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Minimum-uncertainty angular wave packets and quantized mean values

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Uncertainty relations between a bounded coordinate operator and a conjugate momentum operator frequently appear in quantum mechanics. We prove that physically reasonable minimum-uncertainty solutions to such relations have quantized expectation values of the conjugate momentum. This implies, for example, that the mean angular momentum is quantized for any minimum-uncertainty state obtained from any uncertainty relation involving the angular-momentum operator and a conjugate coordinate. Experiments specifically seeking to create minimum-uncertainty states localized in angular coordinates therefore must produce packets with integer angular momentum.

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The use of angular-coordinate and phase operators in quantum mechanics requires more care than perhaps might be expected. Consider the relatively simple example of a particle moving on a circle of unit radius. Classically, a point particle is necessarily located at a single value of the periodic angular coordinate $\phi_p \in (-\pi,\pi]$. The corresponding quantum wave function, however, is an object extended around the circle and so can be directly affected by the nontrivial topology. A simple consequence is that, in contrast to the continuous spectrum of the linear momentum of a free particle on a (topologically trivial) line, the angular momentum $L \equiv -i\partial_\phi$ (in units with $\hbar=1$) on the circle has a point spectrum imposed by the dual requirements of continuity and periodicity of the eigenstates. A more subtle consequence is difficulty in defining an angular-coordinate operator. The direct use at the quantum level of the classical coordinate ϕ_p causes trouble at $\phi_p=\pi$, where any derivatives of ϕ_p acquire δ-function contributions from the discontinuity. For example, the Dirac-type [1,2] commutator relation $[L,\phi]=-i$ is problematic for $\phi\equiv\phi_p$. The attempt to circumvent this by using instead a continuous variable $\phi\equiv\phi_c \in(-\infty,\infty)$ is also unsatisfactory because single-valuedness restricts the Hilbert space to the subspace of 2π-periodic functions, which *inter alia* excludes the coordinate ϕ_c as an observable.

Many of the difficulties arising from the use of ϕ_p or ϕ_c can be sidestepped by selecting instead angular coordinates that are *both* periodic and continuous. However, a single such quantity cannot uniquely specify a point on the circle because periodicity implies extrema, which excludes a one-to-one correspondence and hence is incompatible with uniqueness. A relatively simply choice [3] is to adopt *two* angular-coordinate operators $\hat{\cos}\phi$ and $\hat{\sin}\phi$, defined to satisfy the commutation relations

$$[L,\hat{\cos}\phi]=i\ \hat{\sin}\phi, \quad [L,\hat{\sin}\phi]=-i\ \hat{\cos}\phi. \tag{1}$$

Classically, this would correspond to the identification $(x,y)\rightarrow(\cos\phi,\sin\phi)$ on the unit circle.

Even with periodic and continuous coordinates, some difficulties may remain. In the Hilbert space of square-integrable functions on the circle, where the angular-momentum operator is unbounded below and above, the action of the operators $\hat{\cos}\phi$ and $\hat{\sin}\phi$ on a state can be defined by multiplication by $\cos\phi$ and $\sin\phi$, respectively. This implies the commutator $[\hat{\cos}\phi,\hat{\sin}\phi]=0$. However, in a more general context where the operator conjugate to the coordinates is bounded below or above, the introduction of suitable coordinate operators involves further subtleties. An example is the harmonic-oscillator number operator N, for which the coordinate operators $\hat{\cos}\phi$ and $\hat{\sin}\phi$ defined by analogs of Eq. (1) do not commute [4–12]. Moreover, the use of cosine and sine operators may in general be inadequate to treat all physically interesting quantities [13].

