Exact uncertainty relations

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Abstract

The Heisenberg inequality $\Delta X \Delta P \geq \hbar/2$ can be replaced by an exact equality, for suitably chosen measures of position and momentum uncertainty, which is valid for all wavefunctions. The statistics of complementary observables are thus connected by an “exact” uncertainty relation. Results may be generalised to angular momentum and phase, photon number and phase, time and frequency, and to states described by density operators. Connections to energy bounds, entanglement, Wigner functions, and optimal estimation of an observable from the measurement of a second observable are also given.
I INTRODUCTION

One of the most striking features of quantum mechanics is the property that certain observables cannot simultaneously be assigned arbitrarily precise values. This property does not compromise claims of completeness for the theory, since it may consistently be asserted that such observables cannot simultaneously be measured to an arbitrary accuracy \[1\]. The Heisenberg inequality

\[
\Delta X \Delta P \geq \hbar / 2 \tag{1}
\]

is therefore generally taken to reflect an essential incompleteness in the applicability of classical concepts of position and momentum to physical reality.

It was recently noted that this fundamental inequality can be greatly strengthened - the degree to which classical concepts are inapplicable can, surprisingly, be quantified exactly. In particular, one may define a measure of position uncertainty \(\delta X\) (which arises naturally in classical statistical estimation theory), and a measure of nonclassical momentum uncertainty \(\Delta P_{nc}\) (which arises from a natural decomposition of the momentum operator), such that \[2\]

\[
\delta X \Delta P_{nc} = \hbar / 2 \tag{2}
\]

for all wavefunctions. Such an equality may be regarded as an exact uncertainty relation, and may be shown to imply the usual Heisenberg inequality Eq. \((1)\). Thus, perhaps paradoxically, the uncertainty principle of quantum mechanics may be given a precise form.

In Ref. \[2\] the above exact uncertainty relation was merely noted in passing, with the emphasis being on other properties of \(\delta X\) and \(\Delta P_{nc}\). Similarly, while the very existence of an exact form of the uncertainty principle was recently shown to provide a sufficient basis for moving from classical equations of motion to the Schrödinger equation \[3\], the corresponding exact uncertainty relation Eq. \((2)\) was only briefly mentioned. The purpose of this paper, therefore, is to study the physical significance of Eq. \((2)\) in some detail, including its extensions to other pairs of conjugate observables and to general states described by density operators.

In the following section it is shown that quantum observables such as momentum, position, and photon number have a natural decomposition, into the sum of a classical and a nonclassical component. The classical component corresponds to the best possible measurement of the observable, on a given state, which is compatible with measurement of the conjugate observable. Complementarity implies that the classical component cannot be equivalent to the observable itself, i.e., there is in general an nontrivial
nonclassical component. It is this nonclassical component which reflects the mutual incompatibility of pairs of conjugate observables, and the magnitude of which appears in the exact uncertainty relations to be derived [e.g., $\Delta P_{nc}$ in Eq. (2)]. The decomposition into classical and nonclassical components is also related in a natural manner to quantum continuity equations and to quasiclassical properties of the Wigner function.

In Sec. III a measure of uncertainty is defined for continuous random variables such as position, which plays a fundamental role in classical estimation theory and in Gaussian diffusion processes. This measure, the “Fisher length” of the variable, may of course be calculated for quantum observables as well, and appears as $\delta X$ in the exact uncertainty relation in Eq. (2).

The ingredients of classical/nonclassical decompositions and Fisher lengths are combined in Sec. IV to obtain a number of exact uncertainty relations, such as Eq. (2) and the equality

$$\delta \Phi \Delta N_{nc} = 1/2$$

for phase and photon number, valid for all pure states. These relations generalise to inequalities for states described by density operators, and are far stronger than the corresponding Heisenberg-type inequalities. A simple proof is given of the property that localised quantum states have infinite kinetic energy (arising from the contribution of the nonclassical momentum component), and it is shown that a bound on Fisher length leads to an entropic lower bound for the groundstate energies of quantum systems.

In Sec. V it is shown that the decomposition of an observable of a given quantum system into classical and nonclassical components is essentially nonlocal in nature, being dependent in general on manipulations performed on a second system with which the first is entangled. The significance of the relevant exact uncertainty relations is discussed, with particular reference to EPR-type states.

A formal generalisation of exact uncertainty relations, to arbitrary pairs of quantum observables, is noted in Sec. VI. Moreover, it is shown that a result of Ivanovic [4], for complete sets of mutually complementary observables on finite Hilbert spaces (such as the Pauli spin matrices), may be reinterpreted as an exact uncertainty relation for the “collision lengths” of the observables.

Conclusions are given in Sec. VII.
II CLASSICAL AND NONCLASSICAL COMPONENTS OF QUANTUM OBSERVABLES

A Classical momentum

The nonclassical momentum uncertainty $\Delta P_{nc}$ appearing in Eq. (2) is defined via a natural decomposition of the momentum observable $P$ into "classical" and "nonclassical" components,

$$P = P_{cl} + P_{nc}. \quad (3)$$

This decomposition is state-dependent, and will be defined explicitly further below. In particular, it will be shown that the classical component, $P_{cl}$, corresponds to the best possible estimate of momentum, for a given quantum state, which is compatible with a position measurement. It will be seen further below that $P_{cl}$ is also related to the momentum flow in the classical continuity equation for the position probability density, and to an average momentum arising naturally from quasiclassical properties of the Wigner function. However, it is the "best estimate" interpretation above that provides the most general basis for generalisation to other observables.

As a starting point, recall that in classical mechanics one can simultaneously obtain precise values for position and momentum, whereas in quantum mechanics one must choose to accurately measure either one or the other. It is therefore reasonable to ask the following question: If I measure one of these observables precisely, on a known quantum state, then what is the best estimate I can make for the value of the other observable? Such an estimate of momentum from the measurement of position will be called a classical estimate of $P$, since it assigns simultaneous values to $X$ and $P$.

