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DIFFICULTIES FOR THE EVOLUTION OF PURE STATES INTO MIXED STATES

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ABSTRACT

Motivated by Hawking's proposal that the quantum-mechanical density matrix ρ obeys an equation more general than the Schrödinger equation, we study the general properties of evolution equations for ρ. We argue that any more general equation for ρ violates either locality or energy-momentum conservation.

1. Introduction

A recurring question in the attempt to construct a quantum theory of gravity has been that of whether such a theory can be constructed within the conventional framework of quantum mechanics. Recently, Hawking [1] has argued that this cannot be so, and he has proposed a modified set of axioms for quantum field theory to accommodate quantum gravity.* Basically, Hawking's proposal entails allowing pure states to evolve into mixed states. The motivation for this proposal comes from the idea that the final state of black-hole evaporation should be a mixed state, even when the gravitational field of the black hole has been treated as a part of the quantum -mechanical process; this point has been argued particularly strongly by Page.[3] Hawking also envisions modifications of quantum mechanics, however, in apparently less extreme situations: In particular he predicts that they should occur in ordinary, flat space-time, as the result of instanton-like gravitional quantum fluctuations. This proposal is provocative and clearly of fundamental interest; it therefore deserves the closest scrutiny.

In this paper, we will analyze the effects of such violations of quantum mechanics on ordinary quantum field theory. We will show that the effects suggested by Hawking are very dangerous perturbations, leading either to nonlocal interactions, and, thus, to acausal signal propagation, or to large violations of energy-momentum conservation. We will also argue that neither of these consequences is likely to be suppressed by inverse powers of the Planck scale. The magnitude of such quantum-mechanics violation has been analyzed previously by Ellis, Hagelin, Nanopoulos, and Srednicki,[4] who have pointed out serious phe-

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* Some further formal development of this proposal has been made by Alvarez-Gaumé and Gomez[2] .

nomenological constraints. However their picture of thes effects is considerably more benign than the one to be presented here.

We should, properly, note that the precise proposal made in Ref. 1 does not stand on an especially firm theoretical foundation. Hawking introduces it there as an interpretation of negative-frequency poles observed by Hawking, Page and Pope[5] in propagators in the field of certain gravitational instantons. One might alternatively interpret these poles as resulting from the fact that the spaces considered in Ref. 5 are not asymptotically Euclidean. Recent, Gross[6] has constructed a set of gravitational instantons in the Kaluza-Klein theory and has shown in detail that their effects show no such apparently acausal behavior. However, the connection between systems in background gravitational fields and systems at finite temperature makes it intuitively quite reasonable that pure states might evolve into mixed states in quantum gravity. We feel, therefore, that one should criticize this idea on more general grounds.

We note that, while our arguments are motivated by considerations of the theory of gravity, they apply equally well to other modifications of quantum mechanics which would lead to a loss of quantum coherence. They do not apply, however, to theories such as that of Friedberg and Lee[7] in which space-time is replaced with a background which is random but coherent.

Our analysis will proceed as follows: In Section 2, we will argue, following Ellis, Hagelin, Nanopoulos, and Srednicki[4] , that Hawking's proposal can be expressed as the statement that the quantum mechanical density matrix obeys a linear equation of motion more general than the Schrödinger equation. We will then discuss the general features of such equations for ρ. In Section 3, we will give an interpretation for a subclass of these equations which makes intuitively clear that they violate either locality or momentum conservation. In Section 4, we will show how these unfortunate consequences follow for the more general class of equations described in Section 2. In Section 5, we will illustrate our conclusions with a simple model.

