Semiclassical physics and quantum fluctuations

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We investigate theories in which classical and quantum-mechanical degrees of freedom interact dynamically. In commonly used semiclassical theories, such as those used to study inflationary-universe models, quantum fluctuations do not affect the dynamics of the classical variables. We construct a new semiclassical theory in which the quantum and classical fluctuations do affect each other; the Wigner probability function turns out to be a special case. Relevance to calculations of perturbations from inflation are discussed.

I. INTRODUCTION

Quantum mechanics is currently the language used to describe the physical world. Yet, there are many phenomena for which classical physics provides a more convenient description. In this paper we will study the physics of systems which display both quantum-mechanical and classical aspects, and so it is necessary to consider the interaction of quantum-mechanical and classical degrees of freedom. We will call this semiclassical physics. In principle what should be done is to take two interacting quantum-mechanical systems and let one of them become classical. Unfortunately, even the classical limit of a single quantum-mechanical system is not well understood. There are physical theories, for example, general relativity, which do not have a quantum-mechanical formulation. Therefore, we will take the point of view that semiclassical theories should satisfy certain physical and philosophical requirements, which we discuss below and which will lead us to a unique formulation of the structure of such theories.

There are several levels at which one might study semiclassical physics. At the simplest level, one might ignore the dynamics of the classical degrees of freedom and study the physics of Schrödinger's equation with an external source. For example, it is often convenient to treat an electron as a quantum particle in a classical electromagnetic field, rather than solve the full QED problem. (This is what one does when discussing Stern-Gerlach experiments.) The gravitational analogue is to study, say, a scalar field propagating in a fixed curved spacetime. In both cases the back reaction of the quantum field on the classical field is ignored.

In this paper we will consider the dynamics of both the classical and quantum degrees of freedom, since there are many phenomena for which one expects that a semiclassical treatment is useful only if the dynamics of both are considered. For example, the human retina contains approximately 10^8 rod cells, each containing about 4×10^7 photosensitive rhodopsin molecules. A rod cell can be excited by a single photon of green light (500-nm wavelength), which is absorbed by a single rhodopsin molecule (approximately 2 nm in diameter). After a photon is absorbed, retinal, a prosthetic group in the rhodopsin molecule, changes conformation and initiates a well-defined sequence of events. In attempting to describe this system it seems reasonable to treat the photon quantum mechanically, and the rest classically. In this case, a semiclassical theory should predict the probability that a particular rhodopsin molecule in a particular rod cell is excited, given the initial wave function of the photon. Here we must clearly treat the dynamics of the coupled classical and quantum degrees of freedom.

A system which has some similar features is a bubble chamber. In a bubble chamber, an energetic charged particle is incident on a superheated liquid. One observes bubbles forming in the liquid and outlining a trajectory which is described by classical mechanics. The incident ion is described by some wave function (which in general will not look "classical"). Given the (quantum-mechanical) interaction with the liquid, this can be used to calculate the probability that the ion will "follow" one or another classical path, distinguished by, say, the initial position and velocity of the trajectory. The liquid is in a metastable state and macroscopic-sized bubbles of the liquid change into the more stable gaseous state by gaining energy from the ion, and passing the energy barrier. The entire calculation could, in principle, be treated quantum mechanically, but it is more convenient to think of the liquid as being described by thermodynamics in order to understand the phase transition (note that no one has even proved that liquids exist using *ab initio* quantum-mechanical calculations). Here, a semiclassical theory would treat the ion quantum mechanically, and the rest of the system classically, and would certainly need to deal with the dynamics of the coupled degrees of freedom. Such a semiclassical theory should, for example, predict probabilities for different classical trajectories to occur. One would not expect a semiclassical theory to predict a nonzero probability for the event where the ion leaves a nonclassical trajectory, though in the full quantum treatment there would be a small amplitude for such an event.

In the case of interacting gravitational and matter fields, we do not have a quantum theory. Therefore, in situations where the quantum mechanics of the matter fields are important, a semiclassical theory is the best we can do. A thought experiment which is a gravitational analog of Schrödinger's cat is to suppose that the radioactive decay of an atom somewhere on Earth triggers the detonation of a bomb. If the bomb explodes, the Earth shatters and the trajectory of the Moon is changed. Since the moment of decay of the atom is not certain, one would expect a semiclassical theory of gravity to predict the probability that at time t (i) the atom has not decayed and the Moon is on its usual approximately circular trajectory, (ii) the atom has decayed at time t_A and (hence) the Moon is moving on a straight line in direction A, (iii) the atom has decayed at time t_B and the Moon is moving on a straight line in direction B, and so on. One would not expect a semiclassical theory of gravity to predict a nonzero probability for the Moon to be on a circular trajectory at twice the normal radius, corresponding to the gravitational field of the superposition $(1/\sqrt{2})$ (whole Earth + exploded Earth).

Semiclassical gravity may be particularly relevant in cosmology. It may be important to treat the matter as quantum fields in the early Universe, and to include the back reaction of the quantum stress energy on the gravitational field. For example, in inflationary-universe models, the stress energy of a quantum scalar field is thought to dominate other contributions to the stress energy and derive an exponential expansion of the Universe. In the way that these models have previously been studied, the (classical) gravitational field couples to the quantum field only via the expectation value of the stress-energy tensor in some quantum state. The state evolves according to the Schrödinger equation, in which the gravitational field appears as an external source:

$$G_{ab}[g_{cd}]=\langle\psi\,|\,T_{ab}\,|\,\psi\rangle\ , \tag{1.1}$$

$$H[\phi,\pi,g_{cd}]\psi=-\frac{\hbar}{i}\dot{\psi}\ . \tag{1.2}$$

Equations (1.1) and (1.2) are consistent as a system, and thus are one example of what one might mean by a semiclassical theory of gravity. We will see that the analogous semiclassical approximation for systems of harmonic oscillators, which we can solve exactly, gives reliable answers to certain questions for some time periods. However, by coupling the classical and quantum degrees of freedom only via an expectation value, one will never see any effect of quantum fluctuations on the classical system. Consider a purely quantum-mechanical system with $2N$ degrees of freedom x_i, x_I, $i=1,\ldots,N$, $I=N+1,\ldots,2N$, described by a wave function $\Psi(x_i,x_I)$. By "quantum fluctuations" we mean that generally quantum mechanics predicts amplitudes for many different states of the system at a given time t. Suppose, for example, that the x_i's interact arbitrarily among themselves and likewise for the x_I's, but that x_i is coupled to x_I only for $I=N+i$, and that the coupling is independent of i. Let the x_I all start in their ground state (defined with respect to the noninteraction part of the Hamiltonian). As the system evolves, there are (in general) nonzero amplitudes for many different excited states of the x_I. Consider a limit[1] in which the x_I's "become classical" and in which x_I can be thought of as a measuring device which measures some observable O for x_i. Let the eigenvalues of O be λ_n. Then in a measurement of the x_i system by the x_I system the x_I's will "indicate" one of the possible sets of values $\{\lambda_{n_i}\}$, with probability given in the usual way. By "quantum fluctuations" we mean that (for example) even if initially the x_I's indicate a unique set of values $\{\lambda^0_{n_i}\}$, in general, because of interactions at later times there will be no unique set but only a probability distribution for the various sets to occur.

Return to the semiclassical system (1.1) and (1.2). Given initial data for the wave function and metric, there is a unique evolution for the metric. In this sense, quantum fluctuations do not feed back into the metric. In particular, if the metric and state are initially homogeneous and isotropic, then these symmetries are maintained by the evolution—and so there is no generation of spatial variations in the stress energy or gravitational field by quantum fluctuations. We would like a formulation of semiclassical gravity where even if the metric is determined initially, it generally can only be described by a probability distribution at later times. Going back to the exploding-Earth example, when the experiment is initially set up the gravitational field of Earth is definite, but at later times it is only given by a probability distribution because the atom may or may not have decayed.