It will be shown that the best classical estimate of $P$, given the measurement result $X = x$ on a quantum system described by wavefunction $\psi(x)$, is given by

$$P_{cl}(x) = \frac{\hbar}{2i} \left( \frac{\psi'(x)}{\psi(x)} - \frac{\psi''(x)}{\psi^*(x)} \right) = \hbar \arg \psi(x)''. \quad (4)$$

More generally, for a quantum system described by density operator $\rho$, one has

$$P_{cl}(x) := \frac{\langle x|P\rho + \rho P|x\rangle/2}{\langle x|\rho|x\rangle}, \quad (5)$$

which reduces to the first expression for $\rho = |\psi\rangle\langle \psi|$. The experimentalist’s procedure for measuring the classical momentum component for state $\rho$ is thus to (i) prepare the system in state $\rho$; (ii) measure
the position $X$; and (iii) for result $X = x$ calculate $P_{cl}(x)$. Note that this is equivalent to measurement of the Hermitian operator

$$P_{cl} = \int dx \, P_{cl}(x) |x\rangle \langle x|$$

on state $\rho$, which by construction commutes with $X$. Hence the statistics of $P_{cl}$ are determined by those of $X$. As stated above, this procedure yields the best possible estimate of the momentum of the system that is compatible with simultaneous knowledge of the position of the system.

To prove that $P_{cl}(x)$ provides the best classical estimate of $P$, consider some general classical estimate for momentum for state $\rho$. Since this estimate must by definition be compatible with the measurement of $X$, it is formally equivalent to the measurement of some operator $\tilde{P} = \int dx \, \tilde{P}(x) |x\rangle \langle x|$. The average error of the estimate may therefore be quantified by the mean deviation of $\tilde{P}$ from the momentum operator $P$,

$$\mathcal{E}_P := \langle (P - \tilde{P})^2 \rangle,$$

where $\langle A \rangle$ denotes the expectation value $\text{tr}[\rho A]$.

Using the cyclic property of the trace operation and evaluating the trace in the position representation gives

$$\langle \tilde{P}P + P\tilde{P} \rangle = \int dx \, \langle x| \tilde{P}P|\rho \rangle + \rho P\tilde{P}|x\rangle$$

$$= \int dx \, \tilde{P}(x) \langle x| P|\rho \rangle + \rho P|x\rangle$$

$$= 2 \int dx \, \langle x| \rho |x\rangle \tilde{P}(x) P_{cl}(x) = 2 \langle \tilde{P}P_{cl} \rangle,$$

and hence

$$\mathcal{E}_P = \langle P^2 \rangle + \langle \tilde{P}^2 \rangle - 2\langle \tilde{P}P_{cl} \rangle$$

$$= \langle P^2 \rangle - \langle P_{cl}^2 \rangle + \langle (\tilde{P} - P_{cl})^2 \rangle.$$ 

Since the last term is positive, the average error is minimised by the choice $\tilde{P} = P_{cl}$ as claimed.

**B Nonclassical momentum**

The nonclassical momentum component $P_{nc}$ is now defined via Eq. (3), as the difference of the quantum momentum $\hat{P}$ and the classical momentum $P_{cl}$.
From Eq. (5) one finds that the expectation values of the observables $P$ and $P_{cl}$ are always equal (for the corresponding state $\rho$), and so

$$\langle P \rangle = \langle P_{cl} \rangle, \quad \langle P_{nc} \rangle = 0.$$  

(9)

The quantum momentum $P$ in Eq. (3) can therefore also be interpreted as the sum of an average momentum $P_{cl}$, and a nonclassical momentum fluctuation $P_{nc}$.

The magnitude of this nonclassical fluctuation is simply related to the minimum average error for a classical estimate: choosing $\bar{P} = P_{cl}$ in Eqs. (7) and (8) yields

$$\langle P_{nc}^2 \rangle = E_{P}^{\text{min}} = \langle P^2 \rangle - \langle P_{cl}^2 \rangle.$$  

(10)

It will be seen that, as a consequence of the exact uncertainty relation Eq. (2), this minimum error does not vanish for any state (although it may be arbitrarily small), and hence there is always a residual amount of nonclassicality. Note from Eqs. (3) and (10) that the fluctuation strength $\Delta P_{nc}$ in Eq. (2) is a fully operational quantity, as it may be determined from the measured distributions of $P$ and $P_{cl}$ (and hence from the measured distributions of $P$ and $X$).

Finally, since the decomposition into classical and nonclassical components is state dependent, $P_{cl}$ and $P_{nc}$ should, strictly speaking, explicitly indicate their dependence on a given state $\rho$ (e.g., via the notation $P_{cl}^\rho$ and $P_{nc}^\rho$ respectively). This would in particular be necessary if one wished to evaluate expectation values such as $\text{tr}[\sigma P_{cl}^\rho]$, for some density operator $\sigma$ other than $\rho$. However, expectation values will in fact only be evaluated for the corresponding state $\rho$ throughout this paper, and hence explicit notational dependence on the state may be conveniently dispensed with, without leading to ambiguity.

C Physical significance

It is seen that the classical momentum is the closest possible observable momentum observable $P$ (in a statistical sense), under the constraint of being co-measurable with the conjugate position observable $X$. The nonclassical momentum is then simply defined as the difference between the quantum momentum and the classical momentum. A similar approach can be used to define corresponding decompositions of the position, angular momentum, and photon number observables.

The decomposition in Eq. (4) attempts to demarcate classical and nonclassical momentum properties. It is therefore reasonable to hope that the
nonclassical component $P_{\text{nc}}$ in particular might play a fundamental role in describing the essence of what is “quantum” about quantum mechanics. This is indeed the case. A derivation of the Schrödinger equation as a consequence of adding a nonclassical momentum fluctuation to a classical ensemble (with strength inversely proportional to the uncertainty in position), has recently been given [3]. In this paper it will be shown that the nonclassical components of quantum observables satisfy exact uncertainty relations, such as Eq. (2), and hence allow one to precisely quantify the fundamental uncertainty principle of quantum mechanics. It will further be shown that the decomposition of observables into classical and nonclassical components helps to distinguish between local and nonlocal features of quantum entanglement.

Several formal properties further support the physical significance of the decomposition in Eq. (3). First, the classical and nonclassical components are linearly uncorrelated, i.e.,

$$\text{Var} P = \text{Var} P_{\text{cl}} + \text{Var} P_{\text{nc}},$$

as follows immediately from Eqs. (9) and (10). This implies a degree of statistical, and hence physical, independence for $P_{\text{cl}}$ and $P_{\text{nc}}$. The same equations imply that the kinetic energy splits into a classical part, $\langle P_{\text{cl}}^2/(2m) \rangle$ and a nonclassical part, $\langle P_{\text{nc}}^2/(2m) \rangle$. Note from Eq. (4) that the former contribution vanishes for stationary states, leaving only a nonclassical contribution to the kinetic energy of such states.

