Certifying Nonclassical Behavior for Negative Keldysh Quasiprobabilities

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We introduce an experimental test for ruling out classical explanations for the statistics obtained when measuring arbitrary observables at arbitrary times using individual detectors. This test requires some trust in the measurements, represented by a few natural assumptions on the detectors. In quantum theory, the considered scenarios are well captured by von Neumann measurements. These can be described naturally in terms of the Keldysh quasiprobability distribution (KQPD), and the imprecision and backaction exerted by the measurement apparatus. We find that classical descriptions can be ruled out from measured data if and only if the KQPD exhibits negative values. We provide examples based on simulated data, considering the influence of a finite amount of statistics. In addition to providing an experimental tool for certifying nonclassicality, our results bestow an operational meaning upon the nonclassical nature of negative quasiprobability distributions such as the Wigner function and the full counting statistics.

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Introduction.—The theory of quantum mechanics contains ingredients that are absent in classical theories, such as entanglement, wave-function collapse, and superposition of arbitrary states [1–3]. In some scenarios, these ingredients are beneficial (e.g., quantum information [4]), while in other scenarios, they provide limitations (e.g., quantum noise in measurement and amplification [5]). The realm of possibilities that are enabled or prohibited by quantum mechanics is a highly non-trivial subject of current research.

At the heart of this problem lies the question: "which observations cannot be explained by classical theories?" A strong result in this direction is provided by Bell inequalities [6]. With the help of such inequalities, observed data alone can rule out any theory that fulfills a natural definition of locality [7]. While this is an extremely powerful result, locality is a rather specific requirement and does not encompass all classical theories [8].

Another well-established approach for testing for nonclassicality is given by the Glauber-Sudarshan P function in quantum optics [9,10]. If a state is described by a P function that cannot be interpreted as a probability distribution, then some measurable intensity correlators resulting from this state cannot be described by classical electrodynamics [11,12]. In contrast to Bell inequalities, the measurement device thus has to be trusted to produce intensity correlators of light.

Arguably the most striking difference to classical theories is the fact that observables cannot be described using positive probability distributions in quantum mechanics. Leggett-Garg inequalities [13] provide a test for nonclassicality based on this criterion. However, an additional assumption of noninvasive measurability which is not generally justified complicates the conclusions [14].

In this Letter, we provide a test for nonclassicality that rules out any description based on positive probabilities under a few realistic assumptions on the measurement apparatus. To this end, we consider scenarios where observables are measured using individual detectors, see Fig. 1. In quantum theory, such scenarios are well described by von Neumann type measurements [15–18], where observables of interest are coupled to detectors that are subsequently measured projectively. The probability distribution describing the measurement outcomes have a natural description in terms of a quasiprobability distribution that we abbreviate with KQPD due to its reminiscence of the Keldysh path-integral formulation [19,20]. The KQPD depends on the observables of interest and can

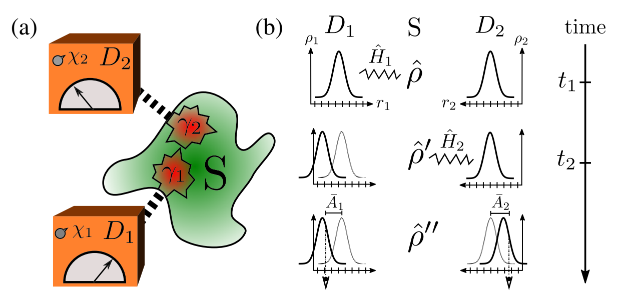

FIG. 1. (a) Sketch of the setup. Two observables are measured by detectors (D_j) coupled to the system (S). The detectors come with a knob (χ_j) and disturb the system (γ_j). (b) Illustration of von Neumann measurements. Detectors are quantum mechanical systems that couple to the system of interest at times t_j via the Hamiltonian $\hat{H}_j$. The interaction shifts the probability distribution ρ_j of the detectors by an amount depending on the system state $\hat{\rho}$. After the interaction, a projective position measurement is performed on the detectors resulting in the outcome $\bar{A}_j$.

