

Generalized Uncertainty Relations: Theory, Examples, and Lorentz Invariance*

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The quantum-mechanical framework in which observables are associated with Hermitian operators is too narrow to discuss measurements of such important physical quantities as elapsed time or harmonic-oscillator phase. We introduce a broader framework that allows us to derive quantum-mechanical limits on the precision to which a parameter—e.g., elapsed time—may be determined via arbitrary data analysis of arbitrary measurements on N identically prepared quantum systems. The limits are expressed as generalized Mandelstam–Tamm uncertainty relations, which involve the operator that generates displacements of the parameter—e.g., the Hamiltonian operator in the case of elapsed time. This approach avoids entirely the problem of associating a Hermitian operator with the parameter. We illustrate the general formalism, first, with nonrelativistic uncertainty relations for spatial displacement and momentum, harmonic-oscillator phase and number of quanta, and time and energy and, second, with Lorentz-invariant uncertainty relations involving the displacement and Lorentz-rotation parameters of the Poincaré group. © 1996 Academic Press, Inc.

1. INTRODUCTION

The goal of quantitative experiments in physics is to determine a set of parameters to some level of confidence. In general this determination entails complex methods of data analysis applied to observed data. From this point of view, the conventional description of measurements in quantum theory, tied to the use of Hermitian operators to represent observable quantities, provides too narrow a framework, because for many experimental parameters, time being an example, there is no suitable Hermitian operator.

In this paper we employ a broader framework for describing the quantum-mechanical determination of parameters such as time [1]. In this framework measurements are described in the most general way permitted by quantum mechanics—in terms of so-called “positive-operator-valued measures” (POVMs). The role of a quantum measurement is to provide data from which one infers the parameter of interest by classical methods of parameter estimation. There is no

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need to associate a Hermitian operator with the parameter, and generally there is no such Hermitian operator. We derive quantum restrictions on determining a parameter by considering optimal measurements and optimal methods of parameter estimation. The quantum restrictions are stated as uncertainty relations that involve the parameter and the operator that generates displacements of the parameter, time and the Hamiltonian operator being an example.

Uncertainty relations are central to the interpretation of quantum theory, yet in many cases of interest it is impossible to formulate an uncertainty relation if one insists that both quantities have an associated Hermitian operator. Hilgevoord and Uffink [2] give an excellent summary of the defects of standard uncertainty relations and of the motivation for parameter-based uncertainty relations. Mandelstam and Tamm [3] derived the first parameter-based uncertainty relation, for time and energy, by treating elapsed time as a parameter to be determined by measurement of a conventional observable that varies with time. Helstrom [4] and Holevo [5] pioneered the modern study of parameter-based uncertainty relations, by considering quantum restrictions on how well one can determine a parameter from the results of general quantum measurements described by POVMs. Other authors [1, 2, 6–8] have formulated parameter-based uncertainty relations in various contexts.

Here we present a general theory of parameter-based uncertainty relations and explore in some detail the question of finding optimal quantum measurements that achieve the lower bound set by the uncertainty relation. We devote Section 2 to summarizing the framework for quantum parameter estimation and the corresponding generalized parameter-based uncertainty relations. Section 2.1 develops the general theory for mixed quantum states (density operators). Section 2.2 specializes the general theory to pure states that are generated by a single-parameter unitary operator, a case that occupies the remainder of the paper. In Section 3 we develop a general description of global optimal measurements that saturate the lower bound in the generalized uncertainty relation. Section 4 illustrates the parameter-based uncertainty relations with various examples of nonrelativistic uncertainty relations: spatial displacement and momentum in Section 4.1, harmonic-oscillator phase and number of quanta in Section 4.2, and time and energy in Section 4.3. Section 5 applies the parameter-based uncertainty relations to the displacement and Lorentz-rotation parameters of the Poincaré group, leading ultimately to relativistically invariant uncertainty relations for the invariant space-time interval of special relativity and the boost and spatial-rotation parameters of Lorentz transformations. Section 6 concludes with a brief discussion.

2. GENERALIZED UNCERTAINTY RELATIONS

2.1. *Uncertainty Relations for Mixed States*

Consider N replicas of a quantum system. Each replica is prepared in the same quantum state (density operator) $\hat{\rho}(X)$, which is parametrized by the single

parameter X . In the following a subscript X on an expectation value denotes an expectation value with respect to $\hat{\rho}(X)$. Braunstein and Caves [1] consider a general smooth path on the space of density operators,

$$\hat{\rho}(X) = \sum_j p_j |j\rangle\langle j|, \quad (1)$$

where both the eigenvalues p_j and the eigenvectors $|j\rangle$ can change along the path. A path is specified by giving the tangent vector

$$\frac{d\hat{\rho}}{dX} = \sum_j \frac{dp_j}{dX} |j\rangle\langle j| - i[\hat{h}, \hat{\rho}] \equiv \hat{\rho}'. \quad (2)$$

The Hermitian operator \hat{h} , which can depend on X , generates the infinitesimal changes in the eigenvectors of $\hat{\rho}(X)$:

$$\hat{\rho}(X + dX) = \hat{\rho}(X) + \hat{\rho}'(X) dX = \sum_j (p_j + dp_j) e^{-idX\hat{h}} |j\rangle\langle j| e^{idX\hat{h}}. \quad (3)$$

Notice that \hat{h} can be replaced by

$$\Delta\hat{h} \equiv \hat{h} - \langle \hat{h} \rangle_X \quad (4)$$

in Eqs. (2) and (3) without changing the path.

The most general measurement permitted by quantum mechanics [5, 9, 10] can be described by a set of bounded, nonnegative, Hermitian operators $\hat{E}(\xi) d\xi$ (generalizations of projection operators), which are complete in the sense that

$$\int d\xi \hat{E}(\xi) = \hat{1} = (\text{unit operator}). \quad (5)$$

The quantity ξ labels the “results” of the measurement; written here as a single continuous real variable, it can be discrete or multivariate. The operators $\hat{E}(\xi) d\xi$ make up what is called a “positive-operator-valued measure” (POVM). The probability distribution for result ξ , given the parameter X , is

$$p(\xi | X) = \text{tr}(\hat{E}(\xi) \hat{\rho}(X)). \quad (6)$$

The properties of the POVM are just those needed to make $p(\xi | X)$ a normalized probability distribution.

Let ξ_1, \dots, ξ_N denote the results of measurements on the N replicas of our quantum system. A general form of data analysis uses a function

$$X_{\text{est}} = X_{\text{est}}(\xi_1, \dots, \xi_N) \quad (7)$$

to generate an estimate X_{est} for the parameter X , based on the data ξ_1, \dots, ξ_N obtained from the measurements and nothing else.

To characterize how precisely the N measurements are able to determine the parameter X , we need something a bit more complicated than the obvious choice, the variance of the estimator, $\langle (\Delta X_{\text{est}})^2 \rangle_X = \langle (X_{\text{est}} - \langle X_{\text{est}} \rangle_X)^2 \rangle_X$. The reason is that the variance does not take into account two important possibilities. First, even if the estimator has a small variance, it might be systematically biased away from the true parameter value—i.e., $\langle X_{\text{est}} \rangle_X$ might not equal X —and thus give a poor estimate. Second, the estimator might have different “units” from the parameter, thus making it difficult to interpret the variance of the estimator as a measure of precision in determining X . Both the amount of bias and the difference in units can depend on the parameter, i.e., on location along the path. To remedy these difficulties, we quantify the estimate’s deviation from the parameter by [1]

$$\delta X \equiv \frac{X_{\text{est}}}{|d\langle X_{\text{est}} \rangle_X/dX|} - X. \quad (8)$$

The derivative $d\langle X_{\text{est}} \rangle_X/dX$ removes the local difference in the “units” of the estimator and the parameter, and then the units-corrected estimator is compared to the parameter X , not to the mean value of the estimator. As a statistical measure of the precision of the estimation, we use the second moment of δX .

There is a lower bound on the second moment of δX :

$$\langle (\delta X)^2 \rangle_X \geq \frac{1}{NF(X)} \geq \frac{1}{N(ds/dX)^2}. \quad (9)$$

Braunstein and Caves [1] derive the ultimate lower bound in two steps, in contrast to derivations by Helstrom [4] and Holevo [5, Chap. VI.2], both of whom proceed to the ultimate lower bound in a single step that obscures the conditions for achieving the ultimate lower bound. The two steps in the Braunstein–Caves derivation are displayed as the two inequalities in Eq. (9). The first inequality is a bound that applies to all estimators X_{est} for a fixed probability distribution $p(\xi | X)$, i.e., for a fixed quantum measurement. The second inequality is a bound that applies to all quantum measurements.

In the first inequality in Eq. (9),

$$F(X) \equiv \int d\xi \frac{1}{p(\xi | X)} \left(\frac{\partial p(\xi | X)}{\partial X} \right)^2 \quad (10)$$

is the *Fisher information* [11] associated with the probability distribution $p(\xi | X)$. The first inequality is an expression of the Cramér–Rao bound of classical estimation theory [11], which places a lower bound on the variance of *any* estimator X_{est} that is applied to data drawn from the distribution $p(\xi | X)$. An estimator that saturates the first inequality in Eq. (9)—and, hence, attains the Cramér–Rao bound—is called an *efficient* estimator. The lower bound in the first inequality can always be achieved asymptotically for large N by using maximum-likelihood estimation [12], but except for special distributions, there is *no* efficient estimator for finite values of N .

The second inequality in Eq. (9) holds for any POVM $\hat{E}(\xi) d\xi$. The second inequality is written in terms of a line element ds^2 , which defines a “statistical distance” [13] that measures the distinguishability of neighboring quantum states and provides a natural Riemannian geometry on the space of density operators. The explicit form that Braunstein and Caves [1] (see also [4, 5, Chap. VI.2]) find for the line element is

$$ds^2/dX^2 = \langle (\mathcal{L}_\rho(\hat{\rho}'))^2 \rangle_X = \text{tr}(\hat{\rho}' \mathcal{L}_\rho(\hat{\rho}')), \quad (11)$$

where \mathcal{L}_ρ is a super-operator that, in the basis that diagonalizes $\hat{\rho}$, takes the form

$$\mathcal{L}_\rho(\hat{O}) = \sum_{\{j, k \mid p_j + p_k \neq 0\}} \frac{2}{p_j + p_k} O_{jk} |j\rangle\langle k|. \quad (12)$$

If $\hat{\rho}$ has no zero eigenvalues, \mathcal{L}_ρ is the inverse of the super-operator defined by $\mathcal{R}_\rho(\hat{O}) \equiv \frac{1}{2}(\hat{\rho}\hat{O} + \hat{O}\hat{\rho})$; hence, \mathcal{L}_ρ was denoted \mathcal{R}_ρ^{-1} by Braunstein and Caves [1]. Helstrom [4] and Holevo [5, Chap. VI.2] call $\mathcal{L}_\rho(\hat{\rho}')$ the “symmetric logarithmic derivative” of $\hat{\rho}$. The lower bound in the second inequality can be achieved by using a POVM such that the operators $\hat{E}(\xi)$ are one-dimensional projection operators onto orthonormal eigenstates of the Hermitian operator $\mathcal{L}_\rho(\hat{\rho}')$ [1]. The conditions given here and above for achieving the two lower bounds in Eq. (9) are sufficient, although they are not always necessary.

The line element (11) on the space of density operators arises here from quantifying precisely the quantum restrictions on determining a parameter—and, hence, the quantum restrictions on the statistical distinguishability of neighboring density operators $\hat{\rho}(X)$ and $\hat{\rho}(X+dX)$. The same line element can also be gotten by defining a natural metric on density operators in terms of the correlation between pairs of conventional observables. The reader interested in this alternative route to the metric can find it spelled out in [8, 14], together with references to related work.

Although not pointed out by Braunstein and Caves, the lower bound (9) does not improve if one allows measurements that do not factor into separate measurements on each of the N replicas. One can see this by treating the N replicas as a single composite system with density operator

$$\hat{\rho}^{(N)}(X) = \hat{\rho}(X) \otimes \cdots \otimes \hat{\rho}(X). \quad (13)$$

Applied to this composite system, the bound (9) takes a form $\langle (\delta X)^2 \rangle_X \geq (dX/ds^{(N)})^2$ that holds for all quantum measurements on the product space of the composite system. It is not difficult to show, however, that for N -replica product states, the line element on the product space reduces to N times the single-replica line element, i.e.,

$$\frac{(ds^{(N)})^2}{dX^2} = \text{tr} \left(\frac{d\hat{\rho}^{(N)}}{dX} \mathcal{L}_{\hat{\rho}^{(N)}} \left(\frac{d\hat{\rho}^{(N)}}{dX} \right) \right) = N \text{tr} (\hat{\rho}' \mathcal{L}_\rho(\hat{\rho}')), \quad (14)$$

thus giving the same lower bound as in Eq. (9). This result provides a limited answer to a question raised by Peres and Wootters [15]: when a composite system is made up of replicas all prepared in the same quantum state, can measurements on the composite system better distinguish states than can separate measurements on each of the replicas? For the very special case of two neighboring states, the answer is no.

We pause at this point to take stock of what has already been presented. The bound (9), together with Eq. (11), is a general species of uncertainty relation, which restricts one's ability to determine a parameter from the results of quantum measurements. This uncertainty relation applies to mixed quantum states, allows for measurements that are not described by projection operators, and includes the possibility of multiple measurements. On the other hand, precisely because this uncertainty relation is so general, we find it instructive in what follows to specialize in three ways, thus permitting us to make closer contact with standard uncertainty relations.

