Correlation entropy of an interacting quantum field and *H* theorem for the O(*N*) model

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Following the Boltzmann-BBGKY paradigm we propose a correlation entropy (of the *n*th order) for an interacting quantum field. The concept of correlation entropy is useful for addressing issues related to thermalization. As a small yet important step in that direction, we state an *H* theorem for the correlation entropy of a quantum-mechanical O(*N*) model with a closed time path two-particle irreducible effective action at the level of a next-to-leading-order large *N* approximation. This model may be regarded as a field theory in 0 space dimensions. We verify the validity of the proposed *H* theorem in two limiting cases.

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I. INTRODUCTION

The goal of this paper is twofold: the proposal of a correlation entropy for an interacting quantum field, and the statement of an *H* theorem for the quantum-mechanical O(*N*) model [1,2], which may be regarded as a field theory in zero space dimensions. For the former, we follow the paradigm of Boltzmann and Bogoliubov, Born, Green, Kirkwood, and Yvon (BBGKY) [3] and propose a correlation entropy (of the *n*th order) for an interacting quantum field [4–8]. We then derive the closed time path (CTP) [9] two-particle irreducible (2PI) [10] effective action (EA) for this model up to the next-to-leading order (NLO) in 1/*N* [11]. As a useful step towards addressing issues related to the thermalization of interacting quantum fields, we state an *H* theorem for the correlation entropy of a quantum-mechanical O(*N*) model at the CTP 2PI NLO level. We introduce the thermalization issue as a motivation for this study and give a short description of different definitions for the entropy of interacting quantum fields in the next section, followed by the statement of the *H* theorem given in the ensuing sections.[1]

The problem of thermalization in relativistic quantum fields has drawn much attention over time, both in the attempt to understand the origin of macroscopic irreversible behavior from microscopic theories, and for practical considerations of nonequilibrium quantum field processes in the early Universe and in relativistic heavy ion collisions [14].

In the strictest theoretical sense, an isolated system depicted by quantum field theory undergoes unitary evolution and does not thermalize (in the strong sense). However, one can still ask meaningful questions such as whether certain correlation functions may converge to their thermal forms in some well defined physical limit. We may call this a weak thermalization condition. In practical terms, one needs to be careful when addressing the question of even weak thermalization, as its precise meaning is often attached to a chosen level of approximation, such as the *n*PI of the correlation hierarchy, the loop expansion, the 1/*N* expansion, or expansion in powers of a coupling constant, etc.

There have been recent claims based on numerical evidence [15–19] that at the NLO large *N* approximation an interacting quantum field may show signs of thermalization. In a recent report [13], we consider an O(*N*) invariant scalar field of unbroken symmetry, develop the CTP 2PI EA [6] in powers of 1/*N*, retaining up to the next-to-leading order [O(1)] terms, and show that the only time translation invariant solutions are thermal. Our analytic result provides support for similar claims. Here, we present an alternative approach by defining a correlation entropy and verifying the existence of an *H* theorem in the simpler quantum-mechanical O(*N*) model. We first summarize the different ways of defining entropy for a quantum field.

II. ENTROPY OF INTERACTING QUANTUM FIELDS

Entropy reflects and measures the degree of incompleteness in the information one can attain resulting from one's specific way of seeking an approximate description of the features and dynamics of a system, in our case, the quantum field. First, for a unitarily evolving quantum field theory whose dynamics is a closed system (as opposed to an ''effectively open system'') and governed by the quantum Liouville equation, it is well known that the von Neumann entropy of the density matrix,

$$S_{\rm VN} = -\,{\rm Tr}[\rho(t)\ln\rho(t)], \tag{1}$$

is exactly conserved. If there is a justifiable separation of macroscopic and microscopic time scales, one can adopt the theoretical framework of quantum kinetic field theory. If one

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[1]The following descriptive summary in this and the next section is adapted from Chap. 5 of [12], where a preliminary attempt to construct a correlation entropy was made but the proof of the *H* theorem for an interacting quantum field did not materialize, and from [13].

makes the assumption of factorization (equivalently, slaving of the Wigner-transformed four-point function), one obtains the relativistic Boltzmann equation in the binary collision approximation. The Boltzmann entropy S_B defined in terms of the phase-space distribution $f(k,X)$ for quasiparticles can in this case be shown to satisfy a relativistic H theorem [20,6]. We want to generalize this to a correlation entropy for interacting quantum fields.

However, in the case where there does *not* exist such a separation of time scales, how does one define the entropy of a quantum field? For nonperturbative truncations of the dynamics of interacting quantum fields, this is a nontrivial question [21]. Intuitively, one expects that any coarse graining which leads to an effectively open system with irreversible dynamics will also lead to the growth of entropy. Formally these operations can be systematically expressed in terms of the projection operator techniques [22]. A projection operator P projects out the *irrelevant* degrees of freedom (thus going over to an open system) from the total system described by the density operator ρ, yielding the reduced density matrix ρ_R,

$$\rho_R(t) = P\rho(t). \tag{2}$$

There exists a well-developed formalism for deriving the equation of motion of the *relevant* degrees of freedom, and in terms of it, the behavior of the coarse-grained (CG) entropy [22,3]

$$S_{\mathrm{CG}} = -\mathrm{Tr}[\rho_R(t)\ln\rho_R(t)], \tag{3}$$

which will in general not be conserved. The projection operator formalism can be used to express the slaving of higher correlation functions in the correlation hierarchy. From it one can define an entropy in effectively open systems (see, e.g., [23]). (So far it has only been implemented within the framework of perturbation theory.) Another equally powerful method adept to field theory is the Feynman-Vernon influence functional formalism [24,25] which has been used to treat entropy in quantum open systems (see, e.g., [26]).

