Nonequilibrium statistical quantum field theory for open systems

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Recently, a number of authors have begun to study the evolution of quantum fields in the early Universe characterized by a time-dependent density matrix $\rho_s(t)$. All of this work is predicated on the assumption that one's "subsystem" of interest is in some sense "decoupled" from the rest of the Universe, so that ρ_s satisfies a Liouville–von Neumann equation which implies, e.g., an isentropic evolution. Starting from "first principles, "i.e., the Schrodinger equation for the totality of "subsystem" plus surroundings ("bath"), it is shown here how such a picture can be derived as the limiting case of a more complete statistical description. Quite generally, one finds that ρ_s and the "bath" density matrix ρ_B satisfy coupled nonlinear generalizations of the Liouville-von Neumann equation and evidence a nonisentropic evolution. However, in a Vlasov-type approximation, ρ_S and ρ_B satisfy instead much simpler bilinear equations which imply an isentropic evolution. And finally, in the limit that the "back reaction" of ρ_s on ρ_B can be neglected in computing the evolution of ρ_B , one recovers a true Liouville-von Neumann equation for the evolution of ρ_s in an external field.

I. INTRODUCTION

Over the past several years, much attention has been focused on the use of statistical quantum field theory in understanding various physical processes in the early Universe. The general discipline of statistical quantum field theory has indeed a long and successful history, but, unfortunately, its most powerful realization, namely, finite-temperature field theory, is oftentimes inapplicable in a cosmological setting. There is usually no reason a priori to assume that the fields of interest are "at equilibrium" — such an equilibrium should be derived, rather than inserted by hand $-$ and there may in fact be good reason to expect that the fields are not "at equilibrium." The Universe as a whole is expanding, so that, strictly speaking, except for special models like a conformally invariant field theory in a conformally static spacetime, equilibrium cannot even be defined. It is only in the limit that some appropriate "relaxation" or "reaction" time t_R is significantly shorter than the expansion time t_H that an approximate notion of equilibrium can make sense.

For this reason, one seems constrained to return to the full dynamics, working with a Schrödinger equation or its field-theoretic analogue, the Tomonaga-Schwinger equation. This, however, leads to different problems, both conceptual and practical. Given the assumption that there exists but one Universe which is characterized by a single wave function, it seems difficult to impart some concrete meaning to the ordinary ensembles of statistical physics. And, even more pragmatically, given that one is trying to probe, either observationally or theoretically, only a part of the Universe (if nothing else, one is quite likely neglecting the quantum dynamics of the gravitational field), which need not be totally decoupled from the rest of the Universe, there is no obvious sense in which the density matrix ρ_s for one's subsystem of interest can be assumed to satisfy a simple Liouville (or Liouville-von Neumann) equation.

However, despite these uncertainties, one does have the intuition that, at least in certain cases, it may prove reasonable to assume that the evolution of ρ_s is in fact governed by a Liouville equation of the form

$$
\frac{d\rho_S}{dt} = -i\left[\mathcal{H}_S, \rho_S\right],\tag{1.1}
$$

where the brackets denote a commutator and \mathcal{H}_S denotes an appropriate subsystem Harniltonian. This is, e.g., the starting point for the elegant functional Schrödinger approach to statistical quantum field theory in the early Universe being developed by Jackiw and his co-workers' or by Cooper and Mottola.² And moreover, such a Liouville equation also underlies the more simplistic approaches to a Schrödinger evolution predicated on a straightforward mode decomposition.³

The obvious questions are as follows. Is there in fact some mathematically well-defined and physically reasonable limit in which this description is valid? And how, at least in principle, might one go beyond such an approximate description? Thus, e.g., this description is limited in the sense that it implies an isentropic evolution. Indeed, it follows trivially that the "entropy"

$$
S_s = -\operatorname{Tr}_S \rho_S \ln \rho_S \tag{1.2}
$$

(where Tr_S denotes a trace over the subsystem variables) is conserved absolutely, i.e., that the time derivative $dS_S(t)/dt \equiv 0$, although there do exist other useful measures of "entropy" which can exhibit a nontrivial time evolution.