2. Evolution Equations for Density Matrices

In Ref. 1, Hawking suggests the modification of the usual logic for extracting the S matrix from Green's functions. He first derives the evolution formula for the quantum-mechanical density matrix:

$$\rho_{\text{out}} = \not{S} \cdot \rho_{\text{in}} \tag{1}$$

where $\not{S}$ is a linear operator which preserves the Hermiticity, positivity, and normalization

$$tr(\rho) = 1 \tag{2}$$

of the density matrix. The operator $\not{S}$, called the superscattering operator, is normally derivable from the S matrix via the relation

$$\not{S} \cdot \rho = S\rho S^{+} \tag{3}$$

However, Hawking chooses to reject the axiom of the completeness of asymptotic states, the ingredient needed to justify the factorization (3). Instead, he considers eq. (1), supplemented by the requirement of overall energy-momentum conservation, as the basis of quantum dynamics. Thus, he considers a structure in which the usual quantum-mechanical connection between ρ and the results of measurements is retained, but in which there exists no pure state limit in which ρ represents the evolution of a single wavefunction.

If the dynamics which gives rise to $\not{S}$ is local in time, we can represent $\not{S}$ as the integral of a differential equation for ρ[4] :

$$\frac{d}{dt}\rho = \not{H} \cdot \rho \,. \tag{4}$$

In this equation, $\not{S}$ represents an arbitrary linear operator, constrained, as $\not{S}$ was, to preserve the Hermiticity, positivity, and normalization of ρ.

Our strategy in this paper will be to write a convenient canonical form for H and then use it to study the properties of Eq. (4). Before we begin, we should give a few remarks of justification for this approach. Quantum mechanics is well-tested only on time scales long compared to the Planck time and in regions of space-time which are, on average, almost flat. We need only assume, then, that (4) can be derived from (1) in such a situation, by performing a coarse-grained averaging over fluctuations of space-time. We thus will not worry about possible effects nonlocal in time over a few million Planck times. Equation (4) contains the possibility of describing effects nonlocal in space. We will not consider such effects troublesome unless the nonlocality is of nuclear, rather than Planck, size.

Let us now simplify Eq. (4). We first consider the case of a finite-dimensional Hilbert space. Let us write this equation, with indices, as

$$\dot{\rho}^{A}{}_{B} = \not{H}^{A}{}_{BC}{}^{D}\, \rho^{C}{}_{D} \tag{5}$$

For fixed values of B and D, we can expand the matrix $\not{H}^{A}{}_{C}$ in terms of a complete orthogonal set of Hermitian matrices Q^{α}, with $Q^{0} = 1$. The expansion coefficients $H^D_{\alpha B}$ (which are, in general, complex) may now also be expanded into term of the Q^α. This allows us to write (5) in the form

$$\dot{\rho} = -\sum_{\alpha\beta} h_{\alpha\beta} Q^\alpha \rho Q^\beta \ . \tag{6}$$

Hermiticity of $\dot{\rho}$, given the Hermiticity of ρ and the Q^α, requires that $h_{\alpha\beta}$ be Hermitian. Now let us write the condition that the normalization is preserved:

$$\mathrm{tr}\,\dot{\rho} = 0 = -\mathrm{tr}\left\{h_{00}\rho + \sum_{\alpha\neq 0}(h_{0\alpha} + h_{\alpha 0})Q^\alpha \rho + \sum_{\alpha,\beta\neq 0} h_{\alpha\beta} Q^B Q^\alpha \rho\right\} . \tag{7}$$

This equation may be solved for the quantities $(h_{0\alpha} + h_{\alpha 0})$. The other linear combination is undetermined; let us parametrize it as follows:

$$(h_{0\alpha} - h_{\alpha 0})Q^\alpha = -2i\,H_0 \tag{8}$$

where H is some Hermitian operator. Then we have cast (4) into the form:

$$\dot{\rho} = -i\,[H_0, \rho] - \frac{1}{2}\sum_{\alpha\beta\neq 0}(Q^\beta Q^\alpha \rho + \rho Q^\beta Q^\alpha - 2Q^\alpha \rho Q^\beta) \ . \tag{9}$$

