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Correlations in the wave function of the Universe

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The Everett-type interpretations of quantum mechanics and quantum cosmology proposed independently by Hartle, Geroch, and Wada are discussed. They essentially involve regarding a strong peak in the wave function as a definite prediction. Wave functions in quantum cosmology are usually peaked about correlations between coordinates and momenta, and methods for identifying such correlations are introduced. The first method involves Wigner's function, a quantum-mechanical analogue of the classical phase-space distribution. The properties of this distribution are discussed and it is shown how it can be of use in describing the emergence of classical behavior from quantum systems. The second method involves a suitably chosen canonical transformation. These methods are applied to harmonic-oscillator examples, which are of relevance to scalar field fluctuations in inflationary universe models. These methods are also applied to WKB wave functions in quantum mechanics and quantum cosmology. The manner in which the wave function becomes peaked about sets of classical solutions is elucidated. This is extended to include inhomogeneous perturbations about minisuperspace in quantum cosmology, and the derivation of the semiclassical Einstein equations, $G_{\mu\nu}=8\pi G\langle T_{\mu\nu}\rangle$, from the Wheeler-DeWitt equation is considered. A condition under which they are valid is derived. It is essentially the requirement that the distribution of $T_{\mu\nu}$, as a function of the matter modes, is strongly peaked about its average value. Some situations in which this condition is satisfied are discussed.

I. INTRODUCTION

The problem of interpretation of the wave function in quantum cosmology appears at first sight to be considerably more difficult than that encountered in conventional quantum mechanics. In conventional quantum mechanics, one envisages an ensemble of identical systems, each described by the state $|\Psi\rangle$, and these systems are observed by an external observer, described by classical physics. It is then assumed that measurement of a variable Q causes the wave function for each system to "collapse" into an eigenstate of Q, $|q\rangle$ say, where $Q|q\rangle=q|q\rangle$, and the measured value of the variable is the eigenvalue q. It is further assumed that the relative frequency with which a given value of q is obtained approaches the value $|\langle\Psi|q\rangle|^2$ as the number of systems in the ensemble approaches infinity. This is how the notion of probability enters the theory—as a relative frequency.

In quantum cosmology, on the other hand, the system under consideration is the whole Universe, for which there is no external observer, for which it is difficult to accept the discontinuous change brought about by the collapse of the wave function, and for which—since it is a single system—the concept of probability has no place. What appears necessary to do, therefore, is to replace the conventional "Copenhagen interpretation" of quantum mechanics, with the interpretation variously known as the "Everett," "relative state," or "many-worlds" interpretation.[1,2] There are a number of different versions of this interpretation, but what they all have in common is that they are based on formulations of quantum mechanics designed to describe correlations internal to an individual, isolated system. For this reason, we shall refer to them generically as the quantum mechanics of individual systems (QMIS).

QMIS begins by discarding all notions of external observer, of collapse of the wave function, and especially, of probability. Some of these notions, such as that of probability, will arise naturally as a result of the formalism of QMIS, but only in situations in which they are appropriate. Now suppose we have an individual system described by the state vector $|\Psi\rangle$. In QMIS one assumes only the following.

If $|\Psi\rangle$ is an eigenstate of the observable Q, i.e., $Q|\Psi\rangle=q|\Psi\rangle$, then observation of Q will yield the eigenvalue q, with certainty. If, however, Q is an observable of which $|\Psi\rangle$ is not an eigenstate, then there is no prediction for the outcome of the observation.

Given the above postulate, it is obviously of paramount importance to determine, for a given system, the observables of which the state vector is an eigenstate. One special case of particular interest is that in which the individual system consists of N identical noninteracting subsystems. Let us write the total wave function for the individual system as

$$\Psi(q_1,\ldots,q_N)=\psi(q_1)\cdots\psi(q_N)\ . \tag{1.1}$$

There is an operator, called the relative-frequency operator f_a^N, which corresponds to measuring the value of q on each subsystem in turn, and then computing the relative frequency with which a given value, $q=a$ say, occurs. It can be shown that in the limit $N\to\infty$, Ψ is an eigenstate of this operator with eigenvalue $|\psi(a)|^2$ (Refs. 2 and 3). That is,

$$f_a^\infty\Psi=|\psi(a)|^2\Psi\ . \tag{1.2}$$

In accordance with the above postulate, measurement of the relative frequency returns the value $|\psi(a)|^2$, with certainty, in the limit of an infinite number of subsystems. It is in this way that the familiar probabilistic interpretation of quantum mechanics is recovered from QMIS.

It must be emphasized that it is the subsystem wave function ψ that is associated with the notion of probability, not the individual system wave function Ψ. The formalism of QMIS does not in any way associate Ψ with probability. Individual systems, such as those encountered in quantum cosmology, will not in general consist of a large number of identical subsystems, in which case the notion of probability does not enter the theory at all.

For those observables of which the quantum state of the individual system is an eigenstate, there is no difficulty in making predictions. However, it is quite possible, if not most probable, that in situations of interest the state is only an approximate eigenstate in some sense. An important example is provided by the case described above. The wave function (1.1) is an exact eigenstate of the relative-frequency operator only in the limit $N \rightarrow \infty$. For the physically realistic case of large but finite N, it will be only an approximate eigenstate. How are we to interpret this?

Let us begin by elaborating on the notion of an approximate eigenstate. Suppose $|\Psi\rangle$ is an eigenstate of an observable Q, $Q|\Psi\rangle=\lambda|\Psi\rangle$. Introduce a complete set of eigenstates of Q, $|q\rangle$ say, where $Q|q\rangle=q|q\rangle$. Then one may write

$$|\Psi\rangle=\int dq\,|q\rangle\langle q|\Psi\rangle\ . \tag{1.3}$$

Since $|\Psi\rangle$ is an eigenstate of Q, $\langle q|\Psi\rangle$ is a δ function $\delta(q-\lambda)$. If, however, $|\Psi\rangle$ was only an approximate eigenstate of Q, then $\langle q|\Psi\rangle$ would be a smooth distribution with a peak of finite height at $q=\lambda$. The question of interpreting such distributions for individual systems has been considered by Hartle,[4] Wada,[5] and Geroch.[6] Hartle offers the following interpretation.

If Ψ is sufficiently peaked about some region in the configuration space, we predict that we will observe the correlations between the observables which characterize this region. If Ψ is small in some region, we predict that observations of the correlations which characterize this region are precluded. Where Ψ is neither small nor sufficiently peaked, we do not predict anything.[4]

The proposal of Wada is very similar.[5] Geroch proposes a version of the Everett interpretation in which all predictions of quantum mechanics are expressed in terms of "precluded regions"—regions in which the wave function is "small." It is then asserted that correlations between the observables which characterize a precluded region will not be observed.[6]

These interpretations hinge very much on the rather vague notions of "sufficiently peaked," "small," and "precluded regions." Naively, one might have thought that in a region in which the wave function was very small, but nonzero, observation of the correlations characterizing this region is not totally impossible. In response to this, I would say that such a belief is based on an understanding of the meaning of the wave function gained from conventional quantum mechanics, in which any configuration for which the wave function is nonzero is not ruled out, since it has nonzero probability. As has already been emphasized, however, one should not in general attempt to associate the wave function with probability in QMIS. In the interpretations of Geroch and Hartle, configurations for which the wave function is "small," even if nonzero, *are* ruled out. They will not be observed. It is perhaps enlightening to quote from Geroch's article at this point: "These precluded regions become the sole 'reality' of the quantum world. Our contact with the quantum world is entirely through an innate understanding we have of precluded configurations."[6]

To conclude this discussion of the interpretation, it is worth remarking that this interpretation of quantum cosmology, in which one takes a peak in the wave function to be a definite prediction, is in fact very much the same as what one does in ordinary quantum mechanics. For in conventional quantum mechanics, one has in practice only a finite number of identical systems, and thus the distribution of the relative frequency operator in the above example is merely peaked about the value $|\psi(a)|^2$. Therefore from the point of view of QMIS, in asserting that $|\psi(a)|^2$ is the probability, one is really taking a peak to be a prediction.

The point of this paper is to apply this type of interpretation to quantum cosmological models of the sort that currently exist in the literature. We shall quite simply look for peaks in the wave function, or in distributions constructed from it. The question of how strongly peaked a distribution has to be before we can regard it as "sufficiently peaked" will not be addressed. The first step in looking for these peaks is the identification of the variables in which one expects the wave function to be peaked, and this we now discuss.

In quantum cosmology the quantum state of the Universe is described by a wave function $\Psi(q)$, which is a solution to the Wheeler-DeWitt equation

$$H\Psi=0\ , \tag{1.4}$$

where H is the Hamiltonian of the system. The "metric representation" is almost always used, in which the variables q are taken to be components of the three-metric h_{ij} and the matter field modes Φ on a three-surface. In this representation, the wave function will not be peaked around particular values of q, unless the model in question possessed static solutions, which are not of cosmological interest. Nor will it be peaked at particular values of p, the momentum conjugate to q, unless the wave function is a plane wave, which is not usually the case. Rather, one would expect that in certain regions the wave function is peaked around a set of classical solutions (in general nonstatic), i.e., around some kind of correlation between p and q. We will discuss methods for identifying such correlations, and this will allow us to see the manner in which the wave function becomes peaked about sets of solutions to the classical field equations. Although the ultimate aim is to discuss quantum cosmology, we will devote some space to discussing some simple examples from quantum mechanics.