The objective here is (a) to derive an exact equation for the evolution of $\rho_s(t)$ which is amenable to approximate analyses and then (b) to show how the implementation of such approximations leads to a Liouville equation for ρ_s .

The basic idea is to start from an isolated system characterized by a wave function ψ and an associated pure-state density matrix ρ , to view this composite sys-

tem as a coupled "subsystem" and "bath," characterized by impure reduced density matrices ρ_s and ρ_b , and then to study the mutual interactions of ρ_s and ρ_b . In so doing, one is implicitly decomposing the total ρ into two pieces, a contribution $\rho_R \equiv \rho_S \rho_B$ which reflects the separate behavior of the subsystem and the bath, and a remaining contribution $\rho_I \equiv \rho - \rho_R$ which reflects the correlations associated with their interactions.

This is a useful paradigm to adopt because of two "natural" approximations that may oftentimes prove justifiable.

(1) Either because the interaction of the subsystem and the bath is weak, or perhaps for some other reason, it may be that the correlations between the subsystem and the bath are small, so that, in the spirit of a Vlasov description, one can approximate $\rho \simeq \rho_R = \rho_S \rho_B$. In this approximation, one finds that ρ_S and ρ_B will satisfy coupled linear equations which constitute an obvious analogue of well-known mean-field equations for the composite system of matter and electromagnetic radiation. Indeed, if ρ_S and ρ_B are reinterpreted as the reduced density matrices for matter and electromagnetic radiation in a system of two-level atoms, the moments of Eqs. (3.1) and (3.2) imply the Bloch-Maxwell equations of quantum optics.⁵

(2) It may further prove that, even though ρ_B has a significant influence on the evolution of ρ_s , the "back reaction" of ρ_S on ρ_B is comparatively weak. In this case, the evolution of ρ_B is governed approximately by a decoupled Liouville equation

$$
\frac{d\rho_B}{dt} = -i[H_B, \rho_B],\qquad(1.3)
$$

the forma1 solution of which will then serve as a source for the time derivative $d\rho_{\rm S}(t)/dt$.

Suppose in particular (a) that the "subsystem" and "bath" refer to the matter and gravitational sectors of a quantum theory of gravity described by a Wheeler-DeWitt equation and (b) that, as suggested by several authors, 6 one can make sense of the Wheeler-DeWitt equation as a time-dependent Schrödinger equation. Assumption (1) then implies a neglect of correlations between the gravitational and matter sectors, and (2) is consistent with the "heavy-light" splitting implicit in the assumption that, to lowest order, the gravitational sector is characterized by a wave function $\chi \approx \exp(iS)$, where S is the classical action associated with some vacuum solution of the Einstein equation.⁷

Section II of this paper uses elementary projection operator techniques to derive exact coupled, nonlinear equations for $d\rho_s/dt$ and $d\rho_B/dt$ which contain no explicit reference to $\rho_I \equiv \rho - \rho_S \rho_B$ except through the propagation of an initial condition $\rho_I(t_0)$. This is simply a transcription into a different setting of an approach first developed by Willis and Picard,⁵ which has already found applications and generalizations in areas extending from stellar dynamics⁸ and galaxy clustering⁹ to "entropy" generation" in the early Universe.^{3,4} Section III then shows that if one neglects the correlations buried in ρ_I , one recovers a linear system for ρ_s and ρ_b , and that if further $\rho_B(t)$ can be viewed as a given function of time, ρ_S will satisfy a Liouville equation with the bath playing the role of an external field.

II. EXACT NONLINEAR EQUATIONS FOR A COUPLED SUBSYSTEM AND BATH

The starting point for the analysis is a wave function ψ , the evolution of which is governed by the Schrödinger equation. This ψ serves to define a (pure state) density matrix ρ , the evolution of which is determined by the Liouville (or Liouville —von Neumann) equation

$$
\frac{d\rho}{dt} = -i[H,\rho] \equiv -L(t)\rho(t) .
$$
 (2.1)

Here H is the (in general time-dependent) Hamiltonian, the square brackets denote a commutator, and $L(t)$ is the so-called Liouville operator. The density matrix is assumed so normalized that $Tr \rho = 1$, where Tr denotes a trace over all the variables.

