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A Minimal Uncertainty Product for One Dimensional Semiclassical Wave Packets

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Happy 60^{th} birthday, Mr. Fritz!

Abstract. Although real, normalized Gaussian wave packets minimize the product of position and momentum uncertainties, generic complex normalized Gaussian wave packets do not. We prove they minimize an alternative product of uncertainties that correspond to variables that are phase space rotations of position and momentum.

1. Introduction

In studying small $\hbar$ asymptotics of solutions to the time–dependent Schrödinger equation, semiclassical wave packets have proven very useful. (See *e.g.*, [**3**] and its references, or more modern works, such as [**1**], [**2**], or [**4**].) In the case of one degree of freedom, for fixed, allowed values of the parameters A, B, $\hbar$, a, and η, these wave packets are an orthonormal basis of $L^2(\mathbb{R}, dx)$ that we denote by $\{\, \varphi_k(A, B, \hbar, a, \eta, x) \,\}$, where $k = 0, 1, \ldots$.

By making a proper choice of the parameters, one can write any normalized, one dimensional complex Gaussian wave packet as $\varphi_0(A, B, \hbar, a, \eta, x)$. Two of the restrictions on the parameters are the conditions $\operatorname{Re} \overline{A}B = 1$ and $\hbar > 0$. By a fairly straightforward calculation, one can prove that the usual position, momentum uncertainty product in the state $\varphi_0(A, B, \hbar, a, \eta, x)$ satisfies $\Delta x \, \Delta p = \dfrac{\hbar}{2} \, |A| \, |B|$. When the complex phases of A and B are the same, $\varphi_0(A, B, \hbar, a, \eta, x)$ is a phase times a real Gaussian, and it is a standard result that this product takes its minimal value $\Delta x \, \Delta p = \dfrac{\hbar}{2}$. When the phases of A and B are different, $|A| \, |B| > 1$, and consequently, $\Delta x \, \Delta p > \dfrac{\hbar}{2}$. As usual, x and p are the position and momentum operators, and we define the uncertainty for a self-adjoint observable X in the state ψ to be $\Delta X = \sqrt{\langle \, \psi, \, X^2 \, \psi \, \rangle - \langle \, \psi, \, X \, \psi \, \rangle^2}$.

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The goal of this paper is to prove an alternative minimum uncertainty product result for the state $\varphi_0(A,\, B,\, \hbar,\, a,\, \eta,\, x)$. We define two "rotated" operators

$$\begin{aligned} \alpha &= \cos(\theta)\; x \;+\; \sin(\theta)\; p \qquad\qquad \text{and} \\ \beta &= -\sin(\theta)\; x \;+\; \cos(\theta)\; p. \end{aligned}$$

We show that in any normalized state,

$$\Delta\alpha\, \Delta\beta \;\geq\; \frac{\hbar}{2},$$

and we show in Theorem 5.2 that by choosing

$$\theta \;=\; \frac{1}{2} \arctan\left(\frac{2\, \mathrm{Im}\,(B\overline{A})}{|B|^2 - |A|^2} \right),$$

one has

$$\Delta\alpha\, \Delta\beta \;=\; \frac{\hbar}{2}$$

in the state $\varphi_0(A,\, B,\, \hbar,\, a,\, \eta,\, x)$. So, general semiclassical wave packets satisfy a minimal uncertainty relation. It is not the usual relation, but the product for the rotated operators.

Remark 1.1. Employing a sort of microlocal intuition, we often like to think heuristically of supports of quantum states in phase space. Weyl asymptotics and Bohr–Sommerfeld rules suggest that a normalized state should occupy a phase space area of $2\pi\hbar$. From this viewpoint, we envision the usual, frequency ω harmonic oscillator ground state as having phase space support of the interior of an ellipse that is centered at the origin and has semiaxes $\sqrt{2\,\hbar/\omega}$ in the x direction and $\sqrt{2\,\hbar\,\omega}$ in the p direction.