We begin in Sec. II by introducing methods whereby correlations between coordinates and momenta may be identified, in the context of nonrelativistic quantum mechanics. The main tool with which this is achieved is Wigner's function, a quantum-mechanical analogue of a classical phase-space distribution. This distribution function has been used before in the literature, but purely as a mathematical device with which to calculate expectation values. Since it can be negative, it has not previously been interpreted as predicting correlations between coordinates and momenta. We show, however, that it can be so interpreted, in certain situations of interest. In order to back up the results derived from Wigner's function, we show how a suitably chosen canonical transformation may also be used to verify a peak about a given region of phase space. These techniques are applied to some simple examples in Sec. III. They are the upside-down harmonic oscillator, the conventional harmonic oscillator, and a set of many harmonic oscillators. It is shown that the methods of Sec. II yield peaks about sets of classical solutions, in the regions where one would expect the behavior to be essentially classical. These results are relevant to the study of scalar field fluctuations in inflationary universe models—they shed some light on the transition from the quantum to the classical regime.

In Sec. IV WKB wave functions—wave functions of the form e^{iS}—are considered. It is shown that these wave functions are peaked around the hypersurface in phase space $p=\partial S/\partial x$. These wave functions are closely related to the minisuperspace wave functions of quantum cosmology, which are discussed in Sec. V. The general formalism of these models is presented. It is shown that a particular solution to the Wheeler-DeWitt equation is peaked around a subset of solutions to the field equations. It is in this way that boundary conditions for the Wheeler-DeWitt equation lead, in the classical limit, to initial conditions on the classical solutions. In Secs. VI and VII we consider perturbations about minisuperspace. The main point of this is to consider the derivation of the semiclassical Einstein equations,

$$G_{\mu\nu}=8\pi G\langle T_{\mu\nu}\rangle \tag{1.5}$$

from the Wheeler-DeWitt equation. Using the interpretation described above, we derive a condition under which the semiclassical Einstein equations are valid. It is essentially that the distribution of $T_{\mu\nu}$, as a function of the matter modes, is strongly peaked when $T_{\mu\nu}$ is equal to its expectation value. Some situations in which this condition is satisfied are discussed. Our conclusions are presented in Sec. VII.

II. CORRELATIONS BETWEEN COORDINATES AND MOMENTA

As already discussed in the Introduction, wave functions in quantum cosmology, in which we are ultimately interested, will be peaked not about particular values of x or p, but about some kind of correlation between them. In this section, therefore, we introduce methods for the identification of correlations between x and p. These methods will be discussed in the familiar context of nonrelativistic quantum mechanics, described by the Schrödinger equation

$$i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+V(x)\Psi\ . \tag{2.1}$$

The generalization to quantum cosmology will be considered in later sections.

A. Wigner's function

The first method we will use to identify the correlations between x and p in the quantum state $\Psi(x,t)$ involves the introduction of a quantum-mechanical analogue of the classical probability distribution on phase space. A candidate for such a distribution is the joint probability distribution of Wigner.[7–9] It is given by

$$F(x,p,t)=\int_{-\infty}^{\infty}du\ \Psi^*(x-\tfrac{1}{2}\hbar u,t)\times e^{-ipu}\Psi(x+\tfrac{1}{2}\hbar u,t)\ . \tag{2.2}$$

It has the properties

$$\int_{-\infty}^{\infty}dp\ F(x,p,t)=|\Psi(x,t)|^2\ , \tag{2.3}$$

$$\int_{-\infty}^{\infty}dx\ F(x,p,t)=|\tilde{\Psi}(p,t)|^2\ , \tag{2.4}$$

where $\tilde{\Psi}(p,t)$ is the Fourier transform of $\Psi(x,t)$. It follows that F may be used to obtain the correct expectation values of any function of the coordinates or momenta. For example, $\langle x\rangle$, the expectation value of x, normally given in terms of the usual inner product by $(\Psi,x\Psi)$, is given in terms of Wigner's function by

$$\langle x\rangle=\int_{-\infty}^{\infty}dx\int_{-\infty}^{\infty}dp\ xF(x,p,t)\ . \tag{2.5}$$

Wigner's function can give incorrect results for quantities of the form $\langle xp\rangle$, unless care is taken with operator ordering, but this will not affect any of the results of this paper. Using (2.1), one may derive the following equation for F:

$$\frac{\partial F}{\partial t}+\frac{p}{m}\frac{\partial F}{\partial x}-\frac{dV}{dx}\frac{\partial F}{\partial p}=\frac{\hbar^2}{24}\frac{d^3V}{dx^3}\frac{\partial^3F}{\partial p^3}+\cdots\ . \tag{2.6}$$

In deriving (2.6), it was assumed that $V(x)$, the potential in the Schrödinger equation, could be expanded in a Taylor series. The ellipsis indicates higher-order terms in this series, involving higher powers of $\hbar$ and higher derivatives of V and F.

The existence of a quantum-mechanical probability distribution on phase space may be a little surprising at first sight, bearing in mind that one cannot measure x and p simultaneously. However, although F is real, it may take negative values, so it is not a genuine probability distribution. It is because of this property that previous authors have declined to interpret Wigner's function as a physically significant probability distribution on phase space. Rather, they regarded it merely as a mathematical object in terms of which one could develop an alternative formulation of quantum mechanics.[8] Consider however, the equation for F, (2.6). If either (i) the third and higher derivatives of V were identically zero, or (ii) terms of order $\hbar^2$ were neglected, then (2.6) would be precisely the continuity equation for a *classical* probability distribution on phase space. In this paper we will be considering quadratic potentials, for which (i) is certainly true, or we will work in the WKB approximation, for which (ii) is true. Moreover, F will turn out to be positive in the cases we consider. It follows therefore, that in these cases, one *can* regard F as a physically significant joint probability distribution on phase space, and this is indeed what we shall do here.

The natural way to interpret this joint probability distribution is as follows: if F is of the form $F_1(x,t)F_2(p,t)$, then we shall say that the wave function predicts no correlation between x and p; if, on the other hand, F is strongly peaked about some region of phase space, $p=g(x)$ say, then we shall say that the wave function predicts this particular correlation between the coordinates and momenta. The expression $p=g(x)$ typically turns out to be a first integral of the equations of motion.

B. Canonical transformation

A second method for showing that the wave function is peaked about a particular region of phase space is to perform a canonical transformation. Classically, one may transform from the variables x,p to new canonical variables $\bar{x},\bar{p}$ using the generating function $G_0(x,\bar{p})$:

$$p=\frac{\partial G_0}{\partial x}, \quad \bar{x}=\frac{\partial G_0}{\partial \bar{p}} . \tag{2.7}$$

In quantum mechanics the transformation from the wave function $\Psi(x,t)$ to the new wave function $\chi(\bar{p},t)$ is given by

$$\chi(\bar{p},t)=\int_{-\infty}^{\infty} dx \exp\left[-\frac{i}{\hbar}G(x,\bar{p})\right]\Psi(x,t) . \tag{2.8}$$

The quantum-mechanical generating function G may be determined by demanding that $\chi(\bar{p},t)$ satisfies the Schrödinger equation derived from the new variables $\bar{x},\bar{p}$, given that $\Psi(x,t)$ satisfies that derived from the old variables x,p. One thus finds that $G=G_0+\hbar G_1+\cdots$ where G_0 is the classical generating function. We will work only to leading order in $\hbar$ when using this method, so G_1 will not be required.[10]

The idea now is to choose the new canonical variables so that the region of phase space of interest is given by $\bar{p}=0$. The new wave function (2.8) will then indicate the extent to which there is a peak about this region. This method is less powerful than the previous one, in that it is necessary to anticipate the correlation in advance in order to choose correctly the canonical transformation. It will be used merely to back up the results obtained using Wigner's function.

III. SIMPLE QUANTUM-MECHANICAL EXAMPLES

In order to fix ideas and demonstrate the usefulness of Wigner's function, we apply the methods of the previous section to some simple exactly soluble models, with a quadratic potential.

A. The upside-down simple harmonic oscillator

The first example is the upside-down simple harmonic oscillator (USHO), i.e., a particle moving in one dimension with the potential

$$V(x)=-\tfrac{1}{2}kx^2, \quad k>0 . \tag{3.1}$$

This model has previously been used by Guth and Pi to discuss the "slow roll down" of the scalar field in inflationary universe models.[11] The Schrödinger equation for the model is

$$i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}-\tfrac{1}{2}kx^2\Psi . \tag{3.2}$$

It may be solved by the ansatz

$$\Psi(x,t)=A(t)\exp[-B(t)x^2] . \tag{3.3}$$

The wave function is taken to be a Gaussian at $t=0$, centered at $x=0$; thus $B(t)$ is real at $t=0$. The normalized solution satisfying this initial condition is

$$B(t)=\frac{(mk)^{1/2}}{2\hbar}\frac{\sin 2\phi-i\sinh 2\omega t}{\cos 2\phi+\cosh 2\omega t} , \tag{3.4}$$

$$A(t)=\left[\frac{(mk)^{1/2}\sin 2\phi}{2\pi\hbar}\right]^{1/4}[\cos(\phi-i\omega t)]^{-1/2} , \tag{3.5}$$

where ϕ is an arbitrary real constant and $\omega=(k/m)^{1/2}$. ϕ is restricted in such a way that $\sin 2\phi>0$ for $\mathrm{Re}B>0$ and so for (3.3) to be square integrable.

Before looking for the peaks in this wave function, consider first the classical solutions. Classically, $x(t)$ satisfies the equation $\ddot{x}-\omega^2x=0$ which has solution $x(t)\approx De^{\omega t}$ for $t\gg 0$, for some constant D. Since $p=m\dot{x}$, this corresponds to the path in phase space

$$p\approx(mk)^{1/2}x . \tag{3.6}$$

We now calculate Wigner's function for the USHO. Inserting (3.3) into (2.2), one obtains

$$F(x,p,t)=\exp\left[\frac{-p^2-4\hbar^2|B|^2x^2+2i\hbar(B-B^*)xp}{B+B^*}\right] . \tag{3.7}$$

Here, the normalization $(\Psi,\Psi)=1$ has been used to eliminate $A(t)$. Since the exponent is real, F is positive.