reduce to the Wigner function [21] or the full counting statistics [22]. Other applications include quantum thermodynamics [23–28], quantum optics [29], generalized Wigner functions [30], weak values [19] (see also Refs. [31–33]), and nonequilibrium phenomena in quantum systems [20]. Importantly, the KQPD can become negative, indicating nonclassical behavior [18,29,34–39]. Here we put this nonclassical feature on a firmer footing by taking an operational approach. To this end, we put forward a classical model for measurements based on individual detectors. This model is based on a few natural assumptions on the detectors and results in an experimentally accessible inequality. We show that within quantum theory, negativity in the KQPD is a necessary and sufficient condition to violate the inequality, ruling out a classical description. Just like negativity in the P function rules out an explanation by classical electrodynamics (as long as the detectors can be trusted to produce intensity correlators), negativity in the KQPD rules out an explanation based on positive probabilities, as long as the measurement apparatus can be trusted to fulfill the assumptions specified below.

In contrast to Leggett-Garg inequalities, noninvasiveness of the measurement is not required. The proposed experimental test of nonclassical behavior is therefore not subject to a *clumsiness* [14] or a *finite precision* loophole [40,41]. The model is not necessarily local or noncontextual [42–44].

Before we introduce the classical model, we provide the quantum mechanical (QM) description of the scenario under investigation, sketched in Fig. 1. While we assume this to be the correct description, we stress that our test for nonclassicality does not rely on the QM model.

The KQPD.—The QM model relies on the KQPD which is discussed in detail in Ref. [19]. It encodes the joint fluctuations of multiple observables of interest. For simplicity, we consider the situation where we are interested in two observables $\hat{A}_1$ and $\hat{A}_2$ at times t_1 and t_2, respectively. The generalization to more observables is straightforward. Let us further consider the situation where t_2 either comes immediately after t_1 (subsequent measurements) or where $t_1 = t_2$ (simultaneous measurements). The KQPD is then defined as ($\hbar = 1$)

$$\mathcal{P}(\boldsymbol{A}|\boldsymbol{\gamma}) = \int \frac{d\boldsymbol{\lambda}}{(2\pi)^2} e^{i\boldsymbol{\lambda}\cdot\boldsymbol{A}} \mathrm{Tr}\{\hat{Q}(\boldsymbol{\lambda},\boldsymbol{\gamma})\hat{\rho}\hat{Q}^\dagger(-\boldsymbol{\lambda},\boldsymbol{\gamma})\}, \quad (1)$$

where $\hat{Q} = \exp\{-i[(\lambda_2/2)+\gamma_2]\hat{A}_2\}\exp\{-i[(\lambda_1/2)+\gamma_1]\hat{A}_1\}$ for subsequent and $\hat{Q} = \exp[-i\sum_{j=1,2}(\lambda_j/2+\gamma_j)\hat{A}_j]$ for simultaneous measurements. The state before the measurement is denoted by $\hat{\rho}$. We grouped the observables into a vector $\boldsymbol{A} = (A_1, A_2)$ and similarly for $\boldsymbol{\lambda}$ and $\boldsymbol{\gamma}$. As shown below, the variables γ_j are necessary to take into account the backaction exerted by the measurement and can be seen as random variables determined by the detectors. A physical motivation for the definition in Eq. (1) is provided below by Eq. (3).

If $[\hat{A}_1, \hat{A}_2] \neq 0$, the measurement of $\hat{A}_1$ may influence the measurement of $\hat{A}_2$ and a description of the system in terms of predetermined values of A_1 and A_2 is not generally possible. In this case, the KQPD may become negative. It has been shown that such negativity requires the system to be in a superposition of states that correspond to different values for the observable A_1 [39]. Negativity in the KQPD can thus be seen as an indicator for nonclassical behavior. However, in an experiment, the negativity of the KQPD is masked by measurement imprecision and backaction, rendering the measured probability distribution strictly non-negative. The inequality that we introduce below relies on a way to unmask the KQPD experimentally.

