Uncertainty Products for the Anharmonic Morse Oscillator.

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The coherent states for a harmonic oscillator, firstly introduced by SCHröDINGER (1), have been found by GLAUBER (2) to be of utility in the quantum-mechanical description of coherence of the radiation field.

Apart from other properties, these states minimize the position-momentum uncertainty relation

\[(\Delta x)^2(\Delta p)^2 \geq \hbar^2/4.\]

Although the extension of the concept of coherent states for systems other than the harmonic oscillator have been proposed (3), these have only been applied to systems with equal-level spacing (4). For general potentials a definition of the coherent states has been proposed by NIETO and SIMMONS (4). These authors claim that the appropriate generalization of the harmonic-oscillator coherent states are a subset of the states which minimize eq. (1).

In a recent paper NIETO and SIMMONS (6) apply their definition of coherent state to the anharmonic Morse oscillator and obtain an analytic expression for the Morse ground-state uncertainty relation.

The purpose of this paper is to give general analytic expressions for the Morse position-momentum uncertainty products. The matrix elements involved in the definition of the uncertainty product

\[(\Delta x)^2(\Delta p) = \langle x^2 \rangle_n - \langle x \rangle_n^2 + \langle p^2 \rangle_n - \langle p \rangle_n^2,\]

apart from the utility in generalizing the concept of coherent states, are of current interest in modelling the interaction of intense electromagnetic fields with molecules (6).
For the Morse oscillator of reduced mass $\mu$, characterized by the parameters $D_e$, $a$ and $x_e$, the eigenstates are well known (7) to be given by

$$\varphi_n(x) = N_n \exp \left[ -\frac{x}{2} \right] x^{b/2} L_n^b(x),$$

where $L_n^b(x)$ are the generalized Laguerre polynomials defined by

$$L_n^b(x) = \sum_{i=0}^{n} \binom{n}{i} \left( \frac{-x}{a} \right)^i \frac{i!}{i!},$$

and

$$x = k \exp \left[ -a(x - x_e) \right],$$

$$k = 2(2\mu D_e)^{1/(ka)},$$

$$b = k - 2n - 1,$$

$$N_n^2 = \frac{abn!}{\Gamma(b + n + 1)}.$$

**Position uncertainty.** The position $(x - x_e)^i$ matrix elements between general Morse eigenstates are given by

$$X_{mn}^{(i)} = \langle m | (x - x_e)^i | n \rangle = \frac{N_m N_n}{a} \int_0^\infty \exp \left[ -\frac{x}{2} \right] x^{b/2} \ln^i \left( \frac{\ln k}{a} - \frac{\ln x}{a} \right) L_m^b(x) L_n^b(x) \, dx,$$

where $b' = k - 2m - 1$. After substituting the generalized Laguerre polynomials by their definition eq. (4) and making the variable change to $y = x/k$, one is left with integrals of the general form

$$I(x, \beta; l) = \int_0^\infty \exp \left[ -xy \right] y^{\beta-1} \ln y^l \, dy,$$

$$I(x, \beta; l) = \left( \frac{d}{d\beta} \right)^l \int_0^\infty \exp \left[ -xy \right] y^{\beta-1} \, dy = \left( \frac{d}{d\beta} \right)^l \left[ \frac{\Gamma(\beta)}{\alpha^\beta} \right].$$

This integral, which extends some results presented in ref. (5), in particular gives

$$X_{mn}^{(1)} = \frac{N_m N_n}{a^2} \sum_{i=0}^{m} \sum_{j=0}^{n} \left( -1 \right)^{i+j} \binom{b + m}{m - i} \binom{b + n}{n - j} \ln k - \psi(t),$$

$$X_{mn}^{(2)} = \frac{N_m N_n}{a^3} \sum_{i=0}^{m} \sum_{j=0}^{n} \left( -1 \right)^{i+j} \binom{b + m}{m - i} \binom{b + n}{n - j} \ln k - \psi(t) - \psi^{(1)}(t),$$

where \( t = k + i + j - n - m - 1 \) and \( \psi(t) = (d/dt)[\ln \Gamma(t)] \) and \( \psi^{(1)}(t) = (d/dt)\psi(t) \) are the digamma and trigamma functions, respectively (*). From these equations the results for the ground state \( \langle x \rangle_0 \) and \( \langle x^2 \rangle_0 \) given in ref. (5) can be easily obtained by setting \( m = n = 0 \).

