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# Bosonic field equations from an exact uncertainty principle

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## Abstract

A Hamiltonian formalism is used to describe ensembles of fields in terms of two canonically conjugate functionals (one being the field probability density). The postulate that a classical ensemble is subject to nonclassical fluctuations of the field momentum density, of a strength determined solely by the field uncertainty, is shown to lead to a unique modification of the ensemble Hamiltonian. The modified equations of motion are equivalent to the quantum equations for a bosonic field, and thus this exact uncertainty principle provides a new approach to deriving and interpreting the properties of quantum ensembles. The examples of electromagnetic and gravitational fields are discussed. In the latter case, the exact uncertainty approach specifies a unique operator ordering for the Wheeler–DeWitt and Ashtekar–Wheeler–DeWitt equations.

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## 1. Introduction

The Heisenberg uncertainty relation

$$\Delta x \Delta p \geq \hbar/2 \quad (1)$$

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

$$\delta x \Delta p^{nc} = \hbar/2 \quad (2)$$

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

The surprising fact that quantum particles 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 [2]. A brief overview of exact uncertainty properties of quantum particles is provided by the conference paper in [3].

The aim of this paper is to show that the exact uncertainty principle may be successfully generalized to derive the equations of motion for bosonic fields with Hamiltonians quadratic in the field momenta (e.g., scalar, electromagnetic and gravitational fields). This ‘exact uncertainty’ approach is extremely minimalist in nature: unlike canonical quantization, it does not use nor make any assumptions about the existence of operators, Hilbert spaces, complex amplitudes, inner products, linearity, superposition, or the like. The sole ‘nonclassical’ element needed is the addition of fluctuations to the momentum density of members of a classical ensemble of fields, with the fluctuation statistics assumed to be determined by the ensemble statistics. The exact uncertainty approach is thus conceptually very simple, being based on the core notion of statistical uncertainty (intrinsic to any interpretation of quantum theory). As a bonus, the exact uncertainty approach further implies a unique operator ordering for the Schrödinger equation associated with the quantum ensemble—something which the canonical quantization procedure is unable to do.

It is remarkable that the basic underlying concept—the addition of ‘nonclassical’ momentum fluctuations to a classical ensemble—carries through from quantum particles to quantum fields, without creating conceptual difficulties (although significant technical generalizations are needed). This logical consistency and range of applicability is a further strength of the exact uncertainty approach.

In the next section the equations of motion for a classical ensemble of fields are expressed in Hamiltonian form, via two canonically conjugate functionals (the probability density and the Hamilton–Jacobi functional). In section 3 it is shown that the classical ensemble Hamiltonian is modified by the addition of nonclassical momentum density fluctuations, in a manner uniquely specified by the exact uncertainty principle, leading to modified equations of motion equivalent to the quantum field equations.

In sections 4 and 5 the examples of the electromagnetic and gravitational fields are discussed. In the former case it is shown that the exact uncertainty approach is equivalent to adding nonclassical fluctuations to the electric field  $\mathbf{E}$ , of a strength determined by the inherent uncertainty of the vector potential  $\mathbf{A}$ . In the latter case it is shown that the exact uncertainty approach leads to a unique operator ordering for the Wheeler–DeWitt and Ashtekar–Wheeler–DeWitt equations. This ordering is, moreover, consistent with Vilenkin’s ‘tunnelling’ boundary condition for inflationary cosmology [4]. Results are discussed in section 6, and necessary

elements from classical field theory and functional analysis, and the proof of the main theorem of section 3, are given in the appendices.

## 2. 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  $H[f, g, t]$ . For example,  $f$  may denote the electromagnetic field  $A \equiv (A^\mu)$ , or some collection of interacting fields labelled by the index  $a$ . Spatial coordinates will be denoted by  $x$  (irrespective of dimension), and the values of field components  $f^a$  and  $g^b$  at position  $x$  will be denoted by  $f_x^a$  and  $g_x^b$  respectively.

There are three canonical approaches to describing the evolution of an *individual* field, based on the (related) Lagrangian, Hamiltonian and Hamilton–Jacobi formalisms respectively. We choose the latter here, as it provides a straightforward mechanism for adding momentum fluctuations to an *ensemble* of fields (equation (8) below). The Hamilton–Jacobi formalism also leads to an elegant ‘ensemble Hamiltonian’ representation for the dynamics of an ensemble of fields, in terms of two canonically conjugate functionals (equation (5) below).

First, the equation of motion for an individual classical field is given by the Hamilton–Jacobi equation

$$\frac{\partial S}{\partial t} + H[f, \delta S/\delta f, t] = 0 \tag{3}$$

where  $S[f]$  denotes the Hamilton–Jacobi functional, and  $\delta/\delta f$  denotes the functional derivative with respect to  $f$  (see appendices A and B). The momentum density associated with field  $f$  is given by  $g = \delta S/\delta f$ , and hence  $S$  will also be referred to as the *momentum potential*.

