Exact uncertainty properties of bosonic fields

Michael J. W. Hall and Kailash Kumar

Theoretical Physics, IAS,

Australian National University,

Canberra ACT 0200, Australia

Marcel Reginatto

Physikalisch-Technische Bundesanstalt,

Bundesallee 100

38116 Braunschweig, Germany

Abstract

The momentum density conjugate to a bosonic quantum field splits naturally into the sum of a classical component and a nonclassical component. It is shown that the field and the nonclassical component of the momentum density satisfy an *exact* uncertainty relation, i.e., an equality, which underlies the Heisenberg-type uncertainty relation for fields. This motivates a new approach to bosonic quantum fields based on an exact uncertainty principle. In particular, the postulate that an ensemble of classical fields is subject to nonclassical momentum fluctuations, of a strength determined by the field uncertainty, leads from the classical to the quantum field equations. Examples include scalar, electromagnetic and gravitational fields. For the latter case the exact uncertainty principle specifies a unique (non-Laplacian) operator ordering for the Wheeler-deWitt equation.

PACS numbers: 11.10.Ef, 03.70.+k

I. INTRODUCTION

The Heisenberg uncertainty relation

$$\Delta x \Delta p \geq \hbar/2 \tag{1}$$

for the rms position and momentum uncertainties of a quantum particle is a well known feature of quantum mechanics. It has recently been shown, however, that this relation is a consequence of a more fundamental connection between the statistics of complementary quantum observables.

In particular, the distinguishing "nonclassical" property of complementary observables is that they cannot be simultaneously measured to an arbitrary accuracy. It is therefore natural to consider the decomposition of one such observable, the momentum say, into the sum of a "classical" and a "nonclassical" component:

$$\hat{p} = \hat{p}^{cl} + \hat{p}^{nc} \ ,$$

where the classical component, $\hat{p}^{cl}$, is defined as that observable *closest* to $\hat{p}$ (in a statistical sense) which *is* simultaneously measurable with the complementary observable $\hat{x}$ [1].

It turns out that such decompositions do indeed, in a number of ways, neatly separate classical and nonclassical properties of quantum observables. For example, for one-dimensional particles the *nonclassical* component of the momentum satisfies the uncertainty relation

$$\delta x \Delta p^{nc} = \hbar/2 \tag{2}$$

for *all* pure states, where δx denotes a measure of position uncertainty from classical statistics called the Fisher length [1, 2]. This *exact* uncertainty relation is far stronger than (and implies) the corresponding Heisenberg uncertainty relation in Eq. (1).

The surprising fact that quantum systems satisfy exact uncertainty relations has recently provided the basis for *deriving* much of the quantum formalism, from an exact uncertainty principle. In particular, the assumption that a classical ensemble is subjected to nonclassical momentum fluctuations, of a strength inversely proportional to uncertainty in position, has been shown to lead directly from the classical equations of motion to the Schrödinger equation [3, 4].

The aim of this paper is to show that the abovementioned results can be generalised to bosonic quantum fields. For example, it will be seen in the following Section that a real

scalar field f, with conjugate momentum density g, satisfies an exact uncertainty relation analogous to Eq. (2). In Sec. III it is shown that the quantum field equations follow from an exact uncertainty principle, for the case of bosonic fields with Hamiltonians quadratic in the field momenta (eg, scalar, electromagnetic and gravitational fields). This exact uncertainty principle further implies a unique operator ordering for the Wheeler-deWitt equation (which, moreover, is consistent with Vilenkin's "tunneling" boundary condition for inflationary cosmology [5]). Necessary elements from classical field theory and functional analysis are briefly summarised in the Appendices.

II. EXACT UNCERTAINTY RELATIONS FOR FIELDS

A Heisenberg-type uncertainty relation may be given for scalar fields, in the form of an inequality for the covariance functions of the field and its conjugate momentum density. However, a stronger result follows via a natural decomposition of the momentum density into classical and nonclassical components, and the use of the Fisher covariance function from classical statistical estimation theory. In particular, an *exact* uncertainty relation for scalar fields is obtained in Sec. II.D below, which underlies and implies the corresponding Heisenberg-type uncertainty relation, and which may be generalised to arbitrary bosonic fields.

This derivation of exact uncertainty relations, i.e., precise quantitative connections between the statistics of conjugate fields, from the quantum formalism, is to some extent conceptually reversed in Sec. III, where the quantisation of a large class of classical fields is achieved via the use of an "exact uncertainty" principle.

A. Heisenberg-type relations

We begin with the simplest case: a real scalar field f with conjugate momentum density g. Spatial coordinates will be denoted by x (irrespective of dimension), and the values of f and g at position x by f_x and g_x respectively.

The underlying origin of the field is not at issue here - it could be a relativistic field satisfying the Klein-Gordon equation [6], or a nonrelativistic field describing vibrations of a stretched string [7]. What is important for the purposes of this section is that the corre-

sponding quantised fields $\hat{f}$ and $\hat{g}$ satisfy the equal-time commutation relations [6]

$$[\hat{f}_x, \hat{f}_{x'}] = [\hat{g}_x, \hat{g}_{x'}] = 0, \qquad [\hat{f}_x, \hat{g}_{x'}] = i\hbar\delta(x - x'). \tag{3}$$

Thus, in the Schrödinger representation, where the quantum state of the field at a given time is formally described by a complex amplitude functional $\Psi[f]$, the action of $\hat{f}$ and $\hat{g}$ is given by [8]

$$\hat{f}\Psi = f\Psi, \qquad \hat{g}\Psi = \frac{\hbar}{i}\frac{\delta\Psi}{\delta f}, \tag{4}$$

where $\delta/\delta f$ denotes the usual functional derivative (see also Appendix A).

The non-vanishing commutator in Eq. (3) reflects the complementary nature of $\hat{f}$ and $\hat{g}$: in general one must choose to accurately measure *either* the field *or* its momentum density. This is analogous to the complementary nature of the position and momentum observables $\mathbf{X}$ and $\mathbf{P}$ of a system of quantum particles, with non-vanishing commutator $[X_j, P_k] = i\hbar\delta_{jk}$. In the latter case one has the corresponding Heisenberg uncertainty relation [9]

$$\mathrm{Cov}(\mathbf{X})\ \mathrm{Cov}(\mathbf{P}) \geq (\hbar^2/4)I \tag{5}$$

for the covariance matrices of $\mathbf{X}$ and $\mathbf{P}$, where $[\mathrm{Cov}(\mathbf{A})]_{jk} := \langle A_j A_k\rangle - \langle A_j\rangle\langle A_k\rangle$, and I denotes the identity matrix. Thus, since the covariance matrix vanishes for the dispersion-free case, the complementary observables $\mathbf{X}$ and $\mathbf{P}$ cannot be simultaneously specified.

The covariance *function* of a given field h is defined by

$$[\mathrm{Cov}(h)]_{xx'} := \langle h_x h_{x'}\rangle - \langle h_x\rangle\langle h_{x'}\rangle, \tag{6}$$

where $\langle\ \rangle$ denotes an ensemble average. Thus the diagonal elements of the covariance function (i.e., $x = x'$) represent the variance of the field at each point, and the off-diagonal elements correspond to the degree of linear correlation between field values at different points.

The covariance functions of the conjugate fields f and g satisfy the Heisenberg-type inequality

$$\mathrm{Cov}(f) * \mathrm{Cov}(g) \succeq (\hbar^2/4)\mathbb{1}. \tag{7}$$

analogous to Eq. (5), where we use a matrix-type notation with multiplication $A * B$ defined by

$$[A * B]_{xx'} := \int dx'' A_{xx''} B_{x''x'},$$

multiplicative identity $\mathbb{1}$ defined by

$$\mathbb{1}_{xx'} := \delta(x - x'),$$

and the ordering $A \succeq B$ holds if and only if

$$h^\dagger(A - B)h := \int dxdx' \, (A - B)_{xx'} h_x^* h_{x'} \geq 0$$

for all h. Eq. (7) is clearly a continuous analogue of the Heisenberg inequality in (5), and indeed may be "proved" from the latter inequality by a discretization argument (where the spatial degree of freedom is represented by discrete cells of volume ϵ at positions x_j, the identifications $X_j = f_{x_j}$, $P_j = \epsilon g_{x_j}$, $\epsilon \sum_j = \int dx$ are made, and the limit $\epsilon \to 0$ is taken). A more rigorous proof is given in Sec. II.D below.

Eq. (7) represents a field-theoretic generalisation of the 1-dimensional Heisenberg uncertainty relation in Eq. (1). Moreover, it has the same physical significance: since the covariance function of field h vanishes for the dispersion-free case, the conjugate fields f and g cannot simultaneously be specified. It will be shown in Sec. II. D that this inequality can be replaced by an *exact* uncertainty relation analogous to Eq. (2). However, two concepts must first be introduced: decomposition of the quantum momentum density into "classical" and "nonclassical" components, and the Fisher covariance function.

B. Decomposition of the momentum density

Since, in contrast to classical fields, the quantum momentum density cannot be measured simultaneously with the field, we define the *classical component* of the momentum density to be that observable which is *closest* to $\hat{g}$, statistically speaking, under the constraint of being comeasurable with $\hat{f}$. Thus measurement of the classical component provides the *best possible* estimate of the momentum density compatible with a measurement of the field.