The QM model.—We consider two detectors, one for each observable to be measured. The detectors can be described by canonically conjugate observables $\hat{r}_j$ and $\hat{\pi}_j$, and they are coupled to the system through the Hamiltonian [15]

$$\hat{H}_j = \delta(t - t_j)\chi_j \hat{A}_j \hat{\pi}_j, \quad (2)$$

where $j = 1, 2$, and χ_j denotes the measurement strength. We assume that the time evolution induced by any Hamiltonian other than Eq. (2) can be neglected during (and between) the measurements, noting that it is straightforward to include time evolution between the measurements (for an investigation on detector memory effects, see Ref. [45]). Equation (2) induces a displacement in the detector coordinates $\hat{r}_j$ which depends on the state of the system. After the interaction, a projective measurement of the detectors is performed to complete the measurement of the system observables $\hat{A}_j$. The measured distribution reads [19] (see also Refs. [46,47])

$$P(\boldsymbol{A}|\boldsymbol{\chi}) = \int d\boldsymbol{A}' d\boldsymbol{\gamma} \mathcal{P}(\boldsymbol{A}'|\boldsymbol{\gamma}) \prod_{j=1,2} \mathcal{W}_j(\bar{A}_j - \bar{A}'_j, \bar{\gamma}_j), \quad (3)$$

where $\mathcal{W}_j(r, \pi)$ denotes the Wigner function of detector j and we introduced $\bar{A}_j = \chi_j A_j$ and $\bar{\gamma}_j = \gamma_j/\chi_j$. This equation has a simple interpretation, motivating the definition in Eq. (1). The KQPD describes the intrinsic fluctuations of the observables, containing all the information of the system. These fluctuations are distorted by the measurement process, giving rise to the convolution with the Wigner functions of the detectors. The uncertainty in the position coordinates induces a fuzziness in the measurement (measurement imprecision) and the uncertainty in the momentum coordinates introduces a random kick in the measured observable through Eq. (2) (measurement backaction). Because of the Heisenberg uncertainty relation, there exists a trade-off between imprecision and backaction [5], which ensures that the measured distribution is always positive, even when the KQPD exhibits negativity. For an investigation of the classical limit of von Neumann type measurements, see Ref. [48].

*The classical model.—*We now introduce a classical hidden-variable model that describes the situation sketched in Fig. 1(a). To this end, we assume that the system is described by a probability distribution $S(\boldsymbol{A}|\boldsymbol{\gamma})$. This distribution encodes the (hidden) values of the observables $(\boldsymbol{A})$ and takes into account that the presence of the detectors may modify the system behavior $(\boldsymbol{\gamma})$. The measured distribution can then be written in the completely general form

$$P_{\mathrm{cl}}(\boldsymbol{A}|\boldsymbol{\chi}) = \int d\boldsymbol{A}' d\boldsymbol{\gamma} M(\boldsymbol{A},\boldsymbol{A}',\boldsymbol{\gamma}|\boldsymbol{\chi}) S(\boldsymbol{A}'|\boldsymbol{\gamma}), \tag{4}$$

where $\boldsymbol{\chi}$ describes the (changeable) detector settings. The function M describes the effect of the detectors. We say that an observed probability distribution has a classical explanation if it can be described by the right-hand side of Eq. (4) with positive S and M.

Equation (4) is sufficiently general that it can essentially describe any observations. To rule out a classical explanation, we place some trust in the detectors and make the following assumptions:

1. Uncorrelated detectors:

$$M(\boldsymbol{A},\boldsymbol{A}',\boldsymbol{\gamma}|\boldsymbol{\chi}) = \prod_j M_j(A_j, A'_j, \gamma_j|\chi_j). \tag{5}$$

2. Uncorrelated imprecision and backaction:

$$M_j(A_j, A'_j, \gamma_j|\chi_j) = p_j(\gamma_j|\chi_j) D_j(A_j, A'_j|\chi_j). \tag{6}$$

3. Backaction only affects the other observable:

$$\int dA_k S(\boldsymbol{A}|\gamma_j, \gamma_k = 0) \equiv S(A_j|\gamma_j) = S(A_j). \tag{7}$$

4. Translational invariance:

$$D_j(A_j, A'_j|\chi_j) = D_j(A_j - A'_j|\chi_j). \tag{8}$$

5. Detectors can be detached:

$$\lim_{\chi_j \to 0} p_j(\gamma_j|\chi_j) D_j(A_j - A'_j|\chi_j) = \delta(\gamma_j) U(A_j). \tag{9}$$

