Quantum entanglement and entropy in particle creation

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We investigate the basic theoretical issues in the quantum entanglement of particle pairs created from the vacuum in a time-dependent background field or spacetime. Similar to entropy generation from these processes which depends on the choice of physical variables and how certain information is coarse grained, entanglement dynamics hinges on the choice of measurable quantities and how the two parties are selected as well as the background dynamics of the field or spacetime. We discuss the conditions of separability of quantum states in particle creation processes and point out the differences in how the von Neumann entropy is used as a measure of entropy generation versus for entanglement dynamics. We show by an explicit construction that adoption of a different set of physical variables yields a different entanglement entropy. As an application of these theoretical considerations we show how the particle number and the quantum phase enter the entanglement dynamics in cosmological particle production.

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I. INTRODUCTION

Entanglement is said to be the uniquely distinguishing feature of “quantumness” 1. Despite increasing interest in the recent decade and advances in quantum information sciences, we are still far from fully understanding the nature and dynamics of quantum entanglement – how it is characterized and how it evolves in time – in quantum open systems, i.e., those interacting with their environments. We believe at this stage of development it is important to analyze these basic issues in great detail in simple enough systems, preferably with exact solutions, so that we can understand in depth its behavior to gain much needed valuable insight 2–6.

Usually entanglement is discussed in the framework of nonrelativistic quantum mechanics, but for a quantity to have physical meaning one needs to know how it transforms in different reference frames, e.g., for two observers moving at relative constant speed how is the quantity one observer reports as entanglement between two parties in its system related to that reported by the other observer in its system? To answer this rather rudimentary question one needs to work with Lorentz transformation of entanglement in the framework of relativistic quantum mechanics (see, e.g., 7 for a review). This is the starting point of relativistic quantum information (RQI). When a quantum field is involved, one needs to upgrade the treatment to that of relativistic quantum field theory. This is the platform we have adopted for our research program on RQI. When quantum informational issues arise pertaining to black hole information loss or early universe quantum processes we need to consider them in the extended framework of quantum field theory in curved spacetime 8.

The simplest process which distinguishes a quantum field theoretical process from a quantum mechanical one is particle creation. The investigation of quantum entanglement in the particle creation process – how to define entanglement, between what parties, and how it evolves in time – is the first order of business toward establishing a RQI theory for quantum field processes. This is the goal of this paper, focusing on particle creation in strong and dynamical background fields, such as in the Schwinger effect 9 and in background spacetimes, as in cosmological particle creation 10, 11. In addition to its theoretical value these results are expected to be useful for quantum information experiments and for probes into the very early universe from next generation cosmological observations.

The statistical mechanical properties of particle creation such as entropy generation have been a subject of both theoretical and cosmological interest for quite some time. Since the mid-1980s there are inquiries on finding a viable
measure of entropy for particle creation processes in a free quantum field \cite{12} and from interacting quantum fields \cite{13}. (The most detailed discussion of entropy generation from free field particle creation along the theme of \cite{12} can be found in \cite{14}. For a summary of recent developments see Chapter 9 of \cite{12}.) The free field case is conceptually more intriguing: On the one hand, from a pure quantum field theoretical perspective, one would say categorically there could be no entropy generation because the particle pair is originated from the vacuum which is a pure state. On the other hand, from thermodynamical considerations one sees clearly that entropy is generated in the amount proportional to the number of created particles. This puzzle is what started the inquiries mentioned above which led to the understanding that one could quantify entropy generation by the number of particles created only because one chooses to measure this process in the Fock (number) representation at the sacrifice of the phase information, or effectively imposing a random phase approximation. One also knows that it is only for the spontaneous production of bosons that particle number increases monotonically, a necessary condition to associate it with an entropy function obeying the second law. For fermions and for stimulated creation processes particle number can decrease which invalidates this definition. What this earlier investigation taught us is that the measured entropy associated with the particle creation process depends on quite a few factors: the choice of physical variables (such as using the number basis), the coarse graining one introduces in its measurement (such as the quantum phase) or recognizing that some information is inaccessible to the observer in the process.

We mention prior studies on entropy generation in particle creation processes because the experience we gained (concepts and methods) and the lessons we learned (see above) prove to be useful for our investigations into the quantum entanglement of particle creation because they share certain qualitative similarities. Specifically, quantum entanglement depends crucially on the choice of physical variables and the way the two parties whose entanglement is the object of interest are defined. Quantum entanglement can be measured in many ways \cite{16}. For the bipartite system the von Neumann (vN) entropy is quite commonly used. We will show that the way the vN entropy is used and what results it yields for these two processes, one pertaining to entanglement dynamics, the other for entropy considerations in nonequilibrium statistical mechanics are quite different, both in terms of whether and how coarse graining is introduced, and for what reasons. A particle pair with some 3-momenta \((\vec{k}, -\vec{k})\) created from the vacuum is habitually regarded as perfectly entangled. We show by explicit construction that adoption of a different set of physical variables with the same 3-momenta \((\vec{k}, -\vec{k})\) makes a difference in the entanglement dynamics.