For the first specialization we assume that the eigenvalues of the density operator do not change along the path—i.e., $dp_j = 0$ in Eq. (3)—which simplifies Eq. (2) to

$$\hat{\rho}' = -i[\hat{h}, \hat{\rho}] = -i[\Delta\hat{h}, \hat{\rho}]. \quad (15)$$

This first specialization means that the path is generated by a unitary transformation; keep in mind, however, that we still allow the local generator of the transformation, \hat{h} , to depend on X . As a consequence of this first specialization, we can write

$$\mathcal{L}_{\hat{\rho}}(\hat{\rho}') = 2i \sum_{\{j,k \mid p_j + p_k \neq 0\}} \frac{p_j - p_k}{p_j + p_k} \Delta h_{jk} |j\rangle\langle k| \equiv 2\widehat{\delta h}, \quad (16)$$

where we introduce $\widehat{\delta h}$ as a shorthand for $\frac{1}{2}\mathcal{L}_{\hat{\rho}}(\hat{\rho}')$, and the line element (11) becomes

$$\frac{ds^2}{dX^2} = 4\langle(\widehat{\delta h})^2\rangle_X = 2 \sum_{j,k} (p_j + p_k) \left(\frac{p_j - p_k}{p_j + p_k}\right)^2 |\Delta h_{jk}|^2 \leq 4\langle(\Delta\hat{h})^2\rangle_X. \quad (17)$$

Notice that in this line element we can drop the restriction on the sum, since under any procedure for approaching the boundary on which one or more eigenvalues of $\hat{\rho}$ vanishes, the terms for which $p_j + p_k = 0$ do not contribute.

A consequence of the last inequality in Eq. (17) is a parameter-based uncertainty relation [1, 4, 5, Chaps.III.2, IV.7, and VI.3],

$$\langle(\delta X)^2\rangle_X \langle(\Delta\hat{h})^2\rangle_X \geq \frac{1}{4N}, \quad (18)$$

which, since it involves the variance of \hat{h} , resembles standard uncertainty relations, except that X is a parameter and the relation holds for multiple measurements. The corresponding uncertainty relation involving $\widehat{\delta h}$,

$$\langle (\delta X)^2 \rangle_X \langle (\widehat{\delta h})^2 \rangle_X \geq \frac{1}{4N}, \quad (19)$$

is stricter [1, 5, Chap. VI.3], unless equality holds in Eq. (17). Equality is equivalent to the condition that $p_j p_k |\Delta h_{jk}|^2 = 0$ for all j and k . In particular, equality holds if $\hat{\rho}$ is a pure state, but never holds if $\hat{\rho}$ has no zero eigenvalues (except in the trivial case $\Delta \hat{h} = 0$).

2.2. Uncertainty Relations for Pure States

The second specialization is to assume that $\hat{\rho}(X) = |\psi_X\rangle\langle\psi_X|$ is a pure state. This assumption implies the first one, which is incorporated in Eq. (15), since a path on the pure states must be generated by a unitary transformation. Normalization implies that

$$\begin{aligned} 0 &= \frac{d}{dX} \langle \psi_X | \psi_X \rangle = \langle \psi_X | \left(\frac{d|\psi_X\rangle}{dX} \right) + \left(\frac{d\langle\psi_X|}{dX} \right) | \psi_X \rangle \\ &= 2 \operatorname{Re} \left(\langle \psi_X | \left(\frac{d|\psi_X\rangle}{dX} \right) \right), \end{aligned} \quad (20)$$

but the freedom to multiply $|\psi_X\rangle$ by a phase factor means that $\operatorname{Im}[\langle \psi_X | (d|\psi_X\rangle/dX)]$ can be chosen arbitrarily. Using Eqs. (15) and (20), one can show that

$$\left(\frac{d|\psi_X\rangle}{dX} \right)_\perp \equiv \frac{d|\psi_X\rangle}{dX} - |\psi_X\rangle\langle\psi_X| \left(\frac{d|\psi_X\rangle}{dX} \right) = -i\Delta\hat{h}|\psi_X\rangle, \quad (21)$$

where $(d|\psi_X\rangle/dX)_\perp$ is the projection of $d|\psi_X\rangle/dX$ orthogonal to $|\psi_X\rangle$. Equation (15) can now be written as

$$\hat{\rho}' = -i[\Delta\hat{h}, \hat{\rho}] = \left(\frac{d|\psi_X\rangle}{dX} \right)_\perp \langle\psi_X| + |\psi_X\rangle \left(\frac{d\langle\psi_X|}{dX} \right)_\perp. \quad (22)$$

A convenient phase choice,

$$\langle\psi_X| \left(\frac{d|\psi_X\rangle}{dX} \right) = -i\langle\hat{h}\rangle_X, \quad (23)$$

leads to a Schrödinger-like equation for $|\psi_X\rangle$:

$$\frac{d|\psi_X\rangle}{dX} = -i\hat{h}|\psi_X\rangle. \quad (24)$$

Notice that the phase freedom in $|\psi_X\rangle$ is equivalent to the freedom to add a multiple of the unit operator to \hat{h} .

Applying our second assumption to Eq. (16), one finds that

$$\widehat{\delta h} = \frac{1}{2} \mathcal{L}_{\hat{\rho}}(\hat{\rho}') = -i[\Delta\hat{h}, \hat{\rho}] = \left(\frac{d\langle\psi_X|}{dX} \right)_{\perp} \langle\psi_X| + |\psi_X\rangle \left(\frac{d\langle\psi_X|}{dX} \right)_{\perp} = \hat{\rho}'. \quad (25)$$

Thus, for pure states, the line element (17) for statistical distance reduces to

$$\frac{ds^2}{dX^2} = 4 \left(\frac{d\langle\psi_X|}{dX} \right)_{\perp} \left(\frac{d|\psi_X\rangle}{dX} \right)_{\perp} = 4\langle(\Delta\hat{h})^2\rangle_X, \quad (26)$$

which implies, as indicated above, that we can restrict our attention to the uncertainty relation (18).

One expects statistical distance, which measures the distinguishability of states, to be related to the inner product and thus to the Hilbert-space angle between pure states. The square of the infinitesimal Hilbert-space angle $d\theta$ between neighboring states $|\psi_X\rangle$ and $|\psi_{X+dX}\rangle$ is

$$d\theta^2 = [\cos^{-1}(|\langle\psi_X|\psi_{X+dX}\rangle|)]^2 = 1 - |\langle\psi_X|\psi_{X+dX}\rangle|^2. \quad (27)$$

The line element $d\theta^2$ defines a natural Riemannian metric, called the Fubini–Study metric [16–18], on the manifold of Hilbert-space rays. Using Eq. (20) and the further consequence of normalization,

$$0 = \frac{1}{2} \frac{d^2}{dX^2} \langle\psi_X|\psi_X\rangle = \left(\frac{d\langle\psi_X|}{dX} \right) \left(\frac{d|\psi_X\rangle}{dX} \right) + \text{Re} \left(\langle\psi_X| \left(\frac{d^2|\psi_X\rangle}{dX^2} \right) \right), \quad (28)$$

one finds that

$$\begin{aligned} d\theta^2 &= dX^2 \left[\left(\frac{d\langle\psi_X|}{dX} \right) \left(\frac{d|\psi_X\rangle}{dX} \right) - \left| \langle\psi_X| \left(\frac{d|\psi_X\rangle}{dX} \right) \right|^2 \right] \\ &= dX^2 \left(\frac{d\langle\psi_X|}{dX} \right)_{\perp} \left(\frac{d|\psi_X\rangle}{dX} \right)_{\perp} = \frac{1}{4} ds^2, \end{aligned} \quad (29)$$

which means that Hilbert-space angle is half the statistical distance defined here.

The third and final specialization is to assume that the generator \hat{h} is independent of X . This assumption allows us to integrate Eq. (24) and to write the path on Hilbert space as being generated by a single-parameter unitary operator,

$$|\psi_X\rangle = e^{-iX\hat{h}} |\psi_0\rangle, \quad (30)$$

where $|\psi_0\rangle$ is a fiducial state at $X=0$. Moreover, this assumption guarantees that the expectation value of any function of \hat{h} is independent of X ; thus we can drop

the subscript X from the mean and variance of \hat{h} . In particular, we can write the uncertainty relation (18) as

$$\langle (\delta X)^2 \rangle_X \langle (\Delta \hat{h})^2 \rangle \geq \frac{1}{4N}. \quad (31)$$

It is this parameter-based uncertainty relation that occupies us for the remainder of this paper. As noted above, this uncertainty relation resembles the standard uncertainty relation, except that the relation holds for multiple measurements and X is a parameter, not necessarily corresponding to any Hermitian operator.

3. GLOBAL OPTIMAL MEASUREMENTS

3.1. General Considerations

The chain of inequalities leading to the uncertainty relation (31) consists of the two inequalities leading to the statistical distance in Eq. (9) and the inequality involving the generator \hat{h} in Eq. (17). The first inequality in Eq. (9) can be saturated asymptotically for large N by use of maximum-likelihood estimation, and the inequality in Eq. (17) is saturated for pure states. Thus the question of achieving equality in the uncertainty relation (31), provided one allows for many measurements N , reduces to finding an *optimal measurement*, i.e., one that saturates the second inequality in Eq. (9). Notice that since the variance of \hat{h} is constant as a consequence of our third assumption, optimal measurements lead to a maximum Fisher information that is constant along the path.

As indicated above, one such optimal measurement uses a POVM such that the operators $\hat{E}(\xi)$ are one-dimensional projection operators onto orthonormal eigenstates of the Hermitian operator $\mathcal{L}_\rho(\hat{p}') = 2 \delta \hat{h}$ (cf. Eq. (25)). This measurement has the defect, however, that it generally depends on X , thus requiring one to know the value of the parameter one is trying to estimate before choosing the optimal measurement. Our goal here is to find a *global* measurement, independent of X , that is optimal all along the path. We seek such a global optimal measurement in terms of a POVM $\hat{E}(x) dx$, where the measurement results are labeled by a single real number x that has the same range of values as X . As we discuss further in Section 3.2, we can hope to find an optimal measurement of this form only if the generator \hat{h} is nondegenerate; if the spectrum of \hat{h} has degeneracies, an optimal measurement must acquire information beyond that which can be described by a single real number.

The POVM $\hat{E}(x) dx$ must, of course, be complete, which means that

$$\hat{1} = \int dx \hat{E}(x). \quad (32)$$

The probability density for result x , given the parameter X , is

$$p(x | X) = \langle \psi_X | \hat{E}(x) | \psi_X \rangle = \langle \psi_0 | e^{iX\hat{h}} \hat{E}(x) e^{-iX\hat{h}} | \psi_0 \rangle. \quad (33)$$

As noted above, global optimal measurements lead to a Fisher information (10) that is independent of X . This suggests that we require that $p(x | X)$ be a function only of $x - X$, which means the POVM must satisfy a “displacement” property

$$e^{iX\hat{h}}\hat{E}(x)e^{-iX\hat{h}} = \hat{E}(x - X). \quad (34)$$

Measurements that satisfy properties (32) and (34) are called *covariant* by Holevo [5].

We restrict our search for global optimal measurements to POVMs that have one additional property: the POVM consists of multiples of “projection operators” onto (generally unnormalizable) states $|x\rangle$,

$$\hat{E}(x) dx = \frac{dx}{C} |x\rangle\langle x| \quad (35)$$

(C is a real constant). The motivation for this assumption is that measurements not described by one-dimensional “projectors” have less resolution [19], but it would be useful to make this motivation precise or to investigate whether covariant measurements that do not satisfy property (35) can be optimal. Notice that we do *not* require that the states $|x\rangle$ be orthogonal, and if they are not, they are necessarily *overcomplete*. The constant C could be absorbed into the states $|x\rangle$, but it is useful to leave it free so that these states can be given conventional normalizations in the examples of Section 4.

Without loss of generality we can discard the freedom to rephase the states $|x\rangle$, because the POVM is unaffected by rephasing, and thus replace the displacement property of the POVM with a displacement requirement on the states,

$$e^{-iX\hat{h}} |x\rangle = |x + X\rangle. \quad (36)$$

This displacement property, written as

$$\langle x | e^{-iX\hat{h}} | \psi \rangle = \langle x - X | \psi \rangle = e^{-X\partial/\partial x} \langle x | \psi \rangle, \quad (37)$$

is equivalent to saying that in the x representation, \hat{h} is represented by a derivative:

$$\hat{h} \Leftrightarrow \frac{1}{i} \frac{\partial}{\partial x}. \quad (38)$$

The probability density (33) can be written as

$$p(x | X) = |\psi_x(x)|^2 = |\psi_0(x - X)|^2 \equiv p(x - X), \quad (39)$$

where

$$\psi_x(x) \equiv \frac{1}{\sqrt{C}} \langle x | \psi_x \rangle = \frac{1}{\sqrt{C}} \langle x - X | \psi_0 \rangle = \psi_0(x - X) \quad (40)$$

is the “wave function” of the state vector $|\psi_x\rangle$ in the x representation.

Equations (32), (35), and (36) are the three properties that we require of the POVM $\hat{E}(x) dx$. Holevo [5, Chap. IV.7] considers the same sorts of measurements; his treatment, while more rigorous mathematically than ours, is inaccessible to many physicists. The three properties are preserved by a “gauge transformation,” which replaces the states $|x\rangle$ with states

$$e^{if(\hat{h})} |x\rangle, \quad (41)$$

where f is an arbitrary real-valued function. This gauge freedom plays an important role, as we discuss further in Section 3.2 and in the examples of Section 4.