More formally, let $\hat{g}^{cl}$ denote the classical component of the momentum density $\hat{g}$. The comeasurability of $\hat{f}$ and $\hat{g}^{cl}$ then implies that the action of the latter in the representation of Eq. (4) has the form

$$\hat{g}^{cl}\Psi = g^{cl}[f]\Psi \tag{8}$$

for some real functional $g^{cl}[f]$. Further, for the classical component to be as close as possible to the quantum momentum density, the average deviation of $\hat{g}^{cl}$ and $\hat{g}$ must be as small as

possible, i.e.,

$$\langle\ (\hat{g}_x - \hat{g}_x^{cl})^2\ \rangle_\Psi = \text{minimum} \tag{9}$$

at each position x.

Conditions (8) and (9) determine the classical component of the momentum density uniquely, for each quantum state Ψ: one finds, as shown further below, that

$$g^{cl}[f] = \frac{\hbar}{2i}\left[\frac{1}{\Psi}\frac{\delta\Psi}{\delta f} - \frac{1}{\Psi^*}\frac{\delta\Psi^*}{\delta f}\right]. \tag{10}$$

Thus the classical component depends on Ψ - to make the best possible estimate one needs to have maximal knowledge about the state of the field. Note that the classical component vanishes identically for real amplitude functionals $\Psi[f]$.

It follows that the momentum density of a quantum field admits a natural (state-dependent) decomposition,

$$\hat{g} = \hat{g}^{cl} + \hat{g}^{nc}, \tag{11}$$

into the sum of a classical component $\hat{g}^{cl}$, corresponding to that part of $\hat{g}$ which is comeasurable with $\hat{f}$, and a *nonclassical* component $\hat{g}^{nc}$, corresponding to an intrinsically "quantum" remainder. These components satisfy the relations

$$\langle\hat{g}_x\rangle = \langle\hat{g}_x^{cl}\rangle, \qquad \langle\hat{g}_x^{nc}\rangle = 0, \tag{12}$$

$$(\Delta g_x)^2 = (\Delta g_x^{cl})^2 + (\Delta g_x^{nc})^2, \tag{13}$$

and hence the classical and nonclassical components also represent an "average" part and a "fluctuation" part respectively, the uncertainties of which add in quadrature.

To derive the explicit form in Eq. (10) for the classical component, consider any other field operator $\hat{h}$ comeasurable with $\hat{f}$, so that $\hat{h}\Psi = h[f]\Psi$ in analogy to Eq. (8). Then from Eqs. (4) and (10), and Eq. (A3) of Appendix A (assuming $\langle h\rangle$ is finite), one has

$$\begin{aligned}\langle\hat{g}_x\hat{h}_x + \hat{h}_x\hat{g}_x\rangle &= \frac{\hbar}{i}\int Df\ \Psi^*\left[\frac{\delta(h_x\Psi)}{\delta f_x} + h_x\frac{\delta\Psi}{\delta f_x}\right] \\ &= (\hbar/i)\int Df\,[\Psi^*(\delta\Psi/\delta f_x) - \Psi(\delta\Psi^*/\delta f_x)]h_x \\ &= 2\langle\hat{g}_x^{cl}\hat{h}_x\rangle,\end{aligned}$$

where $\langle\hat{A}\rangle$ is defined as the functional integral $\int Df\ \Psi^*\hat{A}\Psi$ (see Appendix A). Hence

$$\begin{aligned}\langle(\hat{g}_x - \hat{h}_x)^2\rangle &= \langle(\hat{g}_x)^2\rangle + \langle(\hat{h}_x)^2\rangle - 2\langle\hat{g}_x^{cl}\hat{h}_x\rangle \\ &= \langle(\hat{g}_x)^2\rangle - \langle(\hat{g}_x^{cl})^2\rangle + \langle(\hat{h}_x - \hat{g}_x^{cl})^2\rangle.\end{aligned}$$

Since the last term on the right is nonnegative, the lefthand side is minimised for the choice $\hat{h} \equiv \hat{g}^{cl}$, as required by condition (9).

Note that Eq. (12) follows immediately from Eqs. (10) and (11), and Eq. (13) then follows by substituting $\hat{h} \equiv \hat{g}^{cl}$ into the expression immediately above. Eq. (13) in fact corresponds to the diagonal elements of the more general covariance relation

$$\mathrm{Cov}(g) = \mathrm{Cov}(g^{cl}) + \mathrm{Cov}(g^{nc}), \tag{14}$$

which may be derived by explicit calculation of $\mathrm{Cov}(g - g^{cl})$. The classical and nonclassical field components are therefore linearly uncorrelated.

C. Fisher covariance

Many different classical measures of statistical uncertainty, such as variance and entropy, have been used in writing Heisenberg-type inequalities for quantum particles [10]. Similarly, there is a wide degree of freedom in choosing measures of uncertainty for quantum fields - the covariance function $\mathrm{Cov}(f)$ appearing in Eq. (7) only represents one particular choice. An alternative choice is provided by classical statistical estimation theory: the *Fisher* covariance function.

The Fisher covariance function $\mathrm{Cov}_{\mathrm{F}}(f)$ is, like the standard covariance function $\mathrm{Cov}(f)$, a positive and symmetric two-point function which vanishes for dispersion-free ensembles, and is hence a suitable candidate for describing field uncertainty over an ensemble. Its main role in classical statistics is as the *"minimum"* covariance function associated with estimates of translations of the field.

To motivate $\mathrm{Cov}_{\mathrm{F}}(f)$, consider a classical ensemble of fields described by some probability functional $P[f]$, with ensemble average $\langle f \rangle = \int Df\, Pf = 0$. If each member of the ensemble is translated by some amount $\overline{f}$, a new ensemble is obtained, described by $P[f - \overline{f}]$ and having field average $\langle f \rangle = \overline{f}$. The two ensembles thus differ only by the displacement field $\overline{f}$, and hence distinguishing between two such ensembles is equivalent to estimating this relative displacement.

How easily *can* such ensembles be distinguished? The basic answer is that any *unbiased* estimate $\tilde{f}$ of the displacement field (i.e., with $\langle \tilde{f} \rangle = \overline{f}$) has a covariance function greater

than or equal to the Fisher covariance:

$$\mathrm{Cov}(\tilde{f}) \succeq \mathrm{Cov}_{\mathrm{F}}(f). \tag{15}$$

The Fisher covariance therefore characterises the minimum uncertainty of such estimates. For example, the quantity

$$(\Delta_F f_x)^2 := [\mathrm{Cov}_{\mathrm{F}}(f)]_{xx}$$

represents a lower bound for the variance, $(\Delta\tilde{f}_x)^2$, of any unbiased estimate of the displacement field at position x. Roughly speaking, two ensembles differing by displacement field $\overline{f}$ stand a decent chance of being distinguished at position x if the Rayleigh-type criterion $|\overline{f}_x| \geq \Delta_F f_x$ is satisfied.

To explicitly define the Fisher covariance function, let $F(f)$ denote the "Fisher information matrix" of an ensemble described by probability density functional $P[f]$ [9, 11], with

$$[F(f)]_{xx'} := \int Df\, P \frac{\delta \ln P}{\delta f_x} \frac{\delta \ln P}{\delta f_{x'}}. \tag{16}$$

Then $\mathrm{Cov}_{\mathrm{F}}(f)$ is defined as the corresponding matrix inverse, i.e.,

$$\mathrm{Cov}_{\mathrm{F}}(f) * F(f) = F(f) * \mathrm{Cov}_{\mathrm{F}}(f) = \mathbb{1}. \tag{17}$$

Fisher information was introduced in 1925 for one-dimensional statistical variables [12], and Eq. (15) is the continuous matrix version of the Cramer-Rao inequality [11], well known in classical statistics. A particular case corresponds to the choice $\tilde{f} = f$ in Eq. (15), yielding

$$\mathrm{Cov}(f) \succeq \mathrm{Cov}_{\mathrm{F}}(f). \tag{18}$$

The Fisher covariance is therefore also a lower bound for the standard covariance. As this result is needed for establishing the connection between Heisenberg and exact uncertainty relations in Sec. II.D, it is useful to give a direct proof here.