A. Entropy special to choice of basis or representation

We now consider the entropy functions for quantum fields, beginning with the simpler yet more subtle case of a free field. Historically this issue was, to our knowledge, first raised in the context of entropy generation from particle creation for a free quantum field in an expanding Universe [27] due to the parametric amplification of vacuum fluctuations. The focal point is a wave equation with a time-dependent natural frequency for the amplitude function of a normal mode. [The same condition arises for an interacting field (such as the $\lambda\Phi^4$ theory) in the Hartree-Fock approximation or the O(N) field theory at leading order in the large-N expansion [11].] Since the underlying dynamics is clearly unitary and time-reversal invariant in this case, a suitable coarse graining leading to entropy growth is not trivially evident. Hu and Pavon [28] first made the observation that a coarse graining is implicitly incorporated when one chooses to depict particle numbers in the n-particle Fock (or "N") representation or to depict phase coherence in the phase (or "P") representation. Various proposals for coarse graining the dynamics of parametric oscillators have followed [29–33]. The language of squeezed states is particularly useful for describing entropy growth due to parametric particle creation [26,31,34,35]. For our purposes, the essential features of entropy growth due to parametric particle creation which distinguish it from correlational entropy growth (to be discussed below) are that parametric particle creation depends sensitively on the choice of representation for the state space of the parametric oscillators and the specificity of the initial conditions.

B. Entropy from projecting out irrelevant variables

In contrast to entropy growth resulting from parametric *particle creation* from the vacuum, entropy growth due to *particle interactions* in quantum field theory [21] has a very different physical origin. A coarse-graining scheme was proposed by Hu and Kandrup [21] for these processes. Expressing an interacting quantum field in terms of a collection of coupled parametric oscillators, their proposal is to define a reduced density matrix by projecting the full density operator onto each oscillator's single-oscillator Hilbert space in turn,

$$\gamma(\vec{k}) \equiv \mathrm{Tr}_{\vec{k}'\neq\vec{k}}\rho, \tag{4}$$

and defining the reduced density operator as the tensor product Π of the projected single-oscillator density operators $\gamma(\vec{k})$,

$$\rho_R \equiv \Pi_{\vec{k}}\gamma(\vec{k}). \tag{5}$$

The coarse-grained (Hu-Kandrup) entropy is then just given by Eq. (3), from which we obtain

$$S_{\mathrm{HK}} = -\sum_{\vec{k}} \mathrm{Tr}[\gamma(\vec{k})\ln\gamma(\vec{k})]. \tag{6}$$

It is interesting to observe that for a spatially translation-invariant density matrix for a quantum field theory which is Gaussian in the position basis, this entropy is just the von Neumann entropy of the full density matrix, because the spatially translation-invariant Gaussian density matrix separates into a product over density submatrices for each $\vec{k}$ oscillator. This projection (Hu-Kandrup) coarse graining, like the correlation-hierarchy (Calzetta-Hu) coarse-graining scheme, does not choose or depend on a particular representation for the single oscillator Hilbert space. It is sensitive to the establishment of correlations through the explicit couplings.

C. Entropy from slaving the higher correlations: The CTP 2PI effective action

A general procedure has been presented for obtaining coupled equations for correlation functions at any order l in the correlation hierarchy, which involves a truncation of the *master effective action* at a finite order in the loop expansion [7,8]. By working with an l loop-order truncation of the master effective action, one obtains a closed, time-reversal in-

variant set of coupled equations for the first $l+1$ correlation functions, $\hat{\phi}, G, C_3, \ldots, C_{l+1}$. In general, the equation of motion for the highest-order correlation function will be linear, and thus can be formally solved using Green's-function methods. The existence of a unique solution depends on supplying boundary conditions. We have shown elsewhere that this system will manifest noise/fluctuations [7,8] for the case of the slaving of the four-point function to the two-point function in the symmetry-unbroken $\lambda\Phi^4$ field theory. Thus a framework exists for exploring irreversibility and fluctuations within the context of a unitary quantum field theory, using the truncation and slaving of the correlation hierarchy. The effectively open system framework is useful for precisely those situations, where a separation of macroscopic and microscopic time scales (which would permit an effective kinetic theory description) does *not* exist, such as is encountered in the thermalization issue.

While it is certainly not the only coarse-graining scheme which could be applied to an interacting quantum field, the slaving of higher correlation functions to lower-order correlation functions within a particular truncation of the correlation hierarchy, as a particular coarse-graining method, has several important benefits. It can be implemented in a truly nonperturbative fashion. This necessitates a nonperturbative resummation of daisy graphs, which can be incorporated in the truncation/slaving of the correlation hierarchy in a natural way.

III. THE *H* THEOREM FOR THE QUANTUM-MECHANICAL O(N) MODEL

A. The next-to-leading order large *N* approximation

The number N of replicas of essentially identical fields [like the N scalar fields in an O(N) invariant theory, or the N^2-1 gauge fields in a $SU(N)$ invariant non-Abelian gauge theory] suggests using $1/N$ as a natural small parameter, with a well-defined physical meaning. Unlike coupling constants, this is not subjected to renormalization or radiative corrections. By ordering the perturbative expansion in powers of this small parameter, several nonperturbative effects (in terms of coupling constants) may be systematically investigated.

The ability of the $1/N$ framework to address the nonperturbative aspects of quantum field dynamics has motivated a detailed study of the properties of these systems. In nonequilibrium situations, this formalism has been applied to the dynamics of symmetry breaking [11,36–40] and self-consistent semiclassical cosmological models [41–46].

In the case of the O(N) invariant theory, in the presence of a nonzero background field (or an external gravitational or electromagnetic field interacting with the scalar field) we may distinguish the longitudinal quantum fluctuations in the direction of the background field, in field space, from the $N-1$ transverse (Goldstone or pion) fluctuations perpendicular to it. To first order in $1/N$, the longitudinal fluctuations drop out of the formalism, so we effectively are treating the background field as classical. Likewise, quantum fluctuations of the external field are overpowered by the fluctuations of the N scalar fields. In this way, the $1/N$ framework provides a systematics and a quantitative measure of the semiclassical approximation [47].

To leading order (LO), the theory reduces to $N-1$ linear fields with a time-dependent mass, which depends on the background field and on the linear fields themselves through a gap equation local in time. This depiction of the dynamics agrees both with the Gaussian approximation for the density matrix [48,49] and with the Hartree approximation [32]. The LO $1/N$ theory is Hamiltonian [32] and time-reversal invariant. It simply does not thermalize. For example, if we set up conditions where both the background field and the self-consistent mass are space-time independent, then the particle numbers for each fluctuation mode will be conserved. The existence of these conservation laws precludes thermalization [50].