If the POVM $\hat{E}(x) dx$ is an optimal measurement, then it saturates the second inequality in Eq. (9), which simplifies to

$$\int dx \frac{[p'(x)]^2}{p(x)} = F \leq \frac{ds^2}{dX^2} = 4\langle(\Delta\hat{h})^2\rangle. \quad (42)$$

In this inequality we put the Fisher information F in a new form, which applies to a covariant measurement and which is explicitly independent of X .

For a measurement described by the one-dimensional “projectors” $|x\rangle\langle x|$, the necessary and sufficient condition for an optimal measurement, as shown in [1], is that

$$\text{Im} \left(\langle \psi_x | x \rangle \langle x | \left(\frac{d|\psi_x\rangle}{dX} \right)_{\perp} \right) = 0 \quad \text{for all } x \text{ and all } X. \quad (43)$$

Using Eqs. (21) and (34) and writing

$$\frac{1}{\sqrt{C}} \langle x | \psi_0 \rangle = \psi_0(x) = r(x) e^{i\Theta(x)}, \quad (44)$$

$$r(x) = |\psi_0(x)| = \sqrt{p(x)}, \quad (45)$$

one can recast condition (43) as

$$0 = \frac{1}{C} \text{Im} (i \langle \psi_0 | x \rangle \langle x | \Delta\hat{h} | \psi_0 \rangle) = r^2(x) [\Theta'(x) - \langle \hat{h} \rangle] \quad \text{for all } x, \quad (46)$$

which is equivalent to $\Theta(x) = \langle \hat{h} \rangle x + \text{const}$. After discarding the irrelevant overall phase due to the constant, the resulting wave function is

$$\psi_0(x) = r(x) e^{i\langle \hat{h} \rangle x}. \quad (47)$$

The POVM $\hat{E}(x) dx$ thus describes a global optimal measurement if and only if the wave function $\psi_0(x)$ of the fiducial state is (up to an overall phase) an arbitrary real function times a simple phase factor that accounts for the expectation value of \hat{h} . For a fiducial state whose wave function has a phase that is nonlinear

in x for all choices of the states $|x\rangle$, we cannot rule out the existence of a global optimal measurement, but we can say that any measurement that satisfies properties (32), (35), and (36) is not optimal.

We can get at condition (46) directly by calculating the mean and variance of \hat{h} in the x representation, again writing $\psi_0(x)$ as in Eq. (44):

$$\langle \hat{h} \rangle = \int dx \psi_0^*(x) \frac{1}{i} \frac{\partial}{\partial x} \psi_0(x) = \int dx p(x) \Theta'(x), \quad (48)$$

$$\begin{aligned} \langle (\Delta \hat{h})^2 \rangle &= \int dx \left| \left(\frac{\partial}{\partial x} - i \langle \hat{h} \rangle \right) \psi_0(x) \right|^2 \\ &= \frac{1}{4} \int dx \frac{[p'(x)]^2}{p(x)} + \int dx p(x) [\Theta'(x) - \langle \hat{h} \rangle]^2. \end{aligned} \quad (49)$$

This expression for $\langle (\Delta \hat{h})^2 \rangle$ connects the Cramér–Rao bound of classical estimation theory (first inequality in Eq. (9)) to the requirements of quantum theory (second inequality in Eq. (9)). A glance at Eq. (42) reminds one that the first term in $\langle (\Delta \hat{h})^2 \rangle$ is one-quarter of the Fisher information; moreover, one recognizes that for an optimal measurement this first term must attain its maximum value, which is the variance of \hat{h} . Thus, for an optimal measurement, the second term in $\langle (\Delta \hat{h})^2 \rangle$, which is the variance of $\Theta'(x)$ with respect to $p(x)$, must be zero; vanishing of the second term is precisely the condition (46).

It is instructive to consider in some detail a special case of the uncertainty relation (31), because in this special case one finds the closest connection between our parameter-based uncertainty relations and standard uncertainty relations. Before considering this special case, however, it is useful to note that the mean and variance of the measurement result x are given by

$$\langle x \rangle_X = \int dx xp(x - X) = X + \int dx xp(x) = X + \langle x \rangle_0, \quad (50)$$

$$\langle (\Delta x)^2 \rangle_X = \int dx (x - \langle x \rangle_X)^2 p(x - X) = \int dx (x - \langle x \rangle_0)^2 p(x) = \langle (\Delta x)^2 \rangle. \quad (51)$$

The mean value of x with respect to the fiducial state, $\langle x \rangle_0$, globally biases the mean $\langle x \rangle_X$ away from the parameter. The variance of x is independent of X .

To introduce our special case, suppose that one makes N measurements described by the POVM $\hat{E}(x) dx$ and that one estimates the parameter X as the sample mean of the data, with the global bias removed, i.e.,

$$X_{\text{est}} = \frac{1}{N} \sum_{i=1}^N (x_i - \langle x \rangle_0). \quad (52)$$

This estimator is *unbiased*, i.e., $\langle X_{\text{est}} \rangle_X = \langle x \rangle_X - \langle x \rangle_0 = X$, and thus the deviation (8) becomes $\delta X = X_{\text{est}} - X = \Delta X_{\text{est}}$. In addition, the efficiency of this estimator is independent of N , because the mean-square deviation decreases as $1/N$:

$$\langle (\delta X)^2 \rangle = \langle (\Delta X_{\text{est}})^2 \rangle = \langle (\Delta x)^2 \rangle / N. \quad (53)$$

The resulting special case of the uncertainty relation (31) is

$$\langle (\Delta x)^2 \rangle \langle (\Delta \hat{h})^2 \rangle = N \langle (\delta X)^2 \rangle \langle (\Delta \hat{h})^2 \rangle \geq \frac{1}{4}. \quad (54)$$

The uncertainty relation for this estimator is identical to a standard uncertainty relation for the measurement result x , the only difference being that the states $|x\rangle$ are generally not the eigenstates of any Hermitian operator.

Equality in the uncertainty relation (54) requires saturating both inequalities in Eq. (9). Saturating the second inequality—i.e., making $F = 4\langle (\Delta \hat{h})^2 \rangle$ (see Eq. (42))—means that the fiducial wave function $\psi_0(x)$ has the form (47). Saturating the first inequality means that the sample mean (52) is an efficient estimator for all values of N and, in particular, that $x - \langle x \rangle_0$, the measurement result with the global bias removed, is itself an efficient estimator for $N = 1$. We can determine the resulting conditions by specializing the proof of the Cramér–Rao bound to the case of a single measurement with $x - \langle x \rangle_0$ as the estimator. We first write the mean of the estimator in the form

$$\langle x \rangle_X - \langle x \rangle_0 = \int dx (x - \langle x \rangle_0) p(x - X) = X. \quad (55)$$

Differentiating this expression with respect to X and using

$$0 = \frac{d}{dX} \int dx p(x - X) = - \int dx p'(x - X) \quad (56)$$

leads to

$$\begin{aligned} 1 &= - \int dx (x - \langle x \rangle_0) p'(x - X) \\ &= - \int dx (x - \langle x \rangle_0 - X) p'(x - X) \\ &= - \int dx (x - \langle x \rangle_0) p'(x) = - \int dx p(x) (x - \langle x \rangle_0) \frac{d \ln p(x)}{dx}. \end{aligned} \quad (57)$$

Squaring this expression and using the Schwarz inequality yields

$$\begin{aligned} 1 &= \left(\int dx p(x) (x - \langle x \rangle_0) \frac{d \ln p(x)}{dx} \right)^2 \\ &\leq \left(\int dx (x - \langle x \rangle_0)^2 p(x) \right) \left(\int dx p(x) \left(\frac{d \ln p(x)}{dx} \right)^2 \right). \end{aligned} \quad (58)$$

Rewriting the expression for the Fisher information in Eq. (42) as

$$F = \int dx \frac{[p'(x)]^2}{p(x)} = \int dx p(x) \left(\frac{d \ln p(x)}{dx} \right)^2 \quad (59)$$

shows that Eq. (58) is the classical $N=1$ bound on the estimator x :

$$\langle (\Delta x)^2 \rangle = \int dx (x - \langle x \rangle_0)^2 p(x) \geq \frac{1}{F}. \quad (60)$$

The condition for saturating this bound, which comes from the Schwarz inequality in Eq. (58), is that

$$\frac{d \ln p(x)}{dx} = -\lambda(x - \langle x \rangle_0) \Rightarrow p(x) \propto e^{-\lambda(x - \langle x \rangle_0)^2/2}, \quad (61)$$

where λ is a constant.

The result of these considerations is that equality in the uncertainty relation (54) can be achieved if and only if the fiducial wave function has the form (47), with $p(x) = r^2(x)$ being a Gaussian. These Gaussian states are analogous to the minimum-uncertainty states that give equality in the standard uncertainty relation. Thus our formalism of parameter-based uncertainty relations contains within itself, in the special case of the estimator being the sample mean, the standard uncertainty relation and the associated minimum-uncertainty states. Two points deserve mention. First, for most generators \hat{h} , there are restrictions on the form of the wave function; these restrictions, which are discussed in Section 3.2 and in the examples of Section 4, generally prevent one from choosing a Gaussian for $p(x)$ and thus mean that there are no states that yield equality in the uncertainty relation (54). Second, the restriction to Gaussian wave functions is a consequence of using the sample mean as the estimator. If one allows other estimators, the conditions on the fiducial wave function are weaker. Specifically, as we have seen, in the limit of large N , where maximum-likelihood estimation is asymptotically efficient, the condition for saturating the uncertainty relation (31) is that the fiducial wave function have the form (47).

3.2. The x Representation

Up until now, it has not been necessary to construct explicitly states $|x\rangle$ that satisfy the completeness and displacement properties. Such a construction depends on the eigenvalue spectrum of \hat{h} . Suppose that we write the eigenvalue equation for \hat{h} as

$$\hat{h} |h, \alpha\rangle = h |h, \alpha\rangle, \quad (62)$$

where we allow for the possibility of degeneracies by including a degeneracy label α . The orthonormal eigenstates $|h, \alpha\rangle$ satisfy a completeness relation

$$\hat{1} = \sum_{h, \alpha} |h, \alpha\rangle \langle h, \alpha|. \quad (63)$$

The displacement property (36), with $x=0$ and $X=x$, becomes

$$\langle h, \alpha | x \rangle = e^{-ixh} \langle h, \alpha | x=0 \rangle. \quad (64)$$

The displacement property thus relates all the states $|x\rangle$ to a particular state $|x=0\rangle$, which remains arbitrary.

We can now ask whether it is possible to satisfy the completeness property (32) by noting that

$$\int \frac{dx}{C} |x\rangle\langle x| = \sum_{h, h'} \int \frac{dx}{C} e^{-ix(h-h')} \left(\sum_{\alpha, \alpha'} |h, \alpha\rangle\langle h, \alpha | x=0\rangle\langle x=0 | h', \alpha'\rangle\langle h', \alpha'| \right). \quad (65)$$

One can arrange that

$$\int \frac{dx}{C} e^{-ix(h-h')} = \delta_{hh'}, \quad (66)$$

in which case Eq. (65) simplifies to

$$\int \frac{dx}{C} |x\rangle\langle x| = \sum_h \left(\sum_{\alpha, \alpha'} |h, \alpha\rangle\langle h, \alpha | x=0\rangle\langle x=0 | h, \alpha'\rangle\langle h, \alpha'| \right). \quad (67)$$

To make this integral equal to the unit operator requires that

$$\langle h, \alpha | x=0\rangle\langle x=0 | h, \alpha'\rangle = \delta_{\alpha\alpha'} \quad \text{for all } h, \quad (68)$$

which can only be satisfied if the spectrum of \hat{h} has no degeneracies. Thus only for nondegenerate \hat{h} can one hope to find a global optimal measurement in terms of a POVM described by a single real number x . An example of how to proceed for a degenerate \hat{h} can be found in the discussion of time-energy uncertainty relations in Section 4.3.

We now assume explicitly that the generator \hat{h} is nondegenerate, thus allowing us to drop the degeneracy label α from the preceding equations. The form of the completeness relation depends on further properties of the eigenvalue spectrum of \hat{h} . We illustrate the procedure here for the case that the nondegenerate spectrum of \hat{h} is discrete and that the unitary generator $e^{-iX\hat{h}}$ is periodic with smallest period \mathcal{X} , i.e., $e^{-iX\hat{h}} = \hat{1}$ (other nondegenerate eigenvalue spectra are dealt with in the examples of Section 4). This means that all the eigenvalues can be written as

$$h = 2\pi n_h / \mathcal{X}, \quad n_h \text{ an integer}; \quad (69)$$

any discrete spectrum can be approximated in this way for \mathcal{X} sufficiently large. The periodicity allows us to restrict both the parameter X and the measurement results x to the finite interval $[-\mathcal{X}/2, \mathcal{X}/2)$.

The completeness condition (32) now becomes

$$\begin{aligned}\hat{1} &= \int_{-\mathcal{X}/2}^{\mathcal{X}/2} \frac{dx}{C} |x\rangle\langle x| = \sum_{h, h'} |h\rangle\langle h| \langle x=0\rangle\langle x=0| h'\rangle\langle h'| \int_{-\mathcal{X}/2}^{\mathcal{X}/2} \frac{dx}{C} e^{-ix(h-h')} \\ &= \sum_h |h\rangle\langle h| \frac{\mathcal{X}|\langle h|x=0\rangle|^2}{C},\end{aligned}\quad (70)$$

which can be satisfied by choosing $C = \mathcal{X}$ and

$$\langle h|x=0\rangle = e^{if(h)}, \quad (71)$$

where $f(h)$ is an arbitrary real-valued function. The completeness property thus requires that $|x=0\rangle$ have the same magnitude of overlap with all the eigenstates of \hat{h} .