Uncertainty relations involving the angular momentum are affected by the choice of angular-coordinate operators. Define for each operator X and state $|\chi\rangle$ the uncertainty

$$\Delta X \equiv [\langle X^2\rangle - \langle X\rangle^2]^{1/2}. \tag{2}$$

The Robertson-type [14] uncertainty relation

$$\Delta L \Delta\phi_p \geq \tfrac{1}{2} \tag{3}$$

is incorrect for several reasons. For example, since $\Delta\phi_p$ is bounded within a maximum, there is a physically acceptable limit with sufficiently small ΔL that produces a violation of the inequality. An alternative for $\phi\equiv\phi_p$ involves modifying the definition of $\Delta\phi_p$ or taking into account the appearance of δ-function contributions at $\phi_p=\pi$. This yields a more complicated form of the uncertainty relation [15–17]

$$\Delta L \frac{\Delta\phi_p}{1-3(\Delta\phi_p)^2/\pi^2} \geq \tfrac{1}{2} f(\Delta\phi_p), \tag{4}$$

where $f(\Delta\phi_p)$ varies from $f=1$ at $\Delta\phi_p=0$ to $f\simeq 4.375$ at $\Delta\phi_p=\pi/\sqrt{3}$. If instead one chooses the angular coordinates

$\hat{\cos}\phi$ and $\hat{\sin}\phi$, then the commutators (1) result in yet another set of angular-momentum uncertainty relations

$$\Delta L\ \Delta\hat{\cos}\phi \geq \tfrac{1}{2}|\langle\hat{\sin}\phi\rangle|, \quad \Delta L\ \Delta\hat{\sin}\phi \geq \tfrac{1}{2}|\langle\hat{\cos}\phi\rangle|. \quad (5)$$

In the present work, we focus in particular on minimum-uncertainty solutions to uncertainty relations involving angular or phase coordinates [18]. In topologically trivial situations such as the free particle or the harmonic oscillator, minimum-uncertainty solutions to the uncertainty relations for the position and momentum operators X and P exist in the Hilbert space for arbitrary finite expectation values of $\langle X\rangle$ and $\langle P\rangle$. Naively, one might expect that minimum-uncertainty packets for angular coordinates and their conjugate momentum also have continuously adjustable mean values. However, this intuition is incorrect. Although the detailed form of the minimum-uncertainty solutions depends on the particular angular-coordinate uncertainty relations involved, it turns out that minimum-uncertainty packets generically exist only for *quantized* expectation values of the associated conjugate momentum.

In what follows, we provide a detailed proof of this result and discuss some consequences. We begin with a discussion of limitations on the uncertainty of a general self-adjoint operator and then turn our attention to the stronger constraint that follows for certain operators from the requirement of minimum uncertainty imposed via an uncertainty relation. Finally, we discuss some examples and extensions of the results.

The analysis uses a number of basic results in the theory of linear operators on Hilbert spaces [19]. The following summarizes some of our notation. Let A be a self-adjoint operator in a Hilbert space with domain $\mathscr{D}(A)$ and let z be a complex number that is *not* an eigenvalue of A. Then, the associated resolvent operator $R(z,A)\equiv(A-z)^{-1}$ is well defined. The resolvent set ρ is comprised of those values of z for which $R(z,A)$ is bounded. The spectrum of A is $\sigma\equiv\mathscr{C}/\rho$. It contains two components: the point spectrum σ_p, consisting of the eigenvalues of A; and the remainder, which we call the continuum and denote by σ_c. We refer to the spectrum as discrete in the special case where it consists entirely of isolated eigenvalues with finite multiplicities. Also, by definition the extended discrete spectrum of an unbounded operator differs from the spectrum by the addition of the point at infinity.

Consider a self-adjoint operator A on a Hilbert space $\mathscr{H}$. For an element $\psi\in\mathscr{D}(A^2)$, the uncertainty ΔA_ψ defined by Eq. (2) is the norm $\|(A-\langle A\rangle)|\psi\rangle\|$. First, we examine the possibility of varying to zero the uncertainty while keeping fixed the expectation. We are therefore interested in a sequence $\{|n\rangle\}$ of unit-normalized states convergent in the Hilbert space such that $\langle A\rangle\equiv\langle n|A|n\rangle\equiv\alpha\in\mathscr{R}$ is constant and such that $\lim_{n\to\infty}\Delta A_n=0$.

