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

$$(\Delta x)^2(\Delta p)^2 \geqslant \hbar^2/4 . \tag{1}$$

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 (5) 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

$$(\Delta x)_n(\Delta p)_n = [\langle x^2\rangle_n - \langle x\rangle_n^2]^{\frac{1}{2}}[\langle p^2\rangle_n - \langle p\rangle_n^2]^{\frac{1}{2}} , \tag{2}$$

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).

(1) E. SCHRÖDINGER: *Naturwissenschaften*, **14**, 664 (1926).
(2) R. J. GLAUBER: *Phys. Rev.*, **130**, 2529 (1963); **131**, 2766 (1963).
(3) A. O. BARUT and L. GIRARDELLO: *Commun. Math. Phys.*, **21**, 41 (1971); M. PERELEMOV: *Commun. Math. Phys.*, **26**, 222 (1972).
(4) M. M. NIETO and L. M. SIMMONS jr.: *Phys. Rev. Lett.*, **41**, 207 (1978).
(5) M. M. NIETO and L. M. SIMMONS jr.: *Phys. Rev. A*, **19**, 438 (1979).
(6) R. B. WALKER and R. K. PRESTON: *J. Chem. Phys.*, **67**, 2017 (1977).

For the Morse oscillator of reduced mass μ, characterized by the parameters D_e, a and x_e, the eigenstates are well known [7] to be given by

$$\varphi_n(x) = N_n \exp[-z/2] z^{b/2} L_n^b(z)\,, \tag{3}$$

where $L_n^b(z)$ are the generalized Laguerre polinomials defined by

$$L_n^b(z) = \sum_{i=0}^{n} \binom{b+n}{n-i} \frac{(-z)^i}{i!} \tag{4}$$

and

$$\begin{cases} z &= k \exp[-a(x-x_e)]\,, \\ k &= 2(2\mu D_e)^{\frac{1}{2}}/(\hbar a)\,, \end{cases} \tag{5}$$

$$b = k - 2n - 1\,, \tag{6}$$

$$N_n^2 = abn!/\Gamma(b+n+1)\,. \tag{7}$$

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

$$X_{mn}^{(l)} = \langle m|(x-x_e)^l|n\rangle = \frac{N_m N_n}{a} \int_0^\infty \exp[-z] z^{b/2+b'/2-1} \left(\frac{\ln k}{a} - \frac{\ln z}{a}\right)^l L_m^{b'}(z) L_n^b(z)\,\mathrm{d}z\,, \tag{8}$$

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

$$I(\alpha, \beta; l) = \int_0^\infty \exp[-\alpha y] y^{\beta-1} (\ln y)^l\,\mathrm{d}y\,, \tag{9}$$

$$I(\alpha, \beta; l) = \left(\frac{\mathrm{d}}{\mathrm{d}\beta}\right)^l \int_0^\infty \exp[-\alpha y] y^{\beta-1}\,\mathrm{d}y = \left(\frac{\mathrm{d}}{\mathrm{d}\beta}\right)^l \left[\frac{\Gamma(\beta)}{\alpha^\beta}\right]. \tag{10}$$

This integral, which extends some results presented in ref. [8], in particular gives

$$X_{mn}^{(1)} = \frac{N_m N_n}{a^2} \sum_{i=0}^{m} \sum_{j=0}^{n} \frac{(-1)^{i+j}}{i!\,j!} \binom{b'+m}{m-i} \binom{b+n}{n-j} \Gamma(t)[\ln k - \psi(t)]\,, \tag{11}$$

$$X_{mn}^{(2)} = \frac{N_m N_n}{a^3} \sum_{i=0}^{m} \sum_{j=0}^{n} \frac{(-1)^{i+j}}{i!\,j!} \binom{b'+m}{m-i} \binom{b+n}{n-j} \Gamma(t)[(\psi(t) - \ln k)^2 + \psi^{(1)}(t)]\,, \tag{12}$$

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(7) P. M. Morse: *Phys. Rev.*, **34**, 57 (1929); J. Rundgren: *Ark. Fys.*, **30**, 61 (1965).
(8) J. A. C. Gallas: to appear in *Phys. Rev. A*.

where $t = k + i + j - n - m - 1$ and $\psi(t) = (\mathrm{d}/\mathrm{d}t)[\ln \Gamma(t)]$ and $\psi^{(1)}(t) = (\mathrm{d}/\mathrm{d}t)\,\psi(t)$ are the digamma and trigamma functions, respectively [9]. 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 uncertanity. Integrating once by parts it is easy to see that

$$\langle p\rangle_n = \left\langle -i\hbar a z \frac{\mathrm{d}}{\mathrm{d}z}\right\rangle_n = 0\,, \tag{13}$$

due to the vanishing of the factor $\exp[-z]z^b$ at the limits of integration.