On this intuitive level, the region of phase space corresponding to $\varphi_0(A,\, B,\, \hbar,\, a,\, \eta,\, x)$ is such an ellipse that has been rotated through the angle θ and then translated so its center is at $(a,\, \eta)$.

Remark 1.2. The situation in more than one dimension is significantly more complicated. Although we believe an analogous result must be true, and we have received some preliminary calculations from Vidian Rousse [**5**], we have not seen a complete argument. In n dimensions, one would like to find an orthogonal, symplectic matrix depending on A and B that would define rotated operators α_j and β_j for $j = 1,\, 2,\, \cdots,\, n$, such that in the state $\varphi_0(A,\, B,\, \hbar,\, a,\, \eta,\, x)$,

$$\Delta\alpha_j\, \Delta\beta_j \;=\; \frac{\hbar}{2}$$

for each j.

We have tried to generalize the one dimensional proof given in Section 5 to n dimensions. The proof relies on finding the minimum of a function of n^2 variables. (The symplectic orthogonal group is isomorphic to the n^2 dimensional real Lie group $U(n)$.) Using the second derivative test to separate minima, maxima, and saddles becomes exceptionally complicated.

2. Observations about the Angle of Rotation

The particular value of θ may seem rather bizarre, but it is natural. The wave packet $\varphi_0(A,\, B,\, \hbar,\, a,\, \eta,\, x)$ is the ground state of a Hamiltonian that is quadratic in x and p. That Hamiltonian is explicitly

$$H \;=\; \frac{1}{2}\,(\,x \quad p\,)\begin{pmatrix} |B|^2 & \mathrm{Im}\,(B\overline{A}) \\ \mathrm{Im}\,(B\overline{A}) & |A|^2 \end{pmatrix}\begin{pmatrix} x \\ p \end{pmatrix}.$$

In terms of the raising and lowering operators we use below,

$$H \;=\; \frac{\hbar}{2}\;(\mathcal{A}^*\mathcal{A} \,+\, \mathcal{A}\mathcal{A}^*)\,.$$

A rotation through angle θ diagonalizes the real symmetric matrix

$$\frac{1}{2}\begin{pmatrix} |B|^2 & \mathrm{Im}\,(B\overline{A}) \\ \mathrm{Im}\,(B\overline{A}) & |A|^2 \end{pmatrix},$$

whose eigenvalues are

$$\frac{1}{4}\left\{\,(|A|^2+|B|^2) \;\pm\; \sqrt{(|A|^2-|B|^2)^2 \,+\, 4\,(\mathrm{Im}\,(B\overline{A}))^2}\,\right\}.$$

The product of these eigenvalues is the determinant of the matrix for H. The calculation is a bit tedious, but for allowed values of the parameters, the product is $1/4$.

When H is associated with a diagonal matrix, $\theta = 0$, and one is essentially back to considering a standard frequency ω harmonic oscillator Hamiltonian, where $A = \omega^{-1/2}$ and $B = \omega^{1/2}$. In this case, the standard uncertainty product is $\hbar/2$. When considering the matrix associated with H, the value of θ is very natural.

The vectors $\varphi_k(A,\, B,\, \hbar,\, a,\, \eta,\, x)$ also diagonalize the Hamiltonians

$$H_1 \;=\; \hbar\,\mathcal{A}\mathcal{A}^* \qquad \text{and} \qquad H_2 \;=\; \hbar\,\mathcal{A}^*\mathcal{A}.$$

The matrices associated with these quadratic Hamiltonians are

$$\frac{1}{2}\begin{pmatrix} |B|^2 & -\,i\,B\overline{A} \\ i\,A\overline{B} & |A|^2 \end{pmatrix} \qquad \text{and} \qquad \frac{1}{2}\begin{pmatrix} |B|^2 & i\,A\overline{B} \\ -\,i\,B\overline{A} & |A|^2 \end{pmatrix},$$

respectively. In general, these matrices are not real symmetric and do not have real eigenvectors. However, the quadratic forms in the classical variables x and p are the same as the one for H. So, they lead to the same value of θ.