In inflationary cosmological models there has been much work done on the generation of perturbations in the classical mass density by quantum fluctuations during the inflationary period (see, e.g., Ref. 2). Density perturbations are a source for perturbations in the gravitational field, which one hopes will lead to the formation of galaxies by gravitational instabilities. However, there are some problems with this program within the framework of Eqs. (1.1) and (1.2). As just mentioned, in the semiclassical theory of type given by such equations, the classical field does not couple to quantum fluctuations. Therefore, in models where quantum fluctuations are supposed to become classical density perturbations after inflation, the dynamical effect of the quantum fluctuations is put in by hand, in the matching conditions between evolution governed by (1.1) and the evolution according to the fully classical Einstein-scalar field equations. There are problems in justifying this *ad hoc* procedure, as we shall discuss. If instead one was evolving a pure quantum system, or another type of semiclassical theory which shall be presented, there is some justification for this matching. In these cases, essentially the problem is to pick "typical" initial data out of an ensemble and evolve it such that its "statistical meaning" is unchanged.

In the next section we will demonstrate more precisely some problems with the usual semiclassical theories. Then we will look for a semiclassical theory which couples quantum and classical degrees of freedom on a more equal footing, so that quantum fluctuations do act as a source for the classical variables. One possible approach is to consider theories in which the observables are (Hermitian) operator-valued functions on the phase space of the classical variables. The fundamental object is the density matrix ρ, a Hermitian positive-semidefinite operator-valued function with finite integrated trace. It is desired to find a theory such that ρ is (i) Hermitian and satisfies $\int_\Gamma \mathrm{Tr}\rho=1$ at $t=0$ (where Γ is the classical phase space and Tr is the trace over the quantum Hilbert space), (ii) positive (semidefinite) at $t=0$. Furthermore, we require that the evolution of ρ is determined by the Hamiltonian observable in such a way that the resulting equation of motion (iii) is of the form $\dot\rho=[H,\rho]_{\mathrm{SC}}$, where the brackets operation is to be linear in H and ρ, (iv) is invariant under canonical transformations on Γ, (v) is invariant under (constant) unitary transformations on Hilbert space, (vi) reduces to the usual quantum-mechanical and classical equations if there is no interaction between the quantum and classical systems, (vii) preserves Hermiticity of ρ and $\int_\Gamma \mathrm{Tr}\rho=1$, and (viii) preserves positivity of ρ. A theory which satisfies (i)–(viii) would be able to be given a consistent interpretation, as we shall discuss. We will show that conditions (i)–(vii) determine a unique equation of motion for ρ, but in general condition (viii), positivity, is not also satisfied (for reasons similar to the reasons why Wigner's function[3] is not positive).

Another approach to a semiclassical theory is to consider the Hilbert space of states $\mathcal{H}$ defined to be the tensor product of the Hilbert space of square-integrable functions on the classical phase space and the usual quantum Hilbert space of states. Observables are (Hermitian) operators on $\mathcal{H}$. There is a well-defined prescription (used by people who study geometric quantization[4]) for replacing functions on phase space with operators on $\mathcal{H}$ such that the usual Poisson-brackets relations becomes the corresponding commutator relations. In this theory, the fundamental object is the density matrix ρ (a Hermitian finite-trace positive-semidefinite operator on $\mathcal{H}$) whose evolution is taken to be given by Schrödinger's equation. This equation preserves the Hermiticity, finite trace, and positivity conditions. However, there are severe problems with the interpretation, and there does not appear to be a conserved positive energy, in general. In short, in this paper we examine some possibilities for treating semiclassical systems that up to now have not been adequately described physically and we point out the problems associated with each possibility.

II. STANDARD SEMICLASSICAL THEORIES

In this section we will recall a type of semiclassical theory often used, in which the classical degrees of freedom are coupled to certain expectation values of the quantum variables. We will see explicitly that quantum fluctuations do not affect the dynamics of the classical variables, which will be contrasted with two new types of semiclassical theories which we will discuss in the next two sections.

First, consider a purely quantum-mechanical system with dynamical variables x_i, x_I, and conjugate momenta p_i, p_I, where $i=1,\dots,N$ and $I=N+1,\dots,N+N'$. We will study the limit in which the x_I behave "classically" and make a comparison with semiclassical theories. Let the Hamiltonian be $H(x_i,p_i,x_I,p_I)$. Then, the wave function describing the state of the system evolves according to Schrödinger's equation, $H\Psi=-(\hbar/i)\dot\Psi$. The expectation value of an observable O, or Hermitian operator on the Hilbert space of states, evolves according to

$$\frac{d}{dt}\langle O\rangle_{\mathrm{QM}}=\frac{i}{\hbar}\langle [H,O]\rangle_{\mathrm{QM}}+\left\langle\frac{\partial O}{\partial t}\right\rangle_{\mathrm{QM}}$$

where $\langle O\rangle_{\mathrm{QM}}\equiv\langle\Psi\mid O\mid\Psi\rangle_{\mathrm{QM}}$.

Now suppose we want to consider theories (which we shall call semiclassical) with N quantum-mechanical degrees of freedom x_i, and N' classical ones, x_I. In traditional semiclassical theories, the state of the system is described by a point in phase space (x_I,p_I) and by a wave function $\psi(x_i,x_I,p_I)$, which is a Hilbert-space-valued function on phase space. ψ evolves according to a Scrhödinger-type equation:

$$\hat H\psi=-\frac{\hbar}{i}\dot\psi\ , \tag{2.1}$$

where $\hat H=H(x_i,p_i;x_I,p_I)$, and the classical variables evolve according to Hamilton-type equations

$$\frac{d}{dt}x_I=\frac{\partial\tilde H}{\partial p_I}\quad\text{and}\quad\frac{d}{dt}p_I=-\frac{\partial\tilde H}{\partial x_I}\ , \tag{2.2}$$

where $\tilde H=\langle\psi\mid\hat H\mid\psi\rangle$.

In this case, observables are (Hermitian) operator-valued functions on phase space. The evolution of the expectation value of an operator O is given by

$$\frac{d}{dt}\langle O\rangle_{\mathrm{SC}}=\frac{i}{\hbar}\langle[\hat H,O]\rangle_{\mathrm{SC}}-\{\tilde H,O\}_{\mathrm{PB}}+\left\langle\frac{\partial O}{\partial t}\right\rangle_{\mathrm{SC}}\ , \tag{2.3}$$

where $\langle O\rangle_{\mathrm{SC}}=\langle\psi\mid O\mid\psi\rangle_{\mathrm{SC}}$ and $\{\ ,\ \}_{\mathrm{PB}}$ is the Poisson brackets. (Note that if $O=f$ is a function on phase space then $\langle f\rangle_{\mathrm{SC}}=f$.)

The semiclassical gravity equations (1.1) and (1.2) are an example of the type of system described by Eqs. (2.1) and (2.2) (suitably generalized to an infinite number of degrees of freedom).

Is the semiclassical system (2.1) and (2.2) a good approximation to the full quantum-mechanical system? In some cases it will be—if the x_I are well approximated by their mean, and one is interested in "large-scale" behavior. For example, in the Stern-Gerlach experiment it is adequate to consider the (quantum) electron moving in a mean, background magnetic field, and ignore the correction to the electron's motion from the full interaction between the electron and the quantum electromagnetic field. However, if one is interested in those corrections, obviously system (2.1) and (2.2) is not good enough. To be explicit, let us find the effects of quantum fluctuations in a system we can solve. Consider $2N$ coupled harmonic oscillators with

$$H=\frac{1}{2}\left[\frac{1}{m}p_i^2+k_{ij}x_ix_j+\frac{1}{M}p_I^2+K_{IJ}x_Ix_J+\sigma_{Ij}x_Ix_j\right] . \tag{2.4}$$