Now, α is in the point spectrum σ_p, in the continuum σ_c, or in the resolvent ρ. If α is in the point spectrum, there must exist a unit-normalized state $|\psi\rangle\in\mathscr{D}(A)$ such that $A|\psi\rangle=\alpha|\psi\rangle$. It is then in general possible to find convergent sequences of the desired type. In particular, the constant sequence $\{|n\rangle=|\psi\rangle\forall n\}$ satisfies the requirements. Nonconstant convergent sequences may also exist. If, however, α is in the continuum σ_c then there may exist sequences with uncertainty approaching zero, but they cannot converge. This follows from a theorem for self-adjoint operators on Hilbert spaces [19] stating that if there exists a convergent sequence of unit-normalized states such that $(A-\alpha)|n\rangle\to 0$ as $n\to\infty$, then $\alpha\in\sigma_p$. Moreover, if instead α lies in the resolvent ρ, the desired sequences cannot exist. This follows from another theorem for self-adjoint operators [19] stating that for unit-normalized states in the domain of A and for $\alpha\in\rho$ the norm $\|(A-\alpha)|n\rangle\|$ is greater than a positive constant c. One way of seeing this last result is that if such a sequence did exist, then in the limit $\Delta A\to 0$ for which $c\to 0$ the resolvent operator $R(\alpha,A)$ could not be bounded, contradicting the assumption $\alpha\in\rho$.

The above results already establish, independently of any uncertainty relation, that the uncertainty of a self-adjoint operator cannot be dialed to zero while maintaining constant expectation unless the expectation value is an eigenvalue. From the physical viewpoint, however, there are two reasons why this is less restrictive than it might appear. First, the result does not preclude the possibility that for a given situation the uncertainty could be dialed close to zero, i.e., the constant c might be very small. Second, the result assumes convergence of the sequence in the Hilbert space, which may not be the case in all situations of physical interest. For example, the position operator on the line has no point spectrum and therefore by the above argument no constant-expectation packet can be constructed with uncertainty that can be varied to reach zero. Thus, the above argument excludes a freely evolving Gaussian packet because the limiting state is a δ function, which is not a state in the Hilbert space.

We next show that for certain operators the result can be substantially strengthened if we take into account minimum-uncertainty constraints arising from an uncertainty relation. We are interested in particular in the situation of minimum-uncertainty wave packets for which the uncertainty relation connects a bounded operator B with an operator A having a discrete spectrum. Operators of these types frequently occur in physics. For example, B could represent the coordinate operator on a compact manifold without boundary, such as the n sphere, with A being the associated operator for the (angular) momentum.

Consider two self-adjoint operators A and B, defined in a Hilbert space $\mathscr{H}$ and satisfying

$$[A,B]=iC \quad (6)$$

on a subspace of $\mathscr{H}$. We assume A has a discrete spectrum and B is bounded. The uncertainty relation obeyed by these operators for any given state is [20]

$$\Delta A\Delta B\geq\tfrac{1}{2}|\langle C\rangle|. \quad (7)$$

We seek minimum-uncertainty solutions $|\psi\rangle$ of Eq. (7), defined as normalized solutions of the limiting equality. In general, such solutions are called squeezed states [21]. They are in one-to-one correspondence with solutions $|\psi\rangle$ of the equation [20]

$$(A-\alpha)|\psi\rangle=iS(B-\beta)|\psi\rangle, \quad (8)$$

where $\alpha=\langle A\rangle,\beta=\langle B\rangle$, and

$$S \equiv \Delta A/\Delta B = |\langle C\rangle|/2(\Delta B)^2 \tag{9}$$

is a real constant called the squeezing. The reality of α, β, and S follows from the assumption that A, B, and C are self-adjoint (observable).