Second, the classical momentum component commutes with the conjugate observable $X$ while the nonclassical component does not, i.e.,

$$[X, P_{\text{cl}}] = 0, \quad [X, P_{\text{nc}}] = i\hbar.$$  

Hence it is the nonclassical component of $P$ which generates the fundamental quantum property $[X, P] = i\hbar$.

Third, when the decomposition is generalised to more than one dimension (see Sec. V.A), one finds for pure states that the commutativity property $[P_j, P_k] = 0$ for the vector components of momentum is preserved by the decomposition, i.e.,

$$[P_{\text{cl}}^j, P_{\text{cl}}^k] = 0 = [P_{\text{nc}}^j, P_{\text{nc}}^k].$$

Fourth, the classical momentum $P_{\text{cl}}(x)$ associated with position $X = x$ appears in the continuity equation [3]

$$\partial |\psi|^2 / \partial t + (\partial / \partial x) \left[ |\psi|^2 m^{-1} P_{\text{cl}}(x) \right] = 0$$

7
following from the Schrödinger equation, and hence $P_{cl}$ corresponds to the flow momentum of a classical ensemble of particles described by probability density $|\psi|^2$. This property suggests an alternative “dynamical” approach to defining classical/nonclassical decompositions such as Eq. (3). However, such an approach can generally only be applied to systems with Hamiltonians that are quadratic in the observable to be decomposed.

Finally a “quasiclassical” approach to the decomposition in Eq. (3) is noted, based on an analogy between classical phase space distributions and the Wigner function

$$W(x, p) := (2\pi\hbar)^{-1} \int d\xi e^{-i\xi/p}(x - \xi/2|\rho|x + \xi/2),$$

(14)

where the latter behaves, at least to some extent, like a joint probability density for position and momentum [6].

Now, for any true classical joint probability density $w(x, p)$ on phase space, the average classical momentum associated with position $x$ is given by $p_{cl}(x) = \int dp \text{prob}(p|x)$, where prob($p|x$) denotes the conditional probability that the momentum is equal to $p$ at position $x$, i.e., prob($p|x) = w(x, p)/\int dp w(x, p)$. The average classical momentum at position $x$ is thus

$$p_{cl}(x) = \frac{\int dp pw(x, p)}{\int dp w(x, p)}.$$ 

For quantum systems this immediately suggests defining an analogous average classical momentum associated with position $x$, via replacement of $w(x, p)$ by the Wigner function [6], to give

$$P_{cl}(x) := \frac{\int dp pW(x, p)}{\int dp W(x, p)}.$$ 

(15)

Remarkably, as shown elsewhere [6], this is in fact equivalent to the definition in Eq. (3) ! Note that this quasiclassical approach reinforces the interpretation of Eq. (3), that the momentum of a quantum particle comprises a nonclassical fluctuation $P_{nc}$ about a classical average $P_{cl}$.

One may similarly define a corresponding classical component for the position observable $X$, by interchanging the roles of $x$ and $p$ in Eq. (15). This agrees with the analogous definition based on Eq. (3), corresponding to the more generally applicable “best estimate” approach, and also with the definition given in Ref. [2] based on a semiclassical continuity equation.
III FISHER LENGTH

The uncertainty measure \( \Delta P_{nc} \) in Eq. (2) is now well defined - it is the rms uncertainty of the nonclassical momentum component \( P_{nc} \). However, it still remains to define the measure of position uncertainty \( \delta X \) in Eq. (2). This is done below for the general case of observables taking values over the entire set of real numbers, such as position and momentum. Note that \( \delta X \) is a purely classical measure of uncertainty, requiring no reference to quantum theory whatsoever.

For a random variable \( X \) which takes values over the whole range of real numbers, there are of course many possible ways to quantify the spread of the corresponding distribution \( p(x) \). Thus, for example, one may choose the rms uncertainty \( \Delta X \), the collision length \( 1/\int dx p(x)^2 \), or the ensemble length \( \exp[-\int dx p(x) \ln p(x)] \). All of these examples have the desirable properties of having the same units as \( X \), scaling linearly with \( X \), being invariant under translations of \( X \), and vanishing in the limit as \( p(x) \) approaches a delta function.

A further uncertainty measure satisfying the above properties is

\[
\delta X := \left[ \int_{-\infty}^{\infty} dx p(x) \left( \frac{d \ln p(x)}{dx} \right)^2 \right]^{1/2}.
\]  

While this measure may appear unfamiliar to physicists, it is in fact closely related to the well known Cramer-Rao inequality that lies at the heart of statistical estimation theory:

\[
\Delta X \geq \delta X.
\]  

Thus \( \delta X \) provides a lower bound for \( \Delta X \). Indeed, more generally, \( \delta X \) provides the fundamental lower bound for the rms uncertainty of any unbiased estimator for \( X \). The bound in Eq. (17) is tight, being saturated if and only if \( p(x) \) is a Gaussian distribution.

Eq. (17) is more usually written in the form \( \text{Var} X \geq 1/F_X \), where \( F_X = (\delta X)^{-2} \) is the “Fisher information” associated with translations of \( X \). It is hence appropriate to refer to \( \delta X \) as the Fisher length. From Eq. (16) it is seen that the Fisher length may be regarded as a measure of the length scale over which \( p(x) \) [or, more precisely, \( \ln p(x) \)] varies rapidly.

Basic properties of the Fisher length are: (i) \( \delta Y = \lambda \delta X \) for \( Y = \lambda X \); (ii) \( \delta X \to 0 \) as \( p(x) \) approaches a delta function; (iii) \( \delta X \leq \Delta X \) with equality only for Gaussian distributions; and (iv) \( \delta X \) is finite for all distributions.
This last property follows since the integral in Eq. (16) can vanish only if \( p(x) \) is constant everywhere, which is inconsistent with \( \int dx \, p(x) = 1 \).