This quantum-mechanical system can be solved exactly in terms of the normal modes. Further, letting $z_\alpha=(x_i,p_i,x_I,p_I)$, the equations of motion for expectation values of moments of z_α are

$$\frac{d}{dt}\langle z_\alpha\rangle_{\rm QM}=\Lambda_{\alpha\beta}\langle z_\beta\rangle_{\rm QM} \tag{2.5a}$$

and

$$\frac{d}{dt}\langle \Delta z_\alpha z_\beta\rangle_{\rm QM}=\Lambda_{\alpha\gamma}\langle \Delta z_\gamma z_\beta\rangle_{\rm QM}+\Lambda_{\beta\gamma}\langle \Delta z_\alpha z_\gamma\rangle_{\rm QM} , \tag{2.5b}$$

etc., where $\Delta AB\equiv(A-\langle A\rangle)(B-\langle B\rangle)$ and the nonzero components of $\Lambda_{\alpha\beta}$ are given by

$$\Lambda_{i,j+N}=\frac{1}{m}\delta_{ij},\quad \Lambda_{i+N,j}=-k_{ij},\quad \Lambda_{I,J+N}=\frac{1}{M}\delta_{IJ} ,$$

$$\Lambda_{I+N,J}=-K_{IJ},\quad \Lambda_{i+N,J}=\Lambda_{J+N,i}=-\sigma_{iJ} .$$

In the semiclassical version of this theory, using (2.2) and (2.3) we see that the equations of motion for the linear expectation values $\langle z_\alpha\rangle_{\rm SC}$ are identical in form to the quantum-mechanical equations (2.5a), i.e.,

$$\frac{d}{dt}\langle z_\alpha\rangle_{\rm SC}=\Lambda_{\alpha\beta}\langle z_\beta\rangle_{\rm SC} . \tag{2.6a}$$

Therefore, if one starts with the same initial conditions on $\langle z_\alpha\rangle_{\rm SC}$ and $\langle z_\alpha\rangle_{\rm QM}$ at $t=0$, they will remain equal for all time. The dispersions of the two theories are different, however, as the dispersions of the semiclassical theory are zero except for the purely quantum-mechanical ones, where, with $z_a=(x_i,p_i)$,

$$\frac{d}{dt}\langle \Delta z_a z_\beta\rangle_{\rm SC}=\Lambda_{ac}\langle \Delta z_c z_b\rangle_{\rm SC}+\Lambda_{bc}\langle \Delta z_a z_c\rangle_{\rm SC} . \tag{2.6b}$$

Note that this is not of the same form as Eq. (2.5b) with $\alpha=a$ and $\beta=b$ since there is a contribution to (2.5b) with $\gamma\neq c$. Thus, we see explicitly that if the mean is the only quantity of physical interest then the fully quantum-mechanical and the semiclassical theories agree, but the predictions are different if the dispersions are relevant.

Now, think of the x_I as "measuring instruments." Consider the case of symmetric couplings, i.e., $k_{ij}=k_{ij}=k\delta_{ij}$, $K\delta_{IJ}$, $\sigma_{i,N+l+i}=\sigma_l$ independent of i for $l=1,\ldots,N$ ($N+l+i$ being interpreted modulo N). Thus, the N classical sites are equivalent, and the N quantum-mechanical sites are equivalent. It is clear from the equations of motion that if the initial conditions are symmetric, i.e., $\langle x_i\rangle_{t=0}$ and $\langle p_i\rangle_{t=0}$ are independent of i, and $x_I(t=0)$ and $p_I(t=0)$ independent of I, then $x_I(t)$ is independent of I for all time. In the corresponding fully quantum-mechanical system, although $\langle x_I\rangle_{\rm QM}$ would be independent of I for all time, the set of x_I found in any given "measurements" would, in general, not be. This is what we mean by stating that the quantum fluctuations do not feed into the semiclassical system. Unless we put in the inhomogeneities by hand (in the initial data or the couplings), then the motion of the classical variables is the same at each site.

To put this a little more dramatically, suppose we start all the classical oscillators at rest. Are they forced to start oscillating by the quantum fluctuations? By the above argument, if the initial quantum state is either even or odd under each interchange $x_i\to -x_i$, then the classical oscillators remain at rest for all time. (An example of such a state is a product of the Hermite polynomials in x_i.) Thus, in this semiclassical theory, the classical degrees of freedom may or may not be affected by the quantum system.

An analogous situation occurs in field theory (the limit $N\to\infty$) and we see that in the semiclassical gravity system described by Eqs. (1.1) and (1.2), if initially the expectation value of the quantum-mechanical stress-energy tensor and the gravitational field are Robertson-Walker symmetric, then they will be so for all time. One can only get spatial fluctuations in the metric (and hence in the mass density) by putting spatial variations in the initial data. In short, in this semiclassical gravity system it is impossible for quantum fluctuations to be the seed of galaxy formation. Contrast this with what one would expect from a fully quantum-mechanical treatment of a cosmological system.

To highlight some of the above points, consider the special case of Eq. (2.4) with four masses connected by springs, with a Hamiltonian

$$H=\frac{1}{2m}(p_1^2+p_2^2)+\frac{1}{2M}(p_3^2+p_4^2)+\tfrac{1}{2}k(x_1-x_2)^2+\tfrac{1}{2}\sigma[(x_1-x_3)^2+(x_2-x_4)^2] .$$

As discussed above, from Eqs. (2.5a) and (2.6a) we have $\langle x_i\rangle_{\rm QM}(t)=\langle x_i\rangle_{\rm SC}(t)$ for $i=1,2$, and $\langle x_I\rangle_{\rm QM}(t)=x_I(t)$ for $I=3,4$, and similarly for the momenta, if the initial conditions are the same. The solutions have oscillatory pieces plus a piece which grows linearly in time. However, the dispersions differ for the two theories. In the quantum-mechanical case, Eq. (2.5b) shows that there are terms which are oscillatory (with the same periods as for the linear expectation values) and terms which grow linearly and quadratically in time. For the semiclassical theory, however, only the oscillatory terms occur in the dispersions (and with different periods than in the quantum case). Inspecting the solutions in the limit where $m\ll M$ (which is where one would expect a semiclassical treatment to be valid) shows that $\langle \Delta z_a z_b\rangle_{\rm SC}$ differs from $\langle \Delta z_a z_\beta\rangle_{\rm QM}$ by an amount of an order of one after a time $T\sim M/[m(\sigma+2k)]^{1/2}$. In addition, if the full quantum-mechanical system starts in a state where the heavy masses (x_3,x_4) are in coherent ("classical") states, and x_1,x_2 are in any state, then after a time of order T (as above), $\langle \Delta x_I^2\rangle\sim\langle \Delta x_i^2\rangle$, so that this is also the time scale over which the quantum state stops looking classical (in x_3,x_4).

To summarize, then, we have seen that in the semiclassical theory described in this section, quantum fluctuations do not feed into classical system, and there are several gross features of the quantum-mechanical system which are not modeled successfully.

III. NEW SEMICLASSICAL THEORY: OPERATOR-VALUED FUNCTIONS ON PHASE SPACE

In this section we construct a different type of semiclassical theory, in which quantum and classical degrees of freedom are coupled in such a way that fluctuations in one affects the dynamics of the other. We start with a Hilbert space of quantum state $\mathcal{H}$, and a classical phase space Γ. Observables are to be (Hermitian) operator-valued functions on phase space, which operate on vectors in the quantum Hilbert space. The state of the system is to be described by a density matrix ρ, also an operator-valued function on Γ. ρ is to be a generalization of the familiar density matrix in quantum mechanics and probability distribution on Γ in classical mechanics. The time evolution of ρ is determined by the Hamiltonian observable.

We first state properties which we consider to be natural requirements for a semiclassical theory, generalizing the corresponding properties of purely quantum-mechanical or purely classical theories. We require that ρ is (i) Hermitian and satisfies $\int_\Gamma \mathrm{Tr}\rho=1$ at $t=0$ (where Tr is the trace on the Hilbert space) and (ii) positive (semidefinite) at $t=0$. Further, we require that the equation of motion for ρ (iii) is of the form $\dot\rho=[H,\rho]_{\mathrm{SC}}$, where the brackets operation, which is to be defined, is to be linear in H and ρ, (iv) is invariant under canonical transformation on Γ, (v) is invariant under (constant) unitary transformations on Hilbert space, (vi) reduces to the usual quantum-mechanical and classical equations if there is no interaction between the quantum and classical systems, (vii) preserves Hermiticity of ρ and $\int_\Gamma \mathrm{Tr}\rho=1$, and (viii) preserves positivity of ρ.

Conditions (i), (ii), (vii), and (viii) allowed a consistent probability interpretation to be given to ρ. We shall see that conditions (i)–(vii) determine a unique equation of motion for ρ, which, however, fails to preserve positivity of ρ [condition (viii)]. Therefore, a positive theory would have to give up one of the conditions (i)–(vii). The lack of positivity is related to the same problem which occurs in Wigner's function.[3] Indeed, if one drops requirement (iv), then the equation which Wigner's function obeys is a particular case of the allowed equations of motion for ρ. As in the case of the Wigner function, one expects here that for "sharply peaked" density matrices, probabilities of physically interesting quantities are "mostly positive." However, this appears difficult to prove in general, although we shall mention some results in particular cases. Now we construct the theory and examine its properties in more detail.