We still need to implement the requirement that ρ remain positive. One might also insist that the entropy defined by ρ not decrease with time. We do not know what conditions are necessary to insure these properties, but we can state some simple sufficient conditions. ρ remains positive if $h_{\alpha\beta}$ is a positive matrix. To see this, diagonalize $h_{\alpha\beta}$; this produces

$$h_{\alpha\beta}\, Q^\alpha\, Q^\beta = h_\lambda Q^\lambda\, Q^{\dagger\lambda} \tag{10}$$

where the Q^λ are not necessarily Hermitian but are orthogonal in the sense that

$$\mathrm{Tr}\, Q^\lambda Q^{\dagger\mu} = \delta^{\mu\nu} . \tag{11}$$

Now diagonalize ρ, calling its eigenvalues p_i, and consider the situation in where one eigenvalue, say, p_1, becomes zero. Then

$$\frac{d}{dt} p_1 = \dot{\rho}_{11}|_{p_1=0} = \sum_\lambda h_\lambda |Q^\lambda_{1i}|^2 p_i \tag{12}$$

is positive, so that ρ remains positive, if $h_\lambda \geq 0$. Entropy increases if $h_{\alpha\beta}$ is a real symmetric matrix, or, equivalently, if the Q^λ of (10) are Hermitian. Consider, in fact, the evolution of $\mathrm{tr}(\rho)^a$, $a > 1$:

$$\begin{aligned} \frac{d}{dt} \mathrm{tr}\, \rho^\alpha &= -a \sum_\lambda h_\lambda \sum_{ij} p_i^{a-1} \Big(|Q^{+\lambda}_{ij}|^2 p_i - |Q^\lambda_{ij}|^2 p_j \Big) \\ &= -a \sum_\lambda h_\lambda \sum_{\text{pairs } i,j} \Big(|Q^{+\lambda}_{ij}|^2 p_i - |Q^\lambda_{ij}|^2 p_j \Big)\Big(p_i^{a-1} - p_j^{a-1} \Big) . \end{aligned} \tag{13}$$

This is negative if all of the Q^λ are Hermitian; taking $\alpha \to 0$, we find in this case

$$\frac{d}{dt} \mathrm{tr}\,(-\rho \log \rho) \geq 0 . \tag{14}$$

We have shown, then, that a linear evolution equation for ρ can generally be written in the form (9). Assuming that h is positive insures that ρ remains positive; assuming, in addition, that h is real implies that entropy increases. However, it is easy to find examples which show that these last two conditions are not strictly necessary.

3. An Interpretation of the Evolution Equation

The case in which h in Eq. (9) is real and positive is attractive from another point of view: In this case, Eq. (9) possesses a simple physical interpretation. Let us now present that interpretation, and use it to expose some problems with writing (9) as a fundamental equation.

Consider a system described by quantum mechanics evolving under the action of the following Hamiltonian:

$$H(t) = H_0 + \sum_\alpha j_\alpha(t) Q^\alpha \tag{15}$$

where the Q^α are a set of Hermitian operators and the $j_\alpha(t)$ are c-number sources. Let the j_α vary randomly in time, according to Gaussian statistics with covariance

$$\langle j_\alpha(t) j_\beta(t') \rangle = h_{\alpha\beta} \delta(t - t') \ . \tag{16}$$

In (16), $h_{\alpha\beta}$ is real, symmetric, and positive. If $\rho(0)$ is the density matrix of this system at time $t = 0$, the density matrix at time $t = \epsilon$ is given by:

$$\begin{aligned}\rho(\epsilon) = \rho(0) + i \int_0^\epsilon dt' \Big[H_0 + j_\alpha(t') Q^\alpha, \rho(0) \Big] \\ - \int_0^\epsilon dt' \int_0^{t'} dt'' \Big[H_0 + j_\alpha(t') Q^\alpha, \Big[H_0 + j_\beta(t'') Q^\beta, \rho(0) \Big] \Big] + \cdots \ .\end{aligned} \tag{17}$$

Averaging over the j_α, we find

$$\rho(\epsilon) - \rho(0) = -i\epsilon \ [H_0, \rho(0)] - \frac{1}{2} \epsilon h_{\alpha\beta} [Q^\alpha [Q^\beta, \rho(0)]] + O(\epsilon^2) \tag{18}$$

which, since h is symmetric, is identical to (9). Thus, Eq. (9), in this special case, is simply equivalent to ordinary quantum mechanics in the presence of a random source term.