We note that the failure of the LO approximation to describe thermalization is indicative of a more general breakdown of the approximation at later times, where effects of particle interaction dominate. Both the distribution of energy among the field modes and the phase relationships (or lack thereof) among them affect the way quantum fluctuations react on the background or external fields. Therefore, from physical considerations, one can say that a theory which does not describe thermalization becomes unreliable for most other purposes as well [51].

This is where the next to leading order (NLO) approximation enters. It has been applied to quantum mechanics [1,2], classical field theory [52–55], and quantum field theory [17,19,56], being contrasted both to exact numerical simulations of these systems, as well as against other approximations purporting to go beyond LO. The NLO has been shown to be an accurate approximation, even at moderate values of N.

It is crucial to realize that attempts to compute the time evolution in a $1/N$ expansion of the standard 1PI effective action at NLO fail. This happens, in particular, because of the appearance of secular terms which grow with time and can spoil the $1/N$ counting for times of order N (see, e.g., [57,58]). Therefore, it is crucial to resume the standard $1/N$ expansion, which can be done using the 2PI $1/N$ expansion.

The 2PI formalism is also suitable for this question because, provided an auxiliary field is cleverly introduced, the 2PI CTP effective action can be found in closed form at each order in $1/N$ [11,59]. We now begin our study with a concrete model.

B. O(N) λX^4 theory

We summarize in this section some known results on the O(N) λX^4 theory which we shall need below; see [2,16,59].

To fix the physical ideas, we shall discuss the problem in zero space dimensions, namely, the quantum-mechanical O(N) model. The system dynamics is described by the Hamiltonian with variables X_A and their conjugate momenta P^A, where A,B are the O(N) group indices, with

$$H=\frac{1}{2}\left\{P^B P^B + M^2 X_B X_B + \frac{\lambda}{4N}(X_B X_B)^2\right\}. \qquad (7)$$

The classical action

$$S=\int dt\frac{1}{2}\left\{\dot{X}_B\dot{X}_B-M^2X_BX_B-\frac{\lambda}{4N}(X_BX_B)^2\right\} \tag{8}$$

where M_0^2 and λ_0 are the mass parameter and coupling constant. We rescale $X_B\equiv\sqrt{N}x_B$,

$$S=N\int dt\frac{1}{2}\left\{\dot{x}_B\dot{x}_B-M^2x_Bx_B-\frac{\lambda}{4}(x_Bx_B)^2\right\}. \tag{9}$$

Discarding a constant term, we may rewrite the classical action as

$$S=N\int dt\frac{1}{2}\left\{\dot{x}_B\dot{x}_B-\left[\frac{M^2}{\sqrt{\lambda}}+\frac{\sqrt{\lambda}}{2}x_Bx_B\right]^2\right\}. \tag{10}$$

To set up the $1/N$ resummation scheme, it is customary to introduce the auxiliary field χ, writing

$$S=\frac{N}{2}\int\left\{\dot{x}_B\dot{x}_B-\left[\frac{M^2}{\sqrt{\lambda}}+\frac{\sqrt{\lambda}}{2}x_Bx_B\right]^2+\left[\frac{M^2-\chi}{\sqrt{\lambda}}+\frac{\sqrt{\lambda}}{2}x_Bx_B\right]^2\right\} \tag{11}$$

whence

$$S=N\int dt\left\{\frac{1}{2}\dot{x}_B\dot{x}_B-\chi\left[\frac{M^2}{\lambda}+\frac{x_Bx_B}{2}\right]+\frac{1}{2\lambda}\chi^2\right\}. \tag{12}$$

From now on, we consider χ and x_B as fundamental variables on equal footing.

Because of the O(N) symmetry, the symmetric point must be a solution of the equations of motion. For simplicity, we shall assume we are within this symmetric phase, and treat x_B as a quantum fluctuation. We also split the auxiliary field $\chi=\overline{\chi}+\tilde{\chi}$ into a background field $\overline{\chi}$ and a fluctuation field $\tilde{\chi}$. The action becomes

$$S=S_0+S_1+S_2+S_3. \tag{13}$$

S_0 is just the classical action evaluated at $x_B=0$, $\chi=\overline{\chi}$:

$$S_0=\frac{N}{\lambda}\int dt\left\{\frac{1}{2}\overline{\chi}^2-M^2\overline{\chi}\right\}. \tag{14}$$

S_1 contains terms linear in $\tilde{\chi}$ and can be set to zero by a suitable choice of the background field $\overline{\chi}$,

$$S_1=\frac{N}{\lambda}\int dt\{\overline{\chi}-M^2\}\tilde{\chi}. \tag{15}$$

S_2 contains the quadratic terms and yields the tree-level inverse propagators,

$$S_2=N\int dt\left\{\frac{1}{2}\dot{x}_B\dot{x}_B-\frac{\overline{\chi}}{2}x_Bx_B+\frac{1}{2\lambda}\tilde{\chi}^2\right\}. \tag{16}$$