Suppose α is in the resolvent set ρ of A. Then, Eq. (8) can be expressed in terms of the resolvent operator $R(\alpha,A)$ as

$$[iSR(\alpha,A)(B-\beta)-1]|\psi\rangle = 0. \tag{10}$$

This is an eigenvalue equation for the operator $X \equiv iSR(\alpha,A)(B-\beta)$. Since A has discrete spectrum and since the spectrum $\sigma(R)$ of the resolvent operator $R(\alpha,A)$ can be obtained [22] from the extended spectrum $\tilde{\sigma}(A)$ of A via the transformation $f(\lambda)=(\lambda-\alpha)^{-1}$ for $\lambda \in \tilde{\sigma}(A)$, it follows that $\sigma(R)$ is bounded and consists of isolated eigenvalues of finite multiplicity possibly accumulating only at zero. The resolvent operator $R(\alpha,A)$ is therefore compact. Since by assumption B is bounded, it follows that X itself is also compact. Thus, the spectrum of X is also bounded and consists of isolated eigenvalues with finite multiplicity that can accumulate only at zero. Since one must be an eigenvalue of X, this means that there can be at most a finite number of squeezed states with fixed α and β for which S lies below any given value. In fact, not only are such solutions finite in number by they are also generically rare: they are in one-to-one correspondence with the eigenvalues of $R(\alpha,A)(B-\beta)$ lying on the imaginary axis of the complex plane.

For $\langle A\rangle \in \rho$, the above argument excludes the existence of squeezed states allowing the dialing of S and hence of ΔA to zero. In fact, the same argument shows there is no possibility in *any* interval of dialing the minimum-uncertainty values ΔA at constant $\langle A\rangle$, unless $\langle A\rangle$ is in the spectrum of A. For an operator that has a spectrum without a continuum, it follows that any physically reasonable minimum-uncertainty wave packet must have quantized mean value. In particular, the angular momentum of a minimum-uncertainty wave packet on the circle must be integer valued.

With the main proof completed, we can illustrate some of the ideas via an explicit example. Consider the special case of circular squeezed states (CSS) used in Ref. [23] for the construction of elliptical squeezed states following a classical keplerian orbit in a planar Rydberg atom. The CSS are minimum-uncertainty states in the Hilbert space $\mathscr{H}=L^2(S^1)$ on the circle, determined from the uncertainty relations (7) with the identifications $A \equiv L = -i\partial_\phi$, $B \equiv \hat{\sin}\phi$, and $C \equiv \hat{\cos}\phi$, where $\hat{\sin}\phi$ and $\hat{\cos}\phi$ are defined via multiplication by $\sin\phi$ and $\cos\phi$, respectively. To obtain a packet centered about the point with $x=1$ on the unit circle, we impose $\langle\hat{\sin}\phi\rangle=0$ and $\langle\hat{\cos}\phi\rangle>0$. The solution of Eq. (8) is

$$|S\rangle = \left(\frac{1}{2\pi I_0(2S)}\right)^{1/2} \exp(S\cos\phi + i\langle L\rangle\phi), \tag{11}$$

where S is the squeezing. In the limit $S\to 0$,

$$|S\rangle \to |S_0\rangle = \left(\frac{1}{2\pi}\right)^{1/2} \exp(i\langle L\rangle\phi), \tag{12}$$

which is an angular-momentum eigenstate with eigenvalue $\langle L\rangle$. According to our result, $\langle L\rangle$ must be integer for the solutions $|S\rangle$ to exist. In the context of the limit in Eq. (12), this agrees with the usual requirement of quantized eigenvalues for eigenstates of L. It can also be seen directly from Eq. (11) to be necessary since $|S\rangle$ is required to be periodic in ϕ with period 2π to remain consistently defined [24].

As another example, consider the number operator N for the harmonic oscillator. This operator has a discrete spectrum. Our analysis therefore shows that the expectation $\langle N\rangle$ is integer valued for any state minimizing an uncertainty relation involving N and a (bounded) phase operator.

The stronger constraints we have obtained above make use of the uncertainty relation Eq. (7). For the special case where A is the angular-momentum operator on the circle, the alternative form (4) of the uncertainty relation might be considered instead. In this equation, ΔL may be interpreted as usual, but the definition of $\Delta\phi_p$ involves determining the minimum in a real parameter γ of a functional of ϕ_p:

$$(\Delta\phi_p)^2 \equiv \min_\gamma \int_{-\pi}^{\pi} d\phi_p\ \psi^*(\phi_p+\gamma)\phi_p^2\psi(\phi_p+\gamma). \tag{13}$$

Next, we show that the requirement of discrete $\langle L\rangle$ extends to this case also.