The Fisher length has the unusual feature that it depends on the derivative of the distribution. Moreover, for this reason it vanishes for distributions which are discontinuous - to be expected from the above interpretation of \( \delta X \), since such distributions vary \textit{infinitely} rapidly over a zero length scale (\( \delta X = 0 \) may be shown by replacing such a discontinuity at point \( x_0 \) by a linear interpolation over an interval \([x_0 - \epsilon, x_0 + \epsilon]\) and taking the limit \( \epsilon \to 0 \)). The Fisher length also vanishes for a distribution that is zero over some interval (since \( \ln p(x) \) in Eq. (14) changes from \(-\infty\) to a finite value over any neighbourhood containing an endpoint of the interval). While these features imply that \( \delta X \) is not a particularly useful uncertainty measure for such distributions (similarly, \( \Delta X \) is not a particularly useful measure for the Cauchy-Lorentz distribution \((a/\pi)(a^2 + x^2)^{-1}\)), they are precisely the features that lead to a simple proof that the momentum uncertainty is infinite for any quantum system with a position distribution that is discontinuous or vanishes over some interval (as will be shown in Sec. IV).

One further property of Fisher length worthy of note is its alternative interpretation as a “robustness length”. In particular, suppose that a variable described by \( p(x) \) is subjected to a Gaussian diffusion process, i.e.,
\[
\dot{p} = \gamma p'' + \sigma p'
\]
for diffusion constant \( \gamma \) and drift velocity \( \sigma \). It then follows from Eq. (16) and de Bruijn’s identity (13) that the rate of entropy increase is given by
\[
\dot{S} = \gamma/\delta X^2.
\] (18)
Since a high rate of entropy increase corresponds to a rapid spreading of the distribution, and hence nonrobustness to diffusion, this inverse-square law implies that the Fisher length \( \delta X \) is a direct measure of robustness. Hence \( \delta X \) may also be referred to as a \textit{robustness length}. This characterisation of robustness is explored for quantum systems in Ref. [2].

Finally, note that Fisher length is not restricted to position observables, but may be calculated as per Eq. (16) for any observable which takes values over the entire set of real numbers, such as momentum. A Fisher length having similar properties may also be defined for periodic observables such as phase [8].
IV  EXACT UNCERTAINTY RELATIONS

A  Position and momentum

In the previous two sections the quantities $\Delta P_{nc}$ and $\delta X$ have been motivated and discussed on completely independent grounds. One is a measure of uncertainty for the nonclassical component of momentum, while the other is a measure of uncertainty for position that appears naturally in the contexts of classical statistical estimation theory and Gaussian diffusion processes.

It is a remarkable fact that for all pure states these two quantities are related by the simple equality in Eq. (2), repeated here for convenience:

\[
\delta X \Delta P_{nc} = \frac{\hbar}{2}.
\]  

(19)

Thus the Fisher length of position is inversely proportional to the strength of the nonclassical momentum fluctuation. Noting from Eqs. (11) and (17) that $\Delta P \geq \Delta P_{nc}$ and $\Delta X \geq \delta X$ respectively, the Heisenberg uncertainty relation

\[
\Delta X \Delta P \geq \frac{\hbar}{2}
\]

(20)

is an immediate consequence of this exact quantum uncertainty relation.

The existence of an exact uncertainty relation for position and momentum statistics greatly strengthens the usual statement of the uncertainty principle, from inequality to equality, and hence the measures of uncertainty in Eq. (19) may regarded as more fundamental in nature than those in Eq. (20). Moreover, the phase space area $\hbar/2$ is promoted in status, from a mere lower bound on joint uncertainty to an invariant quantity which precisely characterises the joint uncertainty of every wavefunction.

Thus, consider an ensemble of systems described by state $\psi$, on which independent measurements of $X$ and $P$ are made (on different subensembles). From these measurements one can determine the statistics of $X$ and $P$ [and hence also the statistics of $P_{cl}$ and the variance of $P_{nc}$, from Eqs. (3) and (11) respectively]. The Heisenberg uncertainty relation connects these statistics via an inequality - if one calculates $\Delta P$, then one knows only that $\Delta X \geq \hbar/(2\Delta P)$, where the difference between the lefthand and righthand sides depends on the particular wavefunction $\psi$ describing the ensemble. In contrast, the exact uncertainty relation provides an invariant equality connecting the statistics, where if one calculates the nonclassical momentum fluctuation $\Delta P_{nc}$, then one knows immediately that the Fisher length $\delta X$ is precisely equal to $\hbar/(2\Delta P_{nc})$, regardless of the particular wavefunction.

A simple proof of Eq. (19) was given in Ref. (2); a more general result, valid for density operators, is proved below. Before proceeding to the proof,
however, several simple consequences of the exact uncertainty relation in Eq. (19) will be noted.

First, recalling that \( \delta X \) vanishes for position distributions that are discontinuous or are zero over some interval (see Sec. III), it follows immediately from Eq. (19) that \( \Delta P_{\text{nc}} \) is infinite in such cases. From Eq. (11) the momentum uncertainty \( \Delta P \) is then also infinite. Note that this conclusion cannot be derived from the Heisenberg inequality Eq. (20), nor from the entropic uncertainty relation for position and momentum [15]. The exact uncertainty relation Eq. (19) is thus significantly stronger than the latter inequalities.

A second related consequence worth mentioning is a simple proof that any well-localized pure state, i.e., one for which the position distribution vanishes outside some finite interval, has an infinite energy (at least for any potential energy that is bounded below at infinity). This is immediately implied by the property

\[
E = (8m)^{-1}h^2(\delta X)^{-2} + \langle P_{\text{cl}}^2 \rangle / (2m) + \langle V(x) \rangle
\]

(following from Eqs. (10) and (19)), and noting that \( \delta X = 0 \) for such states. Note that this “paradox” of standard quantum mechanics (that there are no states which are both well-localised and have finite energy) is a consequence of the simple external potential model, rather than of some deep incompleteness of the theory. Note also that this property is purely quantum in nature, since the divergent term - the nonclassical part of the kinetic energy - vanishes in the limit \( \hbar \to 0 \).

Third, the property \( \delta X < \infty \) (see Sec. III) immediately implies from the exact uncertainty relation Eq. (19) that \( \Delta P_{\text{nc}} \) can never vanish, i.e.,

\[
\Delta P_{\text{nc}} > 0.
\]

Thus all pure states necessarily have a nonzero degree of nonclassicality associated with them [16]. This result is intuitively appealing, and provides further support for the physical significance of the classical and nonclassical components.