Finally S_3 contains the bare vertex

$$S_3=\left(\frac{-N}{2}\right)\int d^dx\{\tilde{\chi}x_Bx_B\}. \tag{17}$$

To write the 2PI CTP EA we double the degrees of freedom, incorporating a branch label $a=1,2$ [for simplicity, if not explicitly written, we assume that the label a also contains the time branch, i.e., $x^{Aa}\equiv x^{Aa}(t_a)$]. We also introduce propagators $G^{Aa,Bb}$ for the path ordered expectation values

$$G^{Aa,Bb}=\langle x^{Aa}x^{Bb}\rangle \tag{18}$$

and F^{ab} for

$$F^{ab}=\langle\tilde{\chi}^a\tilde{\chi}^b\rangle. \tag{19}$$

Because of symmetry, it is not necessary to introduce a mixed propagator, for $\langle\tilde{\chi}^ax^{Bb}\rangle\equiv 0$. The 2PI CTP EA reads

$$\Gamma=S_0[\overline{\chi}^1]-S_0[\overline{\chi}^2]+\frac{1}{2}\int du\,dv\left\{D_{Aa,Bb}(u,v)G^{Aa,Bb}(u,v)+\frac{N}{\lambda_0}c_{ab}\delta(u,v)F^{ab}(u,v)\right\}-\frac{i\hbar}{2}[\mathrm{Tr}\ln G+\mathrm{Tr}\ln F]+\Gamma_Q, \tag{20}$$

where, if the position variable is explicit, $c_{11}=-c_{22}=1$, $c_{12}=c_{21}=0$,

$$D_{Aa,Bb}(u,v)=N\delta_{AB}[c_{ab}\partial_x^2-c_{abc}\overline{\chi}^c]\delta(u,v), \tag{21}$$

and $c_{abc}=1$ when all entries are 1, $c_{abc}=-1$ when all entries are 2, and $c_{abc}=0$ otherwise. When we use the compressed notation, it is understood that $c_{ab}\equiv c_{ab}\delta(t_a,t_b)$ and $c_{abc}\equiv c_{abc}\delta(t_a,t_b)\delta(t_a,t_c)$. Γ_Q is the sum of all 2PI vacuum bubbles with cubic vertices from S_3 and propagators $G^{Aa,Bb}$ and F^{ab}. Observe that Γ_Q is independent of $\overline{\chi}^c$.

Taking variations of the 2PI CTP EA and identifying $\overline{\chi}^1=\overline{\chi}^2=\overline{\chi}$, we find the equations of motion

$$\frac{N}{2}\delta_{AB}D_{ab}-\frac{i\hbar}{2}[G^{-1}]_{Aa,Bb}+\frac{1}{2}\Pi_{Aa,Bb}=0, \tag{22}$$

$$\frac{N}{2\lambda}c_{ab}-\frac{i\hbar}{2}[F^{-1}]_{ab}+\frac{1}{2}\Pi_{ab}=0, \tag{23}$$

$$\frac{N}{\lambda}\{\overline{\chi}(t)-M^2\}-\frac{N}{2}\delta_{AB}G^{A1,B1}(t,t)=0, \tag{24}$$

where $D_{ab}(u,v)=c_{ab}[\partial_x^2-\overline{\chi}(u)]\delta(u,v)$,

$$\Pi_{Aa,Bb}=2\frac{\delta\Gamma_Q}{\delta G^{Aa,Bb}},\quad \Pi_{ab}=2\frac{\delta\Gamma_Q}{\delta F^{ab}}. \tag{25}$$

We shall seek a solution with the structure

$$G^{Aa,Bb}=\frac{\hbar}{N}\delta^{AB}G^{ab}(u,v), \tag{26}$$

which is consistent with vanishing Noether charges. Then it is convenient to write

$$F^{ab}=\frac{\hbar}{N}H^{ab}, \quad \Pi_{Aa,Bb}=\delta_{AB}P_{ab},$$

$$\Pi_{ab}(x,y)=NQ_{ab}(x,y). \tag{27}$$

The equations become

$$D_{ab}-i[G^{-1}]_{ab}+\frac{1}{N}P_{ab}=0, \tag{28}$$

$$\frac{1}{\lambda}c_{ab}-i[H^{-1}]_{ab}+Q_{ab}=0, \tag{29}$$

$$\frac{1}{\lambda}\{\overline{\chi}(t)-M^2\}-\frac{\hbar}{2}G^{11}(t,t)=0. \tag{30}$$

Observe that

$$P_{ab}=\frac{2}{\hbar}\frac{\delta\Gamma_Q}{\delta G^{ab}}, \quad Q_{ab}=\frac{2}{\hbar}\frac{\delta\Gamma_Q}{\delta H^{ab}}. \tag{31}$$

These are the exact equations we must solve. The successive $1/N$ approximations amount to different constitutive relations expressing P_{ab} and Q_{ab} in terms of the propagators.

The key observation is that in any given Feynman graph each vertex contributes a power of N, each internal line a power of N^{-1}, and each trace over group indices another power of N. We have both G and H internal lines, but the G lines only appear in closed loops. On each loop, the number of vertices equals the number of G lines, so there only remains one power of N from the single trace over group labels. Therefore, the overall power of the graph is the number of G loops minus the number of H lines. Now, since we only consider 2PI graphs, there is a minimum number of H lines for a given number of G loops. For example, if there are two G loops, they must be connected by no fewer than three H lines, and so this graph cannot be higher than NNLO. A graph with three G loops cannot have fewer than five H lines, and so on.

We conclude that Γ_Q vanishes at LO, and therefore $P_{ab}=Q_{ab}=0$. There is only one NLO graph, consisting of a single G loop and a single H line. This graph leads to

$$\Gamma_Q^{\rm NLO}=(-i\hbar)\left(-\frac{1}{2}\right)\left(-\frac{N}{2Z_0\hbar}\right)^2 2N\left(\frac{\hbar}{N}\right)^3 c_{abc}c_{def} \times\int du\,dv H^{ad}(u,v)G^{be}(u,v)G^{cf}(u,v). \tag{32}$$

Therefore, we get

$$P_{ab}=i\hbar c_{acd}c_{bef}H^{ce}G^{df}, \tag{33}$$

$$Q_{ab}=\frac{i\hbar}{2}c_{acd}c_{bef}G^{ce}G^{df}. \tag{34}$$

The theory so constructed belongs to the class of Φ-derivable theories, and therefore is consistent with energy conservation [60].

From quantum field theory it is common knowledge that equations derived from an action principle are necessarily time reversal invariant if the Lagrangian is local. For a nonlocal action, there is no *a priori* justification to this effect. In fact, a *nonlocal* action of the closed time-path kind may lead upon variation to equations of motion containing dissipation and fluctuations with a clear mathematical and physical meaning. (This has been shown in many circumstances both in theory and in practice, with detailed calculations and discussions. See, e.g., Refs. [44,45,61,62]. In the latest example [63], it is shown how a general dissipative and stochastic equation of motion can be derived from a CTP effective action.)