First, let $A[f]$ denote an arbitrary functional of f with $\langle A \rangle < \infty$, and define

$$\begin{aligned} M_{xx'} &:= \left\langle \left(\frac{\delta \ln P}{\delta f_x} - \frac{\delta A}{\delta f_x} \right) \left(\frac{\delta \ln P}{\delta f_{x'}} - \frac{\delta A}{\delta f_{x'}} \right) \right\rangle \\ &= [F(f)]_{xx'} + \left\langle \frac{\delta A}{\delta f_x} \frac{\delta A}{\delta f_{x'}} \right\rangle - \int Df \left(\frac{\delta P}{\delta f_x} \frac{\delta A}{\delta f_{x'}} + \frac{\delta P}{\delta f_{x'}} \frac{\delta A}{\delta f_x} \right) \\ &= [F(f)]_{xx'} + \left\langle \frac{\delta A}{\delta f_x} \frac{\delta A}{\delta f_{x'}} + 2 \frac{\delta^2 A}{\delta f_x \delta f_{x'}} \right\rangle. \end{aligned} \tag{19}$$

Restricting A to have the quadratic form

$$A[f] = -\frac{1}{2}\int dxdx'\, K_{xx'}(f_x - h_x)(f_{x'} - h_{x'}) \tag{20}$$

for some symmetric matrix function K and field h, and noting that $M \succeq 0$ from Eq. (19), then gives

$$F(f) \succeq 2K - K * \mathrm{Cov}(f) * K,$$

where we have chosen $h = \langle f \rangle$ at the end of the calculation. Finally, Eq. (18) follows by choosing K to be the matrix inverse of $\mathrm{Cov}(f)$. Note that equality holds in Eq. (18) if and only if $M \equiv 0$ in Eq. (19), i.e., if and only if $\delta(\ln P)/\delta f \equiv \delta A/\delta f$. Thus this Cramer-Rao inequality is saturated if and only if $P \sim \exp(A)$, i.e., noting Eq. (20), if and only if the ensemble is Gaussian.

It is important to emphasise here that the Fisher covariance function is a purely *classical* quantity, requiring no reference to quantum theory whatsoever for its motivation or definition. However, it plays an important role as a measure of uncertainty in an exact uncertainty relation for quantum fields, to be derived in Sec. II.D.

D. An exact uncertainty relation

It has been shown that the momentum density of a bosonic quantum field admits a natural decomposition into classical and nonclassical components. Moreover, Eqs. (3), (8) and (11) imply that

$$[\hat{f}_x, \hat{g}^{cl}_{x'}] = 0, \qquad [\hat{f}_x, \hat{g}^{nc}_{x'}] = i\hbar\delta(x - x').$$

Hence it is the *nonclassical* component which is responsible for the non-vanishing commutator in Eq. (3). However, this nonclassical component does not merely satisfy a Heisenberg-type inequality analogous to Eq. (7): it satisfies the *exact* uncertainty relation

$$\mathrm{Cov}_{\mathrm{F}}(f) * \mathrm{Cov}(g^{nc}) = (\hbar^2/4)\mathbb{1}. \tag{21}$$

Thus, *the field uncertainty precisely determines the nonclassical momentum uncertainty*, and vice versa. Eq. (21) is the main result of this Section. It is remarkable that natural measures of uncertainty can be chosen which precisely quantify the uncertainty principle for bosonic fields.

To demonstrate Eq. (21), note that for an ensemble of quantum fields described by probability functional $P[f] = |\Psi[f]|^2$, the Fisher information follows from Eq. (16) as

$$\begin{aligned}
[F(f)]_{xx'} &= \int Df\, \Psi^*\Psi \left[\Psi^{-1}\frac{\delta\Psi}{\delta f_x} + c.c\right]\left[\Psi^{-1}\frac{\delta\Psi}{\delta f_{x'}} + c.c.\right] \\
&= \int Df\, \Psi^*\Psi \left[\Psi^{-1}\frac{\delta\Psi}{\delta f_x} - c.c.\right]\left[\Psi^{-1}\frac{\delta\Psi}{\delta f_{x'}} - c.c.\right] \\
&\quad + 2\int Df\, \left[\frac{\delta\Psi^*}{\delta f_x}\frac{\delta\Psi}{\delta f_{x'}} + c.c.\right] \\
&= -(4/\hbar^2)\langle \hat{g}^{cl}_x \hat{g}^{cl}_{x'}\rangle + (4/\hbar^2)\langle \hat{g}_x \hat{g}_{x'}\rangle,
\end{aligned}$$

where the last line follows via Eqs. (4) and (10). Hence, using Eqs. (12) and (14),

$$\mathrm{Cov}(g^{nc}) = (\hbar^2/4)F(f), \tag{22}$$

i.e., *the covariance of the nonclassical momentum density is proportional to the Fisher information of the field*. Eqs. (21) and (22) are equivalent.

The exact uncertainty relation in Eq. (21), being a strict equality for all states of the field, is clearly far stronger in character than the corresponding Heisenberg-type relation in Eq. (7). Moreover, it immediately implies the latter, since $\mathrm{Cov}(g) \succeq \mathrm{Cov}(g^{nc})$ and $\mathrm{Cov}(f) \succeq \mathrm{Cov}_{\mathrm{F}}(f)$ from Eqs. (14) and (18) respectively.

Various applications of such exact uncertainty relations may be made, analogous to those made in Refs. [1, 2] for quantum particles, but will not be pursued here. However, the notion that the momentum density of a bosonic field decomposes into a classical and a nonclassical part, with the uncertainty of the latter determined by the uncertainty of the field, underlies the formulation of a new approach to quantum field theory in Sec. III below.

E. Multicomponent and complex bosonic fields

It is of interest to briefly outline the form of exact uncertainty relations for more general bosonic fields. Thus, let f^a denote a multicomponent bosonic field with conjugate momentum density g^a. For example, f^a may be a complex Klein-Gordon field ϕ, or the electromagnetic field A^μ. This notation also covers the case where the index a labels several interacting bosonic fields.

The non-vanishing equal-time commutation relation is now

$$\left[\hat{f}^a_x, \hat{g}^b_{x'}\right] = i\hbar\delta^{ab}\delta(x - x'), \tag{23}$$

and the momentum density operator decomposes into classical and nonclassical components as before, with

$$\hat{g}^a = \hat{g}^{cl,a} + \hat{g}^{nc,a}, \tag{24}$$

$$g^{cl,a}[f] = \frac{\hbar}{2i}\left[\Psi^{-1}\frac{\delta\Psi}{\delta f^a} - (\Psi^*)^{-1}\frac{\delta\Psi^*}{\delta f^a}\right]. \tag{25}$$

Clearly the components of $\hat{g}^{cl}$ commute with each other; it may also be checked that the components of $\hat{g}^{nc}$ commute (which is necessary for the covariance function $\mathrm{Cov}(g^{nc})$ to be well defined).

The generalised covariance and Fisher information matrices are defined by

$$[\mathrm{Cov}(h)]^{ab}_{xx'} := \langle\ (h^a_x)^* h^b_{x'}\ \rangle - \langle (h^a_x)^*\rangle\langle h^b_{x'}\rangle, \tag{26}$$

$$[F(f)]^{ab}_{xx'} := \int Df\ P \frac{\delta \ln P}{\delta (f^a_x)^*}\frac{\delta \ln P}{\delta f^b_{x'}}, \tag{27}$$

in analogy to Eqs. (6) and (16) respectively, and similarly are purely classical statistical quantities.

Finally, the corresponding exact uncertainty relation has precisely the form of Eq. (21), providing that the definitions of the multiplicative identity and matrix multiplication are replaced by the natural generalisations

$$\mathbb{1}^{ab}_{xx'} := \delta^{ab}\delta(x - x'),$$

$$[A * B]^{ab}_{xx'} := \sum_c \int dx''\ A^{ac}_{xx''} B^{cb}_{x''x'}.$$

respectively.

III. QUANTISATION OF FIELDS FROM AN EXACT UNCERTAINTY PRINCIPLE

It has been shown that the momentum density of a bosonic quantum field splits naturally and neatly into the sum of *classical* and *nonclassical* parts, as per Eq. (11). Moreover, the uncertainty of the nonclassical part is *precisely linked* to the uncertainty of the field itself, as per Eq. (21). These results are more than a mathematical link between the statistics of conjugate quantum fields: they suggest the existence of a new bridge connecting classical field theory to quantum field theory - an exact uncertainty principle.

Indeed, as demonstrated below, the assumption that an ensemble of classical fields is subjected to "nonclassical" momentum fluctuations, of a magnitude determined by the field uncertainty, leads from the classical equations of motion to the equation of motion of a bosonic quantum field. This result is restricted to the case of field Hamiltonians quadratic in the momentum density, but nevertheless covers most classical fields of physical interest, including the Klein-Gordon, electromagnetic and gravitational fields.

A. Classical ensembles

We first consider a real multicomponent classical field $f \equiv (f^a)$ with conjugate momentum density $g \equiv (g^a)$, described by some Hamiltonian functional $H[f, g, t]$. The equations of motion for an *ensemble* of such fields are given by the Hamilton-Jacobi equation

$$\frac{\partial S}{\partial t} + H[f, \delta S/\delta f, t] = 0, \tag{28}$$

and the continuity equation

$$\frac{\partial P}{\partial t} + \sum_a \int dx \, \frac{\delta}{\delta f_x^a} \left(P \, \frac{\delta H}{\delta g_x^a}\bigg|_{g=\delta S/\delta f} \right) = 0, \tag{29}$$

for the momentum potential S and the probability density P, as is reviewed in Appendix B. These equations specify the motion of the ensemble completely, where the momentum density associated with f is given by $g = \delta S/\delta f$.