Fourth, for all real wavefunctions \( \psi(x) \), including energy eigenstates, one has \( P_{\text{cl}} \equiv 0 \) from Eq. (2). Hence the exact uncertainty relation reduces to the simpler identity

\[
\delta X \Delta P = \hbar / 2.
\]

This result holds more generally whenever the phase of \( \psi \) is at most linear in \( x \).
Eq. (19) for pure states will now be proved as a special case of the more general inequality

$$\delta X \Delta P_{nc} \geq \hbar/2,$$  

(24)

holding for states described by density operators. While not an exact uncertainty relation, this inequality is still much stronger than the corresponding Heisenberg inequality in Eq. (1). Not only is it saturated for all pure states (not just the “minimum uncertainty” states), but it implies that generalisations of the above consequences hold for any quantum state.

Inequality (24) is an immediate consequence of Eq. (10) and the relations

$$\frac{\hbar^2}{4(\delta X)^2} + \langle P_{cl}^2 \rangle = \int dx \frac{|\langle x|P\rho|x\rangle|^2}{\langle x|\rho|x\rangle} \leq \langle P^2 \rangle,$$  

(25)

which hold for all density operators \( \rho \). The equality in Eq. (25) is obtained by substituting Eqs. (5) and (6) for the classical momentum component \( P_{cl} \), and the representation

$$\langle x|P\rho - \rho P|x\rangle^2 = \langle x|\rho\rangle \langle x|\rho\rangle,$$  

(26)

for the Fisher length, following from the definition of \( \delta X \) in Eq. (16) and the identity \( (d/dx)\langle x|A|x\rangle = (i/\hbar)\langle x|[P,A]|x\rangle \) (derived by expanding in momentum eigenkets). The inequality in Eq. (25) is obtained by defining the states \( |\mu\rangle = \rho^{1/2}P|x\rangle, \ |
u\rangle = \rho^{1/2}|x\rangle \), and using the Schwarz inequality

$$|\langle x|P\rho|x\rangle|^2 = |\langle \mu|\nu\rangle|^2 \leq \langle \mu|\mu\rangle \langle \nu|\nu\rangle = \langle x|P\rho P|x\rangle \langle x|\rho|x\rangle.$$  

Remarkably, for the special case of a pure state, direct substitution of \( \rho = |\psi\rangle\langle \psi| \) into the integral in Eq. (25) yields equality on the right hand side, and hence the exact uncertainty relation Eq. (19).

Finally, note that whereas the Heisenberg inequality Eq. (20) is symmetric with respect to position and momentum, this symmetry is broken by the exact uncertainty relation Eq. (19). Instead, one has two (symmetrically related) exact uncertainty relations, given by Eq. (19) and the corresponding conjugate equality

$$\Delta X_{nc} \delta P = \hbar/2.$$  

(27)

The latter exact uncertainty relation is proved in a formally equivalent manner; similarly implies the Heisenberg inequality; requires the variance in position to be infinite for states with momentum distributions that are discontinuous or which vanish over a continuous range of momentum values; and implies that the variance of the nonclassical component of position is strictly positive.
B Energy bounds

Eqs. (10) and (24) immediately yield the lower bound

\[ E \geq (8m)^{-1} \hbar^2 (\delta X)^{-2} + \langle V \rangle \]  

(28)

for the average energy \( E \) of any state, where from Eq. (23) one has equality for all real wavefunctions. Thus energy bounds may be obtained via bounds on the Fisher length \( \delta X \).

A number of upper and lower bounds for the Fisher length are given by Dembo et al. [14], and by Romera and Dehesa [17], which hence yield corresponding bounds on energy. For example, the “isoperimetric inequality” \[ \delta X \leq (2\pi e)^{-1/2} e^{-S}, \]  

where \( S = -\int dx p(x) \ln p(x) \) is the position entropy, implies via Eq. (28) the general entropic lower bound

\[ E \geq (4m)^{-1} \pi \hbar^2 e^{-2S} + \langle V \rangle. \]  

(29)

Eq. (29) may be exploited to estimate groundstate energies, by maximising the position entropy for a given value of \( \langle V \rangle \). Note this gives a lower bound on \( E_0 \), in contrast to the usual upper bounds provided by variational methods. For example, for a harmonic oscillator with \( V(x) = m\omega^2 x^2 / 2 \), the entropy is well known to be maximised for a given value of \( \langle x^2 \rangle \) by a Gaussian distribution. Substituting such a distribution into Eq. (29) and minimising with respect to \( \langle x^2 \rangle \) then yields the estimate \( E_0 \geq \hbar \omega / 2 \), where the righthand side is in fact the correct groundstate energy (because the groundstate probability distribution is indeed Gaussian).

As a nontrivial example of Eq. (29), consider a particle bouncing in a uniform gravitational field, with \( V(x) = mgx \) for \( x \geq 0 \). For a fixed value \( \langle x \rangle = \lambda \) one finds that the entropy is maximised by the exponential distribution \( p(x) = \lambda^{-1} \exp(-x/\lambda) \), yielding the lower bound

\[ E \geq \pi \hbar^2 (4m\lambda^2)^{-1} + mg\lambda. \]

Minimising with respect to \( \lambda \) then gives the estimate

\[ E_0 \geq (3/2)[\pi/(2e)]^{1/3} (mg^2\hbar^2)^{1/3} \approx 1.249 (mg^2\hbar^2)^{1/3}, \]

which is comparable to the exact value of \( (mg^2\hbar^2)^{1/3} a_0 \approx 1.856 (mg^2\hbar^2)^{1/3} \) obtained by solving the Schrödinger equation [18], where \( a_0 \) denotes the first Airy function zero.
C  Phase, angular momentum and photon number

The decomposition of angular momentum and photon number into classical and nonclassical components is discussed in detail elsewhere \[8\]. One finds, for example, that the best estimate of photon number on state \(\rho\), which is compatible with a phase measurement result \(\Phi = \phi\), is given by (cf. Eq. (5))

\[
N_{cl}(\phi) = \frac{\langle \phi | N \rho + \rho N | \phi \rangle}{\langle \phi | \rho | \phi \rangle},
\]

where \(N\) is the photon number operator and \(|\phi\rangle\) is the Susskind-Glogower phase state \(\sum_n \exp(in\phi) |n\rangle\). One also has an additivity property \(\text{Var}N = \text{Var}N_{cl} + \text{Var}N_{nc}\) analogous to Eq. (11). A Fisher length \(\delta\Phi\) for the phase distribution is defined analogously to Eq. (16) (where integration is restricted to a reference interval of length \(2\pi\)), and satisfies a modified form of Cramer-Rao inequality \[8\].