Quantum mechanics with a random source, however, differs from the observed behavior of elementary particles in two important respects. First, energy is not conserved; in each realization of the random source, the nontrivial time dependence of the source allows energy to be added or removed. Secondly, in the case of a field theory, there is an irreconcilable conflict between momentum conservation and locality. In field theory, (15) must be generalized to:

$$H = H_0 + \int d^3x j_\alpha(t,x) Q^\alpha(x) . \tag{19}$$

If the sources $j_\alpha(x)$ fluctuate randomly as a function of spatial position, then, in each given realization, the sources will break translational invariance and add momentum to the system. On the other hand, if the fluctuations of the sources are translationally invariant, the sources must go through the same random fluctuations at widely separated points on the same spacelike surface. This will introduce correlations between fields at spacelike-separated points. In general, the range of the spatial correlations of $\langle j_\alpha(\vec{x}) j_\beta(\vec{y})\rangle$ will be just the reciprocal of the size of typical momenta added or subtracted.

4. Some Consequences of the Evolution Equation

The violation of energy conservation and the conflict between locality and momentum conservation, observed in the previous section as properties of a system governed by the Hamiltonian (15), can be readily seen to follow from the general structure of Eq. (9). Let us work out more explicitly how they arise.

The failure of energy conservation can be seen from the following observation: What if the theory did possess some Hermitian operator H (not necessarily equal to H_0) which was conserved by the dynamics. Then any ρ which was a function only of H could not change under the action of (9). However, this is possible only if (9) contains only operators Q which are simultaneously diagonalizable with H. Unless H has highly degenerate eigenvalues (a property which would exclude it as a good candidate for the energy), this is a serious restriction on $h_{\alpha\beta}$, especially if Q_α must be a local operator rather than a global charge.

The conflict between locality and momentum conservation can be seen as follows: Let us generalize (9) to field theory by writing

$$\dot{\rho} = -i\Big[\int d^3x H(x), \rho\Big] - \frac{1}{2}\int d^3x d^2y\, h_{\alpha\beta}(x-y)\Big\{Q^\beta(y)Q^\alpha(x), \rho\Big\} - 2Q^\alpha(x)\rho Q^\beta(y)\,. \tag{20}$$

For the moment, we allow $h(x-y)$ to have some finite spatial extent. In Fourier space, the second term of (20) has the form

$$-\frac{1}{2}\int \frac{d^3p}{(2\pi)^3} h_{\alpha\beta}(\vec{p})\Big[\Big\{Q^{+\beta}(-\vec{p})Q^\alpha(\vec{p}), \rho\Big\} - Q^\alpha(p)\rho Q^{+\beta}(-p)\Big]\,. \tag{21}$$

The operators $Q^\alpha(\vec{p})$ change the total momentum by $\vec{p}$; the size of $\vec{p}$ is restricted only by the fall-off of the Fourier transform of h. Momentum conservation violations can be kept small if $H(\vec{p})$ is concentrated at small values of $\vec{p}$. Let us compare this to the criterion that the evolution of ρ does not introduce long-range correlations. Consider preparing a density matrix ρ_0 in such a way that all correlations among operators fall off at a specified rate:

$$\mathrm{tr}[A(\vec{x})B(\vec{y})\rho_0] < C\, e^{-\mu|\vec{x}-\vec{y}|}; \qquad \mu|\vec{x}-\vec{y}| \gg 1 \ . \tag{22}$$