3. Preliminary Comments about Uncertainty Products

We wish to begin with the standard argument for the Heisenberg uncertainty relation

$$\Delta x\,\Delta p \;\geq\; \frac{\hbar}{2}. \tag{3.1}$$

This is a consequence of the more general result that for any two self-adjoint operators X and Y, and any normalized state ψ, we have

$$\Delta X\,\Delta Y \;\geq\; \frac{1}{2}\;|\,\langle\,\psi,\,[X,\,Y]\,\psi\,\rangle\,|\,. \tag{3.2}$$

(One can take both sides as infinite if ψ is not in the appropriate domains.)

The formal argument for proving this is to note that the square of the norm of

$$\{ (X - \langle \psi, X\psi \rangle) + i\lambda (Y - \langle \psi, Y\psi \rangle) \} \psi$$

must be positive. By explicit calculation, this leads to the inequality

$$\Delta X^2 + \lambda^2 \Delta Y^2 + \lambda \langle \psi, i[X, Y]\psi \rangle \geq 0.$$

The left hand side is minimized by taking $\lambda = -\dfrac{\langle \psi, i[X, Y]\psi \rangle}{2\Delta Y^2}$. Since the inequality is true for this value for λ, we see that

$$\Delta X^2 - \frac{\langle \psi, i[X, Y]\psi \rangle^2}{4\Delta Y^2} \geq 0,$$

and inequality (3.2) follows immediately.

Since $[x, p] = i\hbar$, inequality (3.2) implies inequality (3.1). We then note that for any value of θ, we have

$$\begin{aligned} [\alpha, \beta] &= [x\cos(\theta) + p\sin(\theta), -x\sin(\theta) + p\cos(\theta)] \\ &= \cos^2(\theta)[x, p] - \sin^2(\theta)[p, x] \\ &= i\hbar. \end{aligned}$$

So, by another application of inequality (3.2), we obtain the uncertainty relation that for any normalized state ψ,

$$\Delta\alpha \Delta\beta \geq \frac{\hbar}{2}. \tag{3.3}$$

Our main result is that one actually has equality when $\psi = \varphi_0(A, B, \hbar, a, \eta, x)$ and $\theta = \dfrac{1}{2}\arctan\left(\dfrac{2\,\mathrm{Im}(B\overline{A})}{|B|^2 - |A|^2}\right)$.

4. One Dimensional Semiclassical Wave Packets

The one dimensional semiclassical wave packets are most easily defined by using raising and lowering operators [**3**]: The number $a \in \mathbb{R}$ denotes the mean position of the wave packets. The number $\eta \in \mathbb{R}$ denotes the mean momentum. We assume the semiclassical parameter $\hbar$ is positive, and we choose any two complex numbers A and B that satisfy $\overline{A}B + \overline{B}A = 2$. We then define

$$\varphi_0(A, B, \hbar, a, \eta, x) = \pi^{-1/4}\hbar^{-1/4}A^{-1/2}\exp\left\{-\frac{B(x-a)^2}{2A\hbar} + i\eta(x-a)/\hbar\right\}.$$

(The square root $A^{-1/2}$ can take either sign. In applications, the sign is determined by an initial choice and continuity in time.) We note that this vector is normalized because $\overline{A}B + \overline{B}A = 2$. Also, any complex, normalized Gaussian can be written this way.

In analogy with the usual harmonic oscillator, we define raising and lowering operators by

$$\mathcal{A}(A, B, \hbar, a, \eta)^* = \frac{1}{\sqrt{2\hbar}}\left[\overline{B}(x-a) - i\overline{A}(p-\eta)\right]$$

and

$$\mathcal{A}(A, B, \hbar, a, \eta) = \frac{1}{\sqrt{2\hbar}}\left[B(x-a) + iA(p-\eta)\right].$$

Using the raising operator inductively, starting from $k = 0$, we define

$$\varphi_{k+1}(A,\, B,\, \hbar,\, a,\, \eta,\, x) \;=\; \frac{1}{\sqrt{k+1}}\; \mathcal{A}(A,\, B,\, \hbar,\, a,\, \eta)^*\; \varphi_k(A,\, B,\, \hbar,\, a,\, \eta,\, x).$$