Defining the *ensemble Hamiltonian* $\tilde{H}$ as the functional integral

$$\tilde{H}[P, S, t] := \langle H \rangle = \int Df \, P H[f, \delta S/\delta f, t], \tag{30}$$

the equations of motion for the dynamical variables P and S may be written in the Hamiltonian form

$$\frac{\partial P}{\partial t} = \frac{\delta \tilde{H}}{\delta S}, \qquad \frac{\partial S}{\partial t} = -\frac{\delta \tilde{H}}{\delta P}. \tag{31}$$

The variational derivative of a functional integral such as $\tilde{H}$, with respect to a functional such as P or S, is discussed in Appendix A, and the equivalence of Eqs. (28) and (29) to Eqs. (31) follows directly from Eq. (A6). Hence, in analogy to Eqs. (B1) of Appendix B, *P and S may be regarded as canonically conjugate functionals, which evolve under the ensemble Hamiltonian $\tilde{H}$* [13]. Note from Eq. (30) that $\tilde{H}$ typically corresponds to the mean energy of the ensemble.

In what follows, we will only consider classical fields with Hamiltonian functionals quadratic in the momentum field density, i.e., of the form

$$H[f,g,t] = \sum_{a,b} \int dx\, K_x^{ab}[f] g_x^a g_x^b + V[f]. \tag{32}$$

Here $K_x^{ab}[f] = K_x^{ba}[f]$ is a kinetic factor coupling components of the momentum density, and $V[f]$ is some potential energy functional. The corresponding *ensemble* Hamiltonian is given by Eq. (30). Note that cross terms of the form $g_x^a g_{x'}^b$ with $x \neq x'$ are not permitted in local field theories, and hence are not considered here.

B. Momentum fluctuations ⇒ quantum ensembles

The ensemble Hamiltonian $\tilde{H}[P,S]$ in Eq. (30) is our classical starting point for describing an ensemble of fields. This starting point must be modified in some way if one is to obtain new equations of motion, to be identifed as describing a quantum ensemble of fields. For example, a standard approach is to assume the existence of a complex field functional $\Psi[f,t]$, and write down the Schrödinger equation $i\hbar\partial\Psi/\partial t = H[f, -i\hbar(\delta/\delta f), t]\Psi$ [8]. While this approach can generally be made to work successfully, it provides no explanation of the appearance of the nonclassical objects Ψ, $\hbar$, and of a linear operator equation. Moreover, for cases in which K_x^{ab} in Eq. (32) is dependent on f (eg, gravitational fields), this approach is ambiguous as to the ordering of the functional derivative operator.

In contrast, we take a very different approach, where the only *a priori* nonclassical feature is an assumption that the classical ensemble Hamiltonian $\tilde{H}$ must be modified to take into account the existence of nonclassical fluctuations of the momentum density, with the magnitude of the fluctations determined by the uncertainty in the field. This "exact uncertainty" approach is motivated by the fact that bosonic fields satisfy exact uncertainty relations such as Eq. (21) of Sec. II. It leads to equations of motion equivalent to the Schrödinger equation above, with the added advantage of a *unique* operator ordering.

Suppose then that $\delta S/\delta f$ is in fact an *average* momentum density associated with field f, in the sense that the true momentum density is given by

$$g = \delta S/\delta f + N, \tag{33}$$

where N is a fluctuation field that vanishes on the average for any given field f. Thus the physical meaning of S changes to being an *average* momentum potential. No specific

underlying model for N is assumed or necessary: in the approach to be followed, one may in fact interpret the "source" of the fluctuations as the field uncertainty itself. Thus the nature of the fluctuation field is not important - its main effect is to remove any deterministic connection between f and g.

Since the momentum fluctuations may conceivably depend on the field f, the average over such fluctuations for a given functional $A[f]$ will be denoted by $\overline{A}[f]$, and the average over fluctuations *and* the field by $\langle A \rangle$. Thus $\overline{N} \equiv 0$ by assumption, and in general $\langle A \rangle = \int Df\, P[f]\overline{A}[f]$. Assuming a quadratic dependence on momentum density as per Eq. (32), it follows that when the fluctuations are significant the classical ensemble Hamiltonian $\tilde{H} = \langle H \rangle$ in Eq. (30) should be replaced by

$$\begin{aligned}\tilde{H}' &= \langle\, H[f, \delta S/\delta f + N, t] \,\rangle \\ &= \sum_{a,b} \int Df \int dx\, P K_x^{ab} \overline{(\delta S/\delta f_x^a + N_x^a)(\delta S/\delta f_x^b + N_x^b)} + \langle V \rangle \\ &= \tilde{H} + \sum_{a,b} \int Df \int dx\, P K_x^{ab} \overline{N_x^a N_x^b}. \end{aligned} \tag{34}$$

Thus the momentum fluctuations lead to an additional nonclassical term in the ensemble Hamiltonian, dependent on the covariance matrix $\mathrm{Cov}_x(N)$ of the fluctuations at position x, where

$$[\mathrm{Cov}_x(N)]^{ab} := \overline{N_x^a N_x^b}. \tag{35}$$

The additional term in Eq. (34) is uniquely specified, up to a multiplicative constant, by the following four assumptions:

(1) Causality: $\tilde{H}'$ is an ensemble Hamiltonian for the canonically conjugate functionals P and S, which yields causal equations of motion. Thus no higher than first-order functional derivatives can appear in the additional term, implying that

$$\mathrm{Cov}_x(N) = \alpha(P, \delta P/\delta f_x, S, \delta S/\delta f_x, f_x, t)$$

for some symmetric matrix function α.

(2) Independence: If the system comprises two independent non-interacting subsystems 1 and 2, with factorisable probability density functional $P[f^{(1)}, f^{(2)}] = P_1[f^{(1)}]P_2[f^{(2)}]$, then the dependence of the subsystem fluctuations on P only enters via the corresponding probability densities P_1 and P_2 respectively. Thus

$$\mathrm{Cov}_x(N^{(1)})\Big|_{P_1 P_2} = \mathrm{Cov}_x(N^{(1)})\Big|_{P_1}, \qquad \mathrm{Cov}_x(N^{(2)})\Big|_{P_1 P_2} = \mathrm{Cov}_x(N^{(2)})\Big|_{P_2}$$

for such a system. Note that this assumption implies that ensemble Hamiltonians are additive for independent non-interacting ensembles (as are the corresponding actions [13]).

(3) Invariance: The additional term transforms correctly under linear canonical transformations of the field components. Thus, noting that $f \to \Lambda^{-1} f$, $g \to \Lambda^T g$ is a canonical transformation for any invertible matrix Λ (with transpose Λ^T and coefficients Λ_{ab}), which preserves the quadratic form of H in Eq. (32) and leaves the momentum potential S invariant (since $\delta/\delta f \to \Lambda^T \delta/\delta f$), one has from Eq. (33) that $N \to \Lambda^T N$, and hence that

$$\mathrm{Cov}_x(N) \to \Lambda^T \mathrm{Cov}_x(N) \Lambda \quad \text{for} \quad f \to \Lambda^{-1} f.$$

Note that for single-component fields this reduces to a scaling relation for the variance of the fluctuations at each point x.

(4) Exact uncertainty: The uncertainty of the momentum fluctuations at any given position and time, as characterised by $\mathrm{Cov}_x(N)$, is specified by the field uncertainty at that position and time. Thus, since the field uncertainty is completely determined by the probability density functional P, it follows that $\mathrm{Cov}_x(N)$ cannot depend on S, nor explicitly on t.

It is seen that the first three assumptions are essentially classical in nature, while the fourth assumption is not: it postulates an exact connection between the nonclassical momentum uncertainty and the field uncertainty. Remarkably, these assumptions lead directly to equations of motion of a bosonic quantum field, as shown by the following Theorem and Corollary.

Theorem: *The above assumptions of causality, independence, invariance, and exact uncertainty imply that*

$$\overline{N_x^a N_x^b} = C(\delta P/\delta f_x^a)(\delta P/\delta f_x^b)/P^2, \tag{36}$$

where C is a positive universal constant.