One wishes now to split the composite system described by ρ into two pieces, a "subsystem" characterized abstractly by some set of variables x , and a "bath" characterized by variables y. The associated reduced density matrices $\rho_S(x)$ and $\rho_B(y)$, not themselves corresponding to pure states, take the forms

$$
\rho_S(x) = \mathrm{Tr}_B \rho(x, y)
$$

and

$$
p_B(y) = Tr_S \rho(x, y) \t\t(2.2)
$$

where Tr_B and Tr_S denote, respectively, partial traces over bath and subsystem variables. The total Hamiltonian H decomposes into subsystem and bath contributions, and an additional interaction piece:

$$
H(x,y) = H_S(x) + H_B(y) + \lambda H_I(x,y) \tag{2.3}
$$

Associated with this decomposition are Liouville operators L_s , L_b , and λL_i . The introduction of the parameter λ , not necessarily assumed small, will prove useful below.

The objective now is to implement this splitting into subsystem and bath in a fashion well suited for analyzing the dynamical evolution (2.1). One "natural" way in which to do this is to write ρ in the form $\rho = \rho_R + \rho_I$, where, by definition,

$$
\rho_R(x, y) \equiv \rho_S(x) \rho_B(y) \tag{2.4}
$$

denotes that piece of the total ρ which contains no information about correlations between the subsystem and the bath. Indeed, as will be seen below, the ansatz $\rho \sim \rho_R$ leads to a simple Vlasov description.

As is well known in nonequilibrium statistical mechanics, this sort of decomposition can be rendered "canonical" and "consistent with the dynamics" through the incal" and "consistent with the dynamics" through the in-
roduction of an appropriate "projection operator." This can be done in many different ways. 10 However, the simplest, and perhaps most intuitive, fashion in which to proceed is simply to introduce the operator (cf. Ref. 5)

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$$
P[\rho_R(t)] \equiv P(t) = \rho_S(t) \text{Tr}_S + \rho_B(t) \text{Tr}_B
$$

$$
-\rho_S(t) \rho_B(t) \text{Tr}_S \text{Tr}_B . \tag{2.5}
$$

One then verifies that

$$
P(t)\rho(t) = \rho_R(t) = \rho_S(t)\rho_B(t) , \qquad (2.6)
$$

that

$$
P(t_2)P(t_1)\xi(x,y) = P(t_2)\xi(x,y)
$$
\n(2.7)

for all matrices $\xi(x,y)$ and all times $t_2 \ge t_1$, and that

$$
\left[P(t),\frac{d}{dt}\right]\rho(t)\equiv 0\ .
$$
 (2.8)

Equation (2.6) shows that P serves to "project out" ρ_R from the total ρ , and (2.7) then implies that, at fixed t, P is in fact idempotent, i.e., a real projection operator. This manifests a precise sense in which ρ_R and ρ_I are "orthogonal." Equation (2.8) shows that the operations of projection and time evolution effectively commute, so that the decomposition $\rho = \rho_R + \rho_I$ is consistent with the dynamics.

By acting on (2.1) with the operators P and $(1-P)$, one is then led to a coupled system of the form

$$
\frac{d\rho_R}{dt} + PL\rho_R = -PL\rho_I \tag{2.9}
$$

and

$$
\frac{d\rho_I}{dt} + (1 - P)L\rho_I = -(1 - P)L\rho_R \tag{2.10}
$$

It is straightforward to solve formally for the evolution of $\rho_I(t)$ in terms of an initial condition $\rho_I(t_0)$ and the values of ρ_R at retarded times $t' < t$, and then to insert this solution to (2.10) into Eq. (2.9). The net result is an exact, albeit nonlocal and nonlinear, equation for the time evolution of $\rho_R(t)$ which contains explicit reference to ρ_I only through the propagation of an initial condition $\rho_I(t_0)$. Thus, explicitly, one finds that