Second, the description of an *ensemble* of such fields further requires a probability density functional,  $P[f]$ . The equation of motion for  $P[f]$  corresponds to the conservation of probability, i.e., to the continuity equation

$$\frac{\partial P}{\partial t} + \sum_a \int dx \frac{\delta}{\delta f_x^a} \left( P \left. \frac{\delta H}{\delta g_x^a} \right|_{g=\delta S/\delta f} \right) = 0 \tag{4}$$

as is reviewed in appendix B.

Equations (3) and (4) describe the motion of the ensemble completely, in terms of the two functionals  $P$  and  $S$ . These equations of motion may be written in the ‘Hamiltonian’ form

$$\frac{\partial P}{\partial t} = \frac{\Delta \tilde{H}}{\Delta S} \quad \frac{\partial S}{\partial t} = -\frac{\Delta \tilde{H}}{\Delta P} \tag{5}$$

where  $\tilde{H}$  denotes the functional integral

$$\tilde{H}[P, S, t] := \langle H \rangle = \int Df PH[f, \delta S/\delta f, t] \tag{6}$$

and where variational derivatives such as  $\Delta \tilde{H}/\Delta S$  are discussed in appendix A. The equivalence of equations (3) and (4) to equations (5) follows directly from equation (A6).

The functional integral  $\tilde{H}$  in equation (6) will therefore be referred to as the *ensemble Hamiltonian*, and in analogy to equations (B1) of appendix B,  $P$  and  $S$  may be regarded as *canonically conjugate functionals*. Note from equation (6) that  $\tilde{H}$  typically corresponds to the mean energy of the ensemble. It may be shown that equations (5) follow from the action principle  $\Delta \tilde{A} = 0$ , with action  $\tilde{A} = \int dt [-\tilde{H} + \int Df S(\partial P/\partial t)]$ .

In what follows, we specialize to ensembles for which the associated Hamiltonian functional is *quadratic* in the momentum field density, i.e., of the form

$$H[f, g, t] = \sum_{a,b} \int dx K_x^{ab}[f] g_x^a g_x^b + V[f]. \tag{7}$$

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 equation (6). 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.

### 3. Momentum fluctuations $\Rightarrow$ quantum ensembles

The ensemble Hamiltonian,  $\tilde{H}[P, S, t]$  in equation (6), 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 identified as describing a *quantum* ensemble of fields. Our approach to modifying the ensemble Hamiltonian is based on a single ingredient: the addition of nonclassical fluctuations to the momentum density, with the magnitude of the fluctuations determined by the uncertainty in the field. This ‘exact uncertainty’ approach leads to equations of motion equivalent to those of a bosonic field, with the interpretational advantage of an intuitive statistical picture for quantum field ensembles, and the technical advantage of a unique operator ordering for the associated Schrödinger equation.

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

$$g = \delta S/\delta f + N \quad (8)$$

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 main effect of the fluctuation field 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 quantity  $A[f, N]$  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 equation (7), it follows that when the fluctuations are significant the classical ensemble Hamiltonian  $\tilde{H} = \langle H \rangle$  in equation (6) should be replaced by

$$\begin{aligned} \tilde{H}' &= \langle H[f, \delta S/\delta f + N, t] \rangle \\ &= \sum_{a,b} \int Df \int dx PK_x^{ab} \overline{(\delta S/\delta f_x^a + N_x^a)(\delta S/\delta f_x^b + N_x^b)} + \langle V \rangle \\ &= \tilde{H} + \sum_{a,b} \int Df \int dx PK_x^{ab} \overline{N_x^a N_x^b}. \end{aligned} \quad (9)$$

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

$$[\text{Cov}_x(N)]^{ab} := \overline{N_x^a N_x^b}. \quad (10)$$

The covariance matrix is uniquely determined, 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 in equation (9), implying that

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

for some symmetric matrix function  $\alpha$ . Note that in principle one could also allow the covariance matrix to depend on auxiliary fields and functionals; however, the fourth assumption below immediately removes such a possibility.

(2) Independence. If the ensemble comprises two independent non-interacting subensembles 1 and 2, with a factorizable probability density functional  $P[f^{(1)}, f^{(2)}] = P_1[f^{(1)}]P_2[f^{(2)}]$ , then any dependence of the corresponding subensemble fluctuations  $N^{(1)}$  and  $N^{(2)}$  on  $P$  only enters via the corresponding probability densities  $P_1$  and  $P_2$  respectively. Thus

$$\text{Cov}_x(N^{(1)})|_{P_1 P_2} = \text{Cov}_x(N^{(1)})|_{P_1} \quad \text{Cov}_x(N^{(2)})|_{P_1 P_2} = \text{Cov}_x(N^{(2)})|_{P_2}$$

for such an ensemble. Note that this assumption implies that the ensemble Hamiltonian  $\tilde{H}'$  in equation (9) is *additive* for independent non-interacting ensembles (as is the corresponding action  $\tilde{A}'$ ).