Before we go into detail, let us begin with a description of how information is chosen or coarse-grained in a closed versus an open quantum system. (For a treatment of entropy generation in squeezed open quantum systems with application to inflationary cosmology, see \cite{17} and related work cited therein.) Any quantum state describing a closed (entirely isolated) system is always pure, and the vN entropy is identically zero. In realistic settings a system is rarely closed as it interacts, no matter how weakly, with its environment. The back action of its environment with some coarse graining (in which process noise is engendered) induces dissipation in the dynamics of the system, now rendered open, and mixed states are allowed in the open quantum system. This is one way entropy is generated in the system. Another way this could happen is either by necessity, that some degree of imprecision always exists in realistic measurements (or uncertainty in quantum state tomography), or by choice, that only some physical variables of direct interests are measured (e.g., number rather than phase in particle creation) and others ignored, averaged, or “integrated out” (e.g., the fast-oscillating elements of the density matrix). These procedures either by necessity or by choice would render a pure state mixed in appearance and entropy generation ensues.

The first type of entropy generation is well illustrated in an open quantum system treatment of cosmological particle creation such as is shown in \cite{17}, and more powerfully in the particle creation and backreaction problems, where the gravitational sector is viewed as the (open) system and the quantum field as its environment \cite{18}, whose backreaction causes the dissipation of anisotropy or inhomogeneities \cite{19, 20} of the early universe. One can obtain the entropy generated in the particle creation process in terms of a vacuum viscosity function, even define gravitational entropy \cite{21} of spacetime dynamics associated with these processes. The second type is illustrated clearly in free field particle creation processes \cite{12, 14}, where the choice of a Fock representation is what enables one to relate the amount of entropy generated to the particle numbers created. Considering particle production in a uniform electric field Kluger, Mottola, and Eisenberg (KME) \cite{14} derived a quantum Vlasov equation describing the evolution of the (adiabatic) particle number, and an equation for the evolution of the quantum phase. They then argued that in the case they considered since the quantum phase as well as the off-diagonal elements of the density matrix (the coherence) oscillate rapidly in time, these fast variables are expected to be averaged out in observations and the density matrix would effectively look like a mixed state to such an observer.

Oftentimes these two sources of entropy generation are intermixed, depending on how a problem is formulated and treated. This happens in the interacting field particle creation calculations of \cite{13}. A more recent example is in \cite{22, 23}, where Campo and Parentani studied the self-consistently truncated “Gaussian and homogeneous density matrix” (GHD) for an interacting field. They calculated the vN entropy of the two-mode sector with opposite wave vectors \((\vec{k}, -\vec{k})\) of the GHD and showed that the vN entropy is the only intrinsic property of the field state during inflation, while the entanglement between particles with \(\vec{k}\) and their \(-\vec{k}\) partners depends on the choice of canonical
variables in the same mode pair $\phi_k \phi_{-k}$. Their vN entropy of the two-mode sector plays a double role. On the one hand, it is a consequence of truncation or coarse graining in obtaining the GHDM, effectively by averaging out fast variables. On the other hand, it is a measure of the entanglement between that mode pair $\phi_k \phi_{-k}$ and its environment consisting of all other modes (rather than the entanglement of $k$ and $-k$ particles in the same two-mode sector), by noting that the GHDM is factorized and the two-mode sector with momenta $(k, -k)$ is by itself the reduced density matrix (at least approximately) with other degrees of freedom traced out.

To get rid of such intermixing, we are focusing on the simplest cases with free quantum fields in a dynamical background. In Secs. II and III we describe the particle creation process of real and complex scalar fields, respectively, in the Schrödinger representation. In Sec. II B and Sec. IV we investigate the behavior of particle numbers and the degree of entanglement between them can be calculated accordingly. Based on these results we are able to look into how the particle number and the quantum phase enter the entanglement dynamics in cosmological particle production. We conclude in Sec. VI with a brief summary of the key results reflecting the main themes stated here.