**Momentum uncertainty.** Integrating once by parts it is easy to see that

\[
\langle p \rangle_n = \left( -i\hbar a_n \frac{d}{dz} \right)_n = 0,
\]
due to the vanishing of the factor \( \exp[-z]e^z \) at the limits of integration.

By use of the differential equation for the generalized Laguerre polynomials

\[
z \frac{d^2}{dz^2} L_n^b(z) + (b + 1 - z) \frac{d}{dz} L_n^b(z) + nL_n^b(z) = 0
\]
in the equation obtained by applying the operator \( p^2 \) to \( \varphi_n \), one gets

\[
\langle p^2 \rangle_n = \hbar^2 a_n \sum_n \left[ -\frac{1}{4} J_{n,b}^{(1)} + \left( \frac{b}{2} + n \right) J_{n,b}^{(0)} - \frac{b}{2} \left( \frac{b}{2} - 1 \right) \right] \cdot J_{n,b}^{(-l)} + \int_0^\infty \exp[-z]e^z \left[ L_n^b(z) \frac{d}{dz} L_n^b(z) dz \right],
\]
where, as defined in eq. (2.13) of ref. (4),

\[
J_{n,b}^{(l)} = \int_0^\infty \exp[-t]e^t [L_n^b(t)]^l dt,
\]

\[
J_{n,b}^{(0)} = \frac{\Gamma(b + n + 1)}{\Gamma(n + 1)} \sum_k (-1)^k \frac{\Gamma(n - k - \beta) \Gamma(b + k + 1 + \beta)}{\Gamma(-k - \beta) \Gamma(b + k + 1)} \frac{1}{\Gamma(k + 1) \Gamma(n - k + 1)},
\]

\[
J_{n,b}^{(\beta)} = \frac{\Gamma(b + n + 1)}{\Gamma(n + 1)} \sum_{k=0}^n (-1)^{k+n} \left( \frac{\Gamma(b + k + 1 + \beta)}{\Gamma(\beta + k + n + 1)} \frac{\Gamma(b + k + 1)}{\Gamma(\beta + k + n + 1)} \frac{1}{\Gamma(b + k + 1)} \right),
\]

for \( \text{Re}(b + \beta + 1) > 0 \). Equation (18) was obtained by \( n \) integrations by parts of eq. (16) after having substituted one of the generalized Laguerre polynomials by eq. (4) and the other one by eq. (8.970-1) of Gradshteyn and Ryzhik (10). The particular values of

this integral needed in eq. (15) are

\[
\begin{align*}
J^{(1)}_{n,b} &= (b + 2n + 1) \Gamma(b + n + 1)/n!, \\
J^{(0)}_{n,b} &= \Gamma(b + n + 1)/n!, \\
J^{(-1)}_{n,b} &= \Gamma(b + n + 1)/(bn!).
\end{align*}
\]

The explicit integral appearing in eq. (15), by integrating by parts, can be shown to be

\[
\int_0^\infty \exp[-x] x^k L_n^k(x) \frac{d}{dx} L_n^k(x) dx = \frac{1}{2} [J^{(1)}_{n,b} - bJ^{(-1)}_{n,b}] = 0,
\]

so that, finally, we have

\[
\langle p^2 \rangle_n = \frac{1}{2} \hbar^2 a^2 (n + 1/2)(k - 2n - 1),
\]

which, for the ground state, reduces to the value found by Nieto and Simmons (4).

In concluding it is worth pointing out that, besides the afore-mentioned applications, the matrix elements given by eqs. (11) and (12) and higher-order ones, easily obtained from eq. (10), are of use in the theoretical investigation of the rotation-vibration coupling and intensities in diatomic molecules (11).