In the spirit of the considered scenario, the first assumption allows us to treat the detectors as individual objects (note that this assumption is also present in the Bell scenario). Assumptions 2 and 3 ensure that the backaction of a detector does not interfere with its own measurement; i.e., a detector's output is independent of its backaction on the system. In Eq. (7), we introduced the distribution relevant for measuring a single variable $S(A_j)$, which is assumed to be independent of the backaction of its own detector. In assumption 5, U denotes the uniform distribution and we defined $\gamma_j = 0$ to denote the absence of any backaction of detector j. We note that our assumptions only include the effect of the detectors. On a qualitative level, one can thus replace our assumptions with the notion of having control over measurements of single observables and preventing any cross-talk between the detectors.

*Certifying nonclassicality.—*We denote by $P(A_j|\chi_j)$ the distribution that describes a measurement of a single observable. We further denote the Fourier transform of any distribution with a tilde $\tilde{P}(\lambda) = \int dA \exp(-i\lambda A) P(A)$. We then consider the quantity

$$K = \frac{1}{(2\pi)^2} \int d\boldsymbol{\lambda} e^{i\boldsymbol{\lambda}\cdot\boldsymbol{A}} \tilde{P}(\boldsymbol{\lambda}|\boldsymbol{\chi}) \prod_{j=1,2} \frac{\tilde{P}(\lambda_j|\chi'_j)}{\tilde{P}(\lambda_j|\chi_j)}, \tag{10}$$

where we note that the right-hand side only contains Fourier transforms of *measurable* probability distributions. If the measurement is described by our classical model, we can write this quantity as [49]

$$K_{\mathrm{cl}} = \int d\boldsymbol{A}' d\boldsymbol{\gamma} S(\boldsymbol{A}'|\boldsymbol{\gamma}) \prod_{j=1,2} p_j(\gamma_j|\chi_j) D_j(A_j - A'_j|\chi'_j). \tag{11}$$

This equation is very similar to Eq. (4) (under our assumptions) with the only difference that χ_j is replaced by χ'_j in the measurement imprecision term D_j. Within our assumptions, the measurement imprecision of the detectors can be corrected for. We end up with a distribution where the backaction is determined by χ_j and the imprecision by χ'_j. In our classical model, this still results in a positive distribution

$$K_{\mathrm{cl}} \geq 0. \tag{12}$$

Any violation of this inequality implies that the observed data cannot be explained by Eq. (4) with positive S and M that satisfy the five assumptions. Trusting the detectors (i.e., the assumptions) then allows us to conclude that no explanation in terms of positive probabilities is possible. The assumptions thus introduce loopholes since a violation of Eq. (12) could in principle result from their breakdown.

In quantum mechanics, the delicate interplay between backaction and imprecision is what masks the negativity of the KQPD. This may result in a violation of the inequality. Using detectors with positive Wigner functions that factorize in a position and a momentum part ensures that our assumptions on the detectors are satisfied. The quantity K is then given by an expression analogous to Eq. (11), with S replaced by the KQPD $\mathcal{P}$. This can be seen by plugging Eq. (3), and a similar expression for single observables, into Eq. (10). A positive KQPD then immediately ensures $K \geq 0$. In the limit where $\chi_j \to 0$ and $\chi'_j \to \infty$, we find

$K \to \mathcal{P}$. Whenever the KQPD exhibits negativity, we can thus find $K < 0$, violating the inequality in Eq. (12). Since the assumptions on the detectors are met, this implies that the measured data cannot be explained by positive probability distributions. Negativity in the KQPD is therefore a necessary and sufficient condition for certifying nonclassicality.

Examples.—We now illustrate how our classical model can be ruled out from experimental (in our case, simulated) data by violating the inequality in Eq. (12). We consider two examples: The simultaneous measurement of position and momentum, and two subsequent, noncommuting Stern-Gerlach type spin measurements. For both examples, we consider identical detectors that are described by the Wigner function (throughout, we consider dimensionless units for position and momentum)

$$\mathcal{W}_j(r_j, p_j) = \frac{1}{\pi} e^{-(r_j^2+p_j^2)}/\pi, \tag{13}$$

corresponding to unsqueezed Gaussian states of minimal uncertainty. As demanded by assumption 2, they factorize into distributions for position (imprecision) and momentum (backaction).