II. REAL SCALAR FIELD WITH TIME-VARYING MASS

Without loss of generality, let us work with a free scalar field in Minkowski spacetime with a mass parameter $M(\eta)$ which is time dependent, representing all time-dependent parameters entering into the system (including that from cosmological spacetimes)

$$S = \int d^4x \left[ -\frac{1}{2} \partial_\mu \Phi \partial^\mu \Phi - \frac{1}{2} M^2(\eta) \Phi^2 \right],$$

where we denote time $x^0$ by $\eta$ anticipating cosmological applications later. In Fourier-transformed representation $\Phi(x) = (2\pi)^{-3} \int d^3k e^{ik \cdot x} \phi_k$, the above action becomes

$$S = \int d\eta d^3k (2\pi)^{3} \left[ \frac{1}{2} \partial_\eta \phi_k \partial_\eta \phi_{-k} - \frac{1}{2} \Omega_k^2(\eta) \phi_k \phi_{-k} \right],$$

where $\Omega_k^2(\eta) = k^2 + M^2(\eta)$ and $\phi_{-k} = \phi_k^*$. The momentum conjugate to $\phi_k$ is $P_k = \delta S/\delta (\partial_\eta \phi_k) = \partial_\eta \phi_{-k}$, and the Hamiltonian can be derived straightforwardly by a Legendre transform of $S$.

In Sec. IV A we will see that the theory with a real scalar field in a Friedmann-Robertson-Walker (FRW) spacetime has the above form in conformal time $\eta$.

A. Quantization in Schrödinger representation

Canonical quantization of this theory is achieved by imposing the following equal-time commutation relations,

$$[\phi_k(\eta), P_p(\eta)] = i\hbar (2\pi)^3 \delta^3(k - p),$$

$$[\phi_k(\eta), \phi_p(\eta)] = [P_k(\eta), P_p(\eta)] = 0.$$  \hspace{1cm} (3)

In the Schrödinger representation, $\phi_k$ are viewed as c-number functions and the conjugate momentum operators are given by

$$\hat{P}_k = (2\pi)^3 \frac{\hbar}{i} \frac{\delta}{\delta \phi_k},$$  \hspace{1cm} (4)

to satisfy the above commutation relations. The Hamiltonian operator then reads

$$\hat{H} = \int \frac{d^3k}{(2\pi)^3} \left[ \frac{\hbar^2}{2} (2\pi)^6 \frac{\delta}{\delta \phi_k} \frac{\delta}{\delta \phi_{-k}} + \frac{1}{2} \Omega_k^2(\eta) \phi_k \phi_{-k} \right].$$  \hspace{1cm} (5)
In this representation all physical information of the system is included in the wave functional $\Psi[\phi_k, \eta]$ satisfying the Schrödinger equation

$$i\hbar \partial_\eta \Psi = \hat{H} \Psi.$$  

(6)

The ground state with minimum $\langle \hat{H} \rangle$ is given by the Gaussian state

$$\Psi_0 = s e^{-i \int^\eta d\eta E_0(\eta)/\hbar} \exp \left\{ -\frac{1}{\hbar} \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3p}{(2\pi)^3} \chi_k^{\mathbf{k-p}}(\eta) \phi_p \right\},$$  

(7)

where $s$ is the normalization factor and $E_0$ is the vacuum energy \[36\]. Substituting the above ansatz into (6), one finds that

$$g^{\mathbf{k-p}}(\eta) = \frac{1}{2i} \chi_k^{\mathbf{k'}}(\eta) (2\pi)^3 \delta(\mathbf{k + p})$$  

(8)

so that $\Psi_0 = \prod_k \Psi_{0k}$, where

$$\Psi_{0k} = s_k e^{-i \int^\eta d\eta \mathcal{E}_k^k(\eta)/\hbar} \exp \left\{ i \frac{1}{2\hbar(2\pi)^3 \delta(0)} \chi_k^{\mathbf{k'}}(\eta) \phi_k \phi_{-k}^\dagger \right\},$$  

(9)

with the normalization factor $s_k$ and the “ground state energy” for the $\mathbf{k}$ or $-\mathbf{k}$ modes,

$$\mathcal{E}_k^k \equiv \frac{\hbar}{2} \left[ |\chi_k^\prime|^2 + \Omega_k^2 |\chi_k|^2 \right],$$  

(10)

such that $E_0(\eta) = \sum_k \mathcal{E}_k^k$. Here $\sum_k \equiv \int dk \delta(0)$, a prime denotes taking the derivative with respect to $\eta$, and the mode function amplitudes $\chi_k$ satisfy the equation

$$\chi'_k + \Omega_k^2(\eta) \chi_k = 0,$$  

(11)

so that $\chi_k = \chi_{-k}$. This as we recognize is the classical field equation for the scalar field, and $\chi_k$ is the solution for this field equation subject to the normalization condition

$$\chi_k \chi_k^\prime - \chi_k^\prime \chi_k = i$$  

(12)

at every moment, which requires $\chi_k$ to be complex functions. Note that $\chi_k$ does not have to be classically physical solutions, because boundary conditions for $\chi_k$ will not be fixed by classical considerations. In fact, different $\chi_k$ could correspond to different quantum states. Compared with the ground state for real scalar fields with constant mass in Minkowski space \[26\], one sees that $\chi_k$ should be taken as $\sqrt{1/2\Omega_k} e^{-i \Omega_k \eta}$ there, which is the positive frequency component of the $k$th mode of the free scalar field.