where

 $\frac{d\rho_R}{dt}$ + $PL\rho_R$ = $C[\rho_R]$

$$
C[\rho_R] = -P(t)L(t)G(t,t_0)\rho_I(t_0) + \int_0^{t-t_0} d\tau P(t)L(t)G(t,t-\tau) \times [1-P(t-\tau)]L(t-\tau)\rho_R(t-\tau)
$$
\n(2.11)

and

$$
G(t_2,t_1) = T \exp \left[- \int_{t_1}^{t_2} dt [1 - P(t)] L(t) \right].
$$
 (2.12)

Coupled equations for ρ_S and ρ_B follow immediately from this formal solution by taking partial traces Tr_B and Tr_S . Thus, for example, one sees that

$$
\operatorname{Tr}_{B}\left[\frac{d\rho_{R}}{dt} + PL\rho_{R}\right] = \frac{d\rho_{S}}{dt} + i \operatorname{Tr}_{B}[H_{s}(x) + \lambda H_{I}(x, y), \rho_{S}(x)\rho_{B}(y)] = \frac{d\rho_{S}(x)}{dt} + i\left[\mathcal{H}_{S}(x), \rho_{S}(x)\right],\tag{2.13}
$$

where

$$
\mathcal{H}_S(x) \equiv H_S(x) + \lambda \operatorname{Tr}_B \rho_B(y) H_I(x, y) \tag{2.14}
$$

denotes an "average subsystem Hamiltonian" weighted by the bath density matrix. In terms of $\mathcal{H}_S(x)$ and the corresponding

$$
\mathcal{H}_B(y) \equiv H_B(y) + \lambda \operatorname{Tr}_S \rho_S(x) H_I(x, y) \tag{2.15}
$$

for the bath, straightforward manipulations then lead to equations of the form $¹¹$ </sup>

$$
\frac{d\rho_S(x,t)}{dt} + i \left[\mathcal{H}_S, \rho_S \right]
$$

= $- \text{Tr}_B L(t) G(t,t_0) \rho_I(t_0)$
 $+ \lambda^2 \int_0^{t-t_0} d\tau \text{Tr}_B \Delta(t) G(t,t-\tau) \Delta(t-\tau)$
 $\times \rho_B(t-\tau) \rho_S(t-\tau)$ (2.16)

\n
$$
\mathcal{H}_S(x) \equiv H_S(x) + \lambda \operatorname{Tr}_B \rho_B(y) H_I(x, y)
$$
\n

\n\n (2.14) \n $\mathcal{H}_S(x) \equiv H_S(x) + \lambda \operatorname{Tr}_B \rho_B(y) H_I(x, y)$ \n

\n\n (2.14) \n $\mathcal{H}_B(x) = -\operatorname{Tr}_S L(t) G(t, t_0) \rho_I(t_0)$ \n

\n\n the bath density matrix. In terms of \n $\mathcal{H}_S(x)$ and the
\n asponding\n

\n\n $\mathcal{H}_B(y) \equiv H_B(y) + \lambda \operatorname{Tr}_S \rho_S(x) H_I(x, y)$ \n

\n\n (2.15) \n $\mathcal{H}_B(y) = \mathcal{H}_B(y) + \lambda \operatorname{Tr}_S \rho_S(x) H_I(x, y)$ \n

where, for arbitrary $\xi(x, y)$,

$$
\lambda \Delta(x, y) \xi(x, y) \equiv i [H(x, y) - \mathcal{H}_S(x) - \mathcal{H}_B(y), \xi(x, y)]
$$

\n
$$
= i \lambda [H_I(x, y) - \text{Tr}_B \rho_B(y') H_I(x, y')
$$

\n
$$
- \text{Tr}_S \rho_S(x') H_I(x', y), \xi(x, y)] \quad (2.18)
$$

\n
\nIII. APPROXIMATE EVOLUTION EQUATIONS
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III. APPROXIMATE EVOLUTION EQUATIONS