We first consider a simultaneous measurement of position and momentum on a single-photon Fock state described by the Wigner function

$$\mathcal{W}(x, p) = \frac{1}{\pi}[2(x^2 + p^2) - 1]e^{-(x^2+p^2)}. \tag{14}$$

In this case, our quantum mechanical model reduces to the Arthurs-Kelly model [50]. We note that such a measurement can be implemented by heterodyne detection [51], see Ref. [52] for an experimental realization. As discussed in detail in Ref. [19], the KQPD for the simultaneous position and momentum measurement is given by $\mathcal{W}(x - \gamma_p/2, p + \gamma_x/2)$. Choosing equal measurement strengths $\chi_x = \chi_p = \chi$ and $\chi'_x = \chi'_p = \chi'$ we then find (see Supplemental Material for details [49])

$$K = \frac{1}{\pi(1+g)^3} e^{-[(x^2+p^2)/(1+g)]}[2(x^2+p^2) - 1 + g^2], \tag{15}$$

where $g = (\chi/2)^2 + 1/(\chi')^2$. We note that in the limit $\chi \to 0$ and $\chi' \to \infty$, we have $g \to 0$ and Eq. (15) reduces to Eq. (14). As long as $g < 1$, we find $K < 0$ at the origin, see Fig. 2(a).

Equation (15) implies that the smaller χ, the stronger the negativity in the measurable quantity K. Weaker measurements thus always seem to be preferable. This is only true under the assumption that K can be estimated precisely. Strictly speaking, this requires an infinite amount of data. For a finite and fixed number of measurements, we will find a trade-off between having large negative values in K (requiring small χ) and being able to reliably estimate K (requiring large χ). To estimate K, we consider an experiment with N measurements resulting in outcomes x_j. We define the empirical characteristic function [53]

$$Y_\lambda = \frac{1}{N}\sum_{j=1}^{N} e^{-i\lambda x_j}, \tag{16}$$

which provides an unbiased estimator of the characteristic function (i.e., the Fourier transform of the probability distribution). We note that it is imprecise for large values of λ, where the characteristic function is a small number. For K, we introduce the estimator

$$K_{\mathrm{est}} = \begin{cases} \int_{-\lambda_c}^{\lambda_c} \frac{d\boldsymbol{\lambda}}{(2\pi)^2} e^{i\boldsymbol{\lambda}\cdot\boldsymbol{A}} Y_{\boldsymbol{\lambda}} \frac{Y_{\lambda_x}{}'}{Y_{\lambda_x}} \frac{Y_{\lambda_p}{}'}{Y_{\lambda_p}} & \text{for } |Y_{\lambda_{x/p}}| > c_o, \\ 0 & \text{otherwise}, \end{cases} \tag{17}$$

where $\boldsymbol{\lambda} \cdot \boldsymbol{A} = \lambda_x x + \lambda_p p$. Here the different empirical characteristic functions are labeled by $\boldsymbol{\lambda}$ for the joint