The wave functional in the form (9) with $\chi_k$ the solutions of the classical field equation is almost the same as an infinite product of the wave functions for squeezed Gaussian states of parametric oscillators with frequency $\Omega_k(\eta)$ \[27\], except that the variables in the exponents are mode pairs $\phi_k \phi_{-k}$ for each $k$ rather than the squared “positions” of the oscillators.

The nonvanishing two-point correlators in the vacuum state (10) are

$$\langle \phi_k, \phi_{-k} \rangle = \hbar (2\pi)^3 \delta(\mathbf{k + p}) |\chi_k|^2, \quad \langle \Pi_k, \Pi_{-k} \rangle = \hbar (2\pi)^3 \delta(\mathbf{k + p}) |\chi_k^\prime|^2,$$  

(13)

and $\langle \phi_k, \Pi_{-k} \rangle = \frac{i}{2} \partial_\eta \langle \phi_k, \phi_{-k} \rangle$, where $\langle A, B \rangle = \frac{1}{2} \int d^3x (AB + BA)\Psi$. Then one can write down the covariance matrix $V$ with elements $V_{ij} = \left\langle R_i, R_j \right\rangle$ in $\mathcal{R}_i \equiv \left\langle \phi_k, \Pi_k, \phi_{-k}, \Pi_{-k} \right\rangle$ representation, whose partial transposition $V^{PT} \equiv V|_{\Pi_{-k} \rightarrow -\Pi_{-k}}$ gives the quantity we used in an earlier paper \[23, 27\]

$$\Sigma \equiv \det \left( V_{ij}^{PT} + \frac{1}{2} [R_i, R_j] \right)$$  

$$= \frac{1}{4} \left[ \hbar (2\pi)^3 \delta^3(0) \right]^4 \left[ \partial_\eta |\chi_k|^2 \right]^2 + 1].$$  

(14)

Since this is always positive, the field modes $\phi_k$ and $\phi_{-k}$ are not only separable from other degrees of freedom in the vacuum state (i.e., the von Neumann entropy of the density matrix $\Psi_{0k}^\dagger \Psi_{0k}$ is zero, or in other words, each $\Psi_{0k}$ is always pure and factorizable from $\Psi_0$), but also “separable with each other” at all times.
To see this more clearly, we write the complex $\phi_k$ in terms of two real field variables as $\phi_k = \phi_k^R + i\phi_k^I$ instead, with $\phi_k^R = \phi_k^L$ and $\phi_k^I = -\phi_k^L$ (since $\phi_k^* = \phi_{-k}$). Then one can easily see that (9) can be factorized into a product of $\phi_k^R$ state and $\phi_k^I$ state. So if the observables are ($\phi_k^R$, $\phi_k^I$) fields, they will always be separable with each other and no entanglement measured in terms of these variables will be generated for a free scalar field with time-varying mass, such as the field in an expanding universe.

Nevertheless, quantum entanglement depends on partition as well as the choice of physical variables or measurables. With reference to quantum entanglement, say, in cosmology, foremost one needs to specify which physical observables are being measured there. Obviously $\phi_k^R$ and $\phi_k^I$ are not the correct variables to describe quantum entanglement in cosmological particle creation: Recall that modern cosmological experiments measure the temperature fluctuations $\delta T/T$ of the cosmological microwave background radiation rather than the amplitudes of quantum fields. The former can be related to the energy density perturbation $\delta \rho/\rho$ with the energy density $\rho = \langle \mathcal{H} \rangle \sim \sum_k \langle N_k \rangle / V$, where $\mathcal{H}$ and $N_k$ are the Hamiltonian density and the number operators for $\phi_k$, respectively. The number operator $N_k$ here consists of creation and annihilation operators defining the in/out vacuum at the initial/final moment (or in the adiabatic vacuum). We therefore intend to look at quantum entanglement in terms of these operators. This also suggests that quantum entanglement generation, like cosmological particle creation, manifests only in those physical variables which facilitate a well-defined in/out or adiabatic vacuum.