C. From correlations to the reduced density matrix

The 2PIEA yields equations of motion for the (arbitrary time) two-point functions of the theory. Given a solution of these equations, in principle we may find the expectation values of a large family of composite operators at any given time. Suppose we adopt a coarse-grained description where we choose a certain number of these expectation values as the relevant variables to describe the system. Then there will be a single density matrix which has maximum von Neumann entropy with respect to the class of states reproducing the preferred expectation values. This maximum entropy density matrix is the reduced density matrix for the system, and its entropy its correlation entropy. The H theorem is the statement that the correlation entropy grows in time, when the correlations themselves are evolved using the equations derived from the 2PIEA truncated to some order in the $1/N$ expansion (this statement will be qualified below).

Let us consider first the simplest case where we describe the system by specifying the values of $\langle x_B x_B\rangle$, $\langle x_B p_B + p_B x_B\rangle$, and $\langle p^B p^B\rangle$ ($p^A=N\dot{x}^A$ is the momentum conjugate to x_B) at every moment of time (by symmetry, we assume $\langle x_B x_C\rangle=\delta_{BC}\langle x_B x_B\rangle/N$, and similarly in the other cases). This choice of relevant variables does not utilize or display the full power of the 2PI CTP EA, in the sense that the 2PI CTP EA yields equations of motion which, if carried beyond LO, account for the build-up of non-Gaussian correlations. However, this restriction is assumed explicitly or implicitly in most of the work on thermalization, and the focus is placed on the shape of the spectrum of the two-point functions at different times. The situation is analogous to Boltzmann theory, where the equations of motion can describe the build-up of two-particle correlation functions from an uncorrelated initial state, but the Boltzmann entropy is defined from the one-particle distribution function alone.

At every moment of time we define a maximum entropy density matrix [64,65]

$$\rho(t)=Z^{-1}e^{-H_0}, \tag{35}$$

where

$$H_0=\frac{1}{2}\{\alpha p^B p^B+\beta(x_B p_B+p_B x_B)+\gamma x_B x_B\} \tag{36}$$

and

$$Z=\mathrm{Tr}\, e^{-H_0}=z^N, \tag{37}$$

$$z=\frac{1}{2\sinh\left[\frac{1}{2}\hbar\sigma\right]}, \tag{38}$$

where

$$\sigma^2=\alpha\gamma-\beta^2 \tag{39}$$

(see Appendix A). The parameter σ measures how far the system is from a pure state. To see this, observe that

$$\mathrm{Tr}\,\rho^2=\frac{\mathrm{Tr}\, e^{-2H_0}}{Z^2}=\left[\frac{2\sinh^2\left[\frac{1}{2}\hbar\sigma\right]}{\sinh[\hbar\sigma]}\right]^N$$
$$=\left(\tanh\left[\frac{1}{2}\hbar\sigma\right]\right)^N. \tag{40}$$

So $\sigma\to\infty$ yields a pure state, while the state is mixed for any finite σ. Therefore, to show the H theorem, we must show that $d\sigma/dt<0$.

Let us begin by showing that σ may be written directly in terms of the expectation values for binary products of canonical variables. Indeed, we have

$$-2\frac{\partial}{\partial\alpha}\ln Z=\langle p^B p^B\rangle=\frac{N\hbar}{\tanh\left[\frac{1}{2}\hbar\sigma\right]}\frac{\gamma}{2\sigma}, \tag{41}$$

$$-2\frac{\partial}{\partial\gamma}\ln Z=\langle x_B x_B\rangle=\frac{N\hbar}{\tanh\left[\frac{1}{2}\hbar\sigma\right]}\frac{\alpha}{2\sigma}, \tag{42}$$

$$-2\frac{\partial}{\partial\beta}\ln Z=\langle x_B p_B+p_B x_B\rangle=\frac{-N\hbar}{\tanh\left[\frac{1}{2}\hbar\sigma\right]}\frac{\beta}{\sigma}. \tag{43}$$

Therefore,

$$4\langle p^B p^B\rangle\langle x_B x_B\rangle-\langle x_B p_B+p_B x_B\rangle^2$$
$$=\left(\frac{N\hbar}{\tanh\left[\frac{1}{2}\hbar\sigma\right]}\right)^2. \tag{44}$$

As an aside, these formulas show that

$$\langle H_0\rangle=\frac{N\hbar\sigma}{2\tanh\left[\frac{1}{2}\hbar\sigma\right]}, \tag{45}$$

therefore the von Neumann entropy of the maximum entropy density matrix is

$$S=-\langle\ln\rho\rangle=\langle H_0\rangle+\ln Z$$
$$=\frac{N\hbar\sigma}{2\tanh\left[\frac{1}{2}\hbar\sigma\right]}-N\ln\left(\sinh\left[\frac{1}{2}\hbar\sigma\right]\right)-N\ln 2. \tag{46}$$

Observe that

$$\frac{dS}{d\sigma}=-\frac{N\hbar^2\sigma}{4\sinh^2\left[\frac{1}{2}\hbar\sigma\right]}<0. \tag{47}$$

So again, to obtain an H theorem we must show that σ is nonincreasing in time.

D. The physical basis of the *H* theorem

It is clear that if we could solve the exact evolution, the H theorem would be manifest: Given $\rho(t_0)$ at the initial time t_0, solve the exact Liouville equation up to a time t_1. Let $\overline{\rho}(t_1)$ be the result. We extract the new expectation values from $\overline{\rho}(t_1)$ and use them to construct the new maximum entropy density matrix $\rho(t_1)$. Then $S[\rho(t_1)]\geqslant S[\overline{\rho}(t_1)]$, by definition, and $S[\overline{\rho}(t_1)]=S[\rho(t_0)]$, because the exact evolution is unitary, thus the H theorem.

What we need to determine is whether, given the approximate dynamics for the expectation values provided by the $1/N$ scheme, the H theorem still holds. In fact, we know to LO it does not. From the angle of addressing the thermalization issue, the LO approximation totally misses the point.