The minimal choice, $f(h) = 0$, which we distinguish by using bold-face characters, leads to *canonical* states

$$|\mathbf{x}\rangle = \sum_h |h\rangle e^{-ixh}, \quad (72)$$

whereas an arbitrary choice for $f(h)$ leads to states,

$$|x\rangle = \sum_h |h\rangle e^{if(h)} e^{-ixh} = e^{if(\hat{h})} |\mathbf{x}\rangle, \quad (73)$$

that are a gauge transformation (41) of the canonical states $|\mathbf{x}\rangle$. A gauge transformation corresponds to the freedom to rephase independently each of the eigenstates of \hat{h} —i.e., to replace $|h\rangle$ by $e^{if(h)} |h\rangle$.

The inner product of $|x\rangle$ and $|x'\rangle$ is given by

$$\langle x|x'\rangle = \sum_h e^{i(x-x')h} = \sum_h e^{2\pi i n_h(x-x')/\mathcal{X}}. \quad (74)$$

These states are orthogonal—i.e., they can be given δ function normalization with $\langle x|x'\rangle = \mathcal{X}\delta(x-x')$ —if and only if *all* integers are required to represent the eigenvalue spectrum of \hat{h} ; only if the states are orthogonal—i.e., all integers are present in the eigenvalue spectrum—are they eigenstates of a Hermitian operator.

The x and h representations of a state $|\psi\rangle$ are related by

$$\frac{1}{\sqrt{\mathcal{X}}} \langle x|\psi\rangle = \psi(x) = \frac{1}{\sqrt{\mathcal{X}}} \sum_h e^{ixh} e^{-if(h)} \langle h|\psi\rangle, \quad (75)$$

$$e^{-if(h)} \langle h|\psi\rangle = \frac{1}{\sqrt{\mathcal{X}}} \int_{-\mathcal{X}/2}^{\mathcal{X}/2} dx e^{-ixh} \psi(x). \quad (76)$$

The amplitude $e^{-if(h)} \langle h|\psi\rangle$ is the discrete Fourier coefficient, corresponding to integer n_h , of the function $\psi(x)$, which is periodic with period \mathcal{X} . The wave functions $\psi(x)$ are restricted to periodic functions that have vanishing Fourier coefficients for

the unused integers. By the same token, the expansion of a state $|\psi\rangle$ in terms of the states $|x\rangle$,

$$|\psi\rangle = \int_{-x/2}^{x/2} \frac{dx}{\mathcal{X}} |x\rangle \langle x | \psi \rangle = \frac{1}{\sqrt{\mathcal{X}}} \int_{-x/2}^{x/2} dx \psi(x) |x\rangle, \quad (77)$$

is not unique; one can add to $\psi(x)$ any periodic function $g(x)$ that has nonvanishing Fourier coefficients only for the unused integers, for such a function satisfies

$$\frac{1}{\sqrt{\mathcal{X}}} \int_{-x/2}^{x/2} dx g(x) |x\rangle = 0. \quad (78)$$

This lack of uniqueness expresses the *overcompleteness* of the states $|x\rangle$. Both the overcompleteness and the restrictions on the wave functions $\psi(x)$ are consequences of the lack of orthogonality of the states $|x\rangle$.

For $H = 2\pi n_H/\mathcal{X}$, we can define a “displacement operator”

$$\begin{aligned} \hat{D}(H) &\equiv \int_{-x/2}^{x/2} dx e^{ixH} \hat{E}(x) = \int_{-x/2}^{x/2} \frac{dx}{\mathcal{X}} e^{ixH} |x\rangle \langle x| \\ &= \sum_{h, h'} \delta_{n_H, n_h + n_H} e^{if(h')} |h'\rangle \langle h| e^{-if(h)}, \end{aligned} \quad (79)$$

which displaces eigenstates of \hat{h} , i.e.,

$$\hat{D}(H) e^{if(h)} |h\rangle = e^{if(h+H)} |h+H\rangle, \quad (80)$$

provided H is the difference in eigenvalues. Given a choice of phases for the eigenstates $|h\rangle$, the canonical states $|x\rangle$ are unique in that their displacement operator $\hat{D}(H)$ displaces the eigenstates $|h\rangle$ without the inclusion of any phase factors. Notice that generally $\hat{D}(H)$ is not a unitary operator. For particular eigenvalue spectra of \hat{h} , however, as in the examples of Section 4, the displacement operator acquires additional important properties.

The x and h representations (75) and (76) of a state $|\psi\rangle$ show that the condition (47) for a global optimal measurement, when written in the h representation, with $h = \langle \hat{h} \rangle + u$, becomes

$$e^{if(\langle \hat{h} \rangle + u)} \langle \langle \hat{h} \rangle + u | \psi_0 \rangle = e^{if(\langle \hat{h} \rangle - u)} \langle \langle \hat{h} \rangle - u | \psi_0 \rangle^*. \quad (81)$$

Since the phases in the h representation can be removed by appropriate choice of the function $f(h)$, this condition reduces to

$$|\langle \langle \hat{h} \rangle + u | \psi_0 \rangle|^2 = |\langle \langle \hat{h} \rangle - u | \psi_0 \rangle|^2. \quad (82)$$

To make this condition meaningful requires that whenever $\langle \langle \hat{h} \rangle + u | \psi_0 \rangle$ is non-zero, $\langle \hat{h} \rangle - u$ is an eigenvalue of \hat{h} . For general eigenvalue spectra of \hat{h} , condition (82) can be met by only a very limited class of states, since it requires symmetric excitation of eigenstates $|h\rangle$ symmetrically located about the expectation value of \hat{h} .

4. EXAMPLES OF GENERALIZED UNCERTAINTY RELATIONS

We turn now to examples of generalized uncertainty relations, first dealing, in this section, with nonrelativistic examples and then turning, in Section 5, to Lorentz-invariant versions of uncertainty relations.

4.1. *Spatial Displacement and Momentum*

The first example of a nonrelativistic uncertainty relation is the familiar one of spatial displacements X that are generated by the momentum operator \hat{p} , i.e., $\hat{h} = \hat{p}/\hbar$:

$$|\psi_x\rangle = e^{-iX\hat{p}/\hbar} |\psi_0\rangle. \quad (83)$$

The uncertainty relation (31) takes the form

$$\langle (\delta X)^2 \rangle_x \langle (\Delta \hat{p})^2 \rangle \geq \frac{\hbar^2}{4N}. \quad (84)$$

Helstrom [4] and Holevo [5, Chap. VI.2] have presented parameter-based uncertainty relations for spatial displacement and momentum, and Dembo, Cover, and Thomas [7] have reviewed the basis for such uncertainty relations in the properties of Fisher information.

To investigate the possibilities for optimal POVMs $\hat{E}(x) dx = |x\rangle\langle x| dx/C$, start from the complete set of δ function normalized eigenstates $|p\rangle$ of \hat{p} :

$$\langle p | p' \rangle = 2\pi\hbar \delta(p - p'), \quad (85)$$

$$\hat{1} = \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} |p\rangle\langle p|. \quad (86)$$

The displacement condition (36), with $x=0$ and $X=x$, becomes

$$\langle p | x \rangle = e^{-ixp/\hbar} \langle p | x=0 \rangle, \quad (87)$$

which leads to

$$\langle p | \left(\int_{-\infty}^{\infty} \frac{dx}{C} |x\rangle\langle x| \right) |p' \rangle = \frac{2\pi\hbar |\langle p | x=0 \rangle|^2}{C} \delta(p - p'). \quad (88)$$

Thus the completeness condition (32) can be satisfied by choosing $C=1$ and

$$\langle p | x=0 \rangle = e^{if(p)}, \quad (89)$$

where $f(p)$ is an arbitrary real-valued function. In this case, because the spectrum of \hat{p} covers the entire real line, the states

$$|x\rangle = \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} |p\rangle e^{if(p)} e^{-ixp/\hbar} \quad (90)$$

have δ function normalization,

$$\langle x | x' \rangle = \delta(x - x'), \quad (91)$$

and thus are eigenstates of the Hermitian operator

$$\hat{x} = \int_{-\infty}^{\infty} dx x \hat{E}(x) = \int_{-\infty}^{\infty} dx x |x\rangle \langle x|. \quad (92)$$

The minimal choice, $f(p) = 0$, leads to the canonical position states,

$$|\mathbf{x}\rangle = \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} |p\rangle e^{-ixp/\hbar}, \quad (93)$$

which are eigenstates of the canonical position operator

$$\hat{\mathbf{x}} = \int_{-\infty}^{\infty} dx x \hat{\mathbf{E}}(x) = \int_{-\infty}^{\infty} dx x |\mathbf{x}\rangle \langle \mathbf{x}|. \quad (94)$$

Measurements described by $\hat{\mathbf{E}}(x)$ are thus canonical measurements of position. An arbitrary choice for $f(p)$ leads to the states (90), which, written as

$$|x\rangle = e^{if(\hat{p})} |\mathbf{x}\rangle, \quad (95)$$

are seen to be a gauge transformation (41) of the position eigenstates. The state $|x\rangle$ is an eigenstate, with eigenvalue x , of the operator (92), which can be written as

$$\hat{x} = e^{if(\hat{p})} \hat{\mathbf{x}} e^{-if(\hat{p})} = \hat{\mathbf{x}} + \hbar f'(\hat{p}); \quad (96)$$

measurements described by $\hat{E}(x)$ are measurements of this operator. Notice that \hat{x} and \hat{p} satisfy the canonical commutation relation,

$$[\hat{x}, \hat{p}] = i\hbar, \quad (97)$$

the gauge freedom being precisely the freedom permitted by this commutator.

The operator that displaces momentum eigenstates,

$$\hat{D}(P) = \int_{-\infty}^{\infty} dx e^{ixP/\hbar} |x\rangle \langle x| = e^{i\hat{x}P/\hbar} \quad (98)$$

(cf. Eq. (79)), in this case a unitary operator, acts according to

$$\hat{D}(P) e^{if(p)} |p\rangle = e^{if(p+P)} |p+P\rangle. \quad (99)$$

The canonical states $|\mathbf{x}\rangle$ lead to a displacement operator $\hat{\mathbf{D}}(P)$ that displaces the momentum eigenstates $|p\rangle$ without the inclusion of any phase factors.

Writing the position wave function of the fiducial state as $\psi_0(x) = r(x) e^{i\Theta(x)}$, the general relations (48) and (49) for the mean and variance of \hat{h} become in this case

$$\langle \hat{p} \rangle = \int_{-\infty}^{\infty} dx \psi_0^*(x) \frac{\hbar}{i} \frac{\partial}{\partial x} \psi_0(x) = \int_{-\infty}^{\infty} dx p(x) \hbar \Theta'(x), \quad (100)$$

$$\begin{aligned} \langle (\Delta \hat{p})^2 \rangle &= \int_{-\infty}^{\infty} dx \left| \left(\hbar \frac{\partial}{\partial x} - i \langle \hat{p} \rangle \right) \psi_0(x) \right|^2 \\ &= \frac{\hbar^2}{4} \int_{-\infty}^{\infty} dx \frac{[p'(x)]^2}{p(x)} + \int_{-\infty}^{\infty} dx p(x) [\hbar \Theta'(x) - \langle \hat{p} \rangle]^2. \end{aligned} \quad (101)$$

For the minimal choice [$f(p) = 0$] and its canonical position operator, several authors have drawn attention to the way the momentum variance splits into the sum of the two parts in Eq. (101). Stam [20] noted long ago that the variance of \hat{p} is bounded below by the Fisher information for position measurements, Cohen [21] has discussed and illustrated with examples the split of the momentum variance, and Sipe and Arkani-Hamed [22] have used this split and the similar split of the variance of \hat{x} to contrast the coherence of pure and mixed states.

The condition for a global optimal measurement is that the position wave function of the fiducial state have the form

$$\langle x | \psi_0 \rangle = \psi_0(x) = r(x) e^{i \langle \hat{p} \rangle x / \hbar} \quad (102)$$

(cf. Eq. (47)). Transforming to the momentum representation, with $p = \langle p \rangle + u$,

$$e^{-if(\langle \hat{p} \rangle + u)} \langle \langle \hat{p} \rangle + u | \psi_0 \rangle = \int_{-\infty}^{\infty} dx e^{-ixu/\hbar} r(x), \quad (103)$$

one sees that the optimality condition can be written as

$$e^{-if(\langle \hat{p} \rangle + u)} \langle \langle \hat{p} \rangle + u | \psi_0 \rangle = e^{if(\langle \hat{p} \rangle - u)} \langle \langle \hat{p} \rangle - u | \psi_0 \rangle^* \quad (104)$$

(cf. Eq. (81)). If one is restricted to canonical position measurements, for which $f(p) = 0$, the condition for optimality is that

$$\langle \langle \hat{p} \rangle + u | \psi_0 \rangle = \langle \langle \hat{p} \rangle - u | \psi_0 \rangle^*. \quad (105)$$

If one allows gauge-transformed measurements, then the gauge transformation can be used to remove the phases in the momentum representation, so the condition for optimality is the weaker condition that

$$|\langle \langle \hat{p} \rangle + u | \psi_0 \rangle|^2 = |\langle \langle \hat{p} \rangle - u | \psi_0 \rangle|^2, \quad (106)$$

i.e., that the momentum probability density is symmetric about $\langle \hat{p} \rangle$.

