}. \tag{4.13b}$$

[It is not obvious that the right-hand sides of (4.11) and (4.12) are Hermitian. The calculation necessary to verify this property is explained at the end of this subsection.]

Equations (4.11)–(4.13) are obtained as follows.[15] Use the general expression

$$e^{+\lambda V} Q e^{-\lambda V} = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!}([V,\,)^n Q(\,])^n \equiv \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} Q_n\,, \tag{4.14}$$

where, in the iterated commutator Q_n, the symbol $(\ )^n$ means writing out the quantity enclosed in the parenthesis n times.

Specifically,

$$\begin{aligned} Q_0 &= Q,\\ Q_1 &= [V,Q],\\ Q_2 &= [V,[V,Q]],\\ &\cdot\\ &\cdot\\ &\cdot \end{aligned} \tag{4.15a}$$

and generally

$$Q_{n+1} = [V, Q_n]\,. \tag{4.15b}$$

From Eqs. (4.9) and (4.10), the iterated commutators for X and P can be evaluated recursively for X and P. The algebraic system composed of the operators X_n and P_n, $n = 0, 1, \ldots$, is spanned by the operators $X_0 = X$ and $X_1 = [h, X] \equiv [-H/\mathcal{E}_0 + \lambda^2, X] = (i2/\hbar a^2)P$ with coefficients which are polynomials in the operator h. [$X_2 = X(4h - 1) + (i4/\hbar a^2)P$, and so on.] There follows a three-term recurrence relation for X_n and a similar one for P_n which can be solved. Finally, the operator power series can be formally summed to yield Eqs. (4.11) and (4.12).

In the above calculations, the choice has been made to write X and P to the left of their coefficient polynomials in h. If this order is reversed,[15] a very similar structure results, and the same calculations can be carried out. The expressions for $X(t)$ and $P(t)$ which result are the Hermitian conjugates of the expressions on the right-hand sides of (4.11) and (4.12). Note, therefore, that the phase factor $\exp(-i\omega_0 t)$ in (4.11) and (4.12) is essential for Hermiticity. (An explicit example will be given at the end of Sec. IV B.) Of course, a manifestly Hermitian form of (4.11) and (4.12) can be obtained by taking a symmetric combination of the two orderings. However, the forms given are more convenient for our purposes.

B. Approximate coherent states

Because X involves H in the denominator, the calculation of G and the exact solution to the eigenvalue equation (3.9) can, to our knowledge, only be done approximately. One must either use perturbation theory or an eigenfunction expansion.

Note, however, that for the special coherent state which is the ground state, $H\psi_0 = E_0\psi_0$. Moreover, for relatively large U_0, and for a coherent state with $\langle n\rangle \ll U_0/\mathcal{E}_0$, only relatively few number states [$\sim\Theta(\langle n\rangle^{1/2})$] will have a significant overlap with the coherent state. Then one can approximate $(U_0 - H - \mathcal{E}_0/4)^{-1}$ by $(U_0 - \overline{E} - \mathcal{E}_0/4)^{-1}$, where $\overline{E} = \langle H\rangle$. The above two observations suggest that one approximate X by $\overline{X} = X(H - \overline{E})$. With this approximation the coherent-states analysis can be done analytically, yielding "approximate coherent states."

Consider the operator

$$\overline{X} = e^z - U_0/(U_0 - \overline{E} - \mathcal{E}_0/4)\,, \tag{4.16}$$

where $\overline{E} = \langle H\rangle$ will be given below. Then

$$[\overline{X}, P] = ia^2\hbar e^{2z} \equiv i\overline{G}\,. \tag{4.17}$$

The solution to the eigenvalue equation (3.9) is

$$\psi_{\overline{\mathrm{CS}}} = \hat{N}(C, B)[e^{-(B+1/2)z}]\exp[-Ce^{-z}], \tag{4.18}$$

$$C = B\langle e^z\rangle + i\langle P\rangle/(a^2\hbar) \equiv u + iv. \tag{4.19}$$

Observe that

$$\langle n|\frac{U_0}{U_0 - H - \mathcal{E}_0/4}|n\rangle = \frac{\lambda^2}{(\lambda - n)(\lambda - n - 1)} = \langle n|e^z|n\rangle\,. \tag{4.20}$$