This is possible in a theory whose lightest particle has mass m if $\mu < m$. Then the normal quantum-mechanical evolution of ρ preserves the locality indicated in (22):

$$\begin{aligned}\frac{d}{dt}\,\mathrm{tr}\left\{A(\vec{x})B(\vec{y})\rho(t)\right\}|_{t=0} &= \mathrm{tr}\left\{A(\vec{x})B(\vec{y}) - i\Big[\int d^3z H(z), \rho_0\Big]\right\} \\ &= -i\ \mathrm{tr}\left\{\Big([A(\vec{x}), H]B(\vec{y}) + A(\vec{x})[B(\vec{y}), H]\Big)\rho_0\right\}\end{aligned} \tag{23}$$

since each indicated commutator is a local operator. The second term of (20), however, gives the additional contribution

$$-\frac{1}{2}\,\mathrm{tr}\left\{A(\vec{x})B(\vec{y})\int d^3z d^3w\, h_{\alpha\beta}(z-w)\Big(\Big\{Q^{\beta}(w)Q^{\alpha}(z), \rho_0\Big\} - Q^{\alpha}(z)\rho_0 Q^{\beta}(w)\Big)\right\} . \tag{24}$$

If $|\vec{x}-\vec{y}| \gg \mu$, we can use the commutativity of space-like separated operators, the cluster properties of ρ, and the identity $h_{\alpha\beta}(x-w) = (h_{\beta\alpha}(w-z))^*$ to write this as:

$$
\begin{aligned}
-\frac{1}{2}\mathrm{tr}\Big\{\int & d^3z h_{\alpha\beta}(z-x)\Big[A(x),\int d^3w Q^\beta(w)\Big]B(\vec{y})Q^\alpha(z) \\
&-\int d^3w\, h_{\alpha\beta}(x-w)\Big[A(\vec{x}),\int d^3x\, Q^\alpha(z)\Big]Q^\beta(w)B(\vec{y})\Big\}\rho_0 \\
&+\Big((A,\vec{x})\leftrightarrow(B,\vec{y})\Big) \\
\simeq -2&\Big(\mathrm{tr}\Big[A(x),\int Q^\alpha\Big]\rho_0\Big)\mathrm{Re}\, h_{\alpha\beta}(x-y)\Big(\mathrm{tr}\Big[B(y),\int Q^\beta\Big]\rho_0\Big) \\
&-i\Big[\Big(\mathrm{tr}\Big[A(x),\int Q^\alpha\Big]\rho_0\Big)\int d^3z\,\mathrm{Im}\, h_{\alpha\beta}(x-z)\mathrm{tr}\Big(\Big\{B(y),Q^\beta(z)\Big\}\rho_0\Big) \\
&+(A,\vec{x})\leftrightarrow(B,\vec{y})\Big]\,.
\end{aligned}
\tag{25}
$$

We are free to choose operators A and B so that this expression is nonzero. Equation (25) is only as local as $h(x-y)$. If h falls off fast enough to insure that (22) is maintained, the considerations of the previous paragraph imply that the theory allows violations of momentum conservation of order μ. (We should note that, if $h(x-y)$ is independent of $(x-y)$ and only operators Q^α with vacuum quantum numbers appear in (20), the effect of (25) is only the rather subtle one of violating cluster decomposition.)

5. An Illustrative Model

The arguments we have just given show that violation of energy and momentum conservation is to be expected for operators of the form (9) which preserve locality. We should now offer a few remarks to connect this analysis more concretely to Hawking's proposals for quantum gravity. In the analysis of Ref. 1, Hawking imagines that quantum coherence is violated by the effects of gravitational quantum fluctuations of the size of the Planck scale, m_p^{-1}. In his picture, the fluctuation influences both the left- and right-hand side of the density matrix ρ at the same space-time point (or within m_p^{-1} of this point). This corresponds to an evolution equation of the form (20) with $h(x-y)$ extended only over a distance m_p^{-1}. The locality of $h(x-y)$ is used in a crucial way in Hawking's analysis (and in the more detailed analysis presented in the appendix to Ref. 3) in estimating the size of the proposed quantum incoherence. Under this condition, Eq. (20) would be able to change the total energy and momentum by amounts of order m_p. Hawking proposes to deal with this problem by imposing overall energy-momentum conservation in scattering processes. However, it is not enough to insure that energy-momentum is conserved in transitions from the asymptotic past to the asymptotic future; energy-momentum should remain constant as a function of time, at least after course-grained averaging over time. We have seen, however, that this would entail removing, by hand, most of the operators $Q_\alpha(p)$ in Eq. (20) and, by hand, making this equation nonlocal. The resulting equation would be very different from what one would obtain by literal application of the prescriptions of Ref. 1, and would, in any event, by an equation with its own set of difficulties.