Proof: From the causality and exact uncertainty assumptions one has $\mathrm{Cov}_x(N) = \alpha(P, \delta P/\delta f_x, f_x)$. To avoid issues of regularisation, it is convenient to consider a position-dependent canonical transformation, $f_x \to \Lambda_x^{-1} f_x$, such that $A[\Lambda] := \exp[\int dx \, \ln|\det \Lambda_x|]$ is finite. Then the probability density functional P and the measure Df transform as $P \to AP$ and $Df \to A^{-1} Df$ respectively, and so the invariance assumption requires that

$$\alpha(AP, A\Lambda_x^T u, \Lambda_x^{-1} w) \equiv \Lambda_x^T \alpha(P, u, w) \Lambda_x,$$

where u^a and w^a denote the vectors $\delta P/\delta f_x^a$ and f_x^a respectively, for a given value of x. Since Λ_x can remain the same at a given point x while varying elsewhere, this homogeneity condition must hold for A and Λ_x independently. Thus, choosing Λ_x to be the identity matrix at some point x, one has $\alpha(AP, Au, w) = \alpha(P, u, w)$ for all A, implying that α can involve P only via the combination $v := u/P$. The homogeneity condition for α therefore reduces to

$$\alpha(\Lambda^T v, \Lambda^{-1} w) = \Lambda^T \alpha(v, w) \Lambda \ .$$

Note that this equation is linear, and invariant under multiplication of α by any function of the scalar $J := v^T w$. Moreover, it may easily be checked that if σ and τ are solutions, then so are $\sigma\tau^{-1}\sigma$ and $\tau\sigma^{-1}\tau$. Choosing the two independent solutions $\sigma = vv^T$, $\tau = (ww^T)^{-1}$, it follows that the general solution has the form

$$\alpha(v, w) = \beta(J) vv^T + \gamma(J)(ww^T)^{-1}$$

for arbitrary functions β and γ. For $P = P_1 P_2$ one finds $v = (v_1, v_2)$, $w = (w_1, w_2)$, where the subscripts label corresponding subsystem quantities, and hence the independence assumption reduces to the requirements

$$\beta(J_1 + J_2) v_1 v_1^T + \gamma(J_1 + J_2)(w_1 w_1^T)^{-1} = \beta_1(J_1) v_1 v_1^T + \gamma_1(J_1)(w_1 w_1^T)^{-1},$$

$$\beta(J_1 + J_2) v_2 v_2^T + \gamma(J_1 + J_2)(w_2 w_2^T)^{-1} = \beta_2(J_2) v_2 v_2^T + \gamma_2(J_2)(w_2 w_2^T)^{-1},$$

for the respective subsystem covariance matrices. Thus $\beta = \beta_1 = \beta_2 = C$, $\gamma = \gamma_1 = \gamma_2 = D$ for universal (i.e., system-independent) constants C and D, yielding the general form

$$[\mathrm{Cov}_x(N)]^{ab} = C(\delta P/\delta f_x^a)(\delta P/\delta f_x^b)/P^2 + D W_x^{ab}[f]$$

for the fluctuation covariance matrix, where $W_x[f]$ denotes the inverse of the matrix with ab-coefficient $f_x^a f_x^b$. Note that the latter term is purely a functional of f, and hence merely contributes a classical additive potential term to the ensemble Hamiltonian of Eq. (34). It thus has no nonclassical role, and can be absorbed directly into the classical potential $\langle V \rangle$ (indeed, for fields with more than one component this term is singularly ill-defined, and hence can be discarded on physical grounds). Thus we may take $D = 0$ without loss of generality. Finally, the positivity of C follows from the positivity of the covariance matrix $\mathrm{Cov}_x(N)$, and the theorem is proved. $\diamondsuit$

The above theorem yields a unique form for the additional term in Eq. (34), up to a multiplicative constant C. The classical equations of motion for the ensemble are recovered in the limit of small fluctuations, i.e., in the limit $C \to 0$. Note that one cannot make the identification $N_x^a \sim (\delta P/\delta f_x^a)/P$ from Eq. (36), as this is inconsistent with the fundamental property $\overline{N_x^a} = 0$.

The main result of this section is the following corollary:

Corollary: *The equations of motion corresponding to the ensemble Hamiltonian $\tilde{H}'$ can be expressed as the single complex equation*

$$i\hbar\frac{\partial\Psi}{\partial t} = H[f, -i\hbar\delta/\delta f, t]\Psi = -\hbar^2\left(\sum_{a,b}\int dx\,\frac{\delta}{\delta f_x^a}K_x^{ab}[f]\frac{\delta}{\delta f_x^b}\right)\Psi + V[f]\Psi, \tag{37}$$

where one defines

$$\hbar := 2\sqrt{C}, \qquad \Psi := \sqrt{P}e^{iS/\hbar}. \tag{38}$$

Proof: First, the equations of motion corresponding to the ensemble Hamiltonian $\tilde{H}'$ follow via the theorem and Eqs. (31) as: (a) the continuity equation Eq. (29) as before (since the additional term does not depend on S), which from Eq. (32) has the explicit form

$$\frac{\partial P}{\partial t} + 2\sum_{ab}\int dx\,\frac{\delta}{\delta f_x^a}\left(PK_x^{ab}\frac{\delta S}{\delta f_x^b}\right) = 0; \tag{39}$$

and (b) the modified Hamilton-Jacobi equation

$$\partial S/\partial t = -\delta\tilde{H}'/\delta P = -H[f, \delta S/\delta f, t] - \delta(\tilde{H}' - \tilde{H})/\delta P.$$

Calculating the last term via Eq. (36) and Eq. (A6) of Appendix C, this simplifies to

$$\frac{\partial S}{\partial t} + H[f, \delta S/\delta f, t] - 4CP^{-1/2}\sum_{a,b}\int dx\,\left(K_x^{ab}\frac{\delta^2 P^{1/2}}{\delta f_x^a \delta f_x^b} + \frac{\delta K_x^{ab}}{\delta f_x^a}\frac{\delta P^{1/2}}{\delta f_x^b}\right) = 0. \tag{40}$$

Second, writing $\Psi = P^{1/2}\exp(iS/\hbar)$, multiplying each side of Eq. (37) on the left by Ψ^{-1}, and expanding, gives a complex equation for P and S. The imaginary part is just the continuity equation of Eq. (39), and the real part is the modified Hamilton-Jacobi equation of Eq. (40) above, providing that one identifies C with $\hbar^2/4$. $\diamondsuit$

Eq. (37) may be recognised as the Schrödinger equation for a quantum bosonic field, and hence the goal of deriving this equation, via an exact uncertainty principle for nonclassical momentum fluctuations acting on a classical ensemble, has been achieved. The ensemble of fields corresponding to ensemble Hamiltonian $\tilde{H}'$ will therefore be called the *quantum*

ensemble corresponding to $\tilde{H}$. It is remarkable that the four assumptions of causality, independence, invariance and exact uncertainty lead to a *linear operator* equation.

Note that the exact uncertainty approach specifies the *unique* operator ordering, $(\delta/\delta f_x^a)K_x^{ab}(\delta/\delta f_x^b)$, for the functional derivative operators in Eq. (37). Thus there is no ambiguity in the ordering for cases where K_x^{ab} depends on the field f, in contrast to traditional approaches (eg, the Wheeler-deWitt equation, discussed in Sec. III.D below). The above results generalise straightforwardly to complex classical fields.

Finally, it may be remarked that the equations of motion of a classical ensemble may be subject to some imposed constraint(s) on f, P, S and $\tilde{H}$. For example, each member of an ensemble of electromagnetic fields may have the Lorentz gauge imposed, so as to reduce the gauge degree of freedom (see Sec III.C below). As a guiding principle, we will require that the corresponding *quantum* ensemble is subject to the same constraint(s) on f, P, S and $\tilde{H}'$. This will ensure a meaningful classical-quantum correspondence for the results of field measurements. However, consistency of the quantum equations of motion with a given set of constraints is not guaranteed by the above Theorem and Corollary, and so must be checked independently for each case.

C. Example: Electromagnetic field

The electromagnetic field is described, up to gauge invariance, by a 4-component field A^μ. In the Lorentz gauge all physical fields satisfy $\partial_\mu A^\mu \equiv 0$, and the classical equations of motion in vacuum are given by $\partial^\nu \partial_\nu A^\mu = 0$. These follow, for example, from the Hamiltonian [8]

$$H_{GB}[A,\pi] = (1/2)\int dx\, \eta_{\mu\nu}\left(\pi^\mu\pi^\nu - \nabla A^\mu \cdot \nabla A^\nu\right), \tag{41}$$

where $\eta_{\mu\nu}$ denotes the Minkowski tensor, π^μ denotes the conjugate momentum density, and ∇ denotes the spatial derivative. Here H_{GB} corresponds to the gauge-breaking Lagrangian $L = -(1/2)\int dx\, A^{\mu,\nu}A_{\mu,\nu}$, and is seen to have the quadratic form of Eq. (32) (with $K_x^{\mu\nu} = \eta_{\mu\nu}/2$). Hence the exact uncertainty uncertainty approach immediately implies that a *quantum* ensemble of electromagnetic fields obeys the Schrödinger equation

$$i\hbar(\partial\Psi/\partial t) = H_{GB}[A, -i\hbar(\delta/\delta A)]\Psi, \tag{42}$$

in agreement with the Gupta-Bleuler formalism [8].

Note that the probability of a member of the classical ensemble not satisfying the Lorentz gauge condition $\partial_\mu A^\mu \equiv 0$ is zero by assumption, i.e., the Lorentz gauge is equivalent to the condition that the product $(\partial_\mu A^\mu)P[A]$ vanishes for all physical fields. For the quantum ensemble to satisfy this condition, as per the guiding principle discussed at the end of Section III.B above, one equivalently requires, noting Eq. (38), that

$$(\partial_\mu A^\mu)\Psi[A] = 0.$$

As is well known, this constraint, if initially satisfied, is satisfied for all times [14] (as is the alternative weaker constraint that only the 4-divergence of the positive frequency part of the field vanishes [8]). Hence the evolution of the quantum ensemble is consistent with the Lorentz gauge. It would be of interest to derive the consistency of this constraint directly from the equation of motion Eqs. (39) and (40) for P and S.