(3) Invariance. The covariance matrix transforms correctly under linear canonical transformations of the field components. Thus, noting that  $f \rightarrow \Lambda^{-1}f, g \rightarrow \Lambda^T g$  is a canonical transformation for any invertible matrix  $\Lambda$  with transpose  $\Lambda^T$ , which preserves the quadratic form of  $H$  in equation (7) and leaves the momentum potential  $S$  invariant (since  $\delta/\delta f \rightarrow \Lambda^T \delta/\delta f$ ), one has from equation (8) that  $N \rightarrow \Lambda^T N$ , and hence that

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

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 density fluctuations at any given position and time, as characterized by the covariance matrix of the fluctuations, 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  $\text{Cov}_x(N)$  cannot depend on  $S$ , nor explicitly on  $t$ .

It is seen that the first three assumptions (causality, independence and invariance) are natural on physical grounds, and hence relatively unconstraining. In contrast, the fourth assumption is ‘special’: 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*

$$\overline{N_x^a N_x^b} = C(\delta P / \delta f_x^a)(\delta P / \delta f_x^b) / P^2 \tag{11}$$

where  $C$  is a positive universal constant.

The theorem thus yields a unique form for the additional term in equation (9), 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  $C \rightarrow 0$ . Note that one cannot make the identification  $N_x^a \sim (\delta P / \delta f_x^a) / P$  from equation (11), as this is inconsistent with the fundamental property  $\overline{N_x^a} = 0$ . The proof of the theorem is given in appendix C, and is substantially different from (and stronger than) proofs of an analogous theorem for quantum particles [2, 3] (the latter proofs rely heavily on a ‘scalar’ assumption that does not carry over in a natural manner to fields).

The main result of this section is the following corollary (proved in appendix C):

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

$$i\hbar \frac{\partial \Psi}{\partial t} = H[f, -i\hbar \delta / \delta f, t] \Psi = -\hbar^2 \left( \sum_{a,b} \int dx \frac{\delta}{\delta f_x^a} K_x^{ab}[f] \frac{\delta}{\delta f_x^b} \right) \Psi + V[f] \Psi \quad (12)$$

where one defines

$$\hbar := 2\sqrt{C} \quad \Psi := \sqrt{P} e^{iS/\hbar}. \quad (13)$$

Equation (12) may be recognized as the Schrödinger equation for a quantum bosonic field [5, 6], 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. Note that the exact uncertainty approach specifies a *unique* operator ordering,  $(\delta / \delta f_x^a) K_x^{ab} (\delta / \delta f_x^b)$ , for the functional derivative operators in equation (12). Thus there is no ambiguity in the ordering for cases where  $K_x^{ab}$  depends on the field  $f$ , in contrast to traditional approaches (e.g., the Wheeler–DeWitt equation, discussed in section 5 below). The above results generalize straightforwardly to complex classical fields.

The ensemble of fields corresponding to ensemble Hamiltonian  $\tilde{H}'$  will be called the *quantum ensemble* corresponding to  $\tilde{H}$ . Note from equations (11) and (13) that the role of Planck's constant is to fix the relative scale of the nonclassical fluctuations. It is remarkable that the four assumptions of causality, independence, invariance and exact uncertainty lead to a *linear operator* equation.

Finally, it may be remarked that the equations of motion of a classical ensemble may be subject to some imposed constraint(s) on  $P$  and  $S$ . For example, each member of an ensemble of electromagnetic fields may have the Lorentz gauge imposed (see section 4 below). As a guiding principle, we will require that the corresponding *quantum* ensemble is subject to the same constraint(s) on  $P$  and  $S$ . 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.

## 4. Example: electromagnetic field

### 4.1. Lorentz gauge

The electromagnetic field is described, up to gauge invariance, by a 4-component field  $A \equiv (A^\mu)$ . 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 [6]

$$H_{GB}[A, \pi] = (1/2) \int dx \eta_{\mu\nu} (\pi^\mu \pi^\nu - \nabla A^\mu \cdot \nabla A^\nu) \quad (14)$$

where  $\eta_{\mu\nu}$  denotes the Minkowski tensor,  $\pi^\mu$  denotes the conjugate momentum density, and  $\nabla$  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 equation (7) (with  $K_x^{\mu\nu} \equiv \eta_{\mu\nu}/2$ ).

The exact uncertainty approach therefore immediately implies, via the corollary of the previous section, that the evolution of a *quantum* ensemble of electromagnetic fields is described by the Schrödinger equation

$$i\hbar(\partial\Psi/\partial t) = H_{GB}[A, -i\hbar(\delta/\delta A)]\Psi \quad (15)$$

in agreement with the Gupta–Bleuler formalism [6].