At $t=0$, $B(t)$ is real, hence

$$F(x,p,t)=\exp\left[-\frac{p^2}{B+B^*}\right]\times\exp\left[-\frac{4\hbar^2|B|^2x^2}{B+B^*}\right] . \tag{3.8}$$

The distribution is thus a product of a function of x and a function of p. It follows that there is no correlation between x and p. For $t \gg 0$, on the other hand,

$$B \approx \frac{(mk)^{1/2}}{\hbar}\left[\sin 2\phi e^{-2\omega t} - \frac{i}{2}\right] \tag{3.9}$$

and Wigner's function is then given by

$$F(x,p,t) \approx \exp\left[-\frac{e^{2\omega t}}{2\hbar(mk)^{1/2}\sin 2\phi} \times [p-(mk)^{1/2}x]^2\right] . \tag{3.10}$$

As $t \to \infty$, therefore, the distribution becomes progressively more peaked about the trajectory $p=(mk)^{1/2}x$, the classical trajectory in phase space.

From (3.7) one can see the condition that must be satisfied for F to be peaked around the classical path in phase space. It is $|\text{Re}B| \ll |\text{Im}B|$. This property of Wigner's function—that it allows one to see the conditions under which one may use classical physics—is an advantage over the distribution used by Guth and Pi.[11] They wrote down the distribution $|\Psi(x,t)|^2\delta(p-(mk)^{1/2}x)$ and then justified its use afterwards. They also needed to invoke other arguments to establish its range of validity.

The result that the wave function predicts the peak about a path in phase space may also be derived using the canonical transformation

$$\bar{p} = p-(mk)^{1/2}x, \quad \bar{x} = x . \tag{3.11}$$

This transformation is generated by the generating function $G_0 = x\bar{p} + \frac{1}{2}(mk)^{1/2}x^2$. Inserting (3.3) into (2.8) and taking B to be given by (3.9), one finds that the term proportional to x^2 in G_0 cancels the imaginary part of B. To leading order in $\hbar$, one thus obtains

$$\chi(\bar{p},t) = \int_{-\infty}^{\infty} dx \exp\left[-\frac{i}{\hbar}x\bar{p} - \frac{(mk)^{1/2}\sin 2\phi}{\hbar} \times e^{-2\omega t}x^2\right]$$
$$= \exp\left[-\frac{e^{2\omega t}}{4\hbar(mk)^{1/2}\sin 2\phi}\bar{p}^2\right] . \tag{3.12}$$

This wave function becomes progressively more peaked about $\bar{p}=0$ as $t \to \infty$, so once again we see the peaking around the classical trajectory $p=(mk)^{1/2}x$. Note that although the wave function is peaked about a single path in phase space, this corresponds to a set of classical solutions in configuration space. The wave function is therefore regarded as corresponding to a superposition of classical solutions satisfying the first integral (3.6).

B. The (rightway-up) simple harmonic oscillator

Our second example is the conventional harmonic oscillator, i.e., a particle moving in one dimension in the potential

$$V(x) = +\tfrac{1}{2}kx^2, \quad k>0 . \tag{3.13}$$

Normally one solves the Schrödinger equation for this model by expanding the wave function in eigenfunctions of the Hamiltonian. Here, however, for simplicity, we will again use the ansatz (3.3). This ansatz is appropriate to the situation in which one has a time-dependent SHO which starts out in its ground state, a situation which arises when considering the functional Schrödinger quantization of a scalar field in an inflationary universe model.[11,12]

The general solution for $B(t)$ is

$$B(t) = \frac{(mk)^{1/2}}{2\hbar}\frac{\sinh 2\phi - i\sin 2\omega(t-t_0)}{\cosh 2\phi - \cos 2\omega(t-t_0)} , \tag{3.14}$$

where ϕ is again an arbitrary real constant and $\omega=(k/m)^{1/2}$. We restrict ϕ to be positive, for $\text{Re}B>0$. In the case of the USHO, the correlation between x and p changed in time—the wave function became progressively more peaked about a superposition of classical paths as the particle rolled down the potential. In this case, however, $B(t)$ is oscillatory in t, and the wave function does not change over long time scales $t \gg \omega^{-1}$. For each value of the arbitrary constant ϕ, it is in a particular superposition of energy eigenstates. The precise relation between ϕ and the coefficients of the superposition may be determined by expanding (3.3) in energy eigenstates. For $\phi \gg 0$, one finds that the wave function is essentially in the ground state and Wigner's function is given by

$$F(x,p,t) = \exp\left[-\frac{\hbar p^2}{(mk)^{1/2}}\right]\exp[-\hbar(mk)^{1/2}x^2] . \tag{3.15}$$

x and p are therefore uncorrelated, and there is no peak about a trajectory in phase space. For $\phi \approx 0$, on the other hand, one finds that the wave function is in a superposition of excited states and Wigner's function is then given by

$$F(x,p,t) = \exp\left[-\frac{2\hbar\sin^2\omega(t-t_0)}{(mk)^{1/2}\sinh\phi} \times [p-(mk)^{1/2}\cot\omega(t-t_0)x]^2\right] . \tag{3.16}$$

F is therefore peaked about the correlation

$$p = (mk)^{1/2}\cot\omega(t-t_0)x ,$$

which is a first integral of the equations of motion. Unlike the previous case, this first integral involves the arbitrary constant t_0, because we did not impose an initial condition on the wave function.

C. Many identical harmonic oscillators

In the previous examples, it was shown that the wave function could become peaked around the region of phase space corresponding to a first integral of the equations of motion. On integration, this corresponds to a set of paths in configuration space, e.g., the set $x = De^{\omega t}$, for the USHO case, parametrized by the arbitrary constant D. In the region where the wave function exhibits this behavior, one can then interpret $|\Psi|^2$ as a probability measure on this set of solutions: $|\Psi(x,t)|^2 dx$ is the probability that one of the classical trajectories will pass through the surface t=const between x and $x+dx$ (Ref. 13).

This measure on the classical paths is not very interesting unless it is strongly peaked at some value of x, at each time t. In the previous examples, $|\Psi|^2$ is a Gaussian peaked at $x=0$, but the peak is not very strong. A much more interesting case is that of N identical harmonic oscillators (either SHO or USHO), for large N. The total wave function for this system is

$$\Psi_N(x_1,\ldots,x_N,t)=\Psi(x_1,t)\cdots\Psi(x_N,t) , \tag{3.17}$$

where each wave function $\Psi(x_i,t)$ is taken to be of the form (3.3), with $A(t)$ and $B(t)$ independent of i; thus,

$$\Psi_N(x_1,\ldots,x_N,t)=A^N(t)\exp\left[-B(t)\sum_{i=1}^{N}x_i^2\right] . \tag{3.18}$$

Again the probability of finding the particle between $\{x_i\}$ and $\{x_i+dx_i\}$ at time t is

$$|\Psi_N|^2 dx_1\cdots dx_N , \tag{3.19}$$

which is peaked at $x_i=0$. However, the wave function depends not on the individual x_i's, but only on the variable r, defined by

$$r^2=x_1^2+\cdots+x_N^2 ; \tag{3.20}$$

thus it is of interest to ask for the distribution of r. Change variables, therefore, from $\{x_i\}$ to spherical polars $\{r,\theta_1,\ldots,\theta_{N-1}\}$, where the θ's are angular variables. The probability distribution of r is then given by

$$|\Psi_N|^2 r^{N-1} dr\, d\Omega_{N-1} , \tag{3.21}$$

where $d\Omega_{N-1}$ is a measure over the angular variables on which the wave function does not depend. It is easy to show that the distribution (3.21) is peaked around

$$r=r_p\equiv\left[\frac{N-1}{2(B+B^*)}\right]^{1/2} . \tag{3.22}$$

The significance of this may be seen by computing the rms value of r. It is

$$\langle r^2\rangle^{1/2}=\left[\sum_i\langle x_i^2\rangle\right]^{1/2}=\left[\frac{N}{2(B+B^*)}\right]^{1/2} . \tag{3.23}$$

For large N therefore, the distribution of r is strongly peaked around a value very close to $r=\langle r^2\rangle^{1/2}$.

This result, first outlined by Wada,[5] is a special case of a more general result which is essentially the central limit theorem. Suppose rather than r^2, one has a more general quantity M_N of the form

$$M_N(x_1,\ldots,x_N)=M(x_1)+\cdots+M(x_N) . \tag{3.24}$$

Suppose also that one has a system again with a wave function of the form (3.17), but here with no assumptions made about the wave function for the identical subsystems $\Psi(x_i,t)$. Then $\langle M_N\rangle=N\langle M\rangle$ with $\langle M\rangle$ independent of the subsystem label i. Now let us consider the deviation of M_N from its average value. This is given by the variance ΔM_N. Now

$$\begin{aligned}(\Delta M_N)^2&=\langle M_N{}^2\rangle-\langle M_N\rangle^2\\&=N\langle M^2\rangle+(N^2-N)\langle M\rangle^2-N^2\langle M\rangle^2 .\end{aligned} \tag{3.25}$$

One therefore has

$$\frac{(\Delta M_N)^2}{\langle M_N\rangle^2}=\frac{1}{N}\frac{\langle M^2\rangle-\langle M\rangle^2}{\langle M\rangle^2} \tag{3.26}$$

and this tends to zero as $N\to\infty$. It follows that the distribution of M_N becomes progressively more peaked about its average value as N becomes large.