Finally, it is well known that one can also obtain the classical equations of motion via an alternative Hamiltonian, by exploiting the degree of freedom left by the Lorentz gauge to remove a dynamical coordinate (corresponding to the longitudinal polarisation). In particular, since $\partial_\mu A^\mu$ is invariant under $A^\mu \to A^\mu + \partial^\mu \chi$ for any function χ satisfying $\partial^\nu \partial_\nu \chi = 0$, one may completely fix the gauge in a given Lorentz frame by choosing χ such that $A^0 = 0$. One thus obtains, writing $A^\mu \equiv (A^0, \mathbf{A})$, the radiation gauge $A^0 = 0$, $\nabla \cdot \mathbf{A} = 0$. The classical equations of motion for $\mathbf{A}$ ($\partial^\nu \partial_\nu \mathbf{A} = 0$), follow, for example, from the Hamiltonian

$$H_R[\mathbf{A}, \mathbf{E}] = (1/2) \int dx \, (\mathbf{E} \cdot \mathbf{E} + |\nabla \times \mathbf{A}|^2), \tag{43}$$

where $\mathbf{E}$ denotes the conjugate momentum density. Here H_R corresponds to the standard Lagrangian $L = -(1/4) \int dx \, F^{\mu\nu} F_{\mu\nu}$, with $A^0 \equiv 0$. This Hamiltonian once again has the quadratic form of Eq. (32), and hence the exact uncertainty approach yields the corresponding Schrödinger equation

$$i\hbar(\partial\Psi/\partial t) = H_R[\mathbf{A}, -i\hbar(\delta/\delta\mathbf{A})]\Psi \tag{44}$$

for a quantum ensemble of electromagnetic fields in the radiation gauge (this is also the form of the Schrödinger equation obtained via the Schwinger-Tomonaga formalism [15]). Note that the momentum density $\mathbf{E}$ is in fact the electric field, and hence, in this case, the exact uncertainty approach corresponds to adding nonclassical fluctuations to the electric field components, with the fluctation uncertainty determined by the uncertainty in the vector potential $\mathbf{A}$.

D. Example: Gravitational field

The gravitational field is described, up to arbitrary coordinate transformations, by the metric tensor $g \equiv (g_{\mu\nu})$. The corresponding invariant length may be decomposed as [16]

$$ds^2 = g_{\mu\nu}dx^\mu dx^\nu = -(\alpha^2 - \boldsymbol{\beta}\cdot\boldsymbol{\beta})dt^2 + 2\beta_i dx^i dt + \gamma_{ij}dx^i dx^j,$$

in terms of the lapse function α, the shift function $\boldsymbol{\beta}$, and the spatial 3-metric $\gamma \equiv (\gamma_{ij})$. The equations of motion are the Einstein field equations, which follow from the Hamiltonian functional [16]

$$H[\gamma, \pi, \alpha, \boldsymbol{\beta}] = \int dx\, \alpha \mathcal{H}_G[\gamma, \pi] - 2\int dx\, \beta_i \pi^{ij}{}_{|j}\ , \tag{45}$$

where $\pi \equiv (\pi^{ij})$ denotes the momentum density conjugate to γ, $|j$ denotes the covariant 3-derivative, and the Hamiltonian density $\mathcal{H}_G$ is given by

$$\mathcal{H}_G = (1/2)G_{ijkl}[\gamma]\pi^{ij}\pi^{kl} - 2\,{}^{(3)}R[\gamma](\det\gamma)^{1/2}. \tag{46}$$

Here ${}^{(3)}R$ is the curvature scalar corresponding to γ_{ij}, and

$$G_{ijkl}[\gamma] = (\gamma_{ik}\gamma_{jl} + \gamma_{il}\gamma_{jk} - \gamma_{ij}\gamma_{kl})(\det\gamma)^{-1/2}.$$

The Hamiltonian functional H corresponds to the standard Lagrangian $L = \int dx\,(-\det g)^{1/2}R[g]$, and the momenta π^0 and π^i conjugate to α and β_i respectively vanish identically [16]. However, the lack of dependence of H on π^0 and π^i is consistently maintained only if the rates of change of these momenta also vanish, i.e., noting Eq. (B1) of Appendix B, only if the constraints [16]

$$\delta H/\delta\alpha = \mathcal{H}_G = 0, \qquad \delta H/\delta\beta_i = -2\pi^{ij}{}_{|j} = 0 \tag{47}$$

are satisfied. Thus the dynamics of the field is independent of α and $\boldsymbol{\beta}$, so that these functions may be fixed arbitrarily [16]. Moreover, these constraints immediately yield $H = 0$ in Eq. (45), and hence the system is static, with no explicit time dependence [16].

It follows that in the Hamilton-Jacobi formulation of the equations of motion (see Appendix B), the momentum potential S is independent of α, $\boldsymbol{\beta}$ and t. Noting that $\pi \equiv \delta S/\delta\gamma$ in this formulation, Eqs. (47) therefore yield the corresponding constraints

$$\frac{\delta S}{\delta\alpha} = \frac{\delta S}{\delta\beta_i} = \frac{\partial S}{\partial t} = 0, \qquad \left(\frac{\delta S}{\delta\gamma_{ij}}\right)_{|j} = 0 \tag{48}$$

for S. As shown by Peres [17], a given functional $F[\gamma]$ of the 3-metric is invariant under spatial coordinate transformations if and only if $(\delta F/\delta\gamma_{ij})_{|j} = 0$, and hence the fourth constraint in Eq. (48) is equivalent to the invariance of S under such transformations. This fourth constraint moreover implies that the second term in Eq. (45) may be dropped from the Hamiltonian, yielding the reduced Hamiltonian

$$H_G[\gamma, \pi, \alpha] = \int dx\, \alpha \mathcal{H}_G[\gamma, \pi] \tag{49}$$

in the Hamiltonian-Jacobi formulation [17, 18].

For an *ensemble* of classical gravitational fields, the independence of the dynamics with respect to α, $\boldsymbol{\beta}$ and t implies that members of the ensemble are distinguishable only by their corresponding 3-metric γ. Moreover, it is natural to impose the additional geometric requirement that the ensemble is invariant under spatial coordinate transformations. One therefore has the constraints

$$\frac{\delta P}{\delta\alpha} = \frac{\delta P}{\delta\beta_i} = \frac{\partial P}{\partial t} = 0, \qquad \left(\frac{\delta P}{\delta\gamma_{ij}}\right)_{|j} = 0 \tag{50}$$

for the corresponding probability density functional $P[\gamma]$, analogous to Eq. (48). The first two constraints imply that ensemble averages only involve integration over γ.

Noting Eq. (46), the Hamiltonian H_G in Eq. (49) has the quadratic form of Eq. (32). Hence the exact uncertainty approach is applicable, and immediately leads to the Schrödinger equation

$$i\hbar\partial\Psi/\partial t = \int dx\, \alpha \mathcal{H}_G[\gamma, -i\hbar(\delta/\delta\gamma)]\Psi \tag{51}$$

for a *quantum* ensemble of gravitational fields, as per the Corollary of Sec. III.B.

As discussed at the end of Sec. III.B, we follow the guiding principle that all constraints imposed on the classical ensemble should be carried over to corresponding constraints on the quantum ensemble. Thus, from Eqs. (48) and (50) we require that P and S, and hence Ψ in Eq. (38), are independent of α, $\boldsymbol{\beta}$ and t and invariant under spatial coordinate transformations, i.e.,

$$\frac{\delta\Psi}{\delta\alpha} = \frac{\delta\Psi}{\delta\beta_i} = \frac{\partial\Psi}{\partial t} = 0, \qquad \left(\frac{\delta\Psi}{\delta\gamma_{ij}}\right)_{|j} = 0. \tag{52}$$

Applying the first and third of these constraints to Eq. (51) immediately yields, via Eq. (46), the reduced Schrödinger equation

$$\mathcal{H}_G[\gamma, -i\hbar(\delta/\delta\gamma)]\Psi = (-\hbar^2/2)\frac{\delta}{\delta\gamma_{ij}} G_{ijkl}[\gamma] \frac{\delta}{\delta\gamma_{kl}}\Psi - 2\,{}^{(3)}R[\gamma](\det\gamma)^{1/2}\Psi = 0, \tag{53}$$

which may be recognised as the Wheeler-deWitt equation in the metric representation [16]. The consistency of Eqs. (52) and (53) is well known [16].

A notable feature of Eq. (53) is that the Wheeler-deWitt equation has not only been derived from an exact uncertainty principle: it has, as a consequence of Eq. (37), been derived with a *precisely* defined operator ordering (with G_{ijkl} sandwiched between the two functional derivatives). Thus the exact uncertainty approach does not admit any ambiguity in the description of quantum gravity, unlike the standard approach [16]. Such removal of ambiguity is essential to making definite physical predictions, and hence may be regarded as an advantage of the exact uncertainty approach.