In principle, it is still possible that the violations of energy-momentum conservation could be unobservablly small. A bound on the occurrence of rare but sizeable violations of energy conservation follows from the fact that changes of order 1 MeV would cause α-emitting nuclei to decay. Thus such changes can occur in each nuclear volume only once in the lifetime of the longest-lived α-emitter. This limit is quite stringent, because Hf^{174} is an α-emitter with a half-life of 2.0×10^{15} yrs; converting this to Planck units in the simplest way, this corresponds to a bound of 10^{-125} energy violations/(Planck time)·(Planck length)^3. One might expect effects of quantum gravity to be inhibited in low-energy physics, with rates containing powers of $(1\ GeV/m_p)$. But we will now show, in a simple model calculation, that such a suppression does not appear in this process.

Hawking's argument in Ref. 1 that his predicted quantum incoherence effects are small applies only to particles of spin $\geq \frac{1}{2}$ and uses constraints of helicity conservation or gauge invariance to provide some suppression. Let us, therefore, examine a process which contains this suppression: photon creation by gravitational instantons. Taking the prescriptions of Ref. 1 literally, we represent the coupling of gravitational fluctuations to photons by writing

$$\dot{\rho} = -i[H_0, \rho] + \frac{a}{2m_p^4} \int d^3x \Big[\Big\{ \Big((F_{\mu\nu})^2 \Big)^2 (x), \rho \Big\} - 2(F_{\mu\nu})^2(x) \rho (F_{\mu\nu})^2(x) \Big] \tag{26}$$

where H_0 is the free photon Hamiltonian. The factor m_p^{-1} is inserted for dimensional reasons. In solving (26), we will cut off momentum integrals at a momentum M of order m_p. Let us insert into (26)

$$\rho(t=0) = |\Omega\rangle \langle\Omega| \tag{27}$$

where $|\Omega\rangle$ is the usual free photon vacuum. Then, if $n(\vec{p})$ is the number of photons of momentum $\vec{p}$

$$\frac{d}{dt}\operatorname{tr} n(p)\,\rho(t)|_{t=0} = \frac{a}{m_p^4}\sum_{\lambda_1\lambda_2}\frac{1}{2p}\int\frac{d^3q}{(2\pi)^3 2q}\cdot 8$$

$$\cdot\,[p\cdot q\,\vec{\epsilon}(\lambda_1)\cdot\vec{\epsilon}(\lambda_2)+\vec{p}\cdot\vec{\epsilon}(\lambda_1)\,\vec{q}\cdot\vec{\epsilon}(\lambda_1)]^2$$

$$= \frac{a}{m_p^4}\cdot\frac{8}{3\pi^2}M^2\,p \tag{28}$$

$$= (\text{pure number})\cdot p\ .$$

It is true that few photons are created at small p, but energy nonconservation allows all modes up to m_p to be populated; the high-energy modes are populated without suppression. The photon energy produced per unit volume is given by integrating (28)

$$\frac{d}{dt}\operatorname{tr}\left(\frac{H_0}{V}\right)\rho(t)|_{t=0} = \int\frac{d^3p}{(2\pi)^3}\left(\frac{d}{dt}\operatorname{tr}\left[n(\vec{p})\rho(t)\right]\right)_{t=0}\cdot p$$

$$= \frac{a}{m_p^4}\,\frac{M^9}{15\pi^4} = (\text{pure number})\cdot m_p^5\ . \tag{29}$$

The moral of this exercise is clear. Incoherent perturbations localized in time and space must, by the Heisenberg uncertainty principle, create energy and momentum. Once energy conservation is lost, the enormous volume of phase space for $|\vec{p}| \sim m_p$ makes quantum incoherence a major effect. A sensible theory of quantum gravity must, then, respect the coherence of quantum states, even under strong gravitational perturbations.

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