Further, 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 3 above, one equivalently requires, noting equation (13), that

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

As is well known, this constraint, if initially satisfied, is satisfied for all times [7] (as is the weaker constraint that only the 4-divergence of the positive frequency part of the field vanishes [6]). 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 equations of motion, equations (C1) and (C2) of appendix C, for  $P$  and  $S$ .

#### 4.2. Radiation gauge

It is well known that one can also obtain the classical equations of motion for the electromagnetic field via an alternative Hamiltonian, obtained by exploiting the degree of freedom left by the Lorentz gauge to remove a dynamical coordinate (corresponding to the longitudinal polarization). In particular, since  $\partial_\mu A^\mu$  is invariant under  $A^\mu \rightarrow A^\mu + \partial^\mu \chi$  for any function  $\chi$  satisfying  $\partial^\nu \partial_\nu \chi = 0$ , one may completely fix the gauge in a given Lorentz frame by choosing  $\chi$  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,  $\partial^\nu \partial_\nu \mathbf{A} = 0$ , follow from the Hamiltonian

$$H_R[\mathbf{A}, \boldsymbol{\pi}] = (1/2) \int dx (\boldsymbol{\pi} \cdot \boldsymbol{\pi} / \epsilon_0 + |\nabla \times \mathbf{A}|^2 / \mu_0) \quad (16)$$

where  $\boldsymbol{\pi}$  denotes the conjugate momentum density. Here  $H_R$  corresponds to the standard Lagrangian  $L = -(1/4\mu_0) \int dx F^{\mu\nu} F_{\mu\nu}$ , with  $A^0 \equiv 0$ .

This Hamiltonian has the quadratic form of equation (7), and hence the exact uncertainty approach yields the corresponding Schrödinger equation

$$i\hbar(\partial\Psi/\partial t) = H_R[\mathbf{A}, -i\hbar(\delta/\delta \mathbf{A})]\Psi \quad (17)$$

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 [8]).

Note that the electric field follows via equations (16) and (B1) as

$$\mathbf{E} = -\partial\mathbf{A}/\partial t = -\delta H_R/\delta \boldsymbol{\pi} = -\boldsymbol{\pi}/\epsilon_0$$

and is therefore directly proportional to the classical momentum density  $\boldsymbol{\pi}$ . Fluctuations of the momentum density thus correspond to fluctuations of the electric field  $\mathbf{E}$ . Further, the constraint  $\nabla \cdot \mathbf{A} = 0$  implies that there is a one–one relation between  $\mathbf{A}$  and the magnetic field  $\mathbf{B} = \nabla \times \mathbf{A}$  (up to an additive constant). Uncertainty in the vector potential thus corresponds to uncertainty in the magnetic field  $\mathbf{B}$ . Hence, in the radiation gauge, *the exact uncertainty approach corresponds to adding nonclassical fluctuations to the electric field components of an ensemble of electromagnetic fields, with the fluctuation strength determined by the uncertainty in the magnetic field components.*



## 5. Example: gravitational field

### 5.1. Hamilton–Jacobi constraints

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 [9]

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

in terms of the lapse function  $\alpha$ , the shift function  $\beta$  and the spatial 3-metric  $\gamma \equiv (\gamma_{ij})$ . The equations of motion are the Einstein field equations, which follow from the Hamiltonian functional [9]

$$H[\gamma, \pi, \alpha, \beta] = \int dx \alpha \mathcal{H}_G[\gamma, \pi] - 2 \int dx \beta_i \pi_{|j}^{ij} \quad (18)$$

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

$$\mathcal{H}_G = (1/2)G_{ijkl}[\gamma]\pi^{ij}\pi^{kl} - 2^{(3)}R[\gamma](\det \gamma)^{1/2}. \quad (19)$$

Here  $^{(3)}R$  is the curvature scalar corresponding to  $\gamma_{ij}$ , 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  $L = \int dx (-\det g)^{1/2} R[g]$ , where the momenta  $\pi^0$  and  $\pi^i$  conjugate to  $\alpha$  and  $\beta_i$  respectively vanish identically. However, the lack of dependence of  $H$  on  $\pi^0$  and  $\pi^i$  is consistently maintained only if the rates of change of these momenta also vanish, i.e., noting equation (B1) of appendix B, only if the constraints [9]

$$\delta H / \delta \alpha = \mathcal{H}_G = 0 \quad \delta H / \delta \beta_i = -2\pi_{|j}^{ij} = 0 \quad (20)$$

are satisfied. Thus the dynamics of the field is independent of  $\alpha$  and  $\beta$ , so that these functions may be fixed arbitrarily. Moreover, these constraints immediately yield  $H = 0$  in equation (18), and hence the system is static, with no explicit time dependence.