It is instructive to illustrate these ideas with an extended example based on a specific fiducial state. For this purpose, introduce an “annihilation operator”

$$\hat{a} = \frac{1}{\sqrt{2}} \left(\frac{\hat{\mathbf{x}}}{L} + i \frac{L\hat{p}}{\hbar} \right), \quad (107)$$

where L is a constant that has dimensions of length, and a “vacuum state” $|\text{vac}\rangle$, which is the state annihilated by \hat{a} ,

$$\hat{a} |\text{vac}\rangle = 0. \quad (108)$$

One easily verifies from this equation that in the vacuum state, $\hat{\mathbf{x}}$ and \hat{p} have zero mean, and their covariance matrix is given by

$$\frac{\langle \text{vac} | (\Delta \hat{\mathbf{x}})^2 | \text{vac} \rangle}{L^2} = \frac{L^2 \langle \text{vac} | (\Delta \hat{p})^2 | \text{vac} \rangle}{\hbar^2} = \frac{1}{2}, \quad (109)$$

$$\langle \text{vac} | (\Delta \hat{\mathbf{x}} \Delta \hat{p} + \Delta \hat{p} \Delta \hat{\mathbf{x}}) | \text{vac} \rangle = 0. \quad (110)$$

The vacuum state is thus a minimum-uncertainty state for $\hat{\mathbf{x}}$ and \hat{p} . It is convenient throughout the remainder of this example to use units such that $L = 1$, a choice that gives $\hat{\mathbf{x}}$ and \hat{p}/\hbar equal variances in the vacuum state.

The next step is to introduce the squeeze operator [23]

$$\hat{S} \equiv \exp\left(\frac{1}{2}r(e^{-2i\varphi}\hat{a}^2 - e^{2i\varphi}\hat{a}^{\dagger 2})\right), \quad (111)$$

which is a function of a squeeze parameter $r \geq 0$ and a squeeze angle φ . The squeeze operator has the property [23]

$$\begin{aligned} \hat{S}\hat{a}\hat{S}^\dagger &= \hat{a} \cosh r + \hat{a}^\dagger e^{2i\varphi} \sinh r \\ &= \frac{1}{\sqrt{2}} \left(\hat{\mathbf{x}}(\cosh r + e^{2i\varphi} \sinh r) + i \frac{\hat{p}}{\hbar} (\cosh r - e^{2i\varphi} \sinh r) \right) \equiv \hat{\chi}. \end{aligned} \quad (112)$$

The fiducial state in this example is generated from the vacuum state by the squeeze operator,

$$|\psi_0\rangle = \hat{S} |\text{vac}\rangle, \quad (113)$$

and is sometimes called the squeezed vacuum state. An immediate consequence of the property (112) is that the squeezed vacuum state is annihilated by $\hat{\chi}$:

$$\hat{\chi} |\psi_0\rangle = 0. \quad (114)$$

One can get a better feel for the nature of the squeezed vacuum state and, in particular, its parameters r and φ by considering $\hat{\mathbf{x}}$ and \hat{p}/\hbar to be coordinates on a phase plane and then rotating by angle φ to new canonical coordinates $\hat{\mathbf{x}}'$ and \hat{p}'/\hbar :

$$\frac{1}{\sqrt{2}} (\hat{\mathbf{x}} + i\hat{p}/\hbar) = \hat{a} = \hat{a}' e^{i\varphi} = \frac{1}{\sqrt{2}} (\hat{\mathbf{x}}' + i\hat{p}'/\hbar) e^{i\varphi}. \quad (115)$$

In terms of the rotated coördinates the operator $\hat{\chi}$ assumes the form

$$\hat{\chi} = e^{i\varphi}(\hat{a}' \cosh r + \hat{a}'^\dagger \sinh r) = \frac{1}{\sqrt{2}} e^{i\varphi} \left(\hat{\mathbf{x}}' e^r + i \frac{\hat{p}'}{\hbar} e^{-r} \right), \quad (116)$$

which, together with Eq. (114), implies that in the squeezed vacuum state, \mathbf{x}' and \hat{p}' have zero mean, and their covariance matrix is given by

$$\langle \psi_0 | (\Delta \hat{\mathbf{x}}')^2 | \psi_0 \rangle e^{2r} = \frac{\langle \psi_0 | (\Delta \hat{p}')^2 | \psi_0 \rangle}{\hbar^2} e^{-2r} = \frac{1}{2}, \quad (117)$$

$$\langle \psi_0 | (\Delta \hat{\mathbf{x}}' \Delta \hat{p}' + \Delta \hat{p}' \Delta \hat{\mathbf{x}}') | \psi_0 \rangle = 0. \quad (118)$$

The squeezed vacuum state is thus a minimum-uncertainty state for the rotated coördinates $\hat{\mathbf{x}}'$ and \hat{p}' ; relative to the vacuum state, $\hat{\mathbf{x}}'$ has uncertainty reduced by a factor e^{-r} , and \hat{p}' has uncertainty increased by a factor e^r . Figure 1 depicts the squeezed vacuum state on a phase-plane diagram.

If one rotates to any other orthogonal axes, the position variance gets bigger than the variance of $\hat{\mathbf{x}}'$ (recall that $r \geq 0$), because the reduced variance of $\hat{\mathbf{x}}'$ is

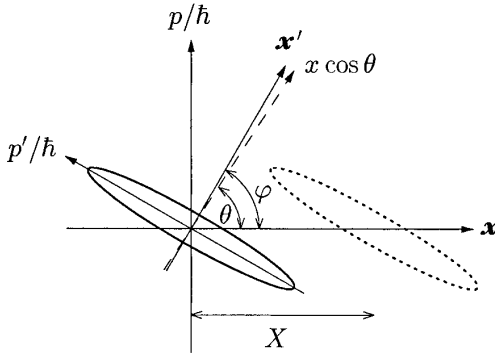


FIG. 1. Phase-plane representation of optimal measurements of displacement of a squeezed vacuum state. The squeezed vacuum state $|\psi_0\rangle = \hat{S}|\text{vac}\rangle$ is represented by a solid "uncertainty ellipse" centered at the origin. The principal axes of the ellipse are oriented along the directions defined by the uncorrelated coördinates \mathbf{x}' and p' , which are rotated by an angle φ relative to the axes defined by the canonical position \mathbf{x} and the momentum p ; the principal radii of the ellipse are given by the uncertainties $\langle \psi_0 | (\Delta \hat{\mathbf{x}}')^2 | \psi_0 \rangle^{1/2} = e^{-r}/\sqrt{2}$ and $\langle \psi_0 | (\Delta \hat{p}')^2 | \psi_0 \rangle^{1/2}/\hbar = e^r/\sqrt{2}$. The dotted uncertainty ellipse depicts the state obtained by displacing the squeezed vacuum state a distance X along the \mathbf{x} axis. The global optimal measurement for distinguishing displaced squeezed states corresponds to measuring a variable x (see Eq. (131)), which is a rescaled position variable along an axis rotated by angle θ from the axis of the canonical position variable \mathbf{x} . The optimal measurement represents a compromise between maximal "signal," which would be obtained by measuring the canonical position variable \mathbf{x} , and minimal "noise," which would be obtained by measuring the rotated position variable \mathbf{x}' (see Eq. (134)).

contaminated by the increased variance of \hat{p}' . Indeed, the covariance matrix of the original canonical coördinates, obtained directly from Eq. (114) or by rotating back to the original coördinates, is given by [23]

$$\langle \psi_0 | (\Delta \hat{\mathbf{x}})^2 | \psi_0 \rangle = \frac{1}{2} (e^{-2r} \cos^2 \varphi + e^{2r} \sin^2 \varphi) = \frac{1}{2 \operatorname{Re}(\gamma)}, \quad (119)$$

$$\frac{\langle \psi_0 | (\Delta \hat{p})^2 | \psi_0 \rangle}{\hbar^2} = \frac{1}{2} (e^{-2r} \sin^2 \varphi + e^{2r} \cos^2 \varphi) = \frac{1}{2 \operatorname{Re}(\gamma^{-1})}, \quad (120)$$

$$\begin{aligned} \frac{\frac{1}{2} \langle \psi_0 | (\Delta \hat{\mathbf{x}} \Delta \hat{p} + \Delta \hat{p} \Delta \hat{\mathbf{x}}) | \psi_0 \rangle}{\hbar} &= -\frac{1}{2} \sinh 2r \sin 2\varphi \\ &= -\frac{\operatorname{Im}(\gamma)}{2 \operatorname{Re}(\gamma)} = \frac{\operatorname{Im}(\gamma^{-1})}{2 \operatorname{Re}(\gamma^{-1})}, \end{aligned} \quad (121)$$

where

$$\gamma = \frac{\cosh r + e^{2i\varphi} \sinh r}{\cosh r - e^{2i\varphi} \sinh r} = \frac{1 + i \sinh 2r \sin 2\varphi}{\cosh 2r - \sinh 2r \cos 2\varphi} = \frac{\cosh 2r + \sinh 2r \cos 2\varphi}{1 - i \sinh 2r \sin 2\varphi} \quad (122)$$

is a complex constant. This covariance matrix can also be gotten from the wave function of the fiducial state in the canonical position representation [23],

$$\Psi_0(x) = \langle \mathbf{x} | \psi_0 \rangle = \left(\frac{\operatorname{Re}(\gamma)}{\pi} \right)^{1/4} \exp \left(-\frac{\gamma x^2}{2} \right), \quad (123)$$

which follows from integrating the differential equation that represents Eq. (114) in the canonical position representation. An irrelevant phase factor is set equal to unity in the wave function (123) (Schumaker [23] has given a consistent set of phases for squeezed-state wave functions).

It is now straightforward to find the optimal measurement. The wave function in the momentum basis is given by

$$\langle p | \psi_0 \rangle = \int_{-\infty}^{\infty} dx e^{-ixp/\hbar} \Psi_0(x) = \sqrt{|\gamma|/\gamma} (4\pi \operatorname{Re}(\gamma^{-1}))^{1/4} \exp \left(-\frac{p^2/\hbar^2}{2\gamma} \right), \quad (124)$$

where $\sqrt{|\gamma|/\gamma}$ is an overall phase factor. According to the optimality condition (104), choosing $f(p)$ to cancel the imaginary part of this complex Gaussian, i.e.,

$$f(p) = -\frac{1}{2} \operatorname{Im}(\gamma^{-1}) p^2/\hbar^2, \quad (125)$$

yields an optimal measurement, corresponding to measuring the operator

$$\hat{x} = \hat{\mathbf{x}} + \hbar f'(\hat{p}) = \hat{\mathbf{x}} - \operatorname{Im}(\gamma^{-1}) \hat{p}/\hbar. \quad (126)$$

The distinguishing feature of using a squeezed state as the fiducial state is that the optimal measurement is a *linear* combination of \hat{x} and \hat{p} . Transforming to the x representation yields a real wave function

$$\psi_0(x) = \langle x | \psi_0 \rangle = \sqrt{|\gamma|/\gamma} \left(\frac{1}{\pi \operatorname{Re}(\gamma^{-1})} \right)^{1/4} \exp \left(-\frac{x^2}{2 \operatorname{Re}(\gamma^{-1})} \right), \quad (127)$$

aside from the overall phase factor $\sqrt{|\gamma|/\gamma}$, in accordance with the general condition for an optimal measurement.

One feature of the optimal measurement in this case, which follows from the fact that $\psi_0(x)$ is a Gaussian wave function of the sort considered at the end of Section 3.1, deserves emphasis. The probability density of measurements of \hat{x} ,

$$p(x) = |\psi_0(x)|^2 = \left(\frac{1}{\pi \operatorname{Re}(\gamma^{-1})} \right)^{1/2} \exp \left(-\frac{x^2}{\operatorname{Re}(\gamma^{-1})} \right), \quad (128)$$

is a zero-mean Gaussian with variance

$$\langle \psi_0 | (\Delta \hat{x})^2 | \psi_0 \rangle = \frac{1}{2} \operatorname{Re}(\gamma^{-1}) = \frac{1}{2} (e^{-2r} \sin^2 \varphi + e^{2r} \cos^2 \varphi)^{-1} = \frac{\hbar^2}{4 \langle \psi_0 | (\Delta \hat{p})^2 | \psi_0 \rangle}. \quad (129)$$

Generally one must appeal to the large- N asymptotic limit to saturate the first (classical) inequality in Eq. (9)—i.e., to achieve the Cramér–Rao bound—but since the statistics of \hat{x} are Gaussian, no such appeal is necessary. Indeed, for Gaussian statistics the sample mean (52) of the data (here $\langle x \rangle_0 = 0$) provides an efficient estimator for all values of N , as is discussed at the end of Section 3.1. The Gaussian statistics of x for the fiducial state, displaced according to Eq. (33), imply that $\langle X_{\text{est}} \rangle_X = X$ —i.e., the estimator is unbiased—which means that the estimate’s deviation away from the parameter becomes $\delta X = X_{\text{est}} - X = \Delta X_{\text{est}}$. The mean-square deviation is independent of X and reduces to

$$\langle (\delta X)^2 \rangle = \langle (\Delta X_{\text{est}})^2 \rangle = \frac{1}{N} \langle \psi_0 | (\Delta \hat{x})^2 | \psi_0 \rangle = \frac{1}{NF}. \quad (130)$$

The final equality, which shows that X_{est} is an efficient estimator, follows most easily from the form of the Fisher information in Eq. (59). In this case, where an efficient estimator is known, one can proceed directly to equality in the uncertainty relation (84), without going through the Fisher information, by combining Eqs. (129) and (130).