The simple models of this section are relevant to scalar field theory in inflationary universe models, not only for the homogeneous mode—as discussed by Guth and Pi[11]—but also for the inhomogeneous modes. Close to the maximum, or the minimum, of an inflationary potential, the scalar field modes will behave, respectively, like a USHO or an SHO. The above results then allow one to determine the conditions under which it is permissible to replace the quantum-mechanical evolution with classical evolution. Moreover, the results of Sec. III C indicate why one can take $\langle\Phi_{\rm op}{}^2\rangle$ as the initial value for Φ^2, where $\Phi_{\rm op}$ is the operator-valued quantum field and Φ is its classical counterpart. As we shall see in Sec. VII, when expanded in harmonics, Φ decomposes into sets of n^2 identical harmonic oscillators, where n is the mode label. For large n, the distribution of the modes will be peaked very close to their rms value. This quantum to classical transition is discussed further in Refs. 13 and 14.

IV. WKB WAVE FUNCTIONS

In this section, to make the link with quantum cosmology, we apply the methods of the previous section to WKB wave functions, that is, to wave functions of the form

$$\Psi=C(x,t)\exp\left[\frac{i}{\hbar}S(x,t)\right] . \tag{4.1}$$

Wave functions of this type emerge when one solves the Schrödinger equation using the WKB approximation, regarding $\hbar$ as a small parameter, as we now show. Inserting (4.1) into the Schrödinger equation (2.1), one finds that the order-$\hbar^0$ terms yield the Hamilton-Jacobi equation for S:

$$-\frac{\partial S}{\partial t}=\frac{1}{2m}\left[\frac{\partial S}{\partial x}\right]^2+V(x) . \tag{4.2}$$

Similarly, the order-$\hbar^1$ terms yield an equation for C:

$$\frac{1}{m}\frac{\partial S}{\partial x}\frac{\partial C}{\partial x}+\frac{\partial C}{\partial t}=-\frac{1}{2m}\frac{\partial^2 S}{\partial x^2}C . \tag{4.3}$$

Solutions to the Schrödinger equation of the form (4.1), with S real, typically arise in regions in which the behavior is essentially classical. We will show that (4.1) is peaked around the region of phase space described by the equation $p=\partial S/\partial x$. This equation defines a first integral to the classical equations of motion, as may be shown using the Hamilton-Jacobi equation (4.2).

Strictly speaking, one cannot apply the methods of the previous section [i.e., calculate Wigner's function or perform the canonical transformation (2.8)] for wave functions of the form (4.1) because they are not in general square integrable. However, we are assuming that (4.1) is an approximation to a square integrable wave function, valid in some region, and that there are small imaginary corrections to S which will make (4.1) square integrable. In the harmonic oscillators of the previous section, for example, the wave functions are of the form (4.1) for $t \gg 0$ in the USHO case and for $\phi \approx 0$ in the SHO case. In the exact wave functions for these cases there are extra terms in the exponent which would not be noticed by the WKB approximation if S is taken to be real, and these terms are indeed sufficient to make the wave functions square integrable. These extra terms merely spread out the peaks we are looking for—they do not alter their location.

We begin by calculating Wigner's function for (4.1). Inserting (4.1) into (2.2) one obtains

$$F(x,p,t)=\int_{-\infty}^{\infty} du\; C^*(x-\tfrac{1}{2}\hbar u)C(x+\tfrac{1}{2}\hbar u) \times\exp\left[-iup-\frac{i}{\hbar}S(x-\tfrac{1}{2}\hbar u)+\frac{i}{\hbar}S(x+\tfrac{1}{2}\hbar u)\right], \tag{4.4}$$

where the dependence on t has been suppressed. The integral can be evaluated approximately by expanding the integrand to order $\hbar^2$. Since S is real, it follows from (4.3) that C is also, and thus the expansion of the terms involving C in the integrand yields

$$C^*(x-\tfrac{1}{2}\hbar u)C(x+\tfrac{1}{2}\hbar u)=C^2(x)+O(\hbar^2)\ . \tag{4.5}$$

Similarly,

$$S(x+\tfrac{1}{2}\hbar u)-S(x-\tfrac{1}{2}\hbar u)=\hbar u\frac{dS}{dx}(x)+O(\hbar^3)\ . \tag{4.6}$$

Equation (4.4) may thus be evaluated to yield

$$F(x,p,t)=|C(x)|^2\delta(p-\partial S/\partial x) \tag{4.7}$$

plus terms of order $\hbar^2$. There is therefore a peak on the first integral $p=\partial S/\partial x$. The prefactor C gives a probability measure on the set of trajectories in configuration space for which $m\dot{x}=p=\partial S/\partial x$: $|C(x,t)|^2dx$ is the probability that a trajectory $x(t)$ will intersect the surface $t=\text{const}$ between x and $x+dx$. Equation (4.3) guarantees that this probability is independent of the choice of surface $t=\text{const}$, i.e., it expresses conservation of probability.

One can derive the same result by performing a canonical transformation to new variables $\bar{p},\bar{x}$ defined by

$$\bar{p}=p-\frac{\partial S}{\partial x},\quad \bar{x}=x\ . \tag{4.8}$$

This transformation is generated by the generating function $G_0(x,\bar{p})=x\bar{p}+S(x,t)$. To leading order, (2.8) then yields

$$\chi(\bar{p},t)=\delta(\bar{p})\ ; \tag{4.9}$$

hence there is a peak at $\bar{p}=0$. The prefactor C is not included here because it contributes at the same order as the quantum correction G_1 to the classical generating function, and we have not calculated G_1.

It is also of interest to consider the case when S is purely imaginary, $iS=-I$ say, where I is real and positive. This situation arises in regions which are normally regarded as classically forbidden, such as tunneling regions. Wigner's function is then given by

$$F(x,p,t)=\int_{-\infty}^{\infty} du\; C^*(x-\tfrac{1}{2}\hbar u)C(x+\tfrac{1}{2}\hbar u) \times\exp\left[-iup-\frac{1}{\hbar}I(x-\tfrac{1}{2}\hbar u)-\frac{1}{\hbar}I(x+\tfrac{1}{2}\hbar u)\right]. \tag{4.10}$$

The important difference between (4.10) and (4.4) is that the two terms involving I in (4.10) have the same sign, whereas in (4.4) the two terms involving S have opposite signs. To order $\hbar$, (4.10) yields

$$F(x,p,t)=|C(x)|^2\exp\left[-\frac{2}{\hbar}I(x)\right]\delta(p)\ . \tag{4.11}$$

The important feature of this expression is that it is a product of a function of p and a function of x. It follows x and p are uncorrelated. There is therefore no peaking about a set of classical paths, which is consistent with regarding the region under consideration as classically forbidden.

V. QUANTUM COSMOLOGY: MINISUPERSPACE MODELS

The examples of the previous sections have paved the way for the discussion of peaks in the wave function in quantum cosmology, to which we now turn. Quantum cosmology involves the quantization of gravity coupled to matter using the as-yet incomplete formalism of quantum gravity. One represents the quantum state of the Universe by a wave function $\Psi[h_{ij},\Phi]$, a functional on superspace, the space of all three-metrics h_{ij} and matter field configurations on a three-surface, normally taken to be compact.[15] The full superspace formalism of quantum cosmology is very difficult to deal with in practice since it involves functional differential equations—differential equations in an infinite number of variables. Attention has been concentrated, therefore, on simplified models whose configuration space is a finite-dimensional approximation to superspace called minisuperspace. A minisuperspace is defined by restricting the metric and matter fields to a particular functional form in such a way that all but a finite number of modes of the fields are frozen. In a minisuperspace model, therefore, the state of the system is described by a finite number of variables $q^a(t)$, say, where $a=1,2,\ldots,n$. There are clearly many ways in which minisuperspace approximations to the full superspace can be constructed.[16] The most common way is to restrict the fields to be homogeneous. For example, $q^a(t)$, with $a=1,2$, could represent the scale factor of a Robertson-Walker metric and the homogeneous mode of a scalar field. We begin by describing the general formalism of minisuperspace models.

The standard 3 + 1 form of the metric is

$$ds^2=-(N^2-N_iN^i)dt^2+2N_i dx^i dt + h_{ij}dx^i dx^j \ , \qquad (5.1)$$

where $i,j=1,2,3$. N is the lapse function and N_i is the shift vector. It is most common to take N to be homogeneous $N=N(t)$ and $N_i=0$. We shall do that here. For the case in which the matter source is bosonic, a wide range of minisuperspace models are described by an action of the form

$$I=\int L\,dt = M^2\int dt\, N\left[\frac{1}{2N^2}f_{ab}(q^c)\dot q^a\dot q^b-U(q)\right] , \qquad (5.2)$$

where f_{ab} is a metric on minisuperspace and M is the Planck mass. $q^a(t)$ represents certain components of the three-metric h_{ij} and certain modes of the matter fields. This action is obtained by inserting the minisuperspace ansatz for the metric and matter fields into the full action for the gravity-plus-matter system. The gravitational action may be the usual Einstein-Hilbert action but may also include higher derivative terms. [It must be remarked that the field equations derived by varying the action (5.2) will not in general be the same as those obtained by varying the full action and then inserting the minisuperspace ansatz. In most of the minisuperspace models constructed so far, however, this problem does not arise.] The remnant of general covariance in (5.2) is reparametrization invariance, which expresses itself through the arbitrariness of the lapse function $N(t)$.

Variation with respect to q^a yields the field equations

$$\frac{1}{N}\frac{d}{dt}\left[\frac{1}{N}\dot q^a\right]+\frac{1}{N^2}\Gamma^a_{bc}\dot q^b\dot q^c+f^{ab}\frac{\partial U}{\partial q^b}=0 , \qquad (5.3)$$

where f^{ab} is the inverse metric and

$$\Gamma^a_{bc}=\tfrac{1}{2}f^{ad}(f_{db,c}+f_{dc,b}-f_{bc,d}) . \qquad (5.4)$$

Equation (5.3) describes geodesic motion with a forcing term in minisuperspace. Variation with respect to N yields the constraint

$$\frac{1}{2N^2}f_{ab}\dot q^a\dot q^b+U(q)=0 . \qquad (5.5)$$

It is important to note that the general solution to the system (5.3),(5.5) will involve $(2n-1)$ arbitrary parameters. Equations (5.3) and (55.) are equivalent, respectively, to the space-space and time-time components of the Einstein equations.