Physically, we expect to obtain an H theorem because our description of the system is incomplete, in that it ignores higher correlations. We may rightfully call this entropy *correlation entropy*, as explained in the Introduction. The system as described by a finite-order $1/N$ approximation is an open system, in the following sense: Suppose we try to reproduce it in the lab. In order to have the different correlations evolving according to the 2PI $1/N$ equations appropriate to the desired order, rather than the full Schwinger-Dyson hierarchy, we must keep nudging it to conform to this artificially created condition (again, due to our inability to comprehend the complete picture). So there is energy and (in principle) entropy flow in and out of the system besides correlation entropy production. The sum of the entropy produced in the system, and that exchanged with the environment (which keeps the system on course) need not be positive.

In the LO case, as the approximate evolution (described by a quantum Vlasov equation [33]) is unitary, there is no net entropy production and no H theorem. This implies that the two sources of entropy change must cancel exactly. Note that

in such a case, if one works with a Fock representation, for boson fields, the number of particles increases with time and can be used as a measure of field entropy (what Hu and Pavon [28] called an intrinsic measure of field entropy, as described in Sec. II A above; see also [32]). However, this should not be confused with the correlation entropy of the Boltzmann kind under study for which the H theorem is defined.

Of course, we expect better approximations to be closer to the exact dynamics, therefore requiring less external control of (or rather, tampering with) the system. This reduces the entropy loss to the environment. Eventually correlation entropy production becomes the dominant factor, and an H theorem is obtained.

To summarize, the relevant question is not whether there is an H theorem for a given choice of relevant variables, which is obvious, but rather if the NLO approximation is good enough to make it manifest, or if we must go even higher.

We emphasize again that the choice of the set of relevant observables is crucial. If one would e.g. define a maximum entropy density matrix by specifying the system only in terms of $\langle x_B x_B\rangle$ and $\langle p^B p^B\rangle$, while leaving out $\langle x_B p_B + p_B x_B\rangle$, then the entropy would probably not be a constant already at LO and a similar analysis would give an H theorem. At the opposite extremum, the von Neumann entropy of the full density matrix (not the maximum entropy one) remains constant both at LO and NLO.

E. Statement of the *H* theorem

To continue our investigation, first note that

$$\Delta = \frac{d}{dt}\{4\langle p^B p^B\rangle\langle x_B x_B\rangle - \langle x_B p_B + p_B x_B\rangle^2\} = -\left(\frac{N^2\hbar^2}{\tanh\left[\frac{1}{2}\hbar\sigma\right]}\right)\frac{1}{\sinh^2\left[\frac{1}{2}\hbar\sigma\right]}\frac{d\sigma}{dt}. \tag{48}$$

So we must show that the left-hand side is positive. Since the $1/N$ scheme proceeds via taking the expectation values of the canonical equations of motion, we may use them to simplify this expression. The canonical equations are (for simplicity, we use the form without the auxiliary field)

$$\dot{x}^A = \frac{p^A}{N}, \tag{49}$$

$$\dot{p}^A = -N\left[M^2 + \frac{\lambda}{2}(x_B x_B)\right]x^A. \tag{50}$$

Therefore,

$$\frac{d}{dt}\langle x_B x_B\rangle = \frac{1}{N}\langle x_B p_B + p_B x_B\rangle, \tag{51}$$

$$\frac{d}{dt}\langle p^B p^B\rangle = -N\left[M^2\langle x_B p_B + p_B x_B\rangle - \frac{\lambda}{2}\langle (x_C x_C) x_B p_B + p_B x_B (x_C x_C)\rangle\right]. \tag{52}$$

Recall the canonical commutation relations

$$x_B p_B = \frac{1}{2}(x_B p_B + p_B x_B) + \frac{i\hbar}{2}, \tag{53}$$

$$p_B x_B = \frac{1}{2}(x_B p_B + p_B x_B) - \frac{i\hbar}{2}, \tag{54}$$

so

$$\frac{d}{dt}\langle p^B p^B\rangle = -N\left[M^2\langle x_B p_B + p_B x_B\rangle + \frac{\lambda}{4}\langle (x_C x_C)(x_B p_B + p_B x_B) + (x_B p_B + p_B x_B)(x_C x_C)\rangle\right]. \tag{55}$$

Finally,

$$\frac{d}{dt}\langle x_B p_B + p_B x_B\rangle = \frac{2}{N}\langle p^B p^B\rangle - 2N\left[M^2\langle x_B x_B\rangle + \frac{\lambda}{2}\langle (x_C x_C)^2\rangle\right], \tag{56}$$

so

$$\begin{aligned}\Delta &= \frac{d}{dt}\{4\langle p^B p^B\rangle\langle x_B x_B\rangle - \langle x_B p_B + p_B x_B\rangle^2\} \\ &= \lambda N\{2\langle x_B p_B + p_B x_B\rangle\langle (x_C x_C)^2\rangle \\ &\quad - \langle x_B x_B\rangle\langle (x_C x_C)(x_B p_B + p_B x_B) \\ &\quad + (x_B p_B + p_B x_B)(x_C x_C)\rangle\}.\end{aligned} \tag{57}$$

This may be rewritten in the following suggestive way:

$$\begin{aligned}\Delta &= \lambda\left\{2\langle (x_C x_C)^2\rangle\frac{d}{dt}\langle x_B x_B\rangle - \langle x_B x_B\rangle\frac{d}{dt}\langle (x_C x_C)^2\rangle\right\} \\ &= (-\lambda)\langle x_B x_B\rangle^3\frac{d}{dt}\left[\frac{\langle (x_C x_C)^2\rangle}{\langle x_B x_B\rangle^2}\right],\end{aligned} \tag{58}$$

so the H theorem reads

$$\frac{d}{dt}\left[\frac{\langle (x_C x_C)^2\rangle}{\langle x_B x_B\rangle^2}\right] \leqslant 0. \tag{59}$$

Or, equivalently,

$$\frac{d}{dt}\left[\frac{\langle (x_C x_C)^2\rangle - \langle x_B x_B\rangle^2}{\langle x_B x_B\rangle^2}\right] \leqslant 0. \tag{60}$$

Observe that this expression is invariant under a rescaling of the field.