One gains insight into the optimal measurement by writing the measured operator (126) as

$$\hat{x} = \hat{x} + \frac{\hat{p}}{\hbar} \tan \theta = \frac{\hat{x} \cos \theta + (\hat{p}/\hbar) \sin \theta}{\cos \theta}, \quad (131)$$

where

$$\tan \theta = -\operatorname{Im}(\gamma^{-1}) = \frac{\sinh 2r \sin 2\varphi}{\cosh 2r + \sinh 2r \cos 2\varphi}, \quad (132)$$

and regarding \hat{x} as a species of position operator that arises from a rotation in the phase plane by angle θ , followed by rescaling by $1/\cos \theta$. The rescaling means that displacement by X produces the same “signal” in \hat{x} as it does in \hat{x} . The optimal angle θ is not equal to φ , the rotation angle that minimizes the variance of the rotated position; instead, the optimal angle is a compromise between reduced “noise” and reduced signal, both of which come with rotation (see Fig. 1). The rescaling of \hat{x} accounts for the reduced signal, so the variance of \hat{x} ,

$$\begin{aligned} & \langle \psi_0 | (\Delta \hat{x})^2 | \psi_0 \rangle \\ &= \langle \psi_0 | (\Delta \hat{x})^2 | \psi_0 \rangle + 2 \frac{\frac{1}{2} \langle \psi_0 | (\Delta \hat{x} \Delta \hat{p} + \Delta \hat{p} \Delta \hat{x}) | \psi_0 \rangle}{h} \tan \theta \\ & \quad + \frac{\langle \psi_0 | (\Delta \hat{p})^2 | \psi_0 \rangle}{h^2} \tan^2 \theta, \end{aligned} \quad (133)$$

is a noise-to-signal ratio [24]. Indeed, the angle that minimizes this noise-to-signal ratio,

$$\tan \theta = -\frac{\frac{1}{2} \langle \psi_0 | (\Delta \hat{x} \Delta \hat{p} + \Delta \hat{p} \Delta \hat{x}) | \psi_0 \rangle / h}{\langle \psi_0 | (\Delta \hat{p})^2 | \psi_0 \rangle / h^2} = -\operatorname{Im}(\gamma^{-1}), \quad (134)$$

defines the optimal measurement.

4.2. Harmonic-Oscillator Phase and Number of Quanta

For our second example of a nonrelativistic uncertainty relation, consider a harmonic oscillator that has creation and annihilation operators \hat{a}^\dagger and \hat{a} . The “number operator”

$$\hat{n} = \hat{a}^\dagger \hat{a} \quad (135)$$

has eigenstates $|n\rangle$, called “number states,” where $n=0, 1, \dots$ is the number of quanta. Shifts $X=\Phi$ in the phase of the oscillator are generated by the number operator,

$$|\psi_\Phi\rangle = e^{i\Phi\hat{n}} |\psi_0\rangle, \quad (136)$$

i.e., $\hat{h} = -\hat{n}$. The uncertainty relation (31) then reads

$$\langle (\delta\Phi)^2 \rangle_\Phi \langle (\Delta\hat{n})^2 \rangle \geq \frac{1}{4N}. \quad (137)$$

Holevo [5, Chap. III. 9] has considered this sort of phase uncertainty relation. Lane, Braunstein, and Caves [25], in a detailed analysis of phase measurements, have used formula (49), specialized to give the variance of the number operator, to bound the Fisher information for the phase.

A phase shift Φ can be thought of as a dimensionless time (measured in units of (harmonic-oscillator period)/ 2π), so the uncertainty relation (137) is a dimensionless time–energy uncertainty relation, special because of the uniform spacing of the eigenstates of the generator \hat{n} . General time–energy uncertainty relations, corresponding to other energy spectra, are considered in Section 4.3.

Since phase shifts are periodic with period 2π , Φ can be restricted to the interval $-\pi \leq \Phi < \pi$. It might be thought that there is a difficulty with the phase-number uncertainty relation (137) when the fiducial state is a number state, for which $\langle (\Delta \hat{n})^2 \rangle = 0$; the uncertainty relation then forces $\langle (\delta \Phi)^2 \rangle_{\phi} \rightarrow \infty$, even though a sensible estimator Φ_{est} is restricted to the same 2π interval as is Φ . No difficulty arises, however, because for a number state, no measurement can provide any information about the phase shift; thus, any estimator, sensible or not, satisfies $d\langle \Phi_{\text{est}} \rangle / d\Phi = 0$, with the result that the deviation $\delta \Phi$ of Eq. (8) diverges, even if Φ_{est} is restricted to a finite range.

The possibilities for POVMs $\hat{E}(\phi) d\phi = |\phi\rangle\langle\phi| d\phi / C$ ($-\pi \leq \phi < \pi$) are determined by the displacement condition (36), which, with $\phi = 0$ and $\Phi = \phi$, becomes

$$\langle n | \phi \rangle = e^{i\phi n} \langle n | \phi = 0 \rangle, \quad (138)$$

and by the completeness condition (32),

$$\hat{1} = \int_{-\pi}^{\pi} \frac{d\phi}{C} |\phi\rangle\langle\phi| = \frac{2\pi}{C} \sum_{n=0}^{\infty} |\langle n | \phi = 0 \rangle|^2 |n\rangle\langle n|, \quad (139)$$

which can be satisfied by choosing $C = 2\pi$ and

$$\langle n | \phi = 0 \rangle = e^{if(n)}, \quad (140)$$

where $f(n)$ is an arbitrary real-valued function. Since there are no number states for negative integers, the phase states $|\phi\rangle$ are not orthogonal, the inner product being given by [26]

$$\begin{aligned} \langle \phi | \phi' \rangle &= \sum_{n=0}^{\infty} e^{-i(\phi - \phi')n} \\ &= \frac{1}{2} \left(\sum_{n=-\infty}^{\infty} e^{-i(\phi - \phi')n} + \sum_{n=-\infty}^{\infty} \text{sgn}(n) e^{-i(\phi - \phi')n} + 1 \right) \\ &= \pi \delta(\phi - \phi') - \frac{i}{2} \cot \left(\frac{\phi - \phi'}{2} \right) + \frac{1}{2}, \end{aligned} \quad (141)$$

where

$$\text{sgn}(n) \equiv \begin{cases} -1, & n < 0, \\ 0, & n = 0, \\ 1, & n > 0. \end{cases} \quad (142)$$

Hence the states $|\phi\rangle$ are overcomplete and are not the eigenstates of any Hermitian operator. There is no Hermitian phase operator in the infinite-dimensional Hilbert space of a harmonic oscillator [5, 26–29], although one can be constructed if the harmonic-oscillator Hilbert space is truncated to be finite-dimensional [30].

The minimal choice, $f(n) = 0$, leads to the Susskind–Glogower [27] canonical phase states,

$$|\Phi\rangle = \sum_{n=0}^{\infty} |n\rangle e^{i\phi n}, \quad (143)$$

which are eigenstates of the nonunitary number-lowering operator

$$\widehat{e^{i\phi}} \equiv (\hat{n} + 1)^{-1/2} \hat{a} = \hat{a} \hat{n}^{-1/2} = \sum_{n=1}^{\infty} |n-1\rangle \langle n|, \quad (144)$$

i.e.,

$$\widehat{e^{i\phi}} |\Phi\rangle = e^{i\phi} |\Phi\rangle. \quad (145)$$

Helstrom [4] and Holevo [5, Chap. III.9] have considered measurements described by the Susskind–Glogower states. An arbitrary choice for $f(n)$ leads to states,

$$|\phi\rangle = \sum_{n=0}^{\infty} |n\rangle e^{if(n)} e^{i\phi n} = e^{if(\hat{n})} |\Phi\rangle, \quad (146)$$

that are a gauge transformation (41) of the Susskind–Glogower states. The state $|\phi\rangle$ is an eigenstate, with eigenvalue $e^{i\phi}$, of the operator

$$\begin{aligned} e^{if(\hat{n})} \widehat{e^{i\phi}} e^{-if(\hat{n})} &= e^{-i[f(\hat{n}+1) - f(\hat{n})]} \widehat{e^{i\phi}} = \widehat{e^{i\phi}} e^{-i[f(\hat{n}) - f(\hat{n}-1)]} \\ &= \sum_{n=1}^{\infty} e^{if(n-1)} |n-1\rangle \langle n| e^{-if(n)}; \end{aligned} \quad (147)$$

the differences $f(\hat{n}+1) - f(\hat{n})$ and $f(\hat{n}) - f(\hat{n}-1)$ in the exponents are analogous to the derivative $\hbar f'(\hat{p})$ in Eq. (96).

For N an integer the number displacement operator is given by

$$\begin{aligned}
 \hat{D}(N) &\equiv \int_{-\pi}^{\pi} d\phi e^{-i\phi N} \hat{E}(\phi) = \int_{-\pi}^{\pi} \frac{d\phi}{2\pi} e^{-i\phi N} |\phi\rangle\langle\phi| \\
 &= \sum_{n, n'} \delta_{n', n+N} e^{if(n')} |n'\rangle\langle n| e^{-if(n)} \\
 &= \sum_{n=\max(0, -N)}^{\infty} e^{if(n+N)} |n+N\rangle\langle n| e^{-if(n)} \tag{148}
 \end{aligned}$$

(cf. Eq. (79)). Because there are no number states for negative integers, $\hat{D}(N)$ is not unitary; the final form of $\hat{D}(N)$ is a consequence of the regular spacing of the number states. Notice that $\hat{D}(-1) = e^{if(\hat{n})} \widehat{e^{i\phi}} e^{-if(\hat{n})}$ (thus the states $|\phi\rangle$ are eigenstates of $\hat{D}(-1)$) and $\hat{D}(1) = [\hat{D}(-1)]^\dagger = e^{if(\hat{n})} \widehat{e^{i\phi}^\dagger} e^{-if(\hat{n})}$.

The ϕ and n representations of a state $|\psi\rangle$ are related by

$$\frac{1}{\sqrt{2\pi}} \langle\phi|\psi\rangle = \psi(\phi) = \frac{1}{\sqrt{2\pi}} \sum_n e^{-i\phi n} e^{-if(n)} \langle n|\psi\rangle, \tag{149}$$

$$e^{-if(n)} \langle n|\psi\rangle = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} d\phi e^{i\phi n} \psi(\phi), \tag{150}$$

$e^{-if(n)} \langle n|\psi\rangle$ being the Fourier coefficient of the periodic function $\psi(\phi)$. The condition for a global optimal measurement, that the ϕ wave function of the fiducial state have the form

$$\psi_0(\phi) = r(\phi) e^{-i\langle\hat{n}\rangle\phi}, \tag{151}$$

is equivalent to the following requirement on the number-state amplitudes:

$$e^{-if(\langle\hat{n}\rangle+u)} \langle\langle\hat{n}\rangle+u|\psi_0\rangle = e^{if(\langle\hat{n}\rangle-u)} \langle\langle\hat{n}\rangle-u|\psi_0\rangle^* \tag{152}$$

(cf. Eq. (81)). If one is restricted to Susskind-Glogower phase measurements [$f(n)=0$], the condition for optimality is that

$$\langle\langle\hat{n}\rangle+u|\psi_0\rangle = \langle\langle\hat{n}\rangle-u|\psi_0\rangle^*, \tag{153}$$

but if one allows gauge-transformed measurements, the condition for optimality becomes

$$|\langle\langle\hat{n}\rangle+u|\psi_0\rangle|^2 = |\langle\langle\hat{n}\rangle-u|\psi_0\rangle|^2. \tag{154}$$

In either case, the condition for optimality can only be met by a limited class of states; in particular, because of the discreteness of the number states, $\langle\hat{n}\rangle$ must be integral or half-integral, and because of the lower bound at $n=0$, $\langle n|\psi\rangle$ must vanish for $n > 2\langle\hat{n}\rangle$.

Since the optimality conditions appear to be so restrictive, it is worth noting that a large class of “semiclassical” states satisfies them approximately. By a semiclassical state, we mean one that has number amplitudes $\langle n | \psi \rangle$ that are concentrated at large n , rendering the lower bound at $n=0$ irrelevant and are spread over a wide range of values of n , making the discreteness of n unimportant. For semiclassical states measurements described by $\hat{E}(\phi)$ are nearly optimal provided only that the number probabilities $|\langle n | \psi \rangle|^2$ are symmetric about $\langle \hat{n} \rangle$ (cf. Eq. (106)). The extent to which measurements of $\hat{E}(\phi)$ are suboptimal for semiclassical states deserves further investigation.

4.3. Time and Energy

For our final example of a nonrelativistic uncertainty relation, consider the Hilbert-space path traced out by dynamical evolution under the Hamiltonian \hat{H} :

$$|\psi_T\rangle = e^{-iT\hat{H}/\hbar} |\psi_0\rangle. \quad (155)$$

The parameter here is the elapsed time T , and the temporal displacements are generated by $\hat{h} = \hat{H}/\hbar$. The uncertainty relation (31) reads

$$\langle (\delta T)^2 \rangle_T \langle (\Delta \hat{H})^2 \rangle \geq \frac{\hbar^2}{4N}. \quad (156)$$

This inequality means that no matter what measurements are made to determine the elapsed time T and no matter how the data from those measurements are processed to give an estimate of T , the estimator’s mean-square deviation from the actual elapsed time must satisfy Eq. (156).