It follows that, in the *Hamilton–Jacobi* formulation of the equations of motion (see appendix B), the momentum potential  $S$  is independent of  $\alpha$ ,  $\beta$  and  $t$ . Noting that  $\pi \equiv \delta S / \delta \gamma$  in this formulation, equations (20) therefore yield the corresponding constraints

$$\frac{\delta S}{\delta \alpha} = \frac{\delta S}{\delta \beta_i} = \frac{\partial S}{\partial t} = 0 \quad \left( \frac{\delta S}{\delta \gamma_{ij}} \right)_{|j} = 0 \quad (21)$$

for  $S$ . As shown by Peres [10], 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 equation (21) is equivalent to the invariance of  $S$  under such transformations. This fourth constraint moreover implies that the second term in equation (18) may be dropped from the Hamiltonian, yielding the reduced Hamiltonian

$$H_G[\gamma, \pi, \alpha] = \int dx \alpha \mathcal{H}_G[\gamma, \pi] \quad (22)$$

in the Hamiltonian–Jacobi formulation [10, 11].

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

$$\frac{\delta P}{\delta \alpha} = \frac{\delta P}{\delta \beta_i} = \frac{\partial P}{\partial t} = 0 \quad \left( \frac{\delta P}{\delta \gamma_{ij}} \right)_{|j} = 0 \quad (23)$$

for the corresponding probability density functional  $P[\gamma]$ , analogous to equation (21). The first two constraints imply that ensemble averages only involve integration over  $\gamma$ .

5.2. *Quantum ensembles and operator ordering*

Noting equation (19), the Hamiltonian  $H_G$  in equation (22) has the quadratic form of equation (7). Hence the exact uncertainty approach is applicable, and immediately leads to the Schrödinger equation

$$i\hbar \partial \Psi / \partial t = \int dx \alpha \mathcal{H}_G[\gamma, -i\hbar(\delta/\delta\gamma)]\Psi \tag{24}$$

for a *quantum* ensemble of gravitational fields, as per the corollary of section 3.

As discussed at the end of section 3, 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 equations (21) and (23) we require that  $P$  and  $S$ , and hence  $\Psi$  in equation (13), are independent of  $\alpha, \beta$  and  $t$  and invariant under spatial coordinate transformations, i.e.,

$$\frac{\delta \Psi}{\delta \alpha} = \frac{\delta \Psi}{\delta \beta_i} = \frac{\partial \Psi}{\partial t} = 0 \quad \left( \frac{\delta \Psi}{\delta \gamma_{ij}} \right)_{|j} = 0. \tag{25}$$

Applying the first and third of these constraints to equation (24) immediately yields, via equation (19), the reduced Schrödinger equation

$$\mathcal{H}_G[\gamma, -i\hbar(\delta/\delta\gamma)]\Psi = (-\hbar^2/2) \frac{\delta}{\delta \gamma_{ij}} G_{ijkl}[\gamma] \frac{\delta}{\delta \gamma_{kl}} \Psi - 2^{(3)}R[\gamma](\det \gamma)^{1/2} \Psi = 0 \tag{26}$$

which may be recognized as the Wheeler–DeWitt equation in the metric representation [9].

A notable feature of equation (26) is that the Wheeler–DeWitt equation has not only been derived from an exact uncertainty principle: it has, as a consequence of equation (12), 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 ambiguity in this respect, unlike the standard approach [9]. 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 [12] have pointed out that Vilenkin’s prediction of inflation in minisuperspace, from a corresponding Wheeler–DeWitt equation with ‘tunnelling’ boundary conditions [4], 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 [4]

$$\left[ \frac{\partial^2}{\partial a^2} + \frac{p}{a} \frac{\partial}{\partial a} - \frac{1}{a^2} \frac{\partial^2}{\partial \phi^2} - U(a, \phi) \right] \Psi = 0 \tag{27}$$

(for a Friedmann–Robertson–Walker metric coupled to a scalar field  $\phi$ ), Kontoleon and Wiltshire show that Vilenkin’s approach fails for orderings with  $p \geq 1$  [12]. 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 [13].

However, noting that the relevant Hamiltonian functional in equation (2.7) of [4] 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 equation (27). Hence the criticism in [12] is avoided. One also has the nice feature that the associated Wheeler–DeWitt equation can be exactly solved for this ‘exact uncertainty’ ordering [4].