For example, Kontoleon and Wiltshire [19] have pointed out that Vilenkin's prediction of inflation in minisuperspace, from a corresponding Wheeler-deWitt equation with "tunneling" boundary conditions [5], depends critically upon the operator ordering used. In particular, considering the class of orderings defined by an integer power p, with corresponding Wheeler-deWitt equation [5]

$$\left[\frac{\partial^2}{\partial a^2} + \frac{p}{a}\frac{\partial}{\partial a} - \frac{1}{a^2}\frac{\partial^2}{\partial \phi^2} - U(a,\phi)\right]\Psi = 0 \tag{54}$$

(for a Friedmann-Robertson-Walker metric coupled to a scalar field ϕ), Kontoleon and Wiltshire show that Vilenkin's approach fails for orderings with $p \geq 1$ [19]. Moreover, they suggest that the only natural ordering is in fact the "Laplacian" ordering corresponding to $p = 1$, which has been justified on geometric grounds by Hawking and Page [20].

However, noting that the relevant Hamiltonian functional in Eq. (2.7) of Ref. [5] is quadratic in the momentum densities of the metric and the scalar field, the exact uncertainty approach may be applied, and yields the Wheeler-deWitt equation corresponding to $p = -1$ in Eq. (54). Hence the criticism in Ref. [19] is avoided. One also has the nice feature that the associated Wheeler-deWitt equation can be exactly solved for this "exact uncertainty" ordering [5].

IV. DISCUSSION

The two main results of this paper are (i) an exact uncertainty relation, Eq. (21), valid for all bosonic quantum fields, and (ii) the derivation of the quantum equation of motion, Eq. (37), from an exact uncertainty principle, for fields with Hamiltonian functionals quadratic in the momentum density. These results are conceptually connected by the notion of the

momentum density splitting into the sum of classical and nonclassical components, with the uncertainty of the nonclassical component determined by the uncertainty of the field. Moreover, they generalise similar results obtained in Refs. [1–4] for quantum particles.

It is important to emphasise that the exact uncertainty approach in Sec. III.B does *not* assume the existence of a complex amplitude functional $\Psi[f]$, nor the representation of fields by operators, nor the existence of a universal constant $\hbar$ with units of action, nor the existence of a linear operator equation. Only the assumptions of causality, independence, invariance and exact uncertainty are required, plus the guiding principle that constraints imposed on the classical ensemble should carry over to the corresponding quantum ensemble. These assumptions also provide an intuitive picture for the origin of the Schrödinger equation for bosonic fields, as arising from nonclassical fluctuations of the momentum density. Of course this picture has limitations - the fluctuations essentially arise from the uncertainty of the field itself, rather than from some external source, and hence are most certainly "nonclassical" rather than "classical" in nature.

A minimalist interpretation of the exact uncertainty approach, based on Eqs. (33) and (36), is that every *physical* field has an intrinsic uncertainty, the nature of which precludes a deterministic relationship between the field and its conjugate momentum density. However, the *degree* of indeterminism in this relationship *is* precisely quantifiable, in a statistical sense, and is directly connected to the ensemble representation of the inherent field uncertainty.

The exact uncertainty approach is very different to the "causal interpretation" of Bohm and co-workers [21]. In the latter it is assumed that there is a pre-existing complex amplitude functional $\Psi[f] = \sqrt{P}\exp(iS/\hbar)$ obeying a Schrödinger equation, which acts upon a single classical field via the addition of a "quantum potential", $Q[P]$, to the classical Hamiltonian. It is further assumed that the momentum density is precisely $g \equiv \delta S/\delta f$, and that physical ensembles of fields have probability density functional $P = |\Psi|^2$. In contrast, the exact uncertainty approach does not postulate the existence of adjunct amplitudes and potentials, the Schrödinger equation directly represents the evolution of an ensemble rather than of an external amplitude functional acting on individual systems (and is derived rather than postulated), and the basic tenet in Eq. (33) is that $g \neq \delta S/\delta f$.

It is of interest to consider the scope and limitations of the exact uncertainty approach to physical systems. Its applicability to nonrelativistic quantum particles [3, 4, 22], and now to bosonic quantum fields with Hamiltonians quadratic in the momentum density (which

include all relativistic integer-spin fields), has been demonstrated. It is also, indirectly, applicable to the non-quadratic Hamiltonian functional of a nonrelativistic boson field (corresponding to second quantisation of the usual nonrelativistic Schrödinger equation), in the sense that this field may be obtained as a low-energy limit of the complex Klein-Gordon field [6] (to which the exact uncertainty approach directly applies).

In this paper the basic Schrödinger equation for bosonic fields has been obtained, with the advantageous feature of a unique operator ordering in cases where other approaches are ambiguous. It would be of interest to consider further issues, such as the representation of general physical observables by operators (addressed for the case of particles in Ref. [3]), boundary conditions, infinities, etc, from the new perspective on the conceptual and technical basis of quantisation offered by the exact uncertainty approach.

Finally, a major question to be addressed in the future is whether the exact uncertainty approach is applicable to fermionic quantum fields. These have two features which present challenges: the corresponding ensemble Hamiltonian is usually linear in the momentum density, and the anticommutation relations make it difficult to connect the equations of motion with corresponding classical equations of motion in the limit as $\hbar \to 0$. One possible approach is to determine whether exact uncertainty relations exist for such fields, analogous to Eq. (21), as these would presumably suggest the statistical properties required by suitable "nonclassical" fluctuations.

Appendix A: Functional derivatives and integrals

Here necessary definitions and properties of functionals are noted, including variational properties of functional integrals. Since manipulations in the paper are of a purely formal character, we avoid discussions of regularisations and discretizations needed to fully define certain quantities.

A functional, $F[f]$, is a mapping from a set of physical fields (assumed to form a vector space) to the real or complex numbers, and the functional derivative of $F[f]$ is defined via the variation of F with respect to f, i.e.,

$$\delta F = F[f + \delta f] - F[f] = \int dx \, \frac{\delta F}{\delta f_x} \, \delta f_x \tag{A1}$$

for arbitrary infinitesimal variations δf. Thus the functional derivative is a field density,

$\delta F/\delta f$, having the value $\delta F/\delta f_x$ at position x. For curved spaces one may explicitly include a volume element in the integral, thus redefining the functional derivative by a multiplicative function of x; however, this is merely a matter of taste and will not be adopted here. The functional derivative is assumed to always exist for the functionals in this paper.

It follows directly from Eq. (A1) that the functional derivative satisfies product and chain rules analogous to ordinary differentiation. The choice $F[f] = f_{x'}$ in Eq. (A1) yields $\delta f_{x'}/\delta f_x = \delta(x - x')$ as required in Eqs. (3) and (4). Moreover, if the field depends on some parameter, t say, then choosing $\delta f_x = f_x(t + \delta t) - f_x(t)$ in Eq. (A1) yields

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \int dx \, \frac{\delta F}{\delta f_x} \frac{\partial f_x}{\partial t} \tag{A2}$$

for the rate of change of F with respect to t.

Functional integrals correspond to integration of functionals over the vector space of physical fields (or equivalence classes thereof). The only property we require for this paper is the existence of a measure Df on this vector space which is *translation invariant*, i.e., $\int Df \equiv \int Df'$ for any translation $f' = f + h$ (which follows immediately, for example, from the discretisation approach to functional integration [6]). In particular, this property implies the useful result

$$\int Df \, \frac{\delta F}{\delta f} = 0 \quad \text{for} \quad \int Df \, F[f] < \infty, \tag{A3}$$

which is used repeatedly below and in the text. Eq. (A3) follows by noting that the finiteness condition and translation invariance imply

$$0 = \int Df \, (F[f + \delta f] - F[f]) = \int dx \, \delta f_x \left(\int Df \, \delta F/\delta f_x \right)$$

for arbitrary infinitesimal translations.

Thus, for example, if $F[f]$ has a finite expectation value with respect to some probability density functional $P[f]$, then Eq. (A3) yields the "integration by parts" formula

$$\int Df \, P(\delta F/\delta f) = -\int Df \, (\delta P/\delta f) F.$$

Moreover, from Eq. (A3) the total probability, $\int Df \, P$, is conserved for any probability flow satisfying a continuity equation of the form

$$\frac{\partial P}{\partial t} + \int dx \, \frac{\delta}{\delta f_x} \, [P V_x] = 0, \tag{A4}$$

providing that the average flow rate, $\langle V_x \rangle$, is finite.

Finally, consider a functional integral of the form

$$I[F] = \int Df\, \xi(F, \delta F/\delta f), \tag{A5}$$

where ξ denotes any function of some functional F and its functional derivative. Variation of $I[F]$ with respect to F then gives, to first order,

$$\begin{aligned}
\delta I = I[F+\delta F] - I[F] \;&=\; \int Df\, \left\{ (\partial\xi/\partial F)\delta F + \int dx\, \left[\partial\xi/\partial(\delta F/\delta f_x)\right] \left[\delta(\delta F)/\delta f_x\right] \right\} \\
&=\; \int Df\, \left\{ (\partial\xi/\partial F) - \int dx\, \frac{\delta}{\delta f_x} \left[\partial\xi/\partial(\delta F/\delta f_x)\right] \right\} \delta F \\
&\quad + \int dx \int Df\, \frac{\delta}{\delta f_x} \left\{ \left[\partial\xi/\partial(\delta F/\delta f_x)\right] \delta F \right\}.
\end{aligned}$$

Assuming that the functional integral of the expression in curly brackets in the last term is finite, this term vanishes from Eq. (A3), yielding the result

$$\delta I = \int Df\, \frac{\delta I}{\delta F}\, \delta F$$

analogous to Eq. (A1), where the variational derivative $\delta I/\delta F$ is defined by

$$\frac{\delta I}{\delta F} = \frac{\partial\xi}{\partial F} - \int dx\, \frac{\delta}{\delta f_x} \left[\frac{\partial\xi}{\partial(\delta F/\delta f_x)} \right]. \tag{A6}$$

A similar result holds for multicomponent fields, with summation over the discrete index a in the second term.