In this picture, the expectation value of an observable O is to be given by

$$\langle O\rangle_{\mathrm{Sc}}=\int_\Gamma \mathrm{Tr}\rho O \tag{3.1}$$

and probabilities are defined as follows. Consider the spectral decomposition of the observable, $O=\sum_n \lambda_n(z)P_n(z)$, where P_n is the projection operator onto the eigenspace of O with eigenvalue $\lambda_n(z)$, both which may depend on the point z in phase space (n may be a continuous index). Then the probability that O takes a value r belonging to some real interval I is given by

$$p_{r\in I}=\sum_n \int_{R_n(I)} \mathrm{Tr}\rho P_n \ , \tag{3.2}$$

where $R_n(I)$ is the region in phase space:

$$R_n(I)=\{z\in\Gamma \mid \lambda_n(z)\in I\} \ .$$

For example, in the case where $O=f(z)$ is just a function on Γ, we have $P_n(z)=$identity, and $R(I)=\{z\in\Gamma \mid f(z)\in I\}$, and

$$p_{r\in I}=\int_{R(I)} \mathrm{Tr}\rho f \ .$$

Now let us turn to the equation of motion for ρ. Let f,g be functions on Γ, and X,Y be operators on Hilbert space with no phase-space dependent. By conditions (iii), (iv), and (v), $[fX,gY]_{\mathrm{SC}}$ can only be a linear combination of the terms $fg(XY\pm YX)$ and $\Omega^{AB}\partial_A f\partial_B g(XY\pm YX)$, where Ω is the symplectic form on Γ. No higher phase-space derivatives appear since these are not invariant under canonical transformations. Equivalently, there is no natural connection. (But if, for example, we assume Γ is a vector space, then there is a natural connection and there are higher derivative terms that are invariant under the restricted set of canonical transformations that leave the connection invariant. A special case of this is what happens with Wigner's function, which we will discuss below.) Assume for the moment that the brackets is antisymmetric. Then condition (vi) now implies that

$$[fX,gY]_{\mathrm{SC}}=-\frac{i}{\hbar}fg[X,Y]\tfrac{1}{2}(XY+YX)+\{f,g\}_{\mathrm{PB}} \ . \tag{3.3}$$

Then for general operators which can be expanded in the form $O=\sum_i f_i X_i$, (3.3) implies

$$[O,O']_{\mathrm{SC}}=-\frac{i}{\hbar}[O,O']+\tfrac{1}{2}\Omega^{AB}(\partial_A O\partial_B O'-\partial_A O'\partial_B O) \ . \tag{3.4}$$

The definition (3.4) ensures that ρ has a Hermitian evolution, but we must check that the trace of ρ remains equal to 1. Indeed,

$$\int_\Gamma \mathrm{Tr}\dot\rho=\int_\Gamma \mathrm{Tr}[H,\rho]_{\mathrm{SC}}=0 \ ,$$

using the cyclic properties of the trace and integration by parts. Thus, condition (vii) is satisfied.

Now, Eq. (3.1) and condition (iii) imply that, for a general operator O,

$$\frac{d}{dt}\langle O\rangle_{\mathrm{SC}}=\frac{i}{\hbar}\langle [H,O]\rangle_{\mathrm{SC}}+\left\langle\frac{\partial O}{\partial t}\right\rangle_{\mathrm{SC}} \ .$$

Thus, for general (time-independent) H and ρ, $(d/dt)\langle H\rangle_{\mathrm{SC}}=0$. If we dropped the condition that the brackets be antisymmetric this would not be true. An example of a term that can arise in Eq. (3.3) for this more general case is $i\lambda\{f,g\}_{\mathrm{PB}}[X,Y]$, with λ real. We will not discuss this class of theories in this paper.

As an example of the general formalism, consider the case of two degrees of freedom, x_1 quantum mechanical and x_2 classical, with

$$H = H_1 + H_2 + V_I(x_1, x_2) \tag{3.5}$$

with

$$H_i = \frac{1}{2}\frac{p_i^2}{m_i} + V_i(x_i) .$$

Then explicitly, the brackets become

$$\begin{aligned}\dot{\rho} &= [H,\rho]_{\rm SC} \\ &= -\frac{i}{\hbar}[H_1,\rho] + \{H_2,\rho\}_{\rm PB} \\ &\quad -\frac{i}{\hbar}[V_I(x_1,x_2) - V_I(x_1',x_2)]\rho \\ &\quad +\frac{1}{2}\left[\frac{\partial V_I(x_1,x_2)}{\partial x_2} + \frac{\partial V_I(x_1',x_2)}{\partial x_2}\right]\frac{\partial \rho}{\partial p_2} ,\end{aligned} \tag{3.6}$$

where $\rho = \rho(x_1, x_1', z)$ and $z = (x_2, p_2)$.

In this system the equations of motion for the expectation values of x_1 and p_1 have exactly the same form as in the full quantum theory. For example,

$$m_j \frac{d^2}{dt^2}\langle x_j \rangle = -\left\langle \frac{\partial V_j}{\partial x_j}\right\rangle - \left\langle \frac{\partial V_I}{\partial x_j}\right\rangle , \tag{3.7}$$

where j runs over *all* the variables. This is different than the old semiclassical theory, where, for example,

$$m_2 d^2/dt^2 x_2 = -\partial V_2/\partial x_2 - \partial\langle V_I \rangle/\partial x_2 .$$

Further, although the quantum dispersions for the previous semiclassical theory did not even qualitatively match those of the full quantum theory, here they obey equations of motion of exactly the same form, except that

$$\frac{d}{dt}\langle \Delta p_1 p_2\rangle_{\rm SC} = \langle \Delta p_1 \{p_2, H\}_{\rm PB}\rangle_{\rm SC} - \frac{i}{\hbar}\langle \Delta p_2 [p_1, H]\rangle_{\rm SC} + \frac{\hbar}{2i}\left\langle \frac{\partial^2 V_I}{\partial x_1 \partial x_2}\right\rangle_{\rm SC} ,$$

the last term (proportional to $\hbar$) being an addition to the usual quantum-mechanical form. In particular, in this semiclassical theory, quantum and classical fluctuations affect each other's dynamics, and in a way consistent with quantum mechanics. Note that these statements about harmonic oscillators could just as well be made about each mode of linearly coupled fields ϕ (quantum) and ψ (classical); the fluctuations $\langle \Delta\phi_k^2 \rangle$ necessarily induce fluctuations $\langle \Delta\psi_k^2 \rangle$.

There is a connection between the ρ discussed here and a semiclassical version of Wigner's function, F_W. Let ρ_Q be the density matrix for a purely quantum-mechanical system with two degrees of freedom. Then let

$$F_W(x_1, x_1', x_2, p_2) = \int dw\, e^{-2ip_2 w/\hbar} \rho_Q(x_1, x_1', x_2 + w, x_2 - w) .$$

This is semiclassical in that the Wigner transform has only been done on one of the variables. Both this and the usual version of the Wigner transform are explicitly not invariant under all canonical transformations on phase space, and this makes the transform difficult or impossible to implement in, for example, general relativity. Wigner's idea was to reformulate quantum mechanics in terms of classical probability distributions on phase space (when the transform is done on all the variables), and indeed one does recover the appropriate expectation values, $\langle O \rangle = \int_\Gamma F_W$, if O is Weyl-ordered product of x and p. However, on both the usual and semiclassical versions of the transform there are serious problems with positivity. First, a positive ρ_Q does not, in general, give a positive F_W (this is what Wigner showed[3]). Second, even if F_W is positive initially, in general, it does not remain positive under evolution in time.