Then, for the lowering operator, we also have

$$\mathcal{A}(A,\, B,\, \hbar,\, a,\, \eta)\; \varphi_0(A,\, B,\, \hbar,\, a,\, \eta,\, x) \;=\; 0$$

and

$$\mathcal{A}(A,\, B,\, \hbar,\, a,\, \eta)\; \varphi_k(A,\, B,\, \hbar,\, a,\, \eta,\, x) \;=\; \sqrt{k}\; \varphi_{k-1}(A,\, B,\, \hbar,\, a,\, \eta,\, x),$$

for $k = 1,\, 2,\, \ldots$.

By using the raising and lowering operators, it is quite easy [**3**] to prove that $\{\, \varphi_k(A,\, B,\, \hbar,\, a,\, \eta,\, x)\,\}$ is an orthonormal basis of $L^2(\mathbb{R},\, dx)$, and that in the state $\varphi_k(A,\, B,\, \hbar,\, a,\, \eta,\, x)$,

$$\Delta x \;=\; \left(\frac{\hbar}{2}\right)^{1/2}\; |A|\; \sqrt{2k+1},$$

and

$$\Delta p \;=\; \left(\frac{\hbar}{2}\right)^{1/2}\; |B|\; \sqrt{2k+1}.$$

The proof we present below for φ_0 generalizes to show that with $\theta \;=\; \dfrac{1}{2} \arctan\left(\dfrac{2\,\mathrm{Im}\,(B\overline{A})}{|B|^2 - |A|^2}\right)$, in the state $\varphi_k(A,\, B,\, \hbar,\, a,\, \eta,\, x)$ we have

$$\Delta\alpha\, \Delta\beta \;=\; \frac{\hbar}{2}\; (2k+1).$$

Our proof of the rotated uncertainty relation (3.3) will make use of the raising and lowering operators to represent $(x-a)$ and $(p-\eta)$. From the definitions above, one easily sees that

$$(x-a) \;=\; \sqrt{\frac{\hbar}{2}}\; \left\{\, A\, \mathcal{A}(A,\, B,\, \hbar,\, a,\, \eta)^* \;+\; \overline{A}\, \mathcal{A}(A,\, B,\, \hbar,\, a,\, \eta)\,\right\} \tag{4.1}$$

and

$$(p-\eta) \;=\; i\, \sqrt{\frac{\hbar}{2}}\; \left\{\, B\, \mathcal{A}(A,\, B,\, \hbar,\, a,\, \eta)^* \;-\; \overline{B}\, \mathcal{A}(A,\, B,\, \hbar,\, a,\, \eta)\,\right\}. \tag{4.2}$$

5. The Rotated Uncertainty Product

We begin with a technical lemma that is proved by simple calculation.

LEMMA 5.1. *If $A(t)$ and $B(t)$ satisfy*

$$\dot{A}(t) \;=\; i\, B(t) \qquad \textit{and} \tag{5.1}$$

$$\dot{B}(t) \;=\; i\, A(t), \tag{5.2}$$

then we have the following time derivatives:

$$\frac{d}{dt}\left(|A(t)|^2\,|B(t)|^2\right) \;=\; 2\left(|A(t)|^2-|B(t)|^2\right)\;Im\,(B(t)\overline{A(t)}), \tag{5.3}$$

$$\frac{d}{dt}\left(Im\,(B(t)\overline{A(t)})\right) \;=\; |A(t)|^2-|B(t)|^2, \qquad \textit{and} \tag{5.4}$$

$$\frac{d}{dt}\left(|A(t)|^2-|B(t)|^2\right) \;=\; -4\,Im\,(B(t)\overline{A(t)}). \tag{5.5}$$

We now state and prove our main result:

THEOREM 5.2. *Let A, B, $\hbar$, a, and η be any allowed values of the parameters. If we choose*

$$\theta \;=\; \frac{1}{2}\,arctan\left(\frac{2\;Im\,(B\overline{A})}{|B|^2-|A|^2}\right),$$

then the state $\varphi_0(A,\,B,\,\hbar,\,a,\,\eta,\,x)$ minimizes the uncertainty product for α and β. I.e.*,*

$$\Delta\alpha\,\Delta\beta \;=\; \frac{\hbar}{2}.$$

PROOF. We can prove this by an explicit, but tedious calculation or by the following more appealing argument.