Canonical momenta are defined in the usual manner:

$$p_a=\frac{\partial L}{\partial \dot a^a}=M^2 f_{ab}\frac{1}{N}\dot q^b . \qquad (5.6)$$

The Hamiltonian is then given by

$$H=p_a\dot q^a-L=N\left[\frac{1}{2M^2}f^{ab}p_ap_b+M^2U(q)\right] . \qquad (5.7)$$

Since N is arbitrary, the Hamiltonian vanishes. One thus obtains the Hamiltonian constraint

$$H=0 \qquad (5.8)$$

which is just the phase space form of (5.5). Strictly, one ought to use the Dirac procedure for constrained Hamiltonian systems to analyze this system, but this is very straightforward and leads to the same conclusions. The Hamilton equations derived from (5.7) lead to the phase-space form of (5.3), which is

$$\frac{1}{N}\frac{dp^a}{dt}+\frac{1}{M^2}\Gamma^a_{bc}p^bp^c+M^2f^{ab}\frac{\partial U}{\partial q^b}=0 . \qquad (5.9)$$

Here the indices on the momenta are raised and lowered using the metric f_{ab}.

Using the substitutions $p_a\to -i\partial/\partial q^a$, the Hamiltonian constraint is quantized to yield the Wheeler-DeWitt equation:

$$\left[-\frac{1}{2M^2}\nabla^2+M^2U\right]\Psi(q^c)=0 \qquad (5.10)$$

(in this and the next section we use units in which $\hbar=1$). We have chosen an operator ordering in (5.10) such that $-f^{ab}p_ap_b$ is replaced by ∇^2, the Laplacian in the metric f_{ab}. Other operator orderings are possible, but this one seems to be the most natural, having the virtue of being invariant under changes of coordinates in minisuperspace. One can also include a curvature term $\mathbb{R}$, the curvature constructed from f_{ab}. These choices relating to operator ordering will not affect the conclusions of this paper. f_{ab} is almost always of hyperbolic signature, in which case the Wheeler-DeWitt equation has the form of a Klein-Gordon equation in an n-dimensional curved space-time, with a space-time-dependent mass term.

On solving the Wheeler-DeWitt equation, one in general finds that there are regions in which the behavior of the wave function is predominantly exponential and regions in which it is predominantly oscillatory. We shall interpret the exponential regions as classically forbidden regions, since, as argued in the previous section, a wave function of this type does not indicate a strong correlation between coordinates and momenta—it is not peaked about a particular path in phase space. It has been argued elsewhere that an exponential wave function corresponds, in the classical limit, not to a Lorentzian four-geometry, but to a Euclidean four-geometry.[17] This argument is in turn based on the assertion that the Wheeler-DeWitt equation is the same if the canonical quantization formalism leading to its derivation is in terms of a Euclidean four-metric rather than the usual Lorentzian one. Not all authors are in agreement on this point, however.[18]

To interpret the wave function in the oscillatory region, one may use the WKB approximation, in which one writes

$$\Psi(q)=\exp[iM^2S_0(q)+iS_1(q)+O(M^{-2})] \ , \qquad (5.11)$$

where S_0 is real and M is regarded as a large parameter. Inserting (5.11) into (5.10), the order M^2 terms yield the Hamilton-Jacobi equation

$$\tfrac{1}{2}f^{ab}\frac{\partial S_0}{\partial q^a}\frac{\partial S_0}{\partial q^b}+U(q)=0 \ . \qquad (5.12)$$

The order-M^0 terms yield an equation for S_1:

$$-i\nabla^2S_0+2f^{ab}\frac{\partial S_0}{\partial q^a}\frac{\partial S_1}{\partial q^b}=0 \ . \qquad (5.13)$$

S_0 is real, so S_1 is purely imaginary and the WKB prefactor $C=e^{iS_1}$ is real.

As in the previous section, we shall argue that the wave function (5.11) is peaked around the hypersurface in phase space

$$p_a=M^2\frac{\partial S_0}{\partial q^a} \ . \qquad (5.14)$$

Before doing this let us show that (5.14) is a solution to the field equations. Clearly the p_a defined by (5.14) satisfy the constraint equation (5.8), by virtue of (5.12). To show that (5.12) satisfies (5.9), differentiate (5.12) with respect to q^c. One thus obtains

$$\tfrac{1}{2}f^{ab}{}_{,c}\frac{\partial S_0}{\partial q^a}\frac{\partial S_0}{\partial q^b}+f^{ab}\frac{\partial S_0}{\partial q^a}\frac{\partial^2 S_0}{\partial q^b\partial q^c}+\frac{\partial U}{\partial q^c}=0 \ . \qquad (5.15)$$

The form of the second term in (5.15) invites the introduction of the vector

$$\frac{d}{d\tau}=f^{ab}\frac{\partial S_0}{\partial q^a}\frac{\partial}{\partial q^b} \qquad (5.16)$$

for some parameter τ. When operated on q^c it implies, via (5.14), the usual relation between velocities and momenta (5.6), provided that τ is identified with proper time $\int N\,dt$. Using (5.14), (5.15) may now be written

$$\frac{dp_c}{d\tau}+\frac{1}{2M^2}f^{ab}{}_{,c}p_ap_b+M^2\frac{\partial U}{\partial q^c}=0 \ . \qquad (5.17)$$

Using f^{ab} to raise the indices on the momenta, after some rearrangement one obtains (5.9), as required.

Consider now the interpretation of the wave function (5.11). As in the previous section, one would expect to be able to show that this wave function predicts correlation between coordinates and momenta of the form (5.14). This can be done by introducing appropriate generalizations of Wigner's function (2.2) and the canonical transformation (2.8). Equation (2.2) becomes

$$F(q^a,p_a)=\int d^nu[-f(u)]^{1/2}\Psi^*(q^a-\tfrac{1}{2}u^a) \times e^{-iu^ap_a}\Psi(q^2+\tfrac{1}{2}u^a) \ , \qquad (5.18)$$

where $f=\det(f_{ab})$, and (2.8) becomes

$$\chi(\bar{p}_a)=\int d^nq[-f(q)]^{1/2}\exp[-iG(q^a,\bar{p}_a)]\Psi(q^a) \ , \qquad (5.19)$$

where $G=q^a\bar{p}_a+S_0(q)$. As in the previous section the WKB wave functions (5.11) are not square integrable. In the case of nonrelativistic quantum mechanics, discussed in the previous section, however, it was argued that this presented no problem because the WKB wave functions were approximations to square-integrable wave functions. Indeed, there is a very good physical reason why they should be square integrable. Nonrelativistic quantum mechanics is the theory of point particles which are localized to a perhaps large, but nevertheless finite region of space: $|\Psi|^2$ must go to zero at infinity. Quantum cosmology, on the other hand, deals with the dynamics of closed universes in superspace. There is no analogous physical reason why $|\Psi|^2$ should go to zero at the boundary of superspace. Unless very special, possibly unphysical, boundary conditions are imposed, the wave function will not in general be square integrable. The expressions (5.18) and (5.19) are therefore ill defined. In the absence of a more complete theory of quantum gravity, there is little we can do about this. However, note that in the previous section it was possible to evaluate Wigner's function and the canonical transformation without actually knowing that the WKB wave functions were approximations to square-integrable wave functions. We shall therefore do the same here. It is possible that the justification of this may come from constructing path-integral versions of (5.18) and (5.19) and then evaluating them in the semiclassical approximation. This is very much in line with the recent suggestion of Hartle, that one should abandon attempts to construct a quantum theory of gravity using the conventional machinery of Hilbert space and work instead solely with the path integral.[4]

Using either (5.18) or (5.19), as in the previous section, it is straightforward to show that the WKB-type wave function (5.11) is indeed peaked on the hypersurface in phase space (5.14). This equation is a set of n first-order differential equations for each solution S_0 of the Hamilton-Jacobi equation, and its solution will therefore involve n arbitrary parameters. Recall, however, that the solution to the full set of field equations involved $(2n-1)$ arbitrary parameters. Now suppose one is given a set of boundary conditions for the Wheeler-DeWitt equation. This will select a particular wave function Ψ, which will in turn pick out a particular solution S_0 of the Hamilton-Jacobi equation. This particular solution Ψ, therefore, is peaked around an n-parameter subset of the $(2n-1)$-parameter general solution to the field equations. In accordance with the interpretational scheme for quantum cosmology outlined in the Introduction, we therefore predict that an observer in the Universe represented by this minisuperspace model will perceive it to be described by one of the solutions to the Einstein field equations satisfying the first integral (5.14).

Finally, note that it has not been necessary to decide how large the peak in the wave function (or in Wigner's function) has to be before it is "sufficiently peaked." This is because the peak is a δ-function peak in the WKB approximation. If we were to go beyond this approximation then the peak would become smeared out and the question of whether or not the peak is sufficiently large would arise. However, in the absence of a more detailed theory of quantum gravity, these minisuperspace models can probably not be trusted beyond the WKB approximation (if at all). The question of the strength of the peak is therefore pushed out into a regime of which we have a poor understanding, and so cannot at present be answered.