[The first equality comes directly from (2.11). The second equality comes from evaluating $(2\lambda/a)N^2(n,\lambda)J^{(-2)}_{n,2\lambda-2n-1}$ by Eq. (2.13).] Equation (4.20) is a verification that $\langle n|X|n\rangle = 0$. This result, compared with (4.18) and (4.19) shows us that to obtain the ground state one needs the special value for the complex parameter $C = B\lambda/(\lambda - 1)$ and one has to restrict the parameter B to be $\lambda - 1$. Thus, one finally has that

$$\psi_{\overline{\mathrm{CS}}} = N(C,\lambda)(e^{-(\lambda-1/2)z})\exp(-Ce^{-z}), \tag{4.21}$$

$$N(C,\lambda) = a^{1/2}[2u]^{\lambda-1/2}/[\Gamma(2\lambda - 1)]^{1/2}\,, \tag{4.22}$$

$$C = (\lambda - 1)\langle e^z\rangle + i\langle P\rangle/\hbar a^2 \equiv u + iv\,. \tag{4.23}$$

$N(C,\lambda)$ can be evaluated by changing variables to $t=\exp(-z)$.

By using integrals of the type we have discussed as well as equation (3.9), one can verify that

$$[(\Delta\overline{X})^2][(\Delta P)^2]=\left(\frac{u^2}{2(\lambda-1)^2(\lambda-\frac{3}{2})}\right)\left(\frac{(\hbar a^2)^2u^2}{2(\lambda-\frac{3}{2})}\right)=\tfrac{1}{4}\langle\overline{G}\rangle^2 . \tag{4.24}$$

[Note that (4.24) also holds for the ground state with X used instead of $\overline{X}$.] Lastly we calculate $\overline{E}$ as

$$\overline{E}=\langle H\rangle_{\overline{\rm CS}}=\mathcal{E}_0\left\{\lambda\left(\lambda-\tfrac{1}{2}\right)\left[\frac{v^2}{u^2}+\left(\frac{\lambda}{u}-1\right)^2\right]+\left(\lambda-\tfrac{1}{4}\right)\right\} . \tag{4.25}$$

For the ground state $C=u+iv=\lambda$, yielding the ground-state energy $\mathcal{E}_0(\lambda-\frac{1}{4})$.

One can decompose these approximate coherent states into number states plus continuum. The expression is

$$\psi_{\overline{\rm CS}}(x)=N(C,\lambda)\sum_{n=0}^{[\lambda-1/2]}N(n,\lambda)\Theta(n,C,\lambda)\psi_n(x)/a \\ +\text{continuum}, \tag{4.26}$$

where the overlap function $\Theta(n,C,\lambda)$ is

$$\Theta(n,C,\lambda)=\sum_{j=0}^{n}\frac{(-1)^j}{j!}\binom{2\lambda-n-1}{n-j}\left(\frac{2}{1+C/\lambda}\right)^{2\lambda-n-1+j}\Gamma(2\lambda-n-1+j) . \tag{4.27}$$

With this decomposition, one can explicitly calculate

$$\langle\overline{\rm CS}|X(t)|\overline{\rm CS}\rangle=\frac{N^2(C,\lambda)}{2a^2}\sum_{n=0}^{[\lambda-1/2-1]}N(n+1,\lambda)N(n,\lambda)D(n,\lambda)\left[\Theta^*(n+1,C,\lambda)\Theta(n,C,\lambda)\exp[i2(\lambda-1-n)\omega_0t]\right. \\ \left.+\Theta(n+1,C,\lambda)\Theta^*(n,C,\lambda)\exp[-i2(\lambda-1-n)\omega_0t]\right]+\text{continuum contribution}. \tag{4.28}$$

The bound-state contribution of (4.28) is real, as it must be if $X(t)$ in the form of Eq. (4.11) is Hermitian. In particular, it would not have been real if there had not been the factor $\exp(-i\omega_0t)$ in Eq. (4.11).

V. DISCUSSION

A. Harmonic-oscillator limit

It is useful to investigate the limit in which the Morse oscillator reduces to the harmonic oscillator. This harmonic-oscillator limit is defined by

$$\lim_{\rm HO}=\lim_{\substack{\lambda\to\infty\\ a\to0\\ \lambda a^2\to m\omega/\hbar}} . \tag{5.1}$$