A certain degree of ambiguity remains, which derives from the need to introduce some sort of regularization scheme to remove divergences arising from the product of two functional derivatives acting at the same point in the Wheeler–DeWitt equation. Such considerations, however, do not play a role in the example that we have just discussed, which concerns minisuperspace quantization involving a finite number of degrees of freedom. It is important to distinguish this regularization problem from the far more difficult one associated with the requirement of ‘Dirac consistency’, i.e., the need to find a choice of operator ordering *and* regularization scheme that will permit mapping the classical Poisson bracket algebra of constraints to an algebra of operators within the context of the Dirac quantization of canonical gravity [14]. Our approach is based on the Hamilton–Jacobi formulation of classical gravity and, as shown by Bergmann [15], the functional form of the Hamilton–Jacobi functional  $S$  is already invariant under the action of the group generated by the constraints.

Finally, note that a similar approach may be applied to the Ashtekar formalism for gravitational fields [16], where again the Hamiltonian is quadratic in the field momentum density (in particular, the two constraints linear in the momentum density  $\tilde{\sigma}$  become constraints on the Hamilton–Jacobi functional  $S$ , corresponding to the invariance of  $S$  under spatial coordinate and internal gauge transformations [17], while the constraint quadratic in  $\tilde{\sigma}$  generates the Ashtekar–Wheeler–DeWitt equation with a unique operator ordering).

## 6. Discussion

The main result of this paper is the derivation of the quantum equation of motion, equation (12), from an exact uncertainty principle, for fields with Hamiltonian functionals quadratic in the momentum density.

It is important to emphasize that the exact uncertainty approach 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 in some Hilbert space. Only the assumptions of causality, independence, invariance and exact uncertainty are required, all formulated in terms of a *single* nonclassical element (the uncertainty introduced by the momentum fluctuation  $N$ ). Since uncertainty is at the conceptual core of quantum mechanics, this is an elegant and pleasing result.

The assumptions used 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 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 equations (8) and (11), is as follows. Every *physical* field has an intrinsic uncertainty, which is modelled by a corresponding statistical ensemble. Further, the nature of this inherent uncertainty is such as to preclude a deterministic relationship between the field and its conjugate momentum density—one must introduce fluctuations into the classical relationship, as per equation (8). However, the *degree* of indeterminism in this relationship is precisely quantifiable, in a statistical sense, being directly specified by the inherent field uncertainty as per equation (11).

The above interpretation may be regarded as a significant sharpening of the so-called ‘statistical interpretation’ of quantum mechanics [18], and is notably very different to the ‘causal interpretation’ of Bohm and co-workers [19]. 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 equation (8) is that  $g \neq \delta S/\delta f$ .

A further strength of the exact uncertainty approach is that the basic underlying concept—the addition of ‘nonclassical’ momentum fluctuations to a classical ensemble—carries through from quantum particles to quantum fields without creating conceptual difficulties. This adds an interpretational strength to the exact uncertainty approach not mirrored in other approaches that rely on connecting the equations of motion of classical and quantum ensembles. For example, the above-mentioned ‘causal interpretation’ of Bohm and co-workers is explicitly non-local, and hence *non-causal*, for relativistic fields [19]. As another example, one cannot simultaneously describe both the electric and the magnetic fields in generalizations of Nelson’s stochastic approach to electromagnetic fields [20].

It is of interest to consider the scope and limitations of the exact uncertainty approach to physical systems. This approach has previously been applied to quantum particles [2, 3], and may be generalized to obtain the Pauli equation for a non-relativistic spin-1/2 particle and the Schrödinger equation for particles with position-dependent mass (where in the latter case one obtains the unique ordering  $\hat{p}[2m(\hat{x})]^{-1}\hat{p} + V(\hat{x})$  for the Hamiltonian operator, corresponding to the ordering parameter  $\alpha = 0$  in [21]). In this paper the approach has been further generalized to bosonic quantum fields with Hamiltonians quadratic in the momentum density (including all relativistic integer-spin fields). It is also, indirectly, applicable to the *non*-quadratic Hamiltonian functional of a non-relativistic Schrödinger field (corresponding to second quantization of the particle Schrödinger equation), in the sense that this field may be obtained as a low-energy limit of the complex Klein–Gordon field [5] (to which the exact uncertainty approach directly applies).

However, a major question to be addressed in the future is whether the exact uncertainty approach is applicable to the derivation of fermionic field equations. 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  $\hbar \rightarrow 0$ . One possible approach is to determine whether exact uncertainty relations exist for such fields, analogous to equation (2), as these might suggest the statistical properties required by suitable ‘nonclassical’ fluctuations (note that the exact uncertainty relations satisfied by bosonic fields are derived in [22]).

Finally, in this paper the basic Schrödinger equation for bosonic fields has been obtained, with the advantageous features of an intuitive picture for the origin of the ‘quantum’ nature of such fields, and 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 [2]), boundary conditions, infinities, etc, from the new perspective on the conceptual and technical basis of quantization offered by the exact uncertainty approach.

## Appendix A. Functional derivatives and integrals

The necessary definitions and properties of functionals are noted here, including variational properties of functional integrals.