First we note that the values of a and η are irrelevant, so we can set them both to zero. Second we note that clockwise rotations of phase space are generated by the standard, frequency 1, classical harmonic oscillator Hamiltonian $(p^2+x^2)/2$. If we propagate with its quantum analog, the state $\varphi_0(A(0),\,B(0),\,\hbar,\,0,\,0,\,x)$ evolves to a new Gaussian $\varphi_0(A(t),\,B(t),\,\hbar,\,0,\,0,\,x)$, where [**3**] $A(t)$ and $B(t)$ are given in equations (5.7) below.

Applying the "counterclockwise" rotation to the quantum operators x and p to obtain α and β is equivalent to keeping the original operators x and p, but rotating the state φ_0 in the clockwise direction. Thus, proving the theorem is equivalent to showing that $\Delta x\,\Delta p = \hbar/2$ in the state $\varphi_0(A(\theta),\,B(\theta),\,\hbar,\,0,\,0,\,x)$.

Since $\Delta x\,\Delta p \;=\; \dfrac{\hbar}{2}\,|A(\theta)|\,|B(\theta)|$, it suffices to show that $|A(\theta)|\,|B(\theta)| \;=\; 1$.

We can find the minimum of $|A(t)|\,|B(t)|$ by setting the derivative of $f(t) \;=\; |A(t)|^2\,|B(t)|^2$ to zero. By formula (5.3), this requires

$$\dot{f}(t) \;=\; 2\left(|A(t)|^2-|B(t)|^2\right)\,\mathrm{Im}\,(B(t)\overline{A(t)}) \;=\; 0.$$

Thus, we must have $\mathrm{Im}\,(B(t)\overline{A(t)}) \;=\; 0$ or $|A(t)|^2-|B(t)|^2 \;=\; 0$.

To obtain a contradiction, suppose a relative minimum occurs with $\mathrm{Im}\,(B(t)\overline{A(t)}) \neq 0$. Then we must have $|A(t)|^2-|B(t)|^2 \;=\; 0$.

From (5.4) and (5.5), we see that the second derivative of f is

$$\ddot{f}(t) \;=\; 2\left(|A(t)|^2-|B(t)|^2\right)^2 \;-\; 8\left(\mathrm{Im}\,(B(t)\overline{A(t)})\right)^2.$$

From our assumptions above, this quantity is strictly negative, and we have found a maximum of f instead of a minimum. Thus, at any minimum of f, we must have

$$\mathrm{Im}\,(B(t)\overline{A(t)}) \;=\; 0. \tag{5.6}$$

Since $\mathrm{Re}\,(B(t)\overline{A(t)}) \;=\; 1$, this condition forces $|A(t)|\,|B(t)| \;=\; 1$, and hence our desired result $\Delta x\,\Delta p \;=\; \dfrac{\hbar}{2}$.

We next note that

$$\begin{aligned} A(t) &= A(0)\,\cos(t) + i\,B(0)\,\sin(t) \\ B(t) &= i\,A(0)\,\sin(t) + B(0)\,\cos(t). \end{aligned} \tag{5.7}$$

We obtain these relations by explicitly solving the linear system of ordinary differential equations (2.16) of [**3**] for this easy special case.