First observe that by simple expansion of (2.1) and (2.11)

$$\lim_{\rm HO}V(x)=\tfrac{1}{2}m\omega^2x^2 , \tag{5.2}$$

$$\lim_{\rm HO}E_n=\hbar\omega(n+\tfrac{1}{2}) . \tag{5.3}$$

Next look at the eigenfunctions. By using the relation on p. 251 of Magnus *et al.*,[8]

$$H_n(x/\sqrt{2})=(-1)^n\,2^{n/2}\Gamma(n+1) \\ \times\lim_{\alpha\to\infty}\left[\alpha^{-n/2}L_n^{(\alpha)}(\sqrt{\alpha}\,x+\alpha)\right], \tag{5.4}$$

then expanding $\exp[-y/2]$ as $\exp[\text{power series in } x]$, and lastly using Stirling's approximation for the gamma functions in $N(n,\lambda)$, one finds that

$$\lim_{\rm HO}\psi_n=\left(\frac{a_0}{\pi^{1/2}2^n\Gamma(n+1)}\right)^{1/2}\exp[-\tfrac{1}{2}a_0^2x^2]H_n(a_0x), \tag{5.5}$$

$$a_0\equiv[m\omega/\hbar]^{1/2} . \tag{5.6}$$

Equations (5.5) and (5.6) are the properly normalized harmonic-oscillator eigenfunctions. Also,

$$\lim_{\rm HO}\begin{Bmatrix}X\\P\end{Bmatrix}=\begin{Bmatrix}ax\\ap\end{Bmatrix} . \tag{5.7}$$

Finally, one similarly can show that

$$\lim_{\rm HO}\psi_{\overline{\rm CS}}=\exp\left(\frac{-i\langle p\rangle}{a\hbar}\right)\left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \\ \times\exp\left[-(x-\langle x\rangle)^2\left(\frac{m\omega}{2\hbar}\right)+\frac{ix\langle p\rangle}{\hbar}\right] . \tag{5.8}$$

That is, up to the phase factor $\exp[-i\langle p\rangle/a\hbar)]$ one obtains Schrödinger's[16] original representation of the harmonic-oscillator coherent states.

B. Uncertainty products

In their interesting paper, Walker and Preston[6] did a numerical study of the one-dimensional

Morse oscillator, with parameters fit to the HF molecule. The system was started in the ground state, and then allowed to interact with a classical electromagnetic field. They found that initially the system was almost in a minimum uncertainty state of x and p:

$$\mathfrak{U} \equiv (\Delta x)(\Delta p) \geq \tfrac{1}{2}\hbar \tag{5.9}$$

had $\mathfrak{U}_0 = 0.503\ \hbar$. (Below we will calculate this number analytically.) After about 5 optical oscillations $\mathfrak{U}$ began growing rapidly with time to a maximum of about 2.4 $\hbar$ by 10 optical cycles. $\mathfrak{U}$ then decreased back to near $\frac{1}{2}\hbar$ after 20 optical cycles. After this the pattern was approximately repeated every 20 optical cycles.

Walker and Preston observed, from analogy to the harmonic oscillator, that $\mathfrak{U}_0 \sim \frac{1}{2}\hbar$ is expected since the Morse ground-state wave function is similar to the harmonic-oscillator ground-state Gaussian. Furthermore, their numerical results showed that the energy absorbed from the external field in about 10 optical cycles was deposited back into the field in the next 10 cycles. [The quantity $\langle x(t) \rangle$ displayed a similar pattern of growth and decay.] Thus $\mathfrak{U}(t)$ could be expected to return to $\sim \frac{1}{2}\hbar$. The pattern then should approximately repeat itself every 20 cycles, as was observed.

Additional understanding of this uncertainty-product oscillation can be gained by further analogy to the harmonic oscillator, also using the results in Secs. III and IV. The electromagnetic field is represented by an interaction proportional to x, where x is the natural variable for the harmonic oscillator: $\langle n \pm 1 | x | n \rangle$ are the only nonzero matrix elements. This is a technical reason that the forced harmonic oscillator remains exactly in a coherent state.[17]

But, as we have seen, it is $X(x)$, defined by Eq. (4.7), which is the natural variable for the Morse oscillator. One immediate consequence is that x produces transitions to all (parity-allowed) states, not just to adjacent eigenstates. Thus the Morse oscillator forced by a time-dependent potential proportional to x is not coherently driven. A feel for this can be seen from Walker and Preston's Figs. 2 and 3. After 10 optical cycles, $\langle n \rangle \sim 2.5$ and $\mathfrak{U} \sim 2.4\ \hbar$. For a harmonic oscillator, $\mathfrak{U}_n = (n + \frac{1}{2})\hbar$, so that for a totally uncoherent harmonic oscillator with $\langle n \rangle \sim 2.5$, one would expect $\mathfrak{U} \sim 3\hbar$.