Now return to our semiclassical theory. Suppose we drop condition (iv), invariance under canonical transformations on Γ. Suppose that we assume that Γ has a vector space structure, and hence a natural derivative operator ∂_A. Then the most general equation of motion consistent with this and with the conditions except for (iv) is

$$\dot{\rho} = \frac{1}{2}\sum_{k=0}^{\infty} \frac{c_k}{k!}\Omega^{a_1 b_1}\cdots\Omega^{a_k b_k}\left[\frac{\partial^k H}{\partial z^{a_1}\cdots\partial z^{a_k}}\frac{\partial^k \rho}{\partial z^{b_1}\cdots\partial z^{b_k}} - \frac{\partial^k \rho}{\partial z^{a_1}\cdots\partial z^{a_k}}\frac{\partial^k H}{\partial z^{b_1}\cdots z^{b_k}}\right] , \tag{3.8}$$

where the constants c_k are arbitrary except that $c_k^* = (-1)^{k+1}c_k$ and $c_0 = 2/i\hbar$, $c_1 = 1$.

The semiclassical F_W satisfies an equation of motion by virtue of the fact that ρ_Q satisfies Schrödinger's equation. For Hamiltonians which are quadratic in the momentum variables this equation can be shown to be a special case of (3.8), with $c_k = (i\hbar/2)^{k-1}$. The Wigner function is the unique function which satisfies certain "natural" conditions. The fact that it is not, in general, positive makes one not surprised that the semiclassical theory of the form outlined is not also positive. It may be, for example, that one should look at nonlinear equations, or systems with dissipation. An example of a nonlinear system, satisfying all the other criteria, is given in the Appendix.

In the case of simple harmonic oscillators, the higher derivative terms ($k \geq 2$) in (3.8) all vanish, and F_W then satisfies precisely $\dot{F}_W = [F_W, H]_{\rm SC}$. Therefore, for quadratic Hamiltonians we know the exact solutions for the density matrix in the new semiclassical theory, since one can solve the full quantum theory for ρ_Q, and hence construct F_W. Since a positive ρ_Q does not, in general, lead to a positive F_W the proper (and laborious) way to implement this is to start with F_W at $t = 0$, do the inverse transform, evolve in time and to the transform back. Further, although ρ (i.e., F_W in this case) will not remain positive for all time, in general, it may be positive if ρ is peaked about a classical path in phase space. Such a ρ is displayed in Appendix, for the Hamiltonian

$$H=\tfrac{1}{2}(p_1^2/m_1+p_2^2/m_2+k_1x_1^2+k_2x_2^2+\sigma x_1x_2) .$$

To see how ρ behaves on Γ, we look at $\mathrm{Tr}\rho=\int dx_1\rho(x_1,x_1,z)$. We find that $\mathrm{Tr}\rho$ is positive definite. In the weak-coupling limit, the expression is sharply peaked about the classical path, with corrections from the interaction: let $\bar{R}=R_2(t)(1-\frac{1}{2}\epsilon^2)+\epsilon R_1(t)$ where $R_i(t)=Q_{i0}\cos[(k_i/m_i)^{1/2}t-\phi_{i0}]$ is the classical path, and

$$\epsilon=\frac{1}{2}\left[\frac{m_1}{m_2}\right]^{1/2}\frac{\sigma}{k_1}\left[1-\left[\frac{k_2}{k_1}\right]\left[\frac{m_1}{m_2}\right]\right]^{-1} \ll 1 .$$

Then we find (letting $k_1=k_2=k$)

$$\mathrm{Tr}\rho(x_2,p_2)=\frac{\sqrt{\pi}}{2}\left[\frac{m_1}{m_2}\right]^{1/8}\frac{\hbar}{\sqrt{m_2k}\,(\Delta x_2)^2}\times\exp\left[-\frac{1}{(\Delta x_2)^2}[x_2-\bar{R}(t)]^2\right]\times\exp\left[-\frac{1}{(\Delta p_2)^2}\left[p_2-m_2\frac{d}{dt}\bar{R}\right]^2\right] ,$$

where

$$(\Delta x_2)^2=\hbar[\sqrt{m_2k}\,(1+\tfrac{1}{2}\epsilon^2)]^{-1} ,$$

$$(\Delta p_2)^2=\hbar[\sqrt{m_2k}\,(1+\epsilon^{3/2})]$$

[and hence $(\Delta x_2)^2(\Delta p_2)^2\geq\hbar^2$].

So there are solutions for ρ that have a sensible behavior on Γ, in much the same way as Wigner's function sometimes does. In these cases one can indeed say what fluctuations are induced in the classical degrees of freedom by the quantum fluctuations.

However, in general, the evolution of the density matrix does not preserve positivity. We will explicitly look at Hamiltonians of the form (3.5). We say that ρ is positive (semidefinite) if for all states $Y\in\mathcal{H}$, and for all $z\in\Gamma$, $\int dx_1dx_1'Y(x_1)Y^*(x_1')\rho(x_1,x_1',z)\geq 0$. To show that this condition is not, in general, preserved the strategy is to find a place where ρ is zero, and where $\dot{\rho}$ is negative, which means that ρ evolves to a negative value there. That is, we seek a (1) $\rho\geq 0$ and an $Y\in\mathcal{H}$, $z_0\in\Gamma$ such that (2) $\int YY^*\rho\,|_{z_0}=0$, and (3) $\int YY^*\dot{\rho}\,|_{z_0}<0$. Now, (1) and (2) imply that $\partial\rho/\partial x_2=0$, $\partial\rho/\partial p_2=0$ at z_0, and similarly that $\int dx_1Y(x_1)\rho(x_1,x_1',z_0)=0$. Therefore, using Eq. (3.6) for ρ, the first three terms in (3) are zero. The last term, however, is a problem and we will have a counterexample if the vector Y also satisfies

$$\int dx_1dx_1'Y(x_1)Y^*(x_1')\left[\frac{\partial V(x_1,x_2)}{\partial x_2}+\frac{\partial V(x_1',x_2)}{\partial x_2}\right]\frac{\partial\rho}{\partial p_2}<0 .$$

One possible choice at $(t=0)$ is to take

$$\rho(x_1,x_1',z)=N\exp\{-[x_1^2+x_1'^2+(x_2-x_2^0)^2+(p_2-p_2^0)^2+\lambda(p_2-p_2^0)(x_1+x_1')]\}$$

with $\lambda^2<2$ (so that ρ is normalizable). Then ρ satisfies conditions (1) and (2) above for $z_0=(x_2^{(0)},p_2^{(0)})$ and for the family of vectors

$$Y_u(x)=\Theta(u-x)\Theta(x)-\frac{E(u)}{E(\infty)-E(u)}\Theta(x-u)\frac{\exp(-x^2)}{\sqrt{2}} ,$$

where Θ is the step function and $E(u)=\int_0^u e^{-x^2}dx$. Further, $\int Y_uY_u^*\dot{\rho}=\lambda g(u)$, where g is not identically zero as a function of u. Hence, we can satisfy condition (3) by a correct choice of the sign of λ.

Even though ρ is not, in general, positive one can ask if probabilities for physically interesting operators to take certain values are positive—for example, is the probability that the energy is $E_0\pm\Delta$ always a positive number? In general, this is a hard question, but there are some partial results along this line. Again let $H=H_1+H_2+H_1$, and suppose that $O=\sigma\lambda_nP_n$ is a purely quantum-mechanical operator which commutes with H_1+H_I. Then the probabilities $p_n=\int_\Gamma\mathrm{Tr}\rho P_n$ have vanishing time derivatives and so, in particular, remain positive if they are so initially. An analogous statement can be made for functions on Γ. For mixed operators, like the energy, the question is much harder.

IV. CLASSICAL OBSERVABLES AS OPERATORS

In this section we will briefly recount an alternative approach to building semiclassical theories. In this approach we first associate operators on a Hilbert space $\mathcal{H}_2$ with each classical observable. $\mathcal{H}_2$ is, for example, square-integrable functions on phase space. We wish to assign an operator f^{op} to each function $f(z)$ on Γ, such that $1^{\mathrm{op}}=1$, and $[f^{\mathrm{op}},g^{\mathrm{op}}]=-(\hbar/i)\{f,g\}_{\mathrm{PB}}^{\mathrm{op}}$.