VI. QUANTUM COSMOLOGY: PERTURBATIONS ABOUT MINISUPERSPACE

The minisuperspace models have been quite successful in their description of cosmology. However, their validity as approximations to a full superspace treatment must be regarded as questionable, since one is effectively restricting attention to a region of superspace of zero volume. Although in the models constructed, this restriction appeared to be physically reasonable, e.g., restricting attention to modes one expects to dominate, one can only test it by comparing the value of the wave function on this zero volume region of superspace with its value in the surrounding region of finite volume. In the case of homogeneous minisuperspace models, for example, this can be done by considering inhomogeneous perturbations. One would hope to find that the wave functions for the inhomogeneous modes are peaked around homogeneity, in which case the minisuperspace approximation seems not unreasonable.

There is a another reason why it is of interest to look at inhomogeneous perturbations. Although the Universe we see is homogeneous and isotropic on very large scales, there are small departures from homogeneity and isotropy caused by galaxies and other large-scale structures. These structures are widely believed to have arisen from small perturbations in density in an otherwise homogeneous universe at early times. In order to study these perturbations, one needs to consider the inhomogeneous modes of the fields.

In this and the next section we extend the minisuperspace formalism of the previous section to include an infinite number of perturbation modes, thereby probing a small but nevertheless finite-volume region of the full superspace. For simplicity we shall assume that the minisuperspace modes q^a are purely gravitational and that the perturbation modes, which we denote by Φ, are matter perturbations. This is not a necessary restriction, but simplifies the formalism, and is sufficient for the discussion of this paper. The more general case, in which some of the q^a are matter modes, and the perturbation modes include gravitational waves, is treated in Ref. 19. A useful example to bear in mind is the case in which q^a is the scale factor of a Robertson-Walker metric and Φ is an inhomogeneous scalar field.[20] The main point of these two sections is to consider the derivation of the semiclassical Einstein equations from the Wheeler-DeWitt equation.

The model will be described by an action $I=I_G+I_M$ where I_G is the minisuperspace action (5.2) and

$$I_M=\int L_M(\Phi,q^a,N)dt \ . \tag{6.1}$$

With this additional term, the field equations (5.3) and (5.5) are modified:

$$\frac{1}{N}\frac{d}{dt}\left[\frac{1}{N}\dot{q}^a\right]+\frac{1}{N^2}\Gamma^a_{bc}\dot{q}^b\dot{q}^c+f^{ab}\frac{\partial U}{\partial q^b}=\frac{1}{M^2}\frac{f_{ab}}{N}\frac{\partial L_M}{\partial q^b} \ , \tag{6.2}$$

$$\frac{1}{2N^2}f_{ab}\dot{q}^a\dot{q}^b+U(q)=\frac{1}{M^2}\frac{\partial L_M}{\partial N} \ . \tag{6.3}$$

The two new terms on the right-hand side of (6.2) and (6.3) are equivalent, respectively, to the space-space and time-time components of the energy-momentum tensor. The Hamiltonian constraint is

$$\begin{aligned} H&=N(H_G+H_M)\\ &=N\left[\frac{1}{2M^2}f^{ab}p_ap_b+M^2U(q)+H_M(q^a,\Phi,\pi_\Phi)\right]\\ &=0 \ , \end{aligned} \tag{6.4}$$

where π_Φ is the momentum conjugate to Φ. Hamilton's equations yield the phase-space form of (6.2):

$$\frac{1}{N}\frac{dp^a}{dt}+\frac{1}{M^2}\Gamma^a_{bc}p^bp^c+M^2f^{ab}\frac{\partial U}{\partial q^b}=-f^{ab}\frac{\partial H_M}{\partial q^b} \ . \tag{6.5}$$

The Wheeler-DeWitt equation for the model is

$$\left[-\frac{1}{2M^2}\nabla^2+M^2U(q)+H_M\left[q^a,\Phi,-i\frac{\partial}{\partial\Phi}\right]\right]\Psi(q^a,\Phi)=0 \ , \tag{6.6}$$

where again ∇^2 is the Laplacian in the metric f_{ab}; it does not operate on the perturbation modes Φ. Equation (6.6) may be solved in the oscillatory region using a WKB-type expansion. One writes

$$\Psi=\exp[iM^2S_0(q)+iS_1(q)+O(M^{-2})]\chi(q,\Phi) \ . \tag{6.7}$$

Inserting (6.7) into (6.6), one finds that the order-M^2 terms again yield the Hamilton-Jacobi equation for S_0, (5.12). S_0 is taken to be real. The order-M^0 terms, however, yield

$$\left[(\nabla S_0)\cdot(\nabla S_1)-\frac{i}{2}\nabla^2 S_0\right]\chi - i(\nabla S_0)\cdot\nabla\chi + H_M\chi = 0 , \tag{6.8}$$

where ∇ denotes $\partial/\partial q^a$ and the dot product is with respect to the metric f_{ab}. It is again convenient to introduce the vector

$$\frac{\partial}{\partial\tau} = (\nabla S_0)\cdot\nabla , \tag{6.9}$$

the tangent vector to the classical trajectories in minisuperspace, where $\tau = \int N\,dt$. We have a single equation, (6.8), for χ and the complex quantity S_1, so there is the freedom to impose the condition

$$\frac{d}{d\tau}(\chi,\chi) = 0 , \tag{6.10}$$

where the inner product is defined by

$$(f,g) = \int d\Phi\, f^*(q,\Phi) g(q,\Phi) . \tag{6.11}$$

Note that the inner product involves an integration over the matter modes Φ, but not the gravitational modes q^a. One would expect this to be well defined because the matter wave functions χ are in general square integrable in Φ. We do not introduce an inner product involving an integration over the gravitational variables, partly because we do not need it, but also because it would not be well defined, since the wave functions will not in general be square integrable in q^a.

Equation (6.10) implies that

$$\left(i\frac{\partial\chi}{\partial\tau},\chi\right) = \left(\chi, i\frac{\partial\chi}{\partial\tau}\right) , \tag{6.12}$$

that is, $(\chi, i\partial\chi/\partial\tau)$ is real. Taking the inner product of (6.8) with χ, one obtains

$$(\nabla S_0)\cdot(\nabla S_1) - \frac{i}{2}\nabla^2 S_0 - \left(\chi, i\frac{\partial\chi}{\partial\tau}\right) + (\chi, H_M\chi) = 0 . \tag{6.13}$$

The imaginary part of (6.13) is

$$(\nabla S_0)\cdot\nabla(\mathrm{Im} S_1) = \tfrac{1}{2}\nabla^2 S_0 , \tag{6.14}$$

where we have assumed that H_M is Hermitian in the inner product (6.11). By comparison with (5.13), it follows that $\mathrm{Im}S_1$ gives the usual WKB prefactor, $C = \exp(-\mathrm{Im}S_1)$, and is unaffected by the perturbations. Putting (6.14) back into (6.8) one obtains

$$\left[H_M + \frac{\partial}{\partial\tau}(\mathrm{Re}S_1)\right]\chi = i\frac{\partial\chi}{\partial\tau} . \tag{6.15}$$

Ignoring for the moment the term $\mathrm{Re}S_1$, (6.15) is a time-dependent Schrödinger equation along the classical minisuperspace trajectories. What we have derived from the Wheeler-DeWitt equation, therefore, is nothing more than the familiar quantum field theory on a fixed background space-time. It is in a perhaps unfamiliar picture, however, namely, the functional Schrödinger picture. Numerous derivations of this type have appeared in the literature.[4,19,21–23]

We next consider the derivation of the semiclassical Einstein equations from the above formalism. This is related to the choice of $\mathrm{Re}S_1$, which is essentially arbitrary. The reason for this is that of order M^0 the Wheeler-DeWitt equation determines only the total phase in (6.7); thus $\mathrm{Re}S_1$ may be divided between χ and the background wave function in any way whatsoever. For example, one may choose $\mathrm{Re}S_1=0$, which is equivalent to absorbing it into the phase of χ. Hartle, however, makes the choice

$$\frac{\partial}{\partial\tau}(\mathrm{Re}S_1) + \langle H_M\rangle = 0 , \tag{6.16}$$

where the average of H_M, $\langle H_M\rangle$, is defined using the inner product (6.10) (Ref. 4). When added to the Hamilton-Jacobi equation (5.12), it yields the semiclassical Hamilton-Jacobi equation

$$\frac{1}{2M^2}[\nabla(\mathrm{Re}S)]^2 + M^2 U + \langle H_M\rangle + O(M^{-2}) = 0 , \tag{6.17}$$

where $S = M^2 S_0 + S_1 + O(M^{-2})$. This will lead to the semiclassical Einstein equations, as desired, if one makes the identification

$$p_a = \frac{\partial}{\partial q^a}(\mathrm{Re}S) = M^2\frac{\partial S_0}{\partial q^a} + \frac{\partial}{\partial q^a}(\mathrm{Re}S_1) . \tag{6.18}$$

A similar derivation was given by Brout *et al.*[23]

While there does not appear to be anything formally wrong with this derivation there are a couple of points about it which are unclear. First, the derivation seems to depend on a very special choice of $\mathrm{Re}S_1$, yet we argued above that $\mathrm{Re}S_1$ could be chosen at will. Second, and more importantly, this derivation does not shed any light on what is perhaps the least understood aspect of the semiclassical Einstein equations—why does the metric couple to the *average value* of the stress tensor $\langle T_{\mu\nu}\rangle$? This is one question that one would hope to get an answer to by deriving the semiclassical Einstein equations from the Wheeler-DeWitt equation.

A possible answer is contained in the ideas introduced in the previous sections concerning correlations in the wave function. In the case of minisuperspace models, it was shown that a wave function of the form e^{iS} predicted a strong correlation between p and $\partial S/\partial q$. Here we have the wave function (6.7) which is similar, but modified by the perturbation wave function χ. The question to ask, therefore, is the following: How is the correlation between p and $\partial S/\partial q$ modified by the presence of this extra term?