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.,

$$\delta F = F[f + \delta f] - F[f] = \int dx \frac{\delta F}{\delta f_x} \delta f_x \quad (\text{A1})$$

for arbitrary infinitesimal variations  $\delta f$ . 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 equation (A1) that the functional derivative satisfies product and chain rules analogous to ordinary differentiation. The choice  $F[f] = f_{x'}$  in equation (A1) yields  $\delta f_{x'}/\delta f_x = \delta(x - x')$ . Moreover, if the field depends on some parameter,  $t$  say, then choosing  $\delta f_x = f_x(t + \delta t) - f_x(t)$  in equation (A1) yields

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \int dx \frac{\delta F}{\delta f_x} \frac{\partial f_x}{\partial t} \quad (\text{A2})$$

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 discretization approach to functional integration [5]). In particular, this property implies the useful result

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

which is used repeatedly below and in the text. Equation (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 equation (A3) yields the ‘integration by parts’ formula

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

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

$$\frac{\partial P}{\partial t} + \int dx \frac{\delta}{\delta f_x} [P V_x] = 0 \quad (\text{A4})$$

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

Finally, consider a functional integral of the form

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

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

$$\begin{aligned}\Delta I &= I[F + \Delta F] - I[F] = \int \text{D}f \left\{ (\partial\xi/\partial F)\Delta F + \int \text{d}x [\partial\xi/\partial(\delta F/\delta f_x)] [\delta(\Delta F)/\delta f_x] \right\} \\ &= \int \text{D}f \left\{ (\partial\xi/\partial F) - \int \text{d}x \frac{\delta}{\delta f_x} [\partial\xi/\partial(\delta F/\delta f_x)] \right\} \Delta F \\ &\quad + \int \text{d}x \int \text{D}f \frac{\delta}{\delta f_x} \{ [\partial\xi/\partial(\delta F/\delta f_x)] \Delta F \}.\end{aligned}$$

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

$$\Delta I = \int \text{D}f \frac{\Delta I}{\Delta F} \Delta F$$

analogous to equation (A1), where the variational derivative  $\Delta I/\Delta F$  is defined by

$$\frac{\Delta I}{\Delta F} := \frac{\partial\xi}{\partial F} - \int \text{d}x \frac{\delta}{\delta f_x} \left[ \frac{\partial\xi}{\partial(\delta F/\delta f_x)} \right]. \quad (\text{A6})$$

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

## Appendix B. Hamilton–Jacobi ensembles

The salient aspects of the Hamilton–Jacobi formulation of classical field theory [23] are collected here, with particular attention to the origin of the associated continuity equation for *ensembles* of classical fields, required in sections 2 and 3.

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

$$\partial f/\partial t = \delta H/\delta g \quad \partial g/\partial t = -\delta H/\delta f. \quad (\text{B1})$$

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

$$\frac{\text{d}G}{\text{d}t} = \frac{\partial G}{\partial t} + \int \text{d}x \left( \frac{\delta G}{\delta f_x} \frac{\delta H}{\delta g_x} - \frac{\delta G}{\delta g_x} \frac{\delta H}{\delta f_x} \right) =: \frac{\partial G}{\partial t} + \{G, H\}$$

where  $\{, \}$  is a generalized 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 equation (B1). Equating the variations of the corresponding actions  $A$  and  $A'$  to zero, it follows that all physical trajectories must satisfy

$$-H + \int \text{d}x g_x (\partial f_x/\partial t) = -H' + \int \text{d}x g'_x (\partial f'_x/\partial t) + \text{d}F/\text{d}t$$

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  $G[f, g', t] = F + \int \text{d}x f'_x g'_x$ , and using equation (A2), then yields

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

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

$$H' = H + \partial G/\partial t \quad g = \delta G/\delta f \quad f' = \delta G/\delta g'. \quad (\text{B2})$$

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 (e.g., to the fields  $f$  and  $g$  at some fixed time  $t_0$ ). From equation (B1) one may choose the corresponding Hamiltonian  $H' \equiv 0$  without loss of generality, and hence from equation (B2) the momentum density and the associated generating functional  $S$  are specified by the functional equations

$$g = \frac{\delta S}{\delta f} \quad \frac{\partial S}{\partial t} + H[f, \delta S/\delta f, t] = 0. \quad (\text{B3})$$

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

Note that along a physical trajectory one has  $g' \equiv \text{constant}$ , and hence from equations (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 [8, 24].

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 equations (B1), an *ensemble* of fields is specified by a probability density functional  $P[f]$ , not by a phase space density functional  $\rho[f, g]$ .