The time-energy uncertainty relation (156) must be used carefully, however. For example, suppose one wishes to estimate elapsed time from the dynamics of a small system decaying into an environment. The inequality (156) places useful limits on such an estimate only if one uses the *total* Hamiltonian of the system and the environment. An alternative approach, which focuses on the dissipative dynamics of the small system, is to use a master equation to describe the dynamics of the small system, to compute ds/dT from the master equation, and then to use the original inequality (9) to place limits on the estimation of elapsed time [31].

Mandelstam and Tamm [3] derived the first parameter-based uncertainty relation, for time and energy, in the following way. They realized that to measure elapsed time T , one measures an observable \hat{A} that changes with time—a clock observable. By defining a time uncertainty

$$\Delta T \equiv \frac{\langle (\Delta \hat{A})^2 \rangle^{1/2}}{|d\langle \hat{A} \rangle/dt|} = \frac{\hbar \langle (\Delta \hat{A})^2 \rangle^{1/2}}{|\langle [\hat{A}, \hat{H}] \rangle|}, \quad (157)$$

they converted the standard operator uncertainty relation for \hat{A} and \hat{H} ,

$$\langle (\Delta \hat{A})^2 \rangle^{1/2} \langle (\Delta \hat{H})^2 \rangle^{1/2} \geq \frac{1}{2} |\langle [\hat{A}, \hat{H}] \rangle|, \quad (158)$$

into a time–energy uncertainty relation

$$\Delta T \langle (\Delta \hat{H})^2 \rangle^{1/2} \geq \frac{\hbar}{2}. \quad (159)$$

The key idea in Mandelstam and Tamm’s work, to regard elapsed time as a parameter to be determined by measuring some other quantity, underlies the formalism of parameter-based uncertainty relations. The technical advances in the present formalism are, first, the use of estimation theory to incorporate easily the possibility of multiple measurements and to quantify precisely the precision with which a parameter can be determined and, second, the use of POVMs to allow for all quantum measurements that might be used to infer the parameter. Helstrom [4] and Holevo [5, Chaps. III.8 and IV.7] pioneered in using these technical advances to formulate time–energy uncertainty relations. Hilgevoord and Uffink [2, 6] have formulated a different sort of parameter-based time–energy uncertainty relation.

For the case of pure-state time evolution, Anandan and Aharonov [16] noted the connection between the Hilbert-space angle (27) and the variance of the Hamiltonian \hat{H} . This connection follows from combining Eqs. (26) and (29):

$$\frac{d\theta}{dT} = \frac{1}{2} \frac{ds}{dT} = \frac{\langle (\Delta \hat{H})^2 \rangle_T^{1/2}}{\hbar}. \quad (160)$$

Knowing that Hilbert-space angle is related to distinguishability through the inner product, Anandan and Aharonov formulated an uncertainty relation by asking for the minimum time for the evolution to proceed to an orthogonal state. Anandan [17] and Uhlmann [32] generalized this approach to mixed states. Our formulation differs in that we also relate Hilbert-space angle to statistical distance and thus to a precise measure of the uncertainty in determining the elapsed time T , i.e., the minimum mean-square deviation $\langle (\delta T)^2 \rangle_T$.

The states $|t\rangle$ that are used to describe global optimal measurements can be obtained from the energy eigenstates $|\varepsilon\rangle$:

$$\hat{H} |\varepsilon\rangle = \varepsilon |\varepsilon\rangle. \quad (161)$$

If the spectrum of energy eigenvalues is discrete and nondegenerate, then the time representation follows immediately from obvious changes in the notation of Section 3. For example, the time states are given by

$$|t\rangle = \sum_{\varepsilon} |\varepsilon\rangle e^{if(\varepsilon)} e^{-it\varepsilon/\hbar}, \quad (162)$$

with the minimal choice, $f(\varepsilon) = 0$, giving the canonical time representation. The states $|t\rangle$, like position eigenstates and phase states, are generally not physical states, as they typically have infinite energy. Holevo [5, Chaps. III.8 and IV.7] has considered the canonical time representation and its application to optimal

measurements and has worked out in detail the example of a free particle, where the energy spectrum is continuous and doubly degenerate. We review the free-particle example here to provide an example of how to proceed when the generator \hat{h} is degenerate.

Consider then a free particle with Hamiltonian

$$\hat{H} = \hat{p}^2/2m. \quad (163)$$

The energy eigenstates coincide with the momentum eigenstates $|p\rangle$, which we normalize as in Eq. (85). The energy eigenstates are, however, doubly degenerate (except for $p=0$), with eigenvalues given by

$$\varepsilon = p^2/2m. \quad (164)$$

A convenient way to deal with the degeneracy is to introduce a degeneracy label

$$\sigma = \text{sgn}(p) \quad (165)$$

($|p| = \sigma p$; cf. Eq (142)), which allows us to write

$$p = \sigma\sqrt{2m\varepsilon}. \quad (166)$$

The energy eigenstates can now be defined as

$$|\varepsilon, \sigma\rangle = (m/2\varepsilon)^{1/4} |p\rangle \Leftrightarrow |p\rangle = (\sigma p/m)^{1/2} |\varepsilon, \sigma\rangle, \quad (167)$$

where σ is used to distinguish degenerate energy eigenstates and where the normalization is chosen so that

$$\langle \varepsilon, \sigma | \varepsilon', \sigma' \rangle = 2\pi\hbar\delta_{\sigma\sigma'}\delta(\varepsilon - \varepsilon'), \quad (168)$$

$$\hat{1} = \sum_{\sigma} \int_0^{\infty} \frac{d\varepsilon}{2\pi\hbar} |\varepsilon, \sigma\rangle\langle \varepsilon, \sigma|. \quad (169)$$

We can now find global optimal measurements in terms of time states $|t, \sigma\rangle$, where the states $|t, +1\rangle$ are constructed as in Eq. (162), but in the $\sigma = +1$ subspace of Hilbert space, and the states $|t, -1\rangle$ are similarly constructed in the $\sigma = -1$ subspace. Notice, however, that because of the degeneracy we have the freedom not only to rephase each of the energy eigenstates independently, but also to use as the basic energy eigenstates any orthonormal linear combination of the states $|\varepsilon, +1\rangle$ and $|\varepsilon, -1\rangle$. In symbols, we have the freedom to choose new energy eigenstates

$$|\varepsilon, \gamma\rangle = \sum_{\sigma} |\varepsilon, \sigma\rangle e^{if(\varepsilon)} U_{\sigma\gamma}(\varepsilon), \quad (170)$$

where $\gamma = \pm 1$ is a new degeneracy label and $U_{\sigma\gamma}(\varepsilon)$ is a 2×2 unitary matrix with unit determinant.

With this freedom in mind, we seek a global optimal measurement in terms of a POVM $\hat{E}(t, \gamma) dt$, where the possible results of the measurement are labeled by the continuous parameter t and the discrete parameter $\gamma = \pm 1$. The POVM satisfies three properties analogous to Eqs. (32), (35), and (36):

$$\hat{E}(t, \gamma) dt = \frac{dt}{C} |t, \gamma\rangle\langle t, \gamma|, \quad (171)$$

$$\hat{1} = \sum_{\gamma} \int_{-\infty}^{\infty} dt \hat{E}(t, \gamma) = \sum_{\gamma} \int_{-\infty}^{\infty} \frac{dt}{C} |t, \gamma\rangle\langle t, \gamma|, \quad (172)$$

$$e^{-iT\hat{H}/\hbar} |t, \gamma\rangle = |t+T, \gamma\rangle. \quad (173)$$

The displacement condition (173), with $t=0$ and $T=t$, becomes

$$\langle \varepsilon, \sigma | t, \gamma\rangle = e^{-it\varepsilon/\hbar} \langle \varepsilon, \sigma | t=0, \gamma\rangle, \quad (174)$$

which leads to

$$\begin{aligned} \langle \varepsilon, \sigma | \left(\sum_{\gamma} \int_{-\infty}^{\infty} \frac{dt}{C} |t, \gamma\rangle\langle t, \gamma| \right) | \varepsilon', \sigma' \rangle \\ = \frac{2\pi\hbar}{C} \delta(\varepsilon - \varepsilon') \sum_{\gamma} \langle \varepsilon, \sigma | t=0, \gamma\rangle \langle t=0, \gamma | \varepsilon, \sigma' \rangle. \end{aligned} \quad (175)$$

Thus the completeness condition (172) can be satisfied by choosing $C=1$ and by requiring that

$$\sum_{\gamma} \langle \varepsilon, \sigma | t=0, \gamma\rangle \langle t=0, \gamma | \varepsilon, \sigma' \rangle = \delta_{\sigma\sigma'}, \quad (176)$$

which, in turn, means that $\langle \varepsilon, \sigma | t=0, \gamma\rangle$ is a 2×2 unitary matrix. By removing the common phase factor from this unitary matrix, it can be written as

$$\langle \varepsilon, \sigma | t=0, \gamma\rangle = e^{if(\varepsilon)} U_{\sigma\gamma}(\varepsilon), \quad (177)$$

where $U_{\sigma\gamma}(\varepsilon)$ is the unit-determinant unitary matrix of Eq. (170). Notice that the new energy eigenstates (170) satisfy $\langle \varepsilon, \gamma | t, \gamma' \rangle = \delta_{\gamma\gamma'} e^{-it\varepsilon/\hbar}$.

Because the energy spectrum is bounded below, the time states

$$|t, \gamma\rangle = \sum_{\sigma} \int_0^{\infty} \frac{d\varepsilon}{2\pi\hbar} | \varepsilon, \sigma \rangle e^{if(\varepsilon)} U_{\sigma\gamma}(\varepsilon) e^{-it\varepsilon/\hbar} = \int_0^{\infty} \frac{d\varepsilon}{2\pi\hbar} | \varepsilon, \gamma \rangle e^{-it\varepsilon/\hbar} \quad (178)$$

are not orthogonal, their inner product being given by

$$\langle t, \gamma | t', \gamma' \rangle = \delta_{\gamma\gamma'} \int_0^{\infty} \frac{d\varepsilon}{2\pi\hbar} e^{i(t-t')\varepsilon/\hbar} = \delta_{\gamma\gamma'} \left(\frac{1}{2} \delta(t-t') + \frac{i}{2\pi} \mathbf{P} \left(\frac{1}{t-t'} \right) \right). \quad (179)$$

The canonical time representation results from choosing $f(\varepsilon) = 0$ and $U_{\sigma\gamma}(\varepsilon) = \delta_{\sigma\gamma}$.

The probability density that a measurement yields results t and γ , given parameter T , is given by

$$p(t, \gamma | T) = |\psi_T(t, \gamma)|^2 = |\psi_0(t - T, \gamma)|^2 = p(t - T, \gamma), \quad (180)$$

where

$$\psi_T(t, \gamma) = \langle t, \gamma | \psi_T \rangle = \langle t - T, \gamma | \psi_0 \rangle = \psi_0(t - T, \gamma) \quad (181)$$

is the wave function of the state $|\psi_T\rangle$ in the time representation. The displacement property (173) implies that in the time representation, \hat{H} is represented by a derivative:

$$\hat{H} \Leftrightarrow \frac{\hbar}{i} \frac{\partial}{\partial t}. \quad (182)$$

Writing the time wave function of the fiducial state as $\psi_0(t, \gamma) = r(t, \gamma) e^{i\Theta(t, \gamma)}$, the general relations (48) and (49) for the mean and variance of \hat{H} become in this case

$$\langle \hat{H} \rangle = \sum_{\gamma} \int_{-\infty}^{\infty} dt \psi_0^*(t, \gamma) \frac{\hbar}{i} \frac{\partial}{\partial t} \psi_0(t, \gamma) = \sum_{\gamma} \int_{-\infty}^{\infty} dt p(t, \gamma) \hbar \Theta'(t, \gamma), \quad (183)$$

$$\begin{aligned} \langle (\Delta \hat{H})^2 \rangle &= \sum_{\gamma} \int_{-\infty}^{\infty} dt \left| \left(\hbar \frac{\partial}{\partial t} - i \langle \hat{H} \rangle \right) \psi_0(t, \gamma) \right|^2 \\ &= \frac{\hbar^2}{4} \sum_{\gamma} \int_{-\infty}^{\infty} dt \frac{[p'(t, \gamma)]^2}{p(t, \gamma)} + \sum_{\gamma} \int_{-\infty}^{\infty} dt p(t, \gamma) [\hbar \Theta'(t, \gamma) - \langle \hat{H} \rangle]^2. \end{aligned} \quad (184)$$

Using this expression for the variance of \hat{H} or using the general condition (43) for an optimal measurement, one can derive that the requirement for a global optimal measurement is that $\Theta(t, \gamma) = \langle \hat{H} \rangle t / \hbar + (\text{const})_{\gamma}$. Discarding an irrelevant overall phase due to the two constants, but retaining the differential phase between the $\gamma = \pm 1$ parts of the wave function, one can write the resulting fiducial wave function for a global optimal measurement as

$$\psi_0(t, \gamma) = e^{i\gamma\mu} r(t, \gamma) e^{i\langle \hat{H} \rangle t / \hbar}, \quad (185)$$

where μ is a constant.