One can attempt to answer this by computing Wigner's function for the wave function (6.8). We are trying to understand how the quantum matter field Φ couples to an almost-classical gravitational field, described by q^a. The appropriate Wigner function to consider, therefore, is $F(q,p,\Phi)$; i.e., we do look for correlations involving p, but we do not look for correlations involving π_Φ, the momentum conjugate to Φ. The extra terms that one gets in the computation of Wigner's function are

$$\chi^*(q^a-\tfrac{1}{2}u^a)\chi(q^a+\tfrac{1}{2}u^a)=|\chi(q^a,\Phi)|^2+\frac{u^b}{2}\left[\chi^*(q^a)\frac{\partial\chi}{\partial q^b}(q^a)-\frac{\partial\chi^*}{\partial q^b}(q^a)\chi(q^a)\right]+\cdots$$
$$=|\chi(q^a,\Phi)|^2\exp\left[\frac{u^a}{2}\frac{\partial}{\partial q^a}(\ln\chi-\ln\chi^*)\right]+\cdots\ . \tag{6.19}$$

Wigner's function is thus given by

$$F(p_a,q^a,\Phi)=|C(q)|^2|\chi(q,\Phi)|^2 \times\delta\left[p_a-M^2\frac{\partial S_0}{\partial q^a}+\frac{i}{2}\frac{\partial}{\partial q^a}(\ln\chi-\ln\chi^*)\right]\ . \tag{6.20}$$

Here we have assumed that $\mathrm{Re}S_1$ has been absorbed into χ. Wigner's function has a peak when p_a, q^a, and Φ satisfy the relation

$$p_a=M^2\frac{\partial S_0}{\partial q^a}-\frac{i}{2}\frac{\partial}{\partial q^a}(\ln\chi-\ln\chi^*)\ . \tag{6.21}$$

This equation indicates how the correlation (5.14) is modified by the presence of the matter perturbations. Note, however, that it involves Φ explicitly, so one would not expect to derive the semiclassical Einstein equations directly from (6.21), because they are independent of Φ. The semiclassical Einstein equations are obtained by replacing the Φ-dependent term in (6.23) by its average value; i.e., one considers the expression

$$p_a=M^2\frac{\partial S_0}{\partial q^a}+\left[\chi,-i\frac{\partial\chi}{\partial q^a}\right]\ . \tag{6.22}$$

Why one should be allowed to replace (6.21) with (6.22) is, of course, the main question we are addressing, and we will return to it in the next section. Equation (6.22) implies

$$\frac{1}{2M^2}f^{ab}p_ap_b=\tfrac{1}{2}M^2(\nabla S_0)^2+\left[\chi,-i\frac{\partial\chi}{\partial\tau}\right]+O(M^{-2})\ . \tag{6.23}$$

Using the Hamilton-Jacobi equation for S_0, (5.12), and the Schrödinger equation for χ, (6.15), Eq. (6.23) becomes

$$\frac{1}{2M^2}f^{ab}p_ap_b+M^2U(q)+(\chi,H_M\chi)+O(M^{-2})=0\ . \tag{6.24}$$

This is the semiclassical version of the Hamiltonian constraint (6.4). To obtain the semiclassical version of (6.5), the remaining Einstein equation in phase space, it is necessary to consider the time evolution along the trajectories defined by (6.22). The tangent vector is no longer (6.9), but the slightly modified vector

$$\frac{d}{d\tilde{\tau}}=(\nabla S_0)\cdot\nabla+\frac{1}{M^2}\left[\chi,-i\frac{\partial\chi}{\partial q^a}\right]f^{ab}\frac{\partial}{\partial q^b}\ . \tag{6.25}$$

q^a and p_a are now related by

$$p_a=M^2f_{ab}\frac{dq^b}{d\tilde{\tau}}\ . \tag{6.26}$$

Applying (6.25) to (6.22), one thus finds, at length, that

$$\frac{dp^a}{d\tilde{\tau}}+\frac{1}{M^2}\Gamma^a_{bc}p^bp^c+M^2f^{ab}\frac{\partial U}{\partial q^b}=-f^{ab}\left[\chi,\frac{\partial H_M}{\partial q^b}\chi\right] \tag{6.27}$$

plus terms of order M^{-2}. This is the desired semiclassical form of (6.5). The details of this derivation are given in the Appendix. We have therefore shown that (6.22) does indeed lead to the semiclassical Einstein equations.

VII. THE PEAK AT THE SEMICLASSICAL EINSTEIN EQUATIONS

It remains to be shown that the Φ-dependent term in (6.21) can be replaced by its average value, as in (6.22). This will not be true in general, but we will show that it is in some situations of interest. Since χ depends on τ, rather than on all the q^a, one has

$$\frac{\partial\chi}{\partial q^a}=\frac{\partial\tau}{\partial q^a}\frac{\partial\chi}{\partial\tau}\ . \tag{7.1}$$

Using the Schrödinger equation (6.15) one may see that our task is then to justify the replacement of the Φ-dependent expression

$$\frac{1}{2}\left[\frac{H_M\chi}{\chi}+\frac{H_M\chi^*}{\chi^*}\right] \tag{7.2}$$

with its average over Φ, which is $\langle H_M\rangle$.

First, one can do this if χ is an eigenfunction of H_M. For then $H_M\chi=\langle H_M\rangle\chi$ (and similarly for the complex conjugate, assuming $H_M^*=H_M$); hence, (7.2) is equal to $\langle H_M\rangle$ exactly. This possibility arises if the background metric is conformally flat and the matter field is conformally invariant. In general, however, this will not be the case, and (7.2) will not be exactly equal to $\langle H_M\rangle$. The next question to ask, therefore, is whether (7.2) can in some sense be close to $\langle H_M\rangle$. The distribution of p_a, q^a, and Φ is given by Wigner's function (6.20), which has a δ-function peak on the hypersurface (6.21). The distribution of q^a and Φ within that hypersurface is then given by the prefactor of Wigner's function. In particular, the distribution of Φ is given, as one would expect, by $|\chi|^2$. We can use this expression to calculate the distribution of the Φ-dependent expression (7.2). In accordance with the interpretation we have been using, if this distribution is strongly peaked when (7.2) is equal to its average value, then we predict that the model will evolve according to (6.24), and hence according to the semiclassical Einstein equations. This, therefore, is the condition under which the semiclassical Einstein equations hold—that the distribution of (7.2) is strongly peaked about its average value. We shall refer to it as condition C.

One case in which condition C will hold is that in which one has a large number of identical noninteracting fields, $\Phi_1, \ldots, \Phi_N$, say, obeying identical boundary conditions. For then (7.2) is a quantity of the form (3.24), with the Φ_i's represented by the x_i's. It follows from the central limit theorem result of Sec. III C that the distribution of (7.2) is peaked about its average value, for large N. That condition C holds in this case is essentially the statement that the leading-order $1/N$ approximation is equivalent to semiclassical gravity.[24]

We next argue that condition C can also hold for the case in which one has a single matter field. To be specific, consider the case of a scalar field $\Phi(\mathbf{x},t)$ with a quadratic potential, in a $k=+1$ Robertson-Walker background, with scale factor a. The standard way to treat this in quantum cosmology is to expand Φ in harmonics on the spatial sections:

$$\Phi(\mathbf{x},t)=\sum_{n=1}^{\infty}\sum_{l=0}^{n-1}\sum_{m=-l}^{l} f_{nlm}(t)Q^n_{lm}(\mathbf{x}) \ . \tag{7.3}$$

Here, the Q^n_{lm} are eigenfunctions of the Laplacian on the three-sphere, ${}^{(3)}\Delta$:

$${}^{(3)}\Delta Q^n_{lm}=-(n^2-1)Q^n_{lm} \ . \tag{7.4}$$

For each n, the degeneracy, labeled by l,m, is n^2 (see Ref. 19 for further details about these harmonics). One may thus expand the matter Hamiltonian in harmonics, with the result

$$H_M=\sum_n H^n_M=\sum_n\sum_{lm}H^{nlm}_M$$
$$=\sum_n\sum_{lm}\tfrac{1}{2}a^{-3}\left[-\frac{\partial^2}{\partial {f_{nlm}}^2}+{\omega_n}^2{f_{nlm}}^2\right] \ . \tag{7.5}$$

The time-dependent frequency ω_n depends on n but not on the degeneracy labels l,m. This has the consequence that each Hamiltonian H^n_M is a sum of n^2 identical Hamiltonians H^{nlm}_M. The natural ansatz to make for the matter wave function is

$$\chi=\prod_n \chi_n=\prod_n\prod_{lm}\chi_{nlm}(f_{nlm},\tau) \ . \tag{7.6}$$

We will make the reasonable assumption that the boundary conditions do not distinguish between different values of the degeneracy labels l,m in the wave functions χ_{nlm}. It follows that for each n we have a set of n^2 systems with identical Hamiltonians and identical boundary conditions.

Using (7.5) and (7.6), (7.2) may now be written

$$\frac{1}{2}\sum_n\left[\frac{H^n_M\chi_n}{\chi_n}+\frac{H^n_M\chi^*_n}{\chi^*_n}\right]\equiv\sum_n h_n \ . \tag{7.7}$$

Each term h_n is then a sum of n^2 terms:

$$h_n=\frac{1}{2}\sum_{lm}\left[\frac{H^{nlm}_M\chi_{nlm}}{\chi_{nlm}}+\frac{H^{nlm}_M\chi^*_{nlm}}{\chi^*_{nlm}}\right] \ . \tag{7.8}$$

The important point now, is that as a consequence of the fact that H^{nlm}_M and χ_{nlm} are independent of l,m, h_n is of the form (3.24) for each n, with $N=n^2$ and the labels i identified with the l,m. It follows that for all but the lower values of n, the distributions of the h_n are peaked about the value $\langle h_n\rangle$. From this we tentatively conclude that condition C is satisfied, and thus the semiclassical Einstein equations hold for a single noninteracting scalar field in a Robertson-Walker background. Wada reached the same conclusion for the special case in which the χ_{nlm} are of the form (3.3) (Ref. 5).