Equations (2.16) and (2.17) constitute a complicated nonlinear system reflecting the detailed effects of correlations between the subsystem and the bath. They do, how-

and

ever, simplify enormously in the limit that these correlations are "weak," so that, in some appropriate sense, the operator $\lambda \Delta$ is small. This will obviously be true if λH_t itself is small. In this case, assuming for simplicity an initial condition $\rho_I(t_0) = 0$, the right-hand sides of (2.16) and (2.17) may be viewed as being of order λ^2 in a λ expansion, and hence small compared with the left-hand sides, which are only of order λ . Indeed, in this case the linear equations

$$
\frac{d\rho_S}{dt} + i[\mathcal{H}_S, \rho_S] = 0 \tag{3.1}
$$

and

$$
\frac{d\rho_B}{dt} + i \left[\mathcal{H}_B, \rho_B \right] = 0 \tag{3.2}
$$

can be viewed formally as equations appropriate in a weak-coupling expansion truncated at $O(\lambda)$.

Even when λH_I is large, $\lambda \Delta$ may be small in a suitable sense. This is, e.g., well known in the theory of Newtonian stellar dynamics.¹² Here the quantum density matrix ρ is replaced by a classical *N*-particle distribution function which satisfies a classical Liouville equation, and the "uncorrelated piece" of this distribution function ρ_R is constructed as a product of N reduced one-particle distribution functions. In this case, λH_i denotes the total gravitational potential energy and the corresponding interaction Liouville operator λL_t involves the total gravitational force acting on each of the stars, a quantity which can in no sense be viewed as small. However, $\lambda \Delta$ involves instead a "fluctuating" gravitational force, from which the "average" Vlasov contribution has been subtracted, and there is a well-defined sense in which this is small. Although pointwise the "fluctuating" force may be large compared with the "true" force, it is small in the sense that its effects are typically manifested only on a very long "relaxation time" t_R .

In any case, the assumption that $\rho \simeq \rho_S \rho_B$ leads immediately to the bilinear system (3.1) and (3.2), which implies an isentropic evolution. Indeed, one verifies immediately that the subsystem and bath "entropies"

$$
S_S = -\text{Tr}_S \rho_S \text{ln} \rho_S \quad \text{and} \quad S_B = -\text{Tr}_B \rho_B \text{ln} \rho_B \tag{3.3}
$$

are both conserved in this Vlasov description: $dS_S/dt \equiv dS_B/dt \equiv 0$. It is only by allowing for changes in the degree of correlations between subsystem and bath that one can generate entropy for either the subsystem or the bath. And never will the total entropy

$$
S \equiv -\operatorname{Tr}\rho \ln \rho \tag{3.4}
$$

of the isolated system change. Equation (2.1) implies that $S \equiv -1$
of the isola
 $dS/dt \equiv 0$.
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If, alternatively, one considers the exact equations (2.16) and (2.17), the entropies S_S and S_B will evidence a nontrivial time dependence. Indeed, if one assumes once again an initial condition $\rho_I(t_0) = 0$, it follows that

$$
S_R \equiv -\operatorname{Tr}\rho_R \ln \rho_R = S_S + S_B \tag{3.5}
$$

the sum of contributions from subsystem and bath,

satisfies an equation

$$
\frac{dS_R}{dt} = \text{Tr} \int_0^{t-t_0} d\tau \rho_R^{-1}(t) \zeta(t) G(t, t-\tau) \zeta(t-\tau) , \qquad (3.5')
$$

where

$$
\zeta \equiv \Delta \rho_R = \Delta \rho_S \rho_B \tag{3.6}
$$

This implies in particular that, as the subsystem and bath interact to generate correlations as reflected by a nonvanishing $\rho_I(t)$, their joint entropy S_R must increase at least initially:

$$
\frac{dS_R(t_0 + \Delta t)}{dt} = \Delta t \operatorname{Tr} \rho_R^{-1}(t_0) \zeta^2(t_0) > 0 . \tag{3.7}
$$