This has been worked out in the context of prequantization[4] and we merely quote the results. Let Ω_{AB} be the symplectic form on Γ with potential θ_A, so $\Omega_{AB}=\nabla_A\theta_B-\nabla_B\theta_A$ (the existence of θ puts some topological restrictions on Γ). Then

$$f^{\mathrm{op}}=\frac{\hbar}{i}\Omega^{AB}\nabla_Bf\left[\nabla_A+\frac{i}{\hbar}\theta_A\right]+f . \tag{4.1}$$

We will work on flat two-dimensional phase space, and choose coordinates (x_2,p_2) with $\theta=-p_2dx_2$. (We use $\Omega_{x_2p_2}=-\Omega_{p_2x_2}=1$ and $\Omega^{AB}\Omega_{CB}=\delta_C^A$.) Then, for example,

$$x_2^{\mathrm{op}}=-\frac{\hbar}{i}\frac{\partial}{\partial p_2}+x_2,\ p_2^{\mathrm{op}}=\frac{\hbar}{i}\frac{\partial}{\partial x_2} ,$$

and

$$H_2^{\mathrm{op}}=\frac{\hbar}{i}\left[\frac{p_2}{m_2}\frac{\partial}{\partial x_2}-\frac{\partial V(x_2)}{\partial x_2}\frac{\partial}{\partial p_2}\right] .$$

With this, one can rewrite classical mechanics in the form of Schrödinger mechanics. The state $\psi(x_2,p_2)$ evolves according to $-(\hbar/i)\dot{\psi}=H_2^{\rm op}\psi$. The density matrix $\rho(z,z')=\psi(z)\psi^*(z')$ then evolves via $\dot{\rho}=-(i/\hbar)[H_2^{\rm op},\rho]$, which implies that the diagonal piece, $\rho(z,z)$ evolves as usual according to the Poisson brackets, $\dot{\rho}(z,z)=\{H_2,\rho\}_{\rm PB}$. So $\rho(z,z)$ can be interpreted as a probability function on phase space.

Although, for example, $\langle x_2\rangle$ and $\langle p_2\rangle$ satisfy the usual equations of motion of classical mechanics, there are interpretational difficulties for $x_2^{\rm op}$. We see that

$$\frac{d^2}{dt^2}\langle x_2^{\rm op}\rangle=-\left\langle\frac{\partial V^{\rm op}}{\partial x}\right\rangle=\left\langle-\frac{\partial V}{\partial x}+\frac{\hbar}{i}\frac{\partial^2 V}{\partial x_2^2}\frac{\partial}{\partial p_2}\right\rangle .$$

If the state is sharply peaked about a trajectory in Γ, $\langle x_2^{\rm op}\rangle$ and $\langle p_2^{\rm op}\rangle$ are *not* sharply peaked about that path. (One can check this explicitly for the simple harmonic oscillator, and verify that the oscillations about this path are *not* suppressed by the factor of $\hbar$ which appears in the equation of motion above.) Thus, the idea is that for a function f on phase space, $\langle f\rangle={\rm Tr}(f\rho)=\int_\Gamma f(z)\rho(z,z)$ gives the expectation value of f (which satisfies the usual equation of motion), and $\langle f^{\rm op}\rangle={\rm Tr}(f^{\rm op}\rho)$ is not interpreted physically. In general, the only operators that are interpreted are the ones that are functions on Γ. In particular, $\rho(z,z')$ is only interpreted for $z=z'$ and it is vital for consistency that the time derivative of $\rho(z,z)$ involve only $\rho(z,z)$, which is true, as mentioned above. This is to be contrasted with the semiclassical extension, discussed next.

It is straightforward to write down a semiclassical Schrödinger system. The Hilbert space is the tensor product $\mathcal{H}=\mathcal{H}_2\otimes\mathcal{H}_2$ (where $\mathcal{H}_1$ is, as before, the space of quantum states) and observables are Hermitian operators on $\mathcal{H}$ which are functions on phase space, $O(x_1,x_1',z)$. From the Hamiltonian we construct $H^{\rm op}$, where each function of the classical degrees of freedom is replaced by its operator according to (4.1). The density matrix $\rho(x_1,x_1',z,z')$ then evolves by

$$\dot{\rho}=-\frac{i}{\hbar}[H^{\rm op},\rho] . \tag{4.2}$$

Since ρ has a unitary evolution, there is no problem with positivity. However, there are severe interpretational difficulties. One can check that if the classical diagonal piece of ρ starts equal to zero, $\rho(x_1,x_1',z)=0$ at $t=0$, then, in general, it does not remain zero. This means that the same classical initial state can have different future evolutions. A second problem is that for general Hamiltonians there is no positive conserved energy. Third, in the semiclassical theory the equations of motion for $\langle x_1\rangle$ and $\langle x_2^{\rm op}\rangle$ have the same form as in the full quantum theory, but this is not very satisfactory since the interpretation of $\langle x_2^{\rm op}\rangle$ is problematic. On the other hand, one could consider instead $\langle x_1\rangle$ and $\langle x_2\rangle$. However, even in the case of two coupled harmonic oscillators, this leads to runaway solutions.

We conclude that whatever one might choose to make out of the interpretation problems, the ambiguity in the evolution of the classical diagonal piece of the density matrix makes this theory an unsatisfactory description.

At this point the reader may wonder why we have only discussed density-matrix formulations, and no wave function approaches. For example, let $\psi(x_1,z)$ evolve as in the previous section, $-(\hbar/i)\dot{\psi}=H^{\rm op}\psi$. Then the diagonal problems of the preceding section do not occur, since we could work with a density matrix that is purely diagonal in the classical variables, $\tilde{\rho}(x_1,x_1',z)=\psi(x_1,z)\psi^*(x_1',z)$. One can easily write down the evolution equation for $\tilde{\rho}$, which turns out *not* to be expressible only in terms of $\tilde{\rho}$. Although that is not fatal to this approach, one also finds that this equation is not invariant under rotations of the wave function by a classical phase, $\psi\rightarrow e^{i\alpha(z)}\psi$. That is a severe problem.

A different approach would be to use H to evolve $\psi(x_1,z)$ rather than $H^{\rm op}$. We know, of course, that this will not yield a density matrix $\psi(x_1,z)\psi^*(x_1',z)$ which satisfies the criteria (i)–(viii) of Sec. III, since the wave function density matrix *would* be positive definite. However, evolutions one might try, such as

$$-\frac{\hbar}{i}\dot{\psi}=H_1\psi+\{H_2,\psi\}_{\rm PB}+\{H_I,\psi\}_{\rm PB} ,$$

have the same phase problems already mentioned.

V. CORRELATIONS AND FLUCTUATIONS IN INFLATION

The generation of perturbations in the (classical) mass density by quantum fluctuations has been much discussed in inflationary scenarios (see, for example, Ref. 2). The idea is that the quantum field, whose mean stress energy drives the inflationary expansion, also has quantum fluctuations about the mean. At some point these fluctuations become classical, and so in effect provide initial conditions $\Delta\rho_{\rm cl}(\mathbf{x},t_0)$ for the future purely classical evolution of the Einstein equation, which should evolve to form galaxies. There are some problems, however, with this program. Inflation happens in the "old" semiclassical theory, Eqs. (1.1) and (1.2). The state and metric are chosen to be de Sitter invariant. Then, as we have seen, the fluctuations in the quantum field do not affect the evolution of the metric; the metric continues to have the de Sitter symmetries. In particular, the metric is homogeneous on each constant time slice. There are no spatial perturbations in the metric, and equivalently, none in the stress energy which is the source for the metric.

What is done is to consider the two-point mass correlation function. For this section only, following standard notation, let ρ be the quantum operator corresponding to the energy density of the field Φ. Let $\rho=\langle\rho\rangle+\delta\rho$, where the expectation value is in the quantum state $|\psi\rangle$, which is, of course, independent of position. The two-point function $\xi(r)=\langle\delta\rho(x)\delta\rho(x+r)\rangle$ does depend on the distance r; the question is, does $\xi(r)$ have anything to do with generating spatial inhomogeneities in the metric (i.e., in the classical mass density) and if so, what? The interpretation which has been made[2] is that there are perturbations in the (classical) mass density of amplitude $|\delta\rho_k|^2$ on the length scale $1/k$, where $|\delta\rho_k|^2$ is the Fourier transform of $\xi(r)$. That is, let us say that for

$t \leq t_0$ the metric evolves according to semiclassical gravity, Eq. (1), and for $t > t_0$, by the purely classical Einstein equations. Choose for initial data on the classical mass density $\rho_{\rm cl}(\mathbf{x},t_0) = \langle \rho \rangle(t_0) + \Delta\rho(\mathbf{x})$ where $\Delta\rho(\mathbf{x})$ is any c-number function that satisfies

$$\frac{1}{V}\int d^3x \; \Delta\rho(\mathbf{x})\Delta\rho(\mathbf{x}+\mathbf{r}) = \langle \delta\rho(\mathbf{x})\delta\rho(\mathbf{x}+\mathbf{r}) \rangle \tag{5.1}$$

(where V is the spatial volume), or, in Fourier space,

$$|\Delta\rho_k|^2 = \langle |\delta\rho_k|^2 \rangle \; . \tag{5.2}$$

That is, the two-point correlation function of the classical perturbation, defined by the spatial average, is to be equal to the quantum two-point function.