IV. CORRELATION ENTROPY PRODUCTION IN WEAKLY COUPLED THEORIES

The results from the last section may be summarized as [cf. Eqs. (47), (48), and (58)]

$$\frac{dS}{dt} = \left(\frac{-\lambda}{4N}\right)\sigma \tanh\left[\frac{1}{2}\hbar\sigma\right]\langle x_B x_B\rangle^3 \frac{d}{dt}\left[\frac{\langle (x_C x_C)^2\rangle}{\langle x_B x_B\rangle^2}\right]. \tag{61}$$

We shall not attempt to give a general proof that this quantity is non-negative, but only check that it is so in some simple cases.

We must first express the expectation value in Eq. (61) to the required order in $1/N$. Recall that the q-number auxiliary field χ was introduced as a formal Gaussian process with correlation functions

$$\langle \chi(t)\rangle_\chi = M^2 + \frac{\lambda}{2} x_B x_B(t), \tag{62}$$

$$\langle \chi(t)\chi(t')\rangle_\chi = \left(M^2 + \frac{\lambda}{2} x_B x_B(t)\right)\left(M^2 + \frac{\lambda}{2} x_B x_B(t')\right) + \frac{i\lambda\hbar}{N}\delta(t-t'), \tag{63}$$

where $\langle\rangle_\chi$ denotes an expectation value with respect to the χ variable alone. Taking a further expectation value over the quantum state of the x fields, we recover Eq. (30) and

$$\frac{\hbar}{N} H^{11}(t,t') = \frac{\lambda^2}{4}[\langle x_B x_B(t) x_B x_B(t')\rangle - \langle x_B x_B(t)\rangle\langle x_B x_B(t')\rangle] + \frac{i\lambda\hbar}{N}\delta(t-t'). \tag{64}$$

Therefore, the H theorem boils down to showing that

$$\frac{4\hbar}{\lambda^2 N}\frac{d}{dt}\frac{[H^{11}(t,t) - i\lambda\,\delta(0)]}{\langle x_B x_B(t)\rangle^2} \leqslant 0. \tag{65}$$

It is clear that there is no correlation entropy production in free theories, so if the H theorem is to hold as a categorical relationship, then it must hold already to lowest order in the coupling constant. Therefore, we may expand $H^{11}(t,t)$ in powers of λ, keeping only the lowest nontrivial order. Iterating the equation of motion

$$H^{ac}(t,t') = i\lambda c^{ac}\delta(t-t') - \lambda\int ds\, c^{ab} Q_{bd}(t,s) H^{dc}(s,t'), \tag{66}$$

we get

$$H^{11}(t,t) = i\lambda\,\delta(0) - i\lambda^2 Q^{11}(t,t) + i\frac{\lambda^3\hbar^2}{4}\Psi, \tag{67}$$

where

$$\Psi = \frac{4}{\hbar^2}\int dt'\{[Q_{11}(t,t')]^2 - [Q_{12}(t,t')]^2\} = \int dt'\{[G^{12}(t,t')]^4 - [G^{11}(t,t')]^4\}. \tag{68}$$

We shall investigate the H theorem in two limiting cases, first at early times for an arbitrary (diagonal in occupation number) initial state, and then at late time for vacuum initial conditions.

A. The *H* theorem at early times

To investigate the meaning of this expression, let us expand the LO propagators in terms of mode functions,

$$f(t) = \frac{1}{\sqrt{2\omega}} e^{-i\omega t}. \tag{69}$$

Concretely, if the initial state is diagonal in occupation number, we have

$$G^{11}(t,t') = \frac{1}{2\omega} e^{-i\omega(t_> - t_<)} + \frac{n}{\omega}\cos\omega(t-t'), \tag{70}$$

$$G^{12}(t,t') = \frac{1}{2\omega} e^{i\omega(t-t')} + \frac{n}{\omega}\cos\omega(t-t'), \tag{71}$$

where $n = \langle a^\dagger a\rangle$. Therefore,

$$\Psi(t) = \frac{i}{8\omega^4}\int_0^t dt'\ \psi(t-t'), \tag{72}$$

$$\psi(t) = 4[2n^3 + 3n^2 - n]\sin 2\omega t + [2(2n^3 + 3n^2) + 4n + 1]\sin 4\omega t \tag{73}$$

(see Appendix B). Since

$$\langle x_B x_B\rangle = \frac{1+2n}{2\omega} \tag{74}$$

is constant, the relevant derivative is $(i)d\Psi/dt$, which is proportional to $d(-\int\psi\,dt)/dt$. The H theorem $[(i)d\Psi/dt < 0]$ will be obtained if $(d/dt)\int\psi\,dt > 0$. Now, since $\psi(0) = 0$,

$$\frac{d}{dt}\int_0^t dt'\ \psi(t-t') = \int_0^t dt' \frac{d}{dt}\psi(t-t')$$

$$= -\int_0^t dt' \frac{d}{dt'}\psi(t-t') = \psi(t), \quad (75)$$

which is indeed positive at short times.

B. The *H* theorem at late times

Let us assume vacuum initial conditions. The lowest-order propagators may be written in terms of mode functions

$$G^{11}(t,t') = F(t_>)F^*(t_<), \quad (76)$$

$$G^{12}(t,t') = F^*(t)F(t'), \quad (77)$$

$$\Psi = \int_0^t dt' \{F^4(t')F^{*4}(t) - F^4(t)F^{*4}(t')\}. \quad (78)$$

We have

$$\langle x_B x_B \rangle = \hbar |F(t)|^2. \quad (79)$$

So the relevant inequality is

$$i\frac{d}{dt}\frac{1}{|F(t)|^4}\int_0^t dt' \{F^4(t')F^{*4}(t) - F^4(t)F^{*4}(t')\} \leqslant 0. \quad (80)$$

Or, equivalently,

$$J = i\frac{d}{dt}\int_0^t dt' \left\{\frac{F^4(t')}{F^4(t)} - \frac{F^{*4}(t')}{F^{*4}(t)}\right\} \leqslant 0. \quad (81)$$