Although the Vlasov description of (3.1) and (3.2) leads to conserved entropies S_S and S_B , energy conservation is more subtle. This for two reasons: (a) If the full Hamiltonian H is time dependent, there can be no fundamental energy conservation; (2) even if H is time independent, so that its expectation value defined with respect to ρ is conserved, there is the possibility of energy exchange between the subsystem and the bath, so that there need be no individually conserved subsystem and bath entropies.

Consistent with these caveats, however, two concrete results can be derived. Provided that H is independent of time, the "mean field energy"

$$
E = \text{Tr}H(x, y)\rho_S(x)\rho_B(y) \tag{3.8}
$$

associated with $\rho_R = \rho_S \rho_B$ will in fact be conserved. And, moreover, in the limit that $\lambda H_I \simeq 0$, i.e., in the absence of any interactions between the subsystem and the bath, there do exist individually conserved quantities

$$
E_S = \text{Tr}_S H_S(x) \rho_S(x) \text{ and } E_B = \text{Tr}_B H_B(y) \rho_B(y) . \quad (3.9)
$$

As noted in the Introduction, this Vlasov description simplifies further in the limit that λH_I has a negligible impact on the evolution of the bath. Indeed, to the extent that one can approximate $\mathcal{H}_B \simeq H_B$, ρ_B will satisfy a closed equation

$$
S_S = -\operatorname{Tr}_S \rho_S \ln \rho_S \quad \text{and} \quad S_B = -\operatorname{Tr}_B \rho_B \ln \rho_B \qquad (3.3) \qquad \frac{d\rho_B}{dt} = -i \left[H_B, \rho_B \right] \equiv -L_B(t) \rho_B(t) \tag{3.10}
$$

so that the formal solution

$$
\rho_B(t) = T \exp\left[-\int_{t_0}^t d\tau L_B(\tau)\right] \rho_B(t_0) \tag{3.11}
$$

allows one to view ρ_B as a known function of t. By inserting this $\rho_B(t)$ back into (3.1), one is then led finally to a Liouville-von Neumann equation for the reduced density matrix of the subsystem, ρ_s now satisfying an evolution equation appropriate in the presence of an external field characterized by a Hamiltonian

$$
H_{\text{ext}}(x) = \lambda \operatorname{Tr}_B H_I(x, y) \rho_B(y) \tag{3.12}
$$

Within the context of the setting suggested in the Introduction, where ρ_S and ρ_B reflect the matter and gravitational sectors of some quantum theory of gravity, the final Liouville equation

$$
\frac{d\rho_S}{dt} = i[H_S + H_{\text{ext}}, \rho_S]
$$
\n(3.13)

would presumably be interpreted as defining a "mean field" theory of matter associated with a gravitational background which need not be dominated by some single semiclassical solution.

One final point should be stressed. Although it has been assumed for conceptual reasons that the composite system of "subsystem" plus "bath" is characterized by a pure state density matrix, this was not used in any of the analysis. The preceding works for any density matrix ρ , either pure or impure, provided only that ρ satisfies the Liouville equation (2.1). This ambivalence reflects an importarit feature of the quantum description which would be lost in the classical limit. In this limit, ρ is reinterpreted as a distribution function, so that a pure state corresponds to a delta function in some appropriate phase space. This means, however, that the reduced distribution functions ρ_S and ρ_B also correspond to delta functions, so that $\rho = \rho_S \rho_B$. It follows, therefore, that

$$
S_R = -\operatorname{Tr}\rho_R \ln \rho_R = -\operatorname{Tr}\rho \ln \rho \tag{3.14}
$$

(where now Tr denotes a phase-space integral}, so that, quite generally, $dS_R/dt \equiv 0$. Only because of "quantum efTects" can a pure state for the composite system lead to a nonisentropic evolution for the subsystem.

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