The time and energy representations of a state $|\psi\rangle$ are related by

$$\begin{aligned} \langle t, \gamma | \psi \rangle &= \psi(t, \gamma) = \sum_{\sigma} \int_0^{\infty} \frac{d\varepsilon}{2\pi\hbar} e^{i\varepsilon t / \hbar} e^{-i f(\varepsilon)} U_{\sigma\gamma}^*(\varepsilon) \langle \varepsilon, \sigma | \psi \rangle \\ &= \int_0^{\infty} \frac{d\varepsilon}{2\pi\hbar} e^{i\varepsilon t / \hbar} \langle \varepsilon, \gamma | \psi \rangle, \end{aligned} \quad (186)$$

$$\langle \varepsilon, \gamma | \psi \rangle = \sum_{\sigma} e^{-i f(\varepsilon)} U_{\sigma\gamma}^*(\varepsilon) \langle \varepsilon, \sigma | \psi \rangle = \int_{-\infty}^{\infty} dt e^{-i\varepsilon t / \hbar} \psi(t, \gamma). \quad (187)$$

These representations show that condition (185) for a global optimal measurement, when written in the energy representation, with $\varepsilon = \langle \hat{H} \rangle + u$, becomes

$$\begin{aligned} \langle \langle \hat{H} \rangle + u, \gamma \mid \psi_0 \rangle &= \sum_{\sigma} e^{-if(\langle \hat{H} \rangle + u)} U_{\sigma\gamma}^* (\langle \hat{H} \rangle + u) \langle \langle \hat{H} \rangle + u, \sigma \mid \psi_0 \rangle \\ &= \sum_{\sigma} e^{if(\langle \hat{H} \rangle - u)} U_{\sigma\gamma} (\langle \hat{H} \rangle - u) \langle \langle \hat{H} \rangle - u, \sigma \mid \psi_0 \rangle^* \\ &= \langle \langle \hat{H} \rangle - u, \gamma \mid \psi_0 \rangle^*, \end{aligned} \quad (188)$$

where we discard the differential phase μ because it can be absorbed into the unitary matrix $U_{\sigma\gamma}$. The condition (188) can be satisfied, by appropriate choices for the function $f(\varepsilon)$ and the unitary matrix $U_{\sigma\gamma}(\varepsilon)$, if and only if

$$\sum_{\sigma} |\langle \langle \hat{H} \rangle + u, \sigma \mid \psi_0 \rangle|^2 = \sum_{\sigma} |\langle \langle \hat{H} \rangle - u, \sigma \mid \psi_0 \rangle|^2, \quad (189)$$

i.e., the total probability density to have energy $\langle \hat{H} \rangle + u$ is the same as the total probability density to have energy $\langle \hat{H} \rangle - u$.

5. LORENTZ-INVARIANT UNCERTAINTY RELATIONS

We now apply the formalism developed in Section 2.2 to formulating Lorentz-invariant uncertainty relations for estimation of the displacement and Lorentz-rotation parameters of the Poincaré group. We deal first with the displacement parameters, where we are seeking a restriction on the estimation of a space–time translation and, hence, on the estimation of the invariant space–time interval. The generator of space–time translations is the operator for the energy–momentum 4-vector

$$\hat{\mathbf{P}} = \hat{P}^{\alpha} \mathbf{e}_{\alpha} = \hat{P}^0 \mathbf{e}_0 + \hat{P}^j \mathbf{e}_j, \quad (190)$$

for whatever fields are used to distinguish translated frames. We write the displacement 4-vector as

$$\mathbf{X} = S \mathbf{n} = S n^{\alpha} \mathbf{e}_{\alpha}, \quad (191)$$

where

$$\mathbf{n} = n^0 \mathbf{e}_0 + \vec{n} = n^0 \mathbf{e}_0 + n^j \mathbf{e}_j \quad (192)$$

is a (timelike or spacelike) unit 4-vector that gives the direction of the space–time translation and S is the invariant interval that parametrizes the translation. The path on Hilbert space is given by

$$|\psi_S\rangle = e^{-iS \mathbf{n} \cdot \hat{\mathbf{P}}/\hbar} |\psi_0\rangle, \quad (193)$$

where

$$\mathbf{n} \cdot \hat{\mathbf{P}} = \eta_{\alpha\beta} n^\alpha \hat{P}^\beta = n^\alpha \hat{P}_\alpha = -n^0 \hat{P}^0 + \vec{n} \cdot \hat{\mathbf{P}}. \quad (194)$$

Here $\|\eta_{\alpha\beta}\| = \text{diag}(-1, +1, +1, +1)$ is the Minkowski metric of special relativity (we adopt units such that the speed of light $c = 1$), and $\vec{n} \cdot \hat{\mathbf{P}} = n^j \hat{P}^j$ is the three-dimensional dot product.

From Eq. (31) the uncertainty relation for estimation of the invariant interval S is

$$\langle (\delta S)^2 \rangle_S \langle (\mathbf{n} \cdot \Delta \hat{\mathbf{P}})^2 \rangle = \langle (\delta S)^2 \rangle_S n^\alpha n^\beta \langle \Delta \hat{P}_\alpha \Delta \hat{P}_\beta \rangle \geq \frac{\hbar^2}{4N}. \quad (195)$$

When \mathbf{n} is timelike, this is a time–energy uncertainty relation for the observer whose 4-velocity is \mathbf{n} , and when \mathbf{n} is spacelike, this is a position-momentum uncertainty relation for an observer whose 4-velocity is orthogonal to \mathbf{n} . In particular, when $\mathbf{n} = \mathbf{e}_0$, the time-energy uncertainty relation takes the form

$$\langle (\delta S)^2 \rangle_S \langle (\Delta \hat{P}^0)^2 \rangle \geq \frac{\hbar^2}{4N}, \quad (196)$$

and when $\mathbf{n} = \vec{n} = n^j \mathbf{e}_j$ is a spatial unit vector, the position-momentum uncertainty relation becomes

$$\langle (\delta S)^2 \rangle_S \langle (\vec{n} \cdot \Delta \hat{\mathbf{P}})^2 \rangle \geq \frac{\hbar^2}{4N}. \quad (197)$$

For illustration, suppose that the relevant field is the free electromagnetic field. When considering the energy-momentum 4-vector as a generator, it is most convenient to decompose the field in terms of plane-wave field modes, for then

$$\hat{\mathbf{P}} = \sum_{\vec{k}, \sigma} \hbar \mathbf{k} \hat{a}_{\vec{k}, \sigma}^\dagger \hat{a}_{\vec{k}, \sigma} \quad (198)$$

is a sum of separate contributions from the various modes. In Eq. (198) $\mathbf{k} = \omega \mathbf{e}_0 + \vec{k} = \omega \mathbf{e}_0 + k^j \mathbf{e}_j$ is a (null) wave 4-vector, with $\omega = |\vec{k}| = k$; the sum runs over all plane-wave field modes, i.e., over all all wave 3-vectors \vec{k} and over the two helicities, denoted by σ . Since the generator $\mathbf{n} \cdot \hat{\mathbf{P}}/\hbar$ for any space–time translation is determined by the number operators for the plane-wave field modes, global optimal measurements will involve measurements of phase shifts of these modes. This is not a surprising conclusion because the effect of a space–time translation is to shift the phase of each plane-wave field mode. Indeed, if only a single plane-wave field mode is excited, the discussion of global optimal measurements of the invariant interval reduces to the analysis of phase measurement in Section 4.2. If many modes are excited, as in a pulse of electromagnetic radiation, the discussion of global optimal measurements is more complicated. Measurements of phase shifts

in the multi-mode case are only beginning to be considered [33–35]. Notice that when many modes are excited, the generator $\mathbf{n} \cdot \hat{\mathbf{P}}/\hbar$ becomes highly degenerate, a situation that cannot be addressed by the general considerations of Section 3.

Turn now to the case of Lorentz transformations, where we seek restrictions on the estimation of the parameters that describe boosts and spatial rotations. The generator of Lorentz transformations is the operator for the antisymmetric angular-momentum two-tensor

$$\hat{\mathbf{J}} = \hat{J}^{\alpha\beta} \hat{\mathbf{e}}_\alpha \otimes \hat{\mathbf{e}}_\beta, \quad (199)$$

whose components are given in terms of the stress-energy tensor by

$$\hat{J}^{\alpha\beta} = \int d^3x (x^\alpha \hat{T}^{\beta 0} - x^\beta \hat{T}^{\alpha 0}). \quad (200)$$

The path on Hilbert space is given by

$$|\psi_\Theta\rangle = \exp\left(-\frac{i}{2\hbar} \Theta \Omega^{\alpha\beta} \hat{J}_{\alpha\beta}\right) |\psi_0\rangle, \quad (201)$$

where Θ is the Lorentz-rotation parameter and $\Omega^{\alpha\beta}$ is an antisymmetric two-tensor that specifies the sense of the Lorentz rotation.

For a boost with velocity v in the direction of a spatial unit vector $\vec{n} = n^j \mathbf{e}_j$, Θ is the velocity parameter corresponding to v , i.e., $\cosh \Theta = (1 - v^2)^{-1/2}$, and the only nonzero components of $\Omega^{\alpha\beta}$ are the time-space components $\Omega^{0j} = -\Omega^{j0} = -n^j$. The path on Hilbert space becomes

$$|\psi_\Theta\rangle = e^{i\Theta \vec{n} \cdot \hat{\mathbf{K}}/\hbar} |\psi_0\rangle, \quad (202)$$

where the boost generator,

$$\hat{\mathbf{K}} = \hat{K}^j \mathbf{e}_j = \hat{J}_0^j \mathbf{e}_j, \quad (203)$$

is an energy-weighted position operator. For a spatial rotation about the spatial unit vector $\vec{n} = n^j \mathbf{e}_j$, Θ is the rotation angle, and the only nonzero components of $\Omega^{\alpha\beta}$ are the space-space components $\Omega^{jk} = \varepsilon^{jkl} n^l$, where ε^{jkl} is the three-dimensional Levi-Civita tensor. The path on Hilbert space becomes

$$|\psi_\Theta\rangle = e^{-i\Theta \vec{n} \cdot \hat{\mathbf{J}}/\hbar} |\psi_0\rangle, \quad (204)$$

where the generator of spatial rotations,

$$\hat{\mathbf{J}} = \hat{J}^j \mathbf{e}_j = \frac{1}{2} \varepsilon^{jkl} \hat{J}_{kl} \mathbf{e}_j, \quad (205)$$

is the angular-momentum operator.

The general form of the uncertainty relation for estimation of the Lorentz-rotation parameter Θ is

$$\langle (\delta\Theta)^2 \rangle_{\Theta} \frac{1}{4} \Omega^{\alpha\beta} \Omega^{\mu\nu} \langle \Delta \hat{J}_{\alpha\beta} \Delta \hat{J}_{\mu\nu} \rangle \geq \frac{\hbar^2}{4N}. \quad (206)$$

For a boost the uncertainty relation,

$$\langle (\delta\Theta)^2 \rangle_{\Theta} \langle (\vec{n} \cdot \Delta \hat{K})^2 \rangle \geq \frac{\hbar^2}{4N}, \quad (207)$$

expresses the quantum-mechanical limitations on determining the velocity parameter Θ . This uncertainty relation is complementary to the relativistic position–momentum uncertainty relation (197). In Eq. (197) the parameter is a spatial displacement, and the operator is the component of 3-momentum which generates the displacement. In Eq. (207) the parameter is related to a velocity change, and the operator is the component of energy-weighted position which generates the change in velocity. For a spatial rotation the uncertainty relation,

$$\langle (\delta\Theta)^2 \rangle_{\Theta} \langle (\vec{n} \cdot \Delta \hat{J})^2 \rangle \geq \frac{\hbar^2}{4N}, \quad (208)$$

expresses the quantum-mechanical limitations on determining a rotation.

To investigate global optimal measurements of a spatial rotation or a boost, it would be wise to decompose the relevant field in terms of angular-momentum modes or “boost modes.” Such an investigation lies outside the scope of the present paper.

6. CONCLUSION

Much ink has been devoted to the problem that many quantities of physical interest, such as time or harmonic-oscillator phase, although determined routinely from measurements, cannot be accommodated within the conventional quantum-mechanical description of measurements, because such quantities have no associated Hermitian operator. The aim of this paper is to show that this problem is only apparent. We eschew tedious discussions of the status of such quantities in quantum theory. Instead we develop a formalism that allows us to derive quantum-mechanical limitations on the determination of such a quantity, without ever having to introduce an operator associated with the quantity, and we illustrate the formalism with numerous examples.

The formalism is founded on the idea that such a quantity should be treated as a parameter, to be determined from the results of measurements. To derive strict quantum-mechanical limits on such a determination, we must be able, first, to describe all measurements permitted by the rules of quantum mechanics—this is

accomplished by using the formalism of POVMs—and, second, to set bounds on all possible ways of estimating the parameter from the results of the measurements—this is accomplished by appealing to the Cramér–Rao bound of classical parameter-estimation theory. The resulting quantum-mechanical limitations are expressed as Mandelstam–Tamm uncertainty relations involving the precision of the parameter estimation and the variance of the operator that generates changes in the parameter. These uncertainty relations take into account naturally the expected improvement in determining the parameter as one is allowed to make measurements on an increasing number of identically prepared systems. Moreover, we are able to derive general conditions for optimal measurements that can achieve the lower bound in the uncertainty relation, although it is generally not known how to perform such optimal measurements. The final result is a formalism that increases considerably the scope and power of uncertainty relations in quantum theory.

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