Now

$$J = -4i\int_0^t dt' \left\{F'(t)\frac{F^4(t')}{F^5(t)} - F^{*'}(t)\frac{F^{*4}(t')}{F^{*5}(t)}\right\}. \quad (82)$$

The mode functions may be expanded in terms of WKB modes

$$F(t) = \alpha(t)f(t) + \beta(t)f^*(t), \quad (83)$$

$$F'(t) = \alpha(t)f'(t) + \beta(t)f^{*'}(t). \quad (84)$$

At long times, the integrals will be dominated by the nonoscillatory terms

$$F^4(t') \sim 6\alpha^2(t)\beta^2(t)|f(t)|^4, \quad (85)$$

$$J \sim \frac{-24it}{|F(t)|^{10}}|f(t)|^4\{F'(t)F^{*5}(t)\alpha^2(t)\beta^2(t)$$

$$-F^{*'}(t)F^5(t)\alpha^{*2}(t)\beta^{*2}(t)\}. \quad (86)$$

We make the analogous approximation

$$F'(t)F^{*5}(t) = \alpha(t)f'(t)F^{*5}(t) + \beta(t)f^{*'}(t)F^{*5}(t)$$

$$\sim 10|f(t)|^4\alpha^{*2}(t)\beta^{*2}(t)\{|\alpha(t)|^2 f'(t)f^*(t) + |\beta(t)|^2 f^{*'}(t)f(t)\} \quad (87)$$

and get

$$J \sim \frac{-240it}{|F(t)|^{10}}|f(t)|^8|\alpha(t)|^4|\beta(t)|^4\{|\alpha(t)|^2 - |\beta(t)|^2\}\{f'(t)f^*(t) - f^{*'}(t)f(t)\}. \quad (88)$$

But

$$|\alpha(t)|^2 - |\beta(t)|^2 = 1, \quad (89)$$

$$f'(t)f^*(t) - f^{*'}(t)f(t) = -i. \quad (90)$$

So

$$J \sim \frac{-240t}{|F(t)|^{10}}|f(t)|^8|\alpha(t)|^4|\beta(t)|^4 < 0. \quad (91)$$

QED.

The existence of an *H* theorem at the NLO is as reassuring as the absence thereof at the LO. It is also interesting to observe that entropy production is (formally) a quantity of the order of N^{-2}; a strict (formal) $1/N$ expansion would neglect such a quantity, but it would be generated in a numerical solution of the full $1/N$ equations of motion. Therefore, it is suggestive that the statistical mechanical description of an interacting quantum field at the NLO level of approximation to a 2PI CTP effective action may permit ''thermalization,'' as claimed by [15–19] based on numerical results. Note that our analysis corroborating this claim is predicated upon the restrictive conditions discussed above. Extension of this work to full field theory in conjunction with the reported results of [13] is under investigation.

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APPENDIX A: COMPUTING THE PARTITION FUNCTION

To compute Z, it is best to diagonalize H_0. Introduce new canonical variables

$$\xi_A = (\cosh u)p_A + (\sinh u)x_A, \tag{A1}$$

$$\eta_A = (\sinh u)p_A + (\cosh u)x_A, \tag{A2}$$

so that $[\xi_A, \eta_B] = [p_A, x_B] = (-i\hbar)\delta_{AB}$. Then

$$p_A = (\cosh u)\xi_A - (\sinh u)\eta_A, \tag{A3}$$

$$x_A = -(\sinh u)\xi_A + (\cosh u)\eta_A, \tag{A4}$$

and

$$H_0 = \left(\frac{1}{2}\right)\{A\xi^B\xi^B + B(\eta_B\xi_B + \xi_B\eta_B) + C\eta_B\eta_B\}, \tag{A5}$$

where

$$A = \alpha\cosh^2 u + \gamma\sinh^2 u - 2\beta\cosh u\sinh u, \tag{A6}$$

$$B = -(\gamma+\alpha)\cosh u\sinh u + \beta(\cosh^2 u + \sinh^2 u), \tag{A7}$$

$$C = \alpha\sinh^2 u + \gamma\cosh^2 u - 2\beta\cosh u\sinh u. \tag{A8}$$

To diagonalize the Hamiltonian, we require $B=0$, namely

$$\tanh 2u = \frac{2\beta}{\gamma+\alpha}. \tag{A9}$$

Now Z is the usual partition function for N harmonic oscillators with frequency $\omega^2 = C/A$ at inverse temperature A.

APPENDIX B: $\psi(t)$

$$\begin{aligned}
\Psi(t) &= \frac{1}{16\omega^4}\int_0^t dt'\{[e^{i\omega(t-t')} + 2n\cos\omega(t-t')]^4 - [e^{-i\omega(t-t')} + 2n\cos\omega(t-t')]^4\} \\
&= \frac{i}{8\omega^4}\int_0^t dt'\{32n^3\cos^3\omega(t-t')\sin\omega(t-t') + 24n^2\cos^2\omega(t-t')\sin 2\omega(t-t') \\
&\quad + 8n\cos\omega(t-t')\sin 3\omega(t-t') + \sin 4\omega(t-t')\} \\
&= \frac{i}{8\omega^4}\int_0^t dt'\{8(2n^3+3n^2)\cos^2\omega(t-t')\sin 2\omega(t-t') + 8n\cos\omega(t-t')\sin 3\omega(t-t') + \sin 4\omega(t-t')\} \\
&= \frac{i}{8\omega^4}\int_0^t dt'\{2(2n^3+3n^2)[2\sin 2\omega(t-t') + \sin 4\omega(t-t')] + 4n[\sin 4\omega(t-t') - \sin 2\omega(t-t')] + \sin 4\omega(t-t')\} \\
&= \frac{i}{8\omega^4}\int_0^t dt'\{4\sin 2\omega(t-t')[2n^3+3n^2-n] + \sin 4\omega(t-t')[2(2n^3+3n^2)+4n+1]\}.
\end{aligned} \tag{B1}$$

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