The corresponding exact uncertainty relations are

\[
\delta\Phi \Delta J_{nc} = \hbar/2, \quad (30)
\]

\[
\delta\Phi \Delta N_{nc} = 1/2, \quad (31)
\]

for phase and angular momentum and for phase and photon number respectively, and are proved exactly as per Eq. (19) above for all pure states. For more general states described by density operators the righthand sides become lower bounds. These exact uncertainty relations are far stronger than the corresponding Heisenberg-type inequalities \[19\].

V  ENTANGLEMENT AND CORRELATION

A  Higher dimensions

Exact uncertainty relations for vector observables are of interest not only because the world is not one-dimensional, but because some physical properties, such as entanglement, require more than one dimension for their very definition. It is therefore indicated here how (4) may be generalised to the case of \(n\)-vectors \(X\) and \(P\). This case has also been briefly considered in Ref. \[2\]. For simplicity only pure states will be considered.

First, one has the vector decomposition

\[
P = P_{cl} + P_{nc} \quad (32)
\]
into classical and nonclassical components, where $\mathbf{P}_{cl}$ commutes with $\mathbf{X}$, and

$$
\mathbf{P}_{cl}(\mathbf{x}) = \langle \mathbf{x} | \mathbf{P}_{cl} | \mathbf{x} \rangle = \frac{\hbar}{2i} \left( \frac{\nabla \psi}{\psi} - \frac{\nabla \psi^*}{\psi^*} \right) = \hbar \nabla \text{[arg} \psi]}
$$

(33)

is the best estimate of $\mathbf{P}$ from measurement value $\mathbf{X} = \mathbf{x}$ for state $\psi$ (one may also derive $\mathbf{P}_{cl}(\mathbf{x})$ from a continuity equation or a Wigner function approach, as per Sec. II.C).

In analogy to Eqs. (9) and (11) one may derive

$$
\langle \mathbf{P} \rangle = \langle \mathbf{P}_{cl} \rangle
$$

and the generalized linear independence property

$$
\text{Cov}(\mathbf{P}) = \text{Cov}(\mathbf{P}_{cl}) + \text{Cov}(\mathbf{P}_{nc}),
$$

(34)

where the $n \times n$ covariance matrix of $n$-vector $\mathbf{A}$ is defined by the matrix coefficients

$$
[Cov(\mathbf{A})]_{jk} = \langle A_j A_k \rangle - \langle A_j \rangle \langle A_k \rangle.
$$

(35)

Note that since the vector components of $\mathbf{P}$ commute, as do the vector components of $\mathbf{P}_{cl}$, then

$$
[P_{nc}^j, P_{nc}^k] = [P^j - P_{cl}^j, P^k - P_{cl}^k] = (\hbar^2 / i) (\partial_j \partial_k - \partial_k \partial_j) \text{[arg} \psi] = 0,
$$

as claimed in Eq. (13).

The notion of Fisher length for one dimension generalises to the matrix inverse

$$
\text{FCov}(\mathbf{X}) := \left\{ \int d^n \mathbf{x} p(\mathbf{x}) [\nabla \ln p(\mathbf{x})] [\nabla \ln p(\mathbf{x})]^T \right\}^{-1},
$$

(36)

where $\mathbf{A}^T$ denotes the vector transpose of $\mathbf{A}$. For the case of one dimension this reduces to the square of the Fisher length $\delta X$, just as the covariance matrix in Eq. (17) reduces to the square of $\Delta A$. Moreover, as per the covariance matrix, the matrix in Eq. (36) is real, symmetric and nonnegative. Finally, the matrix is the inverse of the “Fisher information matrix” of statistical estimation theory [11]. For these reasons $\text{FCov}(\mathbf{X})$ will be referred to as the $\text{Fisher covariance matrix}$ of $\mathbf{X}$. One has the generalized Cramer-Rao inequality

$$
\text{Cov}(\mathbf{X}) \geq \text{FCov}(\mathbf{X}),
$$

(37)

with equality for Gaussian distributions.

One may show, via direct calculation of $\text{Cov}(\mathbf{P}_{cl})$, that the generalized exact uncertainty relation

$$
\text{FCov}(\mathbf{X}) \text{Cov}(\mathbf{P}_{nc}) = (\hbar/2)^2 I_n
$$

(38)
holds for all pure states, where $I_n$ denotes the $n \times n$ unit matrix. This exact uncertainty relation, being a symmetric matrix equality, comprises $n(n + 1)/2$ independent equalities. The corresponding Heisenberg matrix inequality

$$\text{Cov}(X) \text{Cov}(P) \geq (\hbar/2)^2 I_n,$$ (39)

follows immediately from Eqs. (34), (37) and (38).

### B Entangled particles

Consider now the case of two one-dimensional particles, with respective position and momentum observables $(X^{(1)}, P^{(1)})$ and $(X^{(2)}, P^{(2)})$. Such a system corresponds to $n = 2$ above, and the corresponding nonclassical momentum components associated with wavefunction $\psi$ follow from Eqs. (32) and (33) as

$$P_{nc}^{(1)} = P^{(1)} - \hbar \frac{\partial \arg \psi(x_1, x_2)}{\partial x_1}, \quad P_{nc}^{(2)} = P^{(2)} - \hbar \frac{\partial \arg \psi(x_1, x_2)}{\partial x_2}. \quad (40)$$

For entangled states (e.g., a superposition of two product states), it follows that the nonclassical momentum of particle 1 will typically depend on the position observable of particle 2, and vice versa. Hence if some unitary transformation (e.g., a position displacement) is performed on the second particle, then the nonclassical momentum of the first particle is typically changed.

The decomposition into classical and nonclassical components is therefore essentially nonlocal: the decomposition of a single-particle observable typically depends upon actions performed on another particle with which the first is entangled. Conversely, all such decompositions are invariant under actions performed on a second unentangled particle. The nonlocality inherent in quantum entanglement is thus reflected by the nonlocality of classical/nonclassical decompositions.

The exact uncertainty relation corresponding to the decomposition of momentum in Eq. (11) is given by the matrix equality of Eq. (38), with $n = 2$. This leads to three independent inequalities, two of which may be chosen as as generalizations of the exact uncertainty relation in Eq. (2) for each individual particle.