There are two types of questions which arise here. Suppose first that either the evolution was purely quantum mechanical for $t \leq t_0$ and one wanted to match to a classical evolution for $t > t_0$, or that the description was classical probabilistic for $t \leq t_0$ and matched to classical deterministic for $t > t_0$. Then is a criterion such as (5.1) ever a good approximation? The second issue is that we know that quantum fluctuations do not affect the dynamics of the metric in the old semiclassical theory, which describes the inflationary universe for $t \leq t_0$. What then is the justification for deciding that the two-point quantum density correlation function suddenly is a source for the metric at t_0? In a full quantum theory, or in the semiclassical theory of Sec. III, fluctuations in ρ *are* a source for fluctuations in the metric (and vice versa), so in these cases there is some justification for seeking a matching criterion.

Let us start with a purely classical case. Consider a fluid in a box which is coupled to gravity and is heated from below. One solution to the Navier-Stokes equations is the static one, with constant temperature, density, pressure gradient, and zero velocity. If instead there is some inhomogeneity in the density and pressure at $t = 0$, there will be some nonstatic evolution dictated by the competing gravitational and bouyancy forces acting on the perturbations. Suppose that the initial functions $\rho(\mathbf{x},t_0) = \bar{\rho} + \Delta\rho(\mathbf{x})$ are selected from an ensemble, and occur with different probabilities. Then the possible states of the system at a later time are found by evolving each member of the ensemble, and weighting the outcomes by the probability of the initial conditions occurring.

Now, is it possible to choose a "typical" $\rho(\mathbf{x},t_0)$ and evolve, such that one gets "typical" results? This, of course, depends on the underlying probability distribution (the probabilities of different initial density profiles in the example). Typically, if we are interested in a particular physical quantity such as the density, we must first check whether its probability distribution is sharply peaked, and then a "typical" member is one near the peak—choose one. Now, if the physical process is such that averaging over a large spatial volume is like averaging over the ensemble (as for a spin system on a lattice) then the chosen typical member will satisfy $(1/V)\int \rho = \langle \rho \rangle \pm \langle \delta\rho^2 \rangle^{1/2}$. Therefore, in this case it may be sensible to identify the spatial two-point function of the chosen member with the ensemble two-point function, as in (5.1).

Note that if one had chosen $\langle \rho \rangle$ as the typical member, one could get information about the mean temperature, pressure, and velocity, but no information about fluctuations. This is similar to coupling to the expectation value of the stress energy in semiclassical gravity.

It is important to note that condition (5.1) is not maintained by the time evolution of the system in general. This means if the system is evolved by the probabilistic description until some $t_1 > t_0$, then the evolution of the deterministic field from the t_0 matching will not satisfy the two-point correlation function condition that is defined by the ensemble average at t_1. [To see this, consider, for example, systems such as Einstein-fluid or Maxwell, where the evolution of the source J is of the form $\dot{J} = F(\phi, J)$, ϕ representing the other fields. Then, in Fourier space the ensemble two-point function evolves via $(d/dt)\langle J_k J_{-k} \rangle = \langle J_k F_{-k} + J_{-k} F_k \rangle$, whereas the Fourier transform of the spatial two-point function of a single source j evolves according to $(d/dt)(j_k j_{-k}) = j_k F_{-k} + j_{-k} F_k$. These are not the same differential equations, since the ensemble average mixes different k modes.]

Before returning to the question of when the interpretation (5.1) makes sense, especially for semiclassical systems, we note that in general the criterion cannot even be applied consistently. To start the classical evolution, one needs not only the initial density but initial velocities (and metric). However, it is not possible in general to require that the spatial-average two-point function equals the ensemble average two-point function for all the quadratic combinations of position and momenta. Explicitly, let a system be described by the coordinates and momenta x_i, p_i, $i = 1, \ldots, N$ and let $\langle * \rangle$ denote the ensemble average, either quantum mechanical or classical. Define the spatial average of a set of numbers f_i by $\overline{f_i} = (1/N)\sum_{i=1}^{N} f_i$, the two-point function by $\overline{f_i g_j} = (1/N)\sum_{l=1}^{N} f_{i+l} g_{j+l}$, etc., where $f_{i+l} \equiv f_i$. Let the averages $\langle x \rangle_i$, $\langle p \rangle_i$, $\langle x_i x_j \rangle$, $\langle p_i p_j \rangle$, $\langle p_i x_j \rangle$ be given at $t = 0$. Now, can one choose classical numbers y_i, π_i such that $\overline{y_i} = \langle x \rangle_i$, $\langle \pi_i \rangle = \overline{p_i}$, $\overline{y_i y_j} = \langle x_i x_j \rangle$, $\overline{\pi_i \pi_j} = \langle p_i p_j \rangle$, and $\overline{\pi_i y_j} = \langle p_i x_j \rangle$? It is straightforward to check that these conditions can be simultaneously applied only if $\langle y_i \rangle^2 = (1/N)\sum_j \langle y_i y_j \rangle$, and $\langle y_i y_j \rangle \langle \pi_l \pi_i \rangle = \langle y_j \pi_i \rangle \langle y_l \pi_i \rangle = \langle y_j \pi_i \rangle \langle y_i \pi_l \rangle$, which holds only if the sites are independent.

To summarize, suppose we want to evolve the system $O(g) = s(\rho, g)$, $\dot{\rho} = f(g, \rho)$ (where O is some operator and s, f some functions) quantum mechanically, or according to a classical probability distribution for $t \leq t_0$, and then match to a classical deterministic evolution for $t \geq t_0$. Suppose that the probability distribution for ρ is sharply peaked, that the ensemble average is mimicked by the spatial average of individual members of the ensemble, and that both before and after t_0, fluctuations in ρ are a source for g. Then one might sensibly apply the criterion (5.1) to pick out a typical member of the ensemble for initial conditions on the coordinates. However, applying the same criterion to the other two-point functions of the momenta and coordinates leads to a contradiction. Further, the criterion (5.1) is not respected by the time evolution of the system.

Of course, in this example there is a difference in the way the density ρ is a source for g if both are quantum fields than if both are classical. However, at least in either case the fluctuations in ρ and g are dynamically related during both periods of the evolution. The comments of the previous paragraph apply equally well to the new semiclassical theory of Sec. III, if one is working with an initial density matrix which has positive probabilities for the quantities of interest. So, for example, one could study fluctuations of a scalar field coupled to a de Sitter metric in its ground state, since in this case the wave functional is a product of Gaussians, which we have seen has a probability interpretation.

Finally, let us turn to the question of which probability distributions are sharply peaked, making the two-point function criterion sensible for selecting a typical member of the ensemble. Quantum mechanically, perhaps the most interesting distinction is between experiments where there are many events or single events. For example, suppose many radioactive atoms are placed inside a box, the box being divided into collecting bins which indicate a decay product. Then if one plots the number of bins with n events recorded in time T vs n, this distribution is sharply peaked about $\langle n \rangle$, the expected number of decays in T. On the other hand, if a single atom is placed inside the box, the same plot is not sharply peaked about $\langle n \rangle$. The expectation value is a bad indicator for single events, like the occurrence of a string track in a cloud chamber.

Secondly, it is often also important to distinguish between large-scale and small-scale structure. Suppose the probability distribution is a sum of sharply peaked pieces, as for example, when there are degenerate vacua as in inflation. If one is interested in the physics internal to one domain, then a "typical" field configuration should have a mean near *one* of the vacuum values, and dispersion of order the spread around that value. For a large-scale structure, when one averages over many domains, a typical field configuration has a mean near the ensemble average, and dispersion that is characteristic of the ensemble.