B. particle numbers

Continuing our exposition using quantum field theory (QFT) in Minkowski space, we define the annihilation and creation operators $b_k(\eta)$ and $b_k^+(\eta)$ by

$$b_k(\eta) = \frac{-i}{\sqrt{h(2\pi)^3 \delta^3(0)}} (\chi_k^*(\eta)\phi_k - \chi_k^R(\eta)\Pi_{-k}), \quad (15)$$

$$b_k^+(\eta) = \frac{i}{\sqrt{h(2\pi)^3 \delta^3(0)}} (\chi_k^*(\eta)\phi_k - \chi_k^R(\eta)\Pi_{-k}), \quad (16)$$

so that

$$\phi_k = \sqrt{h(2\pi)^3 \delta^3(0)} \left( \chi_k(\eta)b_k(\eta) + \chi_k^R(\eta)b_k^+(\eta) \right), \quad (17)$$

$$\Pi_{-k} = \sqrt{h(2\pi)^3 \delta^3(0)} \left( \chi_k^*(\eta)b_k(\eta) + \chi_k^*(\eta)b_k^+(\eta) \right), \quad (18)$$

are independent of time. The above definition of operators $b_k(\eta)$ and $b_k^+(\eta)$ has the following properties: First, they become the conventional ones in QFT in Minkowski space where $\chi_k = \sqrt{1/2\Omega_k e^{-i\omega_k \eta}}$. Second, the equal-time commutation relations Eq. (3) are equivalent to

$$[b_k, b_k^+] = \delta^3(\mathbf{k} - \mathbf{p})/\delta^3(0). \quad (19)$$

Third, the ground state $\Psi_0$ is the state with the property $b_k\Psi_0 = 0$ for all $k$. Fourth, the “excited states” are analogous to those in simple harmonic oscillators, which are generated by applying these creation and annihilation operators to the ground states, e.g.,

$$\Psi_1(\mathbf{k}) = b_k^+\Psi_0 = \frac{1}{\sqrt{h(2\pi)^3 \delta^3(0)}} \phi_k\Psi_0, \quad (20)$$

$$\Psi_2(\mathbf{k}, -\mathbf{k}) = b_k^+b_{-k}^\dagger\Psi_0 = \left( \frac{1}{h(2\pi)^3 \delta^3(0)} \frac{\phi_k\phi_{-k}}{\chi_k^* \chi_{-k}} \frac{\chi_k}{\chi_{-k}} \right) \Psi_0, \quad etc, \quad (21)$$

are also solutions of the Schrödinger equation. Moreover, all excited states generated in this way, together with the ground state, form a complete set of quantum states for the scalar field.

Note that a proper normalization for $b_k$ and $b_k^+$ has been chosen to make the above excited states satisfy the same normalization conditions for $\Psi_0$. Written in terms of $b_k$ and $b_k^+$, the Hamiltonian operator reads

$$\hat{H} = \sum_k \left\{ \mathcal{E}_k \left( b_k^\dagger b_k + b_k^+b_k^\dagger \right) + \frac{\hbar \delta^3(0)}{2} \left[ (\chi_k^2 + \Omega_k^2 \chi_k^2) b_k b_{-k}^\dagger + H.c. \right] \right\}, \quad (22)$$
where “H.c.” stands for “Hermitian conjugate” and $\mathcal{E}^k_\eta$ is the $k$th component of the ground state energy given in (10). So $\int D\phi \Psi^*_\eta(\eta) \hat{H} \Psi_\eta(\eta) = E_0(\eta)$ is indeed the vacuum energy.

The “number operator” of mode $k$ at the moment $\eta$ is defined as

$$\hat{N}_k(\eta) \equiv \hat{b}^+_k(\eta)\hat{b}_k(\eta).$$

Suppose at the initial moment $\eta_0$ the field is in the vacuum state when the particle-number counter is constructed according to the operator $\hat{N}_k(\eta_0)$. Then, using the same particle-number counter, one finds that the number of the particle created at time $\eta$ by the background spacetime is

$$\langle 0_\eta | \hat{N}_k(\eta_0) | 0_\eta \rangle \equiv \int D\phi \Psi^*_\eta(\eta) \hat{N}_k(\eta_0) \Psi_\eta(\eta) = |\chi_k^*(\eta_0)\chi_k(\eta) - \chi_k(\eta_0)\chi_k^*(\eta)|^2. \tag{24}$$

Since both $\chi_k(\eta_0)$ and $\chi_k(\eta)$ are solutions of (11) and each form a complete set at different times, one may write

$$\chi_k(\eta_0) = \alpha_k(\eta_0, \eta)\chi_k(\eta) + \beta_k(\eta_0, \eta)\chi_k^*(\eta), \tag{25}$$

or equivalently, for $|\alpha_k|^2 - |\beta_k|^2 = 1$, one has

$$\chi_k(\eta) = \alpha_k^*\chi_k(\eta_0) - \beta_k\chi_k^*(\eta_0). \tag{26}$$

Then the Bogoliubov coefficients read

$$\alpha_k = i [\chi_k(\eta_0)\chi_k^*(\eta) - \chi_k(\eta_0)\chi_k^*(\eta)] + i\zeta(\eta)\chi_k(\eta)\chi_k(\eta_0), \tag{27}$$