Let a general wave function on the circle be written as

$$\psi(\phi_p) = r(\phi_p)\exp[i\theta(\phi_p)], \tag{14}$$

with $r(\phi_p)$ and $\theta(\phi_p)$ both real functions, not necessarily positive. Suppose $r(\phi_p)$ is kept fixed, which also fixes $\Delta\phi_p$. Then, the minimum value of ΔL can be obtained by varying with respect to $\theta(\phi_p)$. A short calculation shows that the minimum is attained if $\theta(\phi_p)$ is linear in ϕ_p. The requirement of periodicity on ψ then restricts the possible choices to $\theta(\phi_p)=m\phi_p+k$, where m is integer or half-integer and k is a constant. For these choices, it can also be shown that $\langle L\rangle=m$. This means that any minimum-uncertainty packet based on (4) must also have a discrete value of $\langle L\rangle$.

The case of integer m has been pursued in detail in Ref. [17], where solutions are shown to exist and $f(\Delta\phi_p)$ is numerically computed. In this case, the value of ΔL can be continuously dialed to zero for solutions with fixed integer $\langle L\rangle$. Whether or not solutions exist for half-integer m, they could not have a value of ΔL less than the limiting value. In this case, the limiting value turns out to be $\Delta L=1/2$.

The suggestion has also been made of combining the idea of well-defined angular coordinates with the idea of more complicated uncertainty relations [25]. The uncertainty in the conjugate coordinate to the angular-momentum operator is defined as

$$\Delta\phi \equiv \left(\frac{(\Delta\ \hat{\cos}\phi)^2+(\Delta\ \hat{\sin}\phi)^2}{\langle\hat{\cos}\phi\rangle^2+\langle\hat{\sin}\phi\rangle^2}\right)^{1/2}, \tag{15}$$

which ranges from zero to infinity. The associated uncertainty relation is

$$\Delta L\Delta\phi > \tfrac{1}{2}, \tag{16}$$

a relation that follows directly [5] from the two uncertainty relations (5). In Eq. (16), the value $\frac{1}{2}$ cannot be attained. This is a reflection of the impossibility of simultaneously solving for the two equalities (5), which in turn is a reflection of rotational invariance [23]. Following the construction of the CSS, we can seek a minimum-uncertainty solution centered about $x=1$ by setting $\langle \widehat{\sin\phi} \rangle = 0$. Equation (16) then reduces to a weakened version of the second inequality in Eq. (5), which itself must still hold. So the corresponding minimum-uncertainty solution is again a CSS, which has quantized values of $\langle L \rangle$.

The general result that any minimum-uncertainty state has discrete angular-momentum expectation holds for any macroscopic body viewed as the limit of a large quantum system. Taken to the macroscopic limit this means, for example, that any macroscopic object either has an integer-valued angular momentum or is not in a state of minimum angular uncertainty.

The issue of the physically correct form of the uncertainty relations and its implications is of more than theoretical interest. In recent years, striking results have been found in the behavior of minimum-uncertainty packets. For example, minimum-uncertainty radial electron wave packets in Rydberg atoms have been shown to evolve through a complex sequence of revivals, fractional revivals, and super revivals [26–30]. Specific attention has been given recently to creating in the laboratory packets with minimum uncertainty in an angular coordinate. For example, experimental efforts are presently underway to produce such packets orbiting the nucleus of a Rydberg atom [31,32]. Localized packets with noninteger angular-momentum expectation can certainly be created, for example, by superposing angular-momentum eigenstates with a gaussian weighting of coefficients with noninteger mean value. However, our analysis shows that any such packets cannot have minimum angular uncertainty. Experiments performed to study the classical limit of quantum mechanics via the behavior of minimum-uncertainty angular packets must of necessity involve states with integer angular momentum.

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