By use of the differential equation for the generalized Laguerre polinomials

$$z\frac{\mathrm{d}^2}{\mathrm{d}z^2}L_n^b(z) + (b + 1 - z)\frac{\mathrm{d}}{\mathrm{d}z}L_n^b(z) + nL_n^b(z) = 0 \tag{14}$$

in the equation obtained by applying the operator p^2 to φ_n, one gets

$$\langle p^2\rangle_n = \hbar^2 a N_n^2\left[-\frac{1}{4}J_{n,b}^{(1)} + \left(\frac{b}{2} + n\right)J_{n,b}^{(0)} - \frac{b}{2}\left(\frac{b}{2} - 1\right)\cdot \right.$$
$$\left. \cdot J_{n,b}^{(-1)} + \int_0^\infty \exp[-z]z^b L_n^b(z)\frac{\mathrm{d}}{\mathrm{d}z}L_n^b(z)\,\mathrm{d}z\right], \tag{15}$$

where, as defined in eq. (2.13) of ref. [5],

$$J_{n,b}^{(\beta)} = \int_0^\infty \exp[-t]\,t^{b+\beta}[L_n^b(t)]^2\,\mathrm{d}t\,, \tag{16}$$

$$J_{n,b}^{(\beta)} = \frac{\Gamma(b+n+1)}{\Gamma(n+1)}\sum_{k=0}^{n}(-1)^k\frac{\Gamma(n-k-\beta)}{\Gamma(-k-\beta)}\,\frac{\Gamma(b+k+1+\beta)}{\Gamma(b+k+1)}\,\frac{1}{\Gamma(k+1)\Gamma(n-k+1)}\,, \tag{17}$$

$$J_{n,b}^{(\beta)} = \frac{\Gamma(b+n+1)}{\Gamma(n+1)}\sum_{k=0}^{n}(-1)^{k+n}\cdot$$
$$\cdot\frac{\Gamma(\beta+k+1)}{\Gamma(\beta+k-n+1)}\,\frac{\Gamma(b+k+1+\beta)}{\Gamma(b+k+1)}\,\frac{1}{\Gamma(k+1)\Gamma(n-k+1)}\,, \tag{18}$$

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

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([9]) M. ABRAMOWITZ and I. A. STEGUN (Editors): *Handbook of Mathematical Functions* (New York, N. Y., 1965).

([10]) I. S. GRADSHTEYN and I. M. RYZHIK: *Table of Integrals, Series, and Products*, 4th. ed. (New York, N. Y., 1965).

this integral needed in eq. (15) are

$$(19)\qquad \begin{cases} J^{(1)}_{n,b} = (b+2n+1)\,\Gamma(b+n+1)/n!\,, \\ J^{(0)}_{n,b} = \Gamma(b+n+1)/n!\,, \\ J^{(-1)}_{n,b} = \Gamma(b+n+1)/(bn!)\,. \end{cases}$$

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

$$(20)\qquad \int\limits_0^\infty \exp[-z]\,z^b L^b_n(z)\,\frac{\mathrm{d}}{\mathrm{d}z}L^b_n(z)\,\mathrm{d}z = \frac{1}{2}\,[J^{(0)}_{n,b} - bJ^{(-1)}_{n,b}] = 0\,,$$

so that, finally, we have

$$(21)\qquad \langle p^2\rangle_n = \tfrac{1}{2}\hbar^2 a^2 (n+1/2)(k-2n-1)\,,$$

which, for the ground state, reduces to the value found by NIETO and SIMMONS (5).

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).

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(11) M. BADAWI, N. BESSIS, G. BESSIS and G. HADINGER: *Can. J. Phys.*, **52**, 110 (1974).

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