$$\beta_k = i [\chi_k(\eta_0)\chi_k^*(\eta) - \chi_k(\eta_0)\chi_k^*(\eta)] - i\zeta(\eta)\chi_k^*(\eta_0)\chi_k(\eta_0), \tag{28}$$

with overdots denoting $\partial/\partial\eta|_{\eta=\eta_0}$ and $\zeta \in \mathbb{R}$, whose values will be further fixed by specifying $\chi_k$ or other physical conditions. From (28) it can be seen that we have made the physical choice $\zeta = 0$, which implies $\langle 0_\eta | \hat{N}_k(\eta_0) | 0_\eta \rangle = |\beta_k|^2$.

Note we did not get into the details about how to define an adiabatic particle-number state (which can be found in e.g., [8, 14]) but simply assume that at $\eta_0$ the concept of particle is well defined. Here the Bogolubov coefficients with $\zeta = 0$ are represented explicitly by the Klein-Gordon inner product.

### C. Wigner function and entanglement entropy

Since $\Psi_\eta$ is a pure state, if one divides the degrees of freedom in this model into two parties, then the entanglement between them can be well measured by the von Neumann entropy of the reduced density matrix of one of the two parties. Nevertheless, it is not obvious whether the particles with $k$ and $-k$ are separable as indicated by the positive $\Sigma$ at the end of Sec 11A.

A clearer separability can be seen in the Wigner function of $\Psi_\eta$:

$$\rho(\eta) = \int \prod_{k \in (\mathbb{R}^3 - \{0\})/\mathbb{Z}_2} \left[ d\Delta R d\Delta I e^{i(p^R_k\Delta R + p^I_k\Delta I)/\hbar} \Psi_{0k} \left( \phi^R_k - \frac{\Delta R}{2}, \phi^I_k - \frac{\Delta I}{2} \right) \Psi^*_{0k} \left( \phi^R_k + \frac{\Delta R}{2}, \phi^I_k + \frac{\Delta I}{2} \right) \right]$$

$$= |\tilde{s}|^2 \exp \left[ \frac{2}{\hbar} \int \frac{d^3k}{(2\pi)^3} \left( |\chi_k(\eta)|^2 \phi_k \phi_{-k} + |\chi_k(\eta)|^2 \pi_k \pi_{-k} - \partial_\eta \left( |\chi_k(\eta)|^2 \right) \pi_k \phi_{-k} \right) \right], \tag{29}$$

where we have taken $\phi_k = \phi^R_k + i\phi^I_k$ (with $\phi^R_k = \phi^R_k + \phi^I_k = -\phi^I_k$) and $\pi_k = (p^R_k + ip^I_k)/2$, which are c-numbers here rather than operators. Performing a canonical transformation similar to (17) and (18) as

$$\phi_k = \sqrt{\hbar(2\pi)^3}\delta^3(0) \left( \chi_k(\eta) \tilde{B}_k(\eta) + \chi_k^*(\eta) \tilde{B}^*_k(\eta) \right), \tag{30}$$

$$\pi_k = \sqrt{\hbar(2\pi)^3}\delta^3(0) \left( \chi_k(\eta) \tilde{B}_k(\eta) + \chi_k^*(\eta) \tilde{B}^*_k(\eta) \right), \tag{31}$$

which gives $d\phi_k d\pi_k = d\tilde{B}_k d\tilde{B}^*_k \hbar(2\pi)^3\delta^3(0)$, one ends up with the Wigner function in a Fock representation,

$$\rho(\eta) = |\tilde{s}|^2 \exp \left[ -\frac{2}{\hbar} \sum_k \tilde{B}_k(\eta)\tilde{B}^*_k(\eta) \right]. \tag{32}$$
Here one can easily see that the quantum states of $(\tilde{B}_k, \tilde{B}_k^*)$ and $(\tilde{B}_{-k}, \tilde{B}_{-k}^*)$ for each specific $k$ are separable.

However, in terms of an alternative set of measurables, $k$ and $-k$ particles could be entangled as we will see in the following. From (24) it seems that the physical particle counter should be counting $\tilde{N}_k(\eta_0)$ defined by operators $b_k$ at the initial moment $\eta_0$. Let $B_k \equiv \tilde{B}_k(\eta_0)$ in (30) and (31) at $\eta = \eta_0$, so that

$$\tilde{B}_k(\eta) = \alpha_k B_k + \beta_k^* B_{-k}^*;$$

from (26). Then in terms of $B_k$ with $n_k \equiv |\beta_k|^2$, $c_k \equiv \alpha_k \beta_k$, the Wigner function (32) becomes

$$\rho(\eta) = |\tilde{s}|^2 \exp -2 \sum_k [(2n_k + 1) B_k B_k^* + c_k B_k B_{-k} + c_k^* B_{-k}^* B_{-k}];$$

which gives the “symmetric” particle number

$$\langle B_k^* B_k \rangle = n_k + \frac{1}{2} = \langle 0| b_k^*(\eta_0), b_k(\eta_0) | 0 \rangle.$$