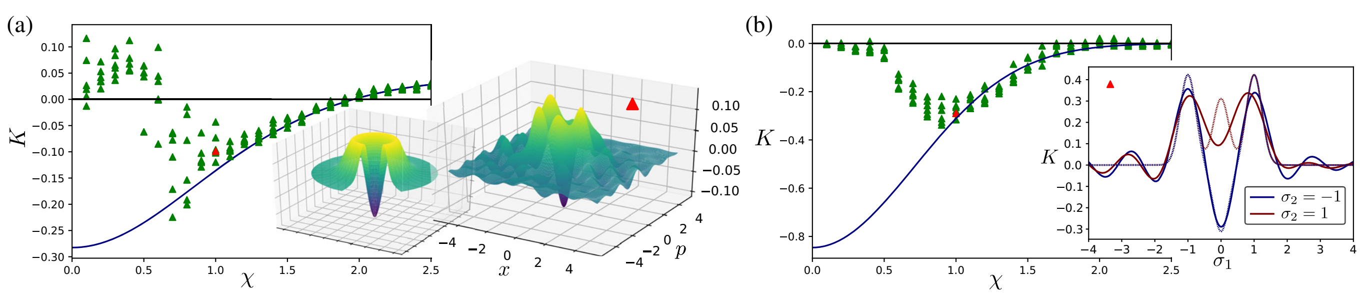

FIG. 2. Certifying nonclassicality. (a) Simultaneous measurement of both quadratures in a single-mode Fock state containing one photon. (b) Two subsequent spin measurements in different directions on a spin one-half particle. The large panels show K for values $\boldsymbol{A}$ that maximize the negativity [$x = 0$, $p = 0$ for (a), $\sigma_1 = 0$, $\sigma_2 = -1$ for (b)]. The solid line corresponds to the exact value of K [Eq. (10)], the triangles to the estimate K_{est} based on numerical simulations [Eq. (17)]. The side panels show the full estimate of K for a single data point. In (a), the small side-panel shows the exact distribution K. In (b), the dashed lines correspond to the exact K. As the measurement strength χ increases, the estimate becomes more reliable but the backaction decreases the negativity in K. The simulations are based on 15 000 individual measurements of the observables and 30 000 joint measurements. Other parameters: (a) $\chi' = 5$, $c_o = 0.011$, $\lambda_c = 10$. (b) $\chi' = 3$, $c_o = 0.01$, $\lambda_c = 12$.

measurement and by a prime for the measurements with strength χ'. Two empirical cutoffs increase the stability of the estimator. The first, c_o, ensures that values of $\boldsymbol{\lambda}$ where we divide by a very small number are not taken into account. The second, λ_c, allows for integrating over a finite domain. The estimator in Eq. (17) is illustrated in Fig. 2(a) for simulated data. For large values of χ, it is both accurate and precise. As χ becomes smaller, the spread of the estimates increases (the precision is reduced). Eventually, the cutoff c_o prevents an accurate estimation because the true characteristic function becomes very small for almost all values of $\lambda_{x/p}$. As expected, we find a trade-off between large χ, where the negativity in K is not very pronounced, and small χ, where it is hard to estimate K.

Our second example is provided by subsequent, noncommuting measurements on a two-level system (for a recent experimental implementation of noncommuting spin measurements, see Ref. [54], for a detailed discussion on simultaneous spin measurements, see Ref. [55]). We consider the system to be in a pure state $|+\rangle$, which is an eigenstate of the Pauli matrix $\hat{\sigma}_x$. We then make a measurement of $\hat{\sigma}_z$ with strength $\chi_1 = \chi$, followed by a projective measurement of $\hat{\sigma}_x$. The KQPD for this system is discussed in Ref. [19] and given in the Supplemental Material [49]. Because it is unavoidable that the first measurement influences the second one, the KQPD exhibits negativity. Since the second measurement is projective, we only correct for the measurement imprecision of the first measurement, choosing $\chi_2 = \chi_2' \to \infty$ in Eq. (10). All distributions can then be given as densities in the continuous variable σ_1 and probabilities in the discrete variable $\sigma_2 = \pm 1$. Certifying nonclassicality of this system is illustrated in Fig. 2(b), where we show both K as well as K_{est}. We find the same qualitative results as for the simultaneous position and momentum measurement. The weaker the first measurement, the more pronounced the negativity but the less reliable is the estimate K_{est}. Detailed calculations can be found in the Supplemental Material [49].

Conclusions.—We introduced a classical model for measurements that use individual detectors for different observables. Under five natural assumptions, we find the inequality $K \geq 0$. Any violation of this inequality implies that either no description in terms of positive probabilities is possible, or one of the assumptions on the detectors is not met. In scenarios which are well described by quantum mechanical von Neumann measurements, we find that K can become negative if and only if the KQPD exhibits negative values. In this case, K provides a way of approximating the KQPD from measurable probability distributions. This is possible because measurement imprecision is a property of the detector alone and can thus be inferred and corrected for. In weak measurements, where backaction becomes small, correcting for the measurement imprecision "unmasks" the KQPD, exposing its negativity.

Our classical model is appropriate whenever individual detectors are used to measure different observables. The introduced operational procedure for certifying nonclassicality is thus of broad experimental relevance and it puts the nonclassical nature of the negative values in the KQPD on a firmer footing.

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