Appendix B: Hamilton-Jacobi field theory

The salient aspects of the Hamilton-Jacobi formulation of classical field theory [7] are collected here, with particular attention to the origin of the associated continuity equation for *ensembles* of classical fields, required in Sec. III.

Two classical fields f, g are canonically conjugate if there is a Hamiltonian functional $H[f, g, t]$ such that

$$\partial f/\partial t = \delta H/\delta g, \qquad \partial g/\partial t = -\delta H/\delta f. \tag{B1}$$

These equations follow from the action principle $\delta A = 0$, with action functional $A = \int dt\, [-H + \int dx\, g_x(\partial f_x/\partial t)]$. The rate of change of an arbitrary functional $G[f, g, t]$ follows from Eqs. (A2) and (B1) as

$$\frac{dG}{dt} = \frac{\partial G}{\partial t} + \int dx\, \left(\frac{\delta G}{\delta f_x}\frac{\delta H}{\delta g_x} - \frac{\delta G}{\delta g_x}\frac{\delta H}{\delta f_x} \right) =: \frac{\partial G}{\partial t} + \{G, H\},$$

where $\{\ ,\ \}$ is a generalised Poisson bracket.

A canonical transformation maps f, g and H to f', g' and H', such that the equations of motion for the latter retain the canonical form of Eq. (B1). Equating the variations of the corresponding actions A and A' to zero, it follows that all physical trajectories must satisfy

$$-H + \int dx\, g_x(\partial f_x/\partial t) = -H' + \int dx\, g'_x(\partial f'_x/\partial t) + dF/dt$$

for some "generating functional" F. Now, any two of the fields f, g, f', g' determine the remaining two fields for a given canonical transformation. Choosing f and g' as the two independent fields, defining the new generating functional $G[f, g', t] = F + \int dx\, f'_x g'_x$, and using Eq. (A2), then yields

$$H' = H + \frac{\partial G}{\partial t} + \int dx\, \left[\frac{\partial f_x}{\partial t}\left(\frac{\delta G}{\delta f_x} - g_x\right) + \frac{\partial g'_x}{\partial t}\left(\frac{\delta G}{\delta g'_x} - f'_x\right)\right]$$

for all physical trajectories. The terms in round brackets therefore vanish identically, yielding the generating relations

$$H' = H + \partial G/\partial t, \qquad g = \delta G/\delta f, \qquad f' = \delta G/\delta g'. \tag{B2}$$

A canonical transformation is thus completely specified by the associated generating functional G.

To obtain the *Hamilton-Jacobi* formulation of the equations of motion, consider a canonical transformation to fields f', g' which are time-independent (eg, to the fields f and g at some fixed time t_0). From Eq. (B1) one may choose the corresponding Hamiltonian $H' \equiv 0$ without loss of generality, and hence from Eq. (B2) the momentum density and the associated generating functional S are specified by the functional equations

$$g = \frac{\delta S}{\delta f}, \qquad \frac{\partial S}{\partial t} + H[f, \delta S/\delta f, t] = 0. \tag{B3}$$

The latter is the desired Hamilton-Jacobi equation. Solving this equation for S is equivalent to solving Eqs. (B1) for f and g.

Note that along a physical trajectory one has $g' \equiv$ constant, and hence from Eqs. (A2) and (B3) that

$$\frac{dS}{dt} = \frac{\partial S}{\partial t} + \int dx\, \frac{\delta S}{\delta f_x}\frac{\partial f_x}{\partial t} = -H + \int dx\, g_x \frac{\partial f_x}{\partial t} = \frac{dA}{dt}.$$

Thus the Hamilton-Jacobi functional S is equal to the action functional A, up to an additive constant. This relation underlies the connection between the derivation of the Hamilton-Jacobi equation from a particular type of canonical transformation, as above, and the derivation from a particular type of variation of the action, as per the Schwinger-Tomonaga formalism [15, 23]. In the latter case the time parameter t is replaced by the multi-time parameter σ.

The Hamilton-Jacobi formulation has the interesting feature that once S is specified, the momentum density is determined by the relation $g = \delta S/\delta f$, i.e., it is a functional of f. Thus, unlike the Hamiltonian formulation of Eqs. (B1), an *ensemble* of fields is specified by a probability density functional $P[f]$, not by a phase space density functional $P[f, g]$. In both cases, the equation of motion for P corresponds to the conservation of probability, i.e., to a continuity equation as per Eq. (A4). In particular, since in the Hamilton-Jacobi formulation the rate of change of the field f follows from Eqs. (B1) and (B3) as the functional

$$V_x[f] = \partial f_x/\partial t = (\delta H/\delta g_x)\,\Big|_{g=\delta S/\delta f}\ ,$$

the associated continuity equation for an ensemble of fields follows from Eq. (A4) as [24]

$$\frac{\partial P}{\partial t} + \int dx\, \frac{\delta}{\delta f_x}\left[P\, \frac{\delta H}{\delta g_x}\bigg|_{g=\delta S/\delta f} \right]. \qquad \text{(B4)}$$

Eqs. (B3) and (B4) generalise immediately to multicomponent fields, and form the basis of the classical starting point in the derivation of the quantum equations of motion for bosonic fields in Sec. III.

---

[1] M.J.W. Hall, Phys. Rev. A **64**, 052103 (2001).

[2] M.J.W. Hall, Phys. Rev. A **62**, 012107 (2000).

[3] M.J.W. Hall and M. Reginatto, J. Phys. A **35**, 3289 (2002).

[4] M.J.W. Hall and M. Reginatto, Fortschr. Phys. **50**, 646 (2002).

[5] A. Vilenkin, Phys. Rev. D **33**, 3560 (1986).

[6] L.S. Brown, *Quantum Field Theory*, (Cambridge, UK, 1992), Chapters 1, 3.

[7] H. Goldstein, *Classical Mechanics*, (Addison-Wesley, USA, 1950), Chapters 8, 9, 11.

[8] S.S. Schweber, *An Introduction to Relativistic Quantum Field Theory*, (Row, Peterson and Co., USA, 1961), Chapter 9.

[9] A. Dembo, T.M. Cover and J.A. Thomas, IEEE Trans. Inf. Theory **37**, 1501 (1991).

[10] J.B.M. Uffink, PhD thesis, University of Utrecht (1990).

[11] D. Dacunha-Castelle and M. Duflo, *Probability and Statistics*, vol. I, (Springer, New York, 1986), Chapter 7.

[12] R.A. Fisher, Proc. Cambridge Philo. Soc. **22**, 700 (1925).

[13] Note that Eqs. (31) follow from the action principle $\delta\tilde{A} = 0$, where the action $\tilde{A}$ is given by $\int dt[-\tilde{H} + \int Df\, S(\partial P/\partial t)]$ (i.e., by the time integal of an ensemble Lagrangian).

[14] P.A.M. Dirac, *Lectures on Quantum Field Theory*, (Academic, New York, 1966), Chapters 14, 15.

[15] J.A. Wheeler, in *Analytical Methods in Mathematical Physics*, edited by R.P. Gilbert and R.G. Newton, (Gordon and Breach, New York, 1970), p. 335.

[16] B.S. de Witt, Phys. Rev. **160**, 1113 (1967).

[17] A. Peres, Nuovo Cim. **26**, 53 (1962).

[18] U.H. Gerlach, Phys. Rev. **177**, 1929 (1969).

[19] N. Kontoleon and D.L. Wiltshire, Phys. Rev. D **59**, 063513 (1999).

[20] S.W. Hawking and D.N. Page, Nucl. Phys. **B264**, 185 (1986).

[21] P.R. Holland, *The Quantum Theory of Motion*, (Cambridge, UK, 1993), section 12.4.

[22] The exact uncertainty approach is also applicable to the Pauli equation (unpublished), and to quantum particles with position-dependent mass (unpublished). In the latter case one obtains a unique operator ordering for the quantum Hamiltonian, analogous to the case of the Wheeler-deWitt equation in Sec. III.D, corresponding to the ordering parameter $\alpha = 0$ in A.R. Plastino, M. Casas and A. Plastino, Phys. Lett. A **281**, 297 (2001).

[23] P. Roman, *Introduction to Quantum Field Theory*, (Wiley, New York, 1969), Chapter 2.

[24] In the Hamiltonian formulation the associated continuity equation for $P[f, g]$ is $\partial P/\partial t + \int dx\, \{(\delta/\delta f_x)[P(\partial f_x/\partial t)] + (\delta/\delta g_x[P(\partial g_x/\partial t)]\} = 0$, which reduces to the Liouville equation $\partial P/\partial t = \{H, P\}$ via Eqs. (B1).