We certainly have not presented any rules for when the two-point function can be used to indicate the amplitude and wavelength or inhomogeneities in a classical source. We have pointed out difficulties which arise, even in matching a classical probabilistic of full quantum-mechanical evolution to a classical deterministic evolution. In the context of standard semiclassical gravity there are further problems, in that the dynamical role of the mass two-point function is different during the semiclassical evolution period and the classical period.

VI. CONCLUSION

There are systems occurring in nature in which some of the interacting components must be described by quantum mechanics, and other parts are apparently adequately described by classical physics. In this paper we have studied the possibility of constructing semiclassical theories, in which quantum-mechanical and classical degrees of freedom are coupled. Of particular interest was to formulate a theory in which the fluctuations in the quantum and classical variables affect the dynamics of each other, which does not occur in the "standard" semiclassical theories. This is relevant to the question, for example, of whether quantum fluctuations in matter fields in the early Universe can generate perturbations in the classical mass density, a computation which is currently done in an *ad hoc* manner.

One approach was to describe the system by a density matrix ρ which is an operator-valued function on phase space. Assuming certain "natural" requirements for the evolution of ρ, one derives a unique equation for the evolution of ρ. However, the density matrix fails to be positive semidefinite, which is necessary for a consistent probabilistic interpretation. It is discussed how in certain "very semiclassical" limits, the density matrix is positive.

In the semiclassical theory which is used to describe the inflationary universe, quantum fluctuations do not affect the dynamics of the (classical) metric. Still, estimates have been made of what this effect would be. We have discussed conditions under which such estimates may be valid; if the underlying probability distribution is not sharply peaked about the physical quantity of interest, the methods currently used to estimate classical perturbations may be misleading. However, the real problem is that one must postulate an abrupt change in the dynamical role of the quantum fluctuations.

So it appears difficult to construct semiclassical theories in which quantum fluctuations cause perturbations in the classical variables. However, one should not be too cocky; we will finish with an example of such a theory, described by a density matrix ρ (as in Sec. III) in which ρ is positive, and satisfies all the other requirements of Sec. III except that the equation of motion for ρ is nonlinear in ρ.

Indeed, as in (3.5) let $H = H_1 + H_2 + V_I$, and let

$$\hat{H} = \int H\,\mathrm{Tr}\rho = H_1 + \langle H_2 \rangle + \int V_I \mathrm{Tr}\rho \ ,$$

$$\tilde{H} = \mathrm{Tr}H \int \rho = \langle H_1 \rangle + H_2 + \mathrm{Tr}V_I \int \rho \ ,$$

so that $\hat{H}$ is an operator and $\tilde{H}$ is a function on phase space. Let the density matrix evolve according to

$$\dot{\rho} = -\frac{i}{\hbar}[\hat{H},\rho] + \{\tilde{H},\rho\}_{\mathrm{PB}} \ . \tag{6.1}$$

This has the correct noninteracting limit, is invariant under transformations on phase space and Hilbert space, and has a Hermitian positive-definite evolution. [To show positivity, let $\rho = \Sigma_A c_A \tilde{\rho}_A \hat{\rho}_A$, where $\tilde{\rho}_A$ is a function and $\hat{\rho}_A$ is an operator. Then (6.1) is satisfied if each of the $\tilde{\rho}_A$ evolves according to the Poisson brackets, and each $\hat{\rho}_A$ evolves according to the commutator.] Now let us look at dispersions. For example, for two coupled harmonic oscillators with $V_I = \sigma x_1 x_2$,

$$\frac{d}{dt}\langle \Delta p_1 p_2 \rangle = -k_1 \langle \Delta x_1 p_2 \rangle - k_2 \langle \Delta x_2 p_1 \rangle \ .$$

This differs from the full quantum-mechanical theory in that the interaction does not enter on the right-hand side; in the full theory, the additional terms $-\sigma\langle\Delta x_2 p_2\rangle-\sigma\langle\Delta p_1 x_1\rangle$ would appear. Hence, here we have a mixing of the quantum and classical fluctuations, but it is independent of the interaction. This is perhaps peculiar, but as has been pointed out, perhaps there is always going to be something peculiar about semiclassical theories.

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APPENDIX

Here we show how to solve for the density matrix of the semiclassical theory of Sec. III when the potential is quadratic,

$$H=\frac{1}{2}\left[\frac{p_1^2}{m_1}+\frac{P_2^2}{m_2}+k_1x_1^2+k_2x_2^2+\sigma x_1x_2\right] . \tag{A1}$$

As explained in Sec. III, for this Hamiltonian the equation of motion for ρ is identical to that for Wigner's function, which is known since we know the solution to the full quantum-mechanical problem for (A1). One expects that a density matrix which is constructed from sharply peaked simple harmonic-oscillator coherent-state wave functions will have the correct positivity properties. Therefore, we will compute Wigner's function (i.e., ρ) constructed from a wave function which is the product of coherent states in the center-of-mass coordinates Q_i [those coordinates which diagonalize (A1)]. Define the transformation A_{ij} between the two sets of coordinates by $Q_i=A_{ij}x_j=\sum U_{ij}\sqrt{m_j}x_j$, where U is unitary. Then the product of the two normal-mode coherent-state wave functions, reexpressed in the x_1,x_2 coordinates, is

$$\Psi(x_1,x_2)=\eta_1\eta_2\exp\{-\tfrac{1}{2}[\alpha_1^2(A_{1j}x_j-\hat{R}_1)^2+\alpha_2^2(A_{2j}x_j-\hat{R}_2)^2]\}\exp[-i(A_{1j}\beta_jx_j+A_{2j}\beta_jx_j+\phi_1+\phi_2)] , \tag{A2}$$

where $\hat{R}_i=Q_{i0}\cos(k_i/m_i)^{1/2}t$, $\beta_i=\hbar^{-1}d/dt\hat{R}_i$, $\alpha_i^2=\hbar^{-1}k_i/m_i$, and $\phi_i(t)=\frac{1}{2}(k_i/m_i)^{1/2}-\frac{1}{4}\alpha_i^2Q_{i0}\sin 2(k_i/m_i)^{1/2}t$, and $\eta_i^2=\alpha_i/\sqrt{\pi}$.

Next one computes Wigner's function $F=\int dw\, e^{-2ip_2w/\hbar}\Psi(x_1,x_2+w)\Psi^*(x_1',x_2-w)$ for the wave function (A2), and therefore we have a solution to (3.6) for ρ (i.e., F), for the Hamiltonian (A1):

$$\begin{aligned}\rho(x_1,x_1',x_2,p_2)=&\frac{1}{2}\left[\frac{\alpha_1\alpha_2m_2}{\sigma}\right]^{1/2}\exp[-i(x_1-x_1')(A_{11}\beta_1+A_{21}\beta_2)]\\&\times\exp\{-\tfrac{1}{2}[\alpha_1^2(A_{11}x_1+A_{12}x_2-\hat{R}_1)^2+\alpha_2^2(A_{21}x_1+A_{22}x_2-\hat{R}_2)^2\\&+\alpha_1^2(A_{11}x_1'+A_{12}x_2-\hat{R}_1)^2+\alpha_2^2(A_{21}x_1'+A_{22}x_2-\hat{R}_2)^2]\}\\&\times\exp\left\{\frac{1}{\sigma}\left[-\left[\frac{p_2}{\hbar}+\gamma\right]^2+m_2\lambda^2(x_1-x_1')^2-2i\lambda\sqrt{m_2}\left[\frac{p_2}{\hbar}+\gamma\right](x_1-x_1')\right]\right\} ,\end{aligned}$$

where $\gamma=(A_{22}\beta_2+A_{12}\beta_1)$, $\sigma=(\alpha_2^2A_{22}^2+\alpha_1^2A_{12}^2)$, and

$$\lambda=-\frac{1}{2}\frac{1}{\sqrt{m_2}}(\alpha_1^2A_{11}A_{12}+\alpha_2^2A_{22}A_{21}) .$$

In the weak-coupling limit, $U_{12}=-U_{21}=\epsilon$, and $U_{11}=U_{22}=1-\frac{1}{2}\epsilon^2$, where ϵ is given in Sec. III. Tracing over the quantum degrees of freedom and taking the weak-coupling limit yields the expression in Sec. III.

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