There are many ways of choosing the third independent inequality. However, one particular choice provides an interesting connection with the Pearson correlation coefficient of classical statistics. The latter coefficient is defined for two compatible observables $A$ and $B$, in terms of the coefficients
of the corresponding covariance matrix \( \text{Cov}(A, B) \), by

\[
 r_P(A, B) := \frac{C_{12}}{(C_{11}C_{22})^{1/2}},
\]

(41)

and provides a measure of the degree to which \( A \) and \( B \) are linearly correlated. It ranges between -1 (a high degree of linear correlation with negative slope) and +1 (a high degree of linear correlation with positive slope). One may analogously define the “Fisher” correlation coefficient in terms of the coefficients \( C_{jk}^F \) of the corresponding Fisher covariance matrix \( \text{FCov}(A, B) \), by

\[
 r_F(A, B) := \frac{C_{12}^F}{(C_{11}^F C_{22}^F)^{1/2}}.
\]

(42)

This also provides a measure of correlation ranging between -1 and +1, and is equal to the Pearson correlation coefficient for all Gaussian distributions.

The third equality may now be chosen as the simple correlation relation

\[
 r_P(P_{nc}^{(1)}, P_{nc}^{(2)}) + r_F(X^{(1)}, X^{(2)}) = 0,
\]

(43)

as may be verified by direct calculation from Eq. (38). It is seen that the exact uncertainty relation in Eq. (38) thus constrains both uncertainty and correlation.

For example, if the nonclassical momentum components of particles 1 and 2 are positively correlated then the position observables are negatively correlated, and vice versa. More generally, the degree of nonclassical momentum correlation is seen to be precisely determined by the degree of position correlation. Note for unentangled particles that Eq. (38) is trivial: both the Pearson and the Fisher correlation coefficients vanish identically. The exact uncertainty relation in Eq. (38) thus reduces in this case to the exact uncertainty relations (19) for each particle.

C EPR correlations

A nice example is provided by the approximate EPR state

\[
 \psi(x_1, x_2) = K e^{-(x_1-x_2-a)^2/4\sigma^2} e^{-(x_1+x_2)^2/4\tau^2} e^{i\theta_0(x_1+x_2)/(2\hbar)},
\]

where \( K \) is a normalisation constant and \( \sigma << 1 << \tau \) in suitable units. One may then calculate

\[
 \langle X^{(1)} - X^{(2)} \rangle = a, \quad \text{Var}(X^{(1)} - X^{(2)}) = \sigma^2 << 1,
\]

\[
 \langle P^{(1)} + P^{(2)} \rangle = p_0, \quad \text{Var}(P^{(1)} + P^{(2)}) = \hbar^2/\tau^2 << 1,
\]

18
and hence $\psi$ is an approximate eigenstate of the relative position and the total momentum, i.e., one may write

$$X^{(1)} - X^{(2)} \approx a, \quad P^{(1)} + P^{(2)} \approx p_0. \quad (44)$$

This state is thus an approximate version of the (nonnormalizable) ket considered by Einstein, Podolsky and Rosen in connection with the completeness of the quantum theory [20].

For state $\psi$ one finds from Eq. (33) that the classical components of momentum are constant, each being equal to $p_0/2$. Hence one has $\text{Cov} P_{nc} = \text{Cov} P$ from Eq. (34). Then, since equality holds in Eq. (37) for Gaussian distributions, the exact uncertainty relation corresponding to $\psi$ follows from Eq. (38) as

$$\text{Cov}(X)\text{Cov}(P) = (\hbar/2)^2 I_n. \quad (45)$$

Eq. (43) reduces to (recalling that $r_P$ and $r_F$ are equivalent for Gaussian distributions) the correlation relation

$$r_P(X) + r_P(P) = 0.$$ 

This latter result is consistent with Eq. (44), which implies that $X^{(1)}$ and $X^{(2)}$ are highly positively correlated for state $\psi$ [$r_P(X) \approx 1$], while $P^{(1)}$ and $P^{(2)}$ are highly negatively correlated [$r_P(P) \approx -1$].

It is of interest to consider the effect of measurements on the approximate EPR state $\psi$. First, for a position measurement on particle 2, with result $X^{(2)} = x$, the state of particle 1 collapses to the wavefunction obtained by substituting $x_2 = x$ and renormalising. It follows that the classical momentum component $P^{(1)}_{cl}$ remains equal to $p_0/2$. Hence the momentum decomposition of particle 1 is not altered by knowledge of $X^{(2)}$.

Conversely, for a momentum measurement on particle 2 with result $P^{(2)} = p$, one finds via straightforward calculation of the appropriate Gaussian integrals that the state of particle 1 collapses to the wavefunction

$$\psi(x_1|P^{(2)} = p) = K' e^{-\left(x_1 + a/2\right)^2/(\sigma^2 + \tau^2)/4} e^{i\bar{p}x_1/\hbar},$$

where $K'$ is a normalisation constant and

$$\bar{p} = \frac{\sigma^2 p + \tau^2 (p_0 - p)}{\sigma^2 + \tau^2} \approx p_0 - p.$$ 

It follows that the classical momentum component $P^{(1)}_{cl}$ is not invariant under a measurement of $P^{(2)}$, changing from $p_0/2$ to $\bar{p}$. Hence there is a “nonlocal”
effect on the classical/nonclassical decomposition of momentum for particle 1, brought about by a measurement of $P^{(2)}$. Thus the strong correlation between $P^{(1)}$ and $P^{(2)}$ for state $\psi$ in Eq. (44) can be considered nonlocal in nature. Similar results hold with respect to the position correlation.

VI OTHER OBSERVABLES

Exact uncertainty relations can be formally extended in a very general way to arbitrary pairs of Hermitian observables. Unfortunately, the physical significance of such an extension is not entirely clear, as will be seen below. However, for the case of a complete set of mutually complementary observables on a finite Hilbert space, such as the Pauli spin matrices, it will be shown that results in the literature provide a very satisfactory form of exact uncertainty relation.

First, consider the case of any two observables $A$ and $B$ represented by Hermitian operators, and for state $\rho$ define

$$B_{cl}^A := \sum_a |a\rangle\langle a| \frac{\langle a|B\rho + \rho B|a\rangle/2}{\langle a|\rho|a\rangle}. \quad (46)$$

Here $|a\rangle$ denotes the eigenket of $A$ with eigenvalue $a$, and the summation is replaced by integration for continuous ranges of eigenvalues.