This justifies $B_k$ as the correct variables corresponding to physical measurements. Suppose we divide the particles into two groups with $k^3 > 0$ and $k^3 < 0$ respectively (that the particles with $k^3 = 0$ are properly divided into these two groups is understood). One may write

$$\rho(\eta) = |\tilde{s}|^2 \exp - \sum_k^+ \left[ (4n_k + 2) (B_k B_k^* + B_{-k} B_{-k}^*) + 4c_k B_k B_{-k} + 4c_k^* B_{-k}^* B_{-k} \right];$$

where $\sum_k^+$ and later $\prod_k^+$ denote summing and multiplying over $k$ with $k^1, k^2 \in \mathbb{R}$ and $k^3 > 0$, respectively. Integrating out $B_{-k}$ and $B_{-k}^*$ in $\rho(\eta)$, one obtains the reduced Wigner function

$$\rho^R(\eta) = \int \prod_k^+ dB_{-k} dB_{-k}^* \rho(\eta)$$

$$= |\tilde{s}|^2 \exp - \sum_k^+ \frac{2B_k B_k^*}{2n_k + 1} \left[ (2n_k + 1)^2 - 4 |c_k|^2 \right]$$

$$= |\tilde{s}|^2 \exp - \sum_k^+ \frac{2B_k B_k^*}{2n_k + 1},$$

which is a mixed state once $|\beta_k| \neq 0$ because the purity

$$P = 2\pi \int dB_k dB_k^* (\rho^R)^2 = \prod_k^+ \frac{1}{2n_k + 1}$$

is less than 1 if any $n_k = |\beta_k|^2 > 0$. This means that the particles measured by “physical particle counter” $\tilde{N}_k(\eta_0)$ with $k$ and $-k$ are entangled. Comparing the above expression for the purity with Eqs. (30) and (31) of Ref. [5], one sees that the von Neumann entropy is

$$S = \sum_k^+ \left[ (n_k + 1) \ln(n_k + 1) - n_k \ln n_k \right]$$

$$= \frac{1}{2} \sum_k^+ \left[ (n_k + 1) \ln(n_k + 1) - n_k \ln n_k \right].$$

(39)

When $n_k \gg 1$ for all $k$, $S \approx \sum_k^+ \ln n_k$.

The vN entropy as an entanglement entropy measures the quantum nonlocal correlations at some moment between the system and some specified party which could be the rest of the world. The latter is traced out at the moment the entanglement entropy is evaluated. Note that “nonlocal” here does not imply “nonlocal in space”: the particles in this paper are actually something similar to plane waves, which are local in momentum space but nonlocal in position space. They are not spacelike separated. Rather, they can occupy the same position space at the same time.
III. COMPLEX SCALAR FIELD WITH TIME-VARYING MASS

One can easily generate the above formulations to a complex field with time-varying mass:

\[
S = \int d^4x \left[ -\frac{1}{2} \partial_{\mu} \Phi \partial^{\mu} \Phi - \frac{1}{2} M^2(\eta) |\Phi|^2 \right],
\]

(40)
or in a Fourier-transformed representation,

\[
S = \int d\eta \frac{d^2k}{(2\pi)^2} \left[ \frac{1}{2} \partial_\eta \phi_\eta \partial_\eta \phi_\eta^* - \frac{1}{2} \Omega_k^2(\eta)|\phi_k|^2 \right],
\]

(41)
The only difference is that now \(\phi_k^*\) is independent of \(\phi_{-k}\), while \(\Pi_k = \partial_\eta \phi_k\). The above action describes scalar QED of a quantum charged scalar field in a classical uniform electric field \([14]\).

The ground state wave function is still in the form of (9), except that the \(\phi_{-k}\) should be replaced by \(\phi_k^*\). But now the particles and antiparticles can be distinguished by their different charges in addition to their momenta. So instead of (17) and (18), one writes

\[
\phi_k = \sqrt{h(2\pi)^3\delta^3(0)} \left( \chi_k(\eta) a_k(\eta) + \chi_k^*(\eta) b_{-k}^*(\eta) \right),
\]

(42)
\[
\Pi_k = \sqrt{h(2\pi)^3\delta^3(0)} \left( \chi_k(\eta) a_k(\eta) + \chi_k^*(\eta) b_{-k}^*(\eta) \right),
\]