In either case, the equation of motion for the probability density corresponds to the conservation of probability, i.e., to a continuity equation as per equation (A4). For example, in the Hamiltonian formulation the associated continuity equation for  $\rho[f, g]$  is

$$\partial\rho/\partial t + \int dx \{(\delta/\delta f_x)[\rho(\partial f_x/\partial t)] + (\delta/\delta g_x[\rho(\partial g_x/\partial t)])\} = 0$$

which reduces to the Liouville equation  $\partial\rho/\partial t = \{H, \rho\}$  via equations (B1).

Similarly, in the Hamilton–Jacobi formulation, the rate of change of the field  $f$  follows from equations (B1) and (B3) as the functional

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

and hence the associated continuity equation for an ensemble of fields described by  $P[f]$  follows via equation (A4) as

$$\frac{\partial P}{\partial t} + \int dx \frac{\delta}{\delta f_x} \left[ P \frac{\delta H}{\delta g_x} \Big|_{g=\delta S/\delta f} \right] = 0. \quad (\text{B4})$$

Equations (B3) and (B4) generalize 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 sections 2 and 3.

**Appendix C. Proofs of the theorem and corollary**

**Proof of theorem** (equation (11)). From the causality and exact uncertainty assumptions in section 3, one has  $\text{Cov}_x(N) = \alpha(P, \delta P / \delta f_x, f_x)$ . To avoid issues of regularization, it is convenient to consider a position-dependent canonical transformation,  $f_x \rightarrow \Lambda_x^{-1} f_x$ , 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  $P \rightarrow AP$  and  $Df \rightarrow A^{-1} Df$  respectively, and so the invariance assumption in section 3 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  $\Lambda_x$  can remain the same at a given point  $x$  while varying elsewhere, this homogeneity condition must hold for  $A$  and  $\Lambda_x$  independently. Thus, choosing  $\Lambda_x$  to be the identity matrix at some point  $x$ , one has  $\alpha(AP, Au, w) = \alpha(P, u, w)$  for all  $A$ , implying that  $\alpha$  can involve  $P$  only via the combination  $v := u/P$ .

The above homogeneity condition for  $\alpha$  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  $\alpha$  by any function of the scalar  $J := v^T w$ . Moreover, it may easily be checked that if  $\sigma$  and  $\tau$  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  $\beta$  and  $\gamma$ .

For  $P = P_1 P_2$  one finds  $v = (v_1, v_2), w = (w_1, w_2)$ , where the subscripts label corresponding subensemble quantities, and hence the independence assumption in section 3 reduces to the requirements

$$\begin{aligned} \beta(J_1 + J_2)v_1v_1^T + \gamma(J_1 + J_2)(w_1w_1^T)^{-1} &= \beta_1(J_1)v_1v_1^T + \gamma_1(J_1)(w_1w_1^T)^{-1} \\ \beta(J_1 + J_2)v_2v_2^T + \gamma(J_1 + J_2)(w_2w_2^T)^{-1} &= \beta_2(J_2)v_2v_2^T + \gamma_2(J_2)(w_2w_2^T)^{-1} \end{aligned}$$

for the respective subensemble 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

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

for the fluctuation covariance matrix, where  $W_x[f]$  denotes the inverse of the matrix with  $ab$ -coefficient  $f_x^a f_x^b$ .

Since  $W_x[f]$  is purely a functional of  $f$ , it merely contributes a classical additive potential term to the ensemble Hamiltonian of equation (9). 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  $\text{Cov}_x(N)$ , and the theorem is proved.  $\square$

**Proof of corollary** (equation (12)). First, the equations of motion corresponding to the ensemble Hamiltonian  $\hat{H}'$  follow via the theorem and equations (5) as (a) the continuity equation (4) as before (since the additional term does not depend on  $S$ ), which from equation (7) has the explicit form

$$\frac{\partial P}{\partial t} + 2 \sum_{a,b} \int dx \frac{\delta}{\delta f_x^a} \left( P K_x^{ab} \frac{\delta S}{\delta f_x^b} \right) = 0 \tag{C1}$$



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 equation (11) and equation (A6) of appendix A, this simplifies to

$$\frac{\partial S}{\partial t} + H[f, \delta S/\delta f, t] - 4CP^{-1/2} \sum_{a,b} \int dx \left( K_x^{ab} \frac{\delta^2 P^{1/2}}{\delta f_x^a \delta f_x^b} + \frac{\delta K_x^{ab}}{\delta f_x^a} \frac{\delta P^{1/2}}{\delta f_x^b} \right) = 0. \quad (\text{C2})$$

Second, writing  $\Psi = P^{1/2} \exp(iS/\hbar)$ , multiplying each side of equation (12) on the left by  $\Psi^{-1}$ , and expanding, gives a complex equation for  $P$  and  $S$ . The imaginary part is just the continuity equation of (C1), and the real part is the modified Hamilton–Jacobi equation of (C2) above, providing that one identifies  $C$  with  $\hbar^2/4$ .  $\square$

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