Clearly the above expression generalises Eqs. (5) and (6), and indeed $B_{cl}^A$ may be interpreted as providing the best estimate of $B$ compatible with measurement of $A$ on state $\rho$. Note that $A_{cl}^A = A$, i.e., $A$ is its own best estimate. One may further define $B_{nc}^A$ via the decomposition

$$B = B_{cl}^A + B_{nc}^A,$$

and obtain the relations

$$\langle B \rangle = \langle B_{cl}^A \rangle, \quad \text{Var}B = \text{Var}B_{cl}^A + \text{Var}B_{nc}^A$$

for state $\rho$, in analogy to Eqs. (3) and (11).

If one is then prepared to define the quantity $\delta_BA$ by

$$(\delta_BA)^{-2} = \sum_a \frac{\langle a|\langle i/\hbar|B,\rho\rangle|a\rangle^2}{\langle a|\rho|a\rangle},$$

in analogy to Eq. (26), then precisely as per the derivation of Eq. (24) one may show that

$$(\delta_BA) \Delta B_{nc}^A \geq \hbar/2, \quad (47)$$

20
with equality for all pure states.

Thus there is a very straightforward generalisation of Eq. (3) to arbitrary pairs of observables. A difficulty is, however, to provide a meaningful statistical interpretation of \( \delta_{B,A} \). Note in particular that, unlike the Fisher length \( \delta X \), this quantity is not a functional of the probability distribution \( \langle a | \rho | a \rangle \) in general. Possibly, noting the commutator which appears in the definition of \( \delta_{B,A} \), one can interpret this quantity as a measure of the degree to which a measurement of \( A \) can distinguish between \( B \)-generated translations of state \( \rho \), i.e., between unitary transformations of the form \( e^{ixB/\hbar} \rho e^{-ixB/\hbar} \) [21]. Here such an attempt will not be made, although it is noted that the case of arbitrary quadrature observables of a single-mode field should provide a simple test.

Finally, it is pointed out that a rather different type of exact uncertainty relation exists for a set of \( n + 1 \) mutually complementary observables \( A_1, A_2, \ldots, A_{n+1} \) on an \( n \)-dimensional Hilbert space. Such sets are defined by the property that the distribution of any member is uniform for an eigenstate of any other member, and are known to exist when \( n \) is a power of a prime number [22]. As an example one may choose \( n = 2 \), and take \( A_1, A_2 \) and \( A_3 \) to be the Pauli spin matrices.

Let \( L \) denote the collision length of probability distribution \( \{ p_1, p_2, \ldots, p_n \} \), defined by [4]

\[
L := 1 / \sum_j (p_j)^2.
\]

Note that \( L \) is equal to 1 for a distribution concentrated on a single outcome, and is equal to \( n \) for a distribution spread uniformly over all \( n \) possible outcomes. It hence provides a direct measure of the spread of the distribution over the space of outcomes [4].

One may show that [4]

\[
\sum_i 1/L_i = 1 + \text{tr}[\rho^2] \leq 2,
\]

where \( L_i \) denotes the collision length of observable \( A_i \) for state \( \rho \). This reduces to strict equality for all pure states, and thus provides an exact uncertainty relation for the collision lengths of any set of \( n + 1 \) mutually complementary observables. For example, if \( L_j = 1 \) for some observable \( A_j \) (minimal uncertainty), then \( L_i = n \) for all \( i \neq j \) (maximal uncertainty). Ivanovic has shown that Eq. (18) can be used to derive an entropic uncertainty relation for the \( A_i \) [4], while Brukner and Zeilinger have interpreted Eq. (18) as an additivity property of a particular “information” measure [23].
VII CONCLUSIONS

The existence of exact uncertainty relations connecting the statistics of complementary observables greatly strengthens the usual statement of the uncertainty principle: the lack of knowledge about an observable, for any wavefunction, is precisely determined by the lack of knowledge about the conjugate observable. The measures of lack of knowledge must of course be chosen appropriately (as the nonclassical fluctuation strength and the Fisher length). What is remarkable is that such measures can be chosen at all.

The decomposition of the momentum observable into classical and nonclassical components has a number of clear physical consequences. The classical component characterises that part of the momentum comeasurable with position, while the nonclassical component successfully characterises the “quantum” nature of the momentum observable $P$ (including the exact uncertainty relation Eq. (2), the nonclassical part of the kinetic energy, and the nonlocality inherent in the momentum correlations of entangled particles). It has been shown elsewhere that the nonclassical position and momentum uncertainties characterises the robustness of quantum systems with respect to Gaussian noise processes [2], and the notion of a nonclassical momentum fluctuation inversely related to position uncertainty has been successfully used as a starting point for deriving the Schrödinger equation [3].

The exact uncertainty relations in Eqs. (2), (30), (31) and (38) are formal consequences of the Fourier transformations which connect the representations of conjugate quantum observables. Hence they may be extended to any domain in which such transformations have physical significance. This includes the time-frequency domain, discussed elsewhere [8] (where the “classical” component of the frequency is essentially the so-called “instantaneous frequency” [24]), as well as Fourier optics and image processing.

It would be of interest to determine whether exact uncertainty relations exist for relativistic systems. One is hampered in direct attempts by difficulties associated with one-particle interpretations of the Klein-Gordon and Dirac equations. It would perhaps therefore be more fruitful to first consider extensions to general field theories.

Finally, note that the definition of the Fisher covariance matrix in Eq. (30) suggests an analogous definition of a “Wigner” covariance matrix $\text{WCov}$, defined via the coefficients of its matrix inverse

\[
[W\text{Cov}^{-1}]_{jk} := \int d^{2n}z W^{-1} \frac{\partial W}{\partial z_j} \frac{\partial W}{\partial z_k}.
\]
Here $W$ denotes the Wigner function of the state, and $z$ denotes the phase space vector $(x, p)$. It would be of interest to determine to what degree this matrix is well-defined, and to what extent its properties characterise nonclassical features of quantum states.

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It was conjectured in Ref. [2] that the joint nonclassicality $\Delta X_{nc}\Delta P_{nc}$ is not only strictly positive, but is bounded below by $\hbar/2$ for the case of pure states. This conjecture is, however, violated by the wavefunction $K \exp[-x^2 + i\alpha x^2]$, where $K$ and $\alpha$ are real constants.

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