Moreover, the Morse ground state is a minimum uncertainty state for the uncertainty product of Eq. (3.8): $(\Delta X)^2 (\Delta P)^2 \geq \frac{1}{4}\langle G \rangle^2$. Thus, one expects $\mathfrak{U}_0 \neq \frac{1}{2}\hbar$. As it happens, for the Morse ground state with the HF parameters used by Walker and Preston, Eq. (3.8) is strikingly close to Eq. (5.9) and the numerical factor in Eq. (5.9) is 0.503 instead of 0.5. To make this statement precise, we now analytically calculate the ground-state uncertainty $\mathfrak{U}_0$ (this yielding 0.503 for the Walker-Preston system), and point out the generalization to higher Morse number states.

The Morse ground state can be written

$$\psi_0 = N(0, \lambda)(2\lambda)^{\lambda - 1/2} [f(2\lambda - 1, \lambda)]^{1/2}\ , \tag{5.10}$$

$$f(\tau, \lambda) = e^{-z\tau} \exp(-2\lambda e^{-z})\ . \tag{5.11}$$

By observing that

$$\frac{d}{d\lambda} f(2\lambda - 1, \lambda) = -2z f(2\lambda - 1, \lambda) - 2f(2\lambda, \lambda) \tag{5.12}$$

and interchanging the order of differentiation and integration, one obtains

$$\langle x \rangle_0 = -a^{-2} N(0, \lambda)^2 (2\lambda)^{2\lambda - 1} \times \left(\frac{1}{2} \frac{d}{d\lambda} F(2\lambda - 1, \lambda) + F(2\lambda, \lambda) \right)\ , \tag{5.13}$$

where

$$F(\tau, \lambda) = \int_{-\infty}^{\infty} dz\, f(\tau, \lambda) = \Gamma(\tau)(2\lambda)^{-\tau}\ . \tag{5.14}$$

The end result is that

$$\langle x \rangle_0 = a^{-1} [\ln(2\lambda) - \Psi(2\lambda - 1)]\ , \tag{5.15}$$

where Ψ is the digamma function.[8] Similarly,

$$\langle x^2 \rangle_0 = a^{-3} N(0, \lambda)^2 (2\lambda)^{2\lambda - 1} \times \left(\frac{1}{4} \frac{d^2}{d\lambda^2} F(2\lambda - 1, \lambda) + \frac{d}{d\lambda} F(2\lambda, \lambda) + F(2\lambda + 1, \lambda) \right) \tag{5.16}$$

$$= a^{-2} \{ \Psi'(2\lambda - 1) + [\ln(2\lambda) - \Psi(2\lambda - 1)]^2 \}\ , \tag{5.17}$$

where Ψ' is the trigamma function. In an easier manner

$$\langle p \rangle_0 = 0\ , \tag{5.18}$$

$$\langle p^2 \rangle_0 = -\hbar^2 a N(0, \lambda)^2\ (2\lambda)^{2\lambda - 1} \times [(\lambda - \tfrac{1}{2})^2 F(2\lambda - 1, \lambda) - 2\lambda^2 F(2\lambda, \lambda) + \lambda^2 F(2\lambda + 1, \lambda)] \tag{5.19}$$

$$= \tfrac{1}{2}\hbar^2 a^2 (\lambda - \tfrac{1}{2})\ . \tag{5.20}$$

Combining Eqs. (5.15)–(5.20)

$$(\Delta x)_0^2 (\Delta p)_0^2 = \tfrac{1}{2}\hbar^2 (\lambda - \tfrac{1}{2}) \Psi'(2\lambda - 1)\ . \tag{5.21}$$

For the HF parameters used by Walker and Preston, $\lambda = 23.87$. This means that to evaluate the trigamma function in Eq. (5.21) we can use the large-

argument expression[8]

$$\Psi'(z)=\frac{1}{z}+\frac{1}{2z^2}+\frac{1}{4z^3}-\frac{1}{30z^5}+\cdots . \tag{5.22}$$

Thus

$$(\Delta x)_0(\Delta p)_0=0.5027\,\hbar. \tag{5.23}$$

Finally we point out that one can similarly calculate the $x-p$ uncertainty product for any other number state, $n\neq 0$. The only difference is that there will be $(n+1)^2$ times as many terms, because there are $n+1$ terms in the polynomial $L_n^{(2\lambda-2n-1)}(y)$.

In later work we will present a discussion of the time evolution of these coherent states.

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