From these relations, we see that

$$\begin{aligned} &\mathrm{Im}\,(B(t)\,\overline{A(t)}) \\ =\;& \mathrm{Im}\,\{\,(i\,A(0)\,\sin(t) + B(0)\,\cos(t))\,\Big(\overline{A(0)}\,\cos(t) - i\,\overline{B(0)}\,\sin(t)\Big) \\ =\;& \mathrm{Im}\,\Big\{i\,(|A(0)|^2 - |B(0)|^2)\cos(t)\sin(t) + B(0)\overline{A(0)}\cos^2(t) + A(0)\overline{B(0)}\sin^2(t)\Big\} \\ =\;& (|A(0)|^2 - |B(0)|^2)\,\cos(t)\,\sin(t) + \mathrm{Im}\,(B(0)\overline{A(0)})\,(\cos^2(t) - \sin^2(t)). \end{aligned}$$

So, equation (5.6) is equivalent to

$$(|A(0)|^2 - |B(0)|^2)\,\sin(2t) + 2\,\mathrm{Im}\,(B(0)\overline{A(0)})\,\cos(2t) = 0,$$

which is satisfied if we choose $t = \theta$. This proves the theorem. □

Remark 5.3. Our comments about the choice of θ in Section 2 relied on operators that were quadratic in the raising and lowering operators. In the spirit of the proof of Theorem 5.2, we can make similar comments that just involve the lowering operator.

Let $U(t)$ denote the propagator for the standard, frequency 1, quantum harmonic oscillator. Choosing $a = 0$ and $\eta = 0$, we have $\mathcal{A}\,\varphi_0(A,\,B,\,\hbar,\,0,\,0,\,x) = 0$. Thus,

$$\begin{aligned} 0 &= U(t)\,\mathcal{A}\,\varphi_0(A,\,B,\,\hbar,\,0,\,0,\,x) \\ &= U(t)\,\mathcal{A}\,U(t)^{-1}\,U(t)\,\varphi_0(A,\,B,\,\hbar,\,0,\,0,\,x) \\ &= [B(x\,\cos(t) + p\,\sin(t)) + iA(-x\,\sin(t) + p\,\cos(t))]\,U(t)\,\varphi_0(A,\,B,\,\hbar,\,0,\,0,\,x) \\ &= [(B\cos(t) - iA\sin(t))x + i(A\cos(t) - iB\sin(t))\,p]\,U(t)\,\varphi_0(A,\,B,\,\hbar,\,0,\,0,\,x). \end{aligned} \tag{5.8}$$

If we choose $t = \theta$, the coefficients of x and p inside the square brackets have the same complex phase. This is equivalent to

$$[\,\gamma\,x + i\,\delta\,p\,]\;U(t)\,\varphi_0(A,\,B,\,\hbar,\,0,\,0,\,x) = 0,$$

where γ and δ are real. This implies $U(t)\,\varphi_0(A,\,B,\,\hbar,\,0,\,0,\,x)$ is a phase times a real Gaussian, and that it consequently minimizes $\Delta x\,\Delta p$. Undoing the rotation of phase space shows that $\varphi_0(A,\,B,\,\hbar,\,0,\,0,\,x)$ minimizes the uncertainty product of $\Delta\alpha\,\Delta\beta$.

Requiring the coefficients in (5.8) to have the same phases is equivalent to solving (5.6) and equivalent to solving the eigenvalue problem of Section 2.

REMARK 5.4. If one is not interested in the value of θ, but only its existence, the portion of the proof after equation (5.6) can be replaced by the following:

It suffices to prove that equation (5.6) is satisfied for some t. All rotations of $\mathbb{R}^2$ are symplectic, and the rotation group $SO(2)$ is compact. So, there exists a value of t at which $g(t) = \left(\mathrm{Im}\,(B(t)\overline{A(t)})\right)^2$ takes its minimum. At that minimum, $\dot{g}(t) = 2\,g(t)\,(|A(t)|^2 - |B(t)|^2)$ must be zero. So, $g(t) = 0$ or $(|A(t)|^2 - |B(t)|^2) = 0$. If $g(t) \neq 0$, we must have $(|A(t)|^2 - |B(t)|^2) = 0$, and in that case, it follows from explicit calculation that $\ddot{g}(t) = -8\,g(t)^2 < 0$. This cannot happen at a minimum, so we conclude that $g(t)$ must be zero.

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