The above argument clearly does not crucially depend on the details of this particular example. It depends only on having a large number of identical systems which in turn depends first, on our assumption about the boundary conditions and second, on the degeneracy of the harmonics. This degeneracy is a consequence of the symmetry of the spatial sections. One would expect, therefore, that this sort of argument will also apply to other types of noninteracting matter field in more complicated backgrounds, providing they have a certain amount of symmetry.

The above conclusion concerning condition C for a single field is only tentative because the quantities we have been dealing with, such as $\langle H_M\rangle$, are formally divergent. Deductions made about the distribution of (7.7) given the distribution of the h_n are therefore questionable. These divergences could be difficult to regularize because the formalism we have been using is noncovariant. One possible way to proceed, however, might be to try and express the condition C in terms of the covariant quantity $T_{\mu\nu}$, the energy-momentum tensor of the matter field. Standard methods may then be used to carry out the regularization. When expressed in terms of $T_{\mu\nu}$, condition C would then be something like the requirement that the distribution of $T_{\mu\nu}$ be strongly peaked about its average value. We have not found the precise relationship between this condition and condition C, however.

Finally, it is of interest to compare this latter condition with the results of Ford, who considered linearized gravity about flat space coupled to a massless scalar field.[25] He showed that the semiclassical Einstein equations are valid if the state satisfies the condition

$$\langle T_{\alpha\beta}(x)T_{\mu\nu}(x')\rangle=\langle T_{\alpha\beta}(x)\rangle\langle T_{\mu\nu}(x')\rangle \ . \tag{7.9}$$

This is essentially the requirement that the variance of the distribution of $T_{\mu\nu}$ vanishes, and hence that the distribution of $T_{\mu\nu}$ is entirely concentrated at $\langle T_{\mu\nu}\rangle$.

VIII. SUMMARY AND DISCUSSION

The main point of this paper was to discuss correlations in the wave functions of quantum mechanics and quantum cosmology and hence, in the latter case, to extract predictions from the wave function, using an interpretation of quantum cosmology of the type proposed by Geroch, Hartle, and Wada in which one regards a strong peak as a definite prediction. The main tool with which this was achieved was Wigner's function, which was used to identify correlations between coordinates and momenta. We saw in Sec. III that Wigner's function proved to be very useful for discussing the emergence of classical behavior in quantum-mechanical systems. This is important in the study of scalar field fluctuations in inflationary universe models.

After a preparatory discussion of WKB wave function in quantum mechanics in Sec. IV, we turned, In Sec. V, to WKB wave functions in quantum cosmology. It was shown that for wave functions of the form Ce^{iS}, Wigner's function is peaked about the hypersurface in phase space $p=\partial S/\partial q$. For a minisuperspace model with n coordinates q^a, a particular solution to the Wheeler-DeWitt equation is thus peaked around an n-parameter subset of the $(2n-1)$-parameter general solution to the minisuperspace field equations. It is in this way that boundary conditions for the wave function of the Universe lead to initial conditions for the classical field equations. The prediction of a given minisuperspace model, with given boundary conditions, is therefore that an observer living in the Universe it describes will perceive it to evolve according to one of the solutions contained in the n-parameter subset. This underscores the need for boundary conditions on the Wheeler-DeWitt equation—a completely general solution to the Wheeler-DeWitt equation will correspond to the $(2n-1)$-parameter general solution to the field equations, so no particular advantage is to be gained by calculating the wave function, except possibly for the location of the classically forbidden regions.

The extension of minisuperspace models to the full superspace was considered in Secs. VI and VII. It was shown that, to first order, the wave function $Ce^{iS}\chi$ is peaked around the minisuperspace trajectories with Hamilton-Jacobi function S, with χ evolving according to the Schrödinger equation along these trajectories. It is in this way that quantum field theory in a classical curved space-time background emerges from quantum cosmology. The main point of this section was to consider the derivation of the semiclassical Einstein equations from the Wheeler-DeWitt equation. This was done by asking how the correlation $p=\partial S/\partial q$ is modified by the presence of the matter perturbations Φ. It was found that the correlation was modified by a term which depended on Φ explicitly, as one would expect. If this term, (7.2), was replaced by its average value, then the semiclassical Einstein equations followed. A condition under which this could be done was derived. It is essentially the requirement that the distribution of $T_{\mu\nu}$ is peaked about its average value. It was argued that this condition holds for the case of a large number of identical noninteracting fields, and also for the case of a single noninteracting field subject to certain restrictions. Some of these conclusions are only tentative since we did not discuss the regularization of divergent quantities. This is currently under investigation.

In the Introduction, we discussed the Everett interpretation of quantum mechanics. This, as already noted, is a formulation of quantum mechanics designed to deal with correlations internal to an isolated system. In particular, it was designed to describe correlations in an isolated system consisting of an observer and an observed subsystem, i.e., to describe the process of measurement in a fully quantum-mechanical manner without having to assume an external observer obeying classical physics, and without having to invoke the collapse of the wave function. In this paper, however, we made no mention of the act of observation in quantum cosmology. A proper treatment ought to include this; one ought to consider models of the Universe which include models of observing apparatus interacting with the rest of the Universe. One could then ask questions about the correlations between the states of the observing apparatus and the state of the rest of the Universe.

Models involving observers would clearly be more complicated than those we have been considering here. What we have attempted to do here is offer an interpretation of the wave functions for the models that currently exist in the literature which do not involve observers. The assumption is that if one were to introduce an observing apparatus into these models, then providing it did not disturb the system very much, one would still find correlations of the form (5.14), say. In a sense, the perturbation modes may be regarded as "measuring" the minisuperspace background. In the classical regime, they respond as if on the classical trajectory $p=\partial S/\partial q$, yet to lowest order, do not affect the background. It would be of interest to develop these ideas further and study the measurement process in quantum cosmology, in the spirit of the Everett interpretation of quantum mechanics.

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APPENDIX: DERIVATION OF EQ. (6.27)

In this appendix we give the details of the derivation of Eq. (6.27).

Applying (6.25) to (6.22), one obtains

$$\frac{dp_a}{d\tilde{\tau}}=M^2\frac{d}{d\tau}\left[\frac{\partial S_0}{\partial q^a}\right]+\left[\chi,-i\frac{\partial x}{\partial q^c}\right]f^{cb}\frac{\partial^2 S_0}{\partial q^b q^a}+\frac{d}{d\tau}\left[\left[\chi,-i\frac{\partial \chi}{\partial q^a}\right]\right]. \tag{A1}$$

Using (5.12) the first term in (A1) becomes

$$M^2\left[-\tfrac{1}{2}f^{bc}{}_{,a}\frac{\partial S_0}{\partial q^b}\frac{\partial S_0}{\partial q^c}-\frac{\partial U}{\partial q^a}\right]. \tag{A2}$$

The third term in (A1) is

$$\left[\frac{\partial \chi}{\partial \tau}, -i\frac{\partial \chi}{\partial q^a}\right] + \left[\chi, -i\frac{\partial}{\partial \tau}\left[\frac{\partial \chi}{\partial q^a}\right]\right] . \tag{A3}$$

From the definition of τ, (6.9),

$$\begin{aligned}\frac{\partial}{\partial \tau}\left[\frac{\partial \chi}{\partial q^a}\right] &= f^{bc}\frac{\partial S_0}{\partial q^b}\frac{\partial}{\partial q^c}\left[\frac{\partial \chi}{\partial q^a}\right] \\ &= \frac{\partial}{\partial q^a}\left[\frac{\partial \chi}{\partial \tau}\right] - f^{bc}{}_{,a}\frac{\partial S_0}{\partial q^b}\frac{\partial \chi}{\partial q^c} \\ &\quad - f^{bc}\frac{\partial^2 S_0}{\partial q^b \partial q^a}\frac{\partial \chi}{\partial q^c} .\end{aligned} \tag{A4}$$

Inserting (A4) into (A3) and using the Schrödinger equation for χ, (A3) becomes

$$-\left[\chi, \frac{\partial H}{\partial q^a}\chi\right] + \frac{\partial^2 S_0}{\partial q^b \partial q^a} f^{bc}\left[\chi, i\frac{\partial \chi}{\partial q^c}\right] + \frac{\partial S_0}{\partial q^b} f^{bc}{}_{,a}\left[\chi, i\frac{\partial \chi}{\partial q^c}\right] . \tag{A5}$$

Inserting (A2) and (A5) into (A1), one obtains

$$\frac{dp_a}{d\tilde{\tau}} = -f^{bc}{}_{,a}\left[M^2\frac{\partial S_0}{\partial q^b}\frac{\partial S_0}{\partial q^c} + 2\left[\chi, -i\frac{\partial \chi}{\partial q^c}\right]\frac{\partial S_0}{\partial q^b}\right] - M^2\frac{\partial U}{\partial q^a} - \left[\chi, \frac{\partial H}{\partial q^a}\chi\right] . \tag{A6}$$

Using the expression (6.22) for p_a, (A6) may now be written

$$\frac{dp_a}{d\tilde{\tau}} + \frac{1}{2M^2}f^{bc}{}_{,a}p_b p_c + M^2\frac{\partial U}{\partial q^a} = -\left[\chi, \frac{\partial H}{\partial q^a}\chi\right] , \tag{A7}$$

where we have neglected terms of order M^{-2}. Using the metric to raise the indices on the momenta, and after some rearrangement, one obtains the desired semiclassical form of (6.5), (6.27).

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