(43)
with

\[
[a_k, a_p^\dagger] = [b_k, b_p^\dagger] = \delta^3(k-p)/\delta^3(0).
\]

(44)
This will make the Wigner function of the vacuum state a product of two copies of (32):

\[
\rho(\eta) = |\tilde{s}|^2 \exp -2 \sum_k \left( \tilde{A}_k(\eta) \tilde{A}_k^*(\eta) + \tilde{B}_k(\eta) \tilde{B}_k^*(\eta) \right),
\]

(45)
where \((\tilde{A}_k, \tilde{B}_k)\) corresponding to \((a_k, b_k)\) are the counterpart of \(\tilde{A}_k\) of the real scalar field. Thus as before one can express them in terms of the ones defined at the initial moment as

\[
\tilde{A}_k(\eta) = \alpha_k A_k + \beta_k^* B_{-k}^*, \quad \tilde{B}_k(\eta) = \beta_k A_k + \alpha_k^* B_{-k}^*,
\]

(46)
according to (25). These imply

\[
\rho(\eta) = |\tilde{s}|^2 \exp -2 \sum_k \left[ (2n_k + 1) (A_k A_k^* + B_k B_{-k}^*) + c_k A_k B_{-k} + A_{-k} B_k + c_k^* (A_k^* B_{-k}^* + A_{-k}^* B_k^*) \right].
\]

(47)
Although a mixing between the particles with \(k\) and the antiparticles with \(-k\) is generated, the vacuum state \(\rho(\eta)\) remains a pure state. Only after one integrates out the antiparticles (particles) associated with \(B_k\) \((A_k)\) will the reduced Wigner function for particles (antiparticles), \(\rho^A\) \((\rho^B)\), become

\[
\rho^C(\eta) = |\tilde{s}|^2 \exp -\sum_k \frac{2C_k C_{-k}}{2n_k + 1},
\]

(48)
with \(C = A, B\). Now \(\rho^C\) is a mixed state. The purity and the von Neumann entropy are those for the real scalar field \([38]\) and \([39]\) with \(\prod_k\) and \(\sum_k^+\) replaced by the usual \(\prod_k\) and \(\sum_k\). So the values of the von Neumann entropy of a complex scalar field between particles and antiparticles are twice the value for a real scalar field, indicated by \([39]\).

IV. PHASE INFORMATION

Observe that the description from (32) to (34) is that of squeezing in a two-mode squeezed state, well known from a squeezed-state description of particle creation (see, e.g., \([17, 28]\)). Writing \(\tilde{B}_k\) in terms of quadrature amplitudes, namely, \(\tilde{B}_k = (\tilde{Q}_k + i\tilde{P}_k)/\sqrt{2}\) with \(\tilde{Q}_k\) and \(\tilde{P}_k\) real, then (32) looks like a direct product of the Wigner functions for the ground states of \(\tilde{Q}_k\) for all \(k\). Now, since \(|\alpha_k|^2 - |\beta_k|^2 = 1\), one is allowed to parametrize \(\alpha_k\) and \(\beta_k\) as

\[
\alpha_k \equiv e^{i\gamma_k} \cosh r_k, \quad \beta_k \equiv -e^{i\theta_k} \sinh r_k.
\]

(49)
Let $B_k \equiv (Q_k + i\tilde{P}_k)/\sqrt{2}$. Then one has
\begin{align}
Q_k &= \cosh r_k \left( Q_k \cos \sigma_k + \tilde{P}_k \sin \sigma_k \right) + \sinh r_k \left( Q_k \cos \theta_k - \tilde{P}_k \sin \theta_k \right), \\
P_k &= \cosh r_k \left( -Q_k \sin \sigma_k + \tilde{P}_k \cos \sigma_k \right) - \sinh r_k \left( Q_k \sin \theta_k + \tilde{P}_k \cos \theta_k \right),
\end{align}
from the relation (53). We see this involves two steps: 1) $(Q_{\pm k}, \tilde{P}_{\pm k})$ are first rotated locally in angles $\sigma_k$ and $-\theta_k$ on the $+k$ and $-k$ modes, respectively, and then 2) squeezed globally in squeeze parameter $r_k$. Local operations do not affect the entanglement measure: The phases $\sigma_k$ and $\theta_k$ are not present in the reduced density matrix (RDM) transformed from (57), neither is any function of the RDM such as the entanglement entropy (59). Here only squeezing which is a global operation is relevant to quantum entanglement.

We now turn to the question of how to obtain the phase information and whether/how it enter into entanglement dynamics considerations.

A. Quantum phase

Mathematically the phase $\theta_k$ of $\beta_k$ in the parametrization (19) can be obtained by evaluating
\begin{equation}
\theta_k = -\frac{i}{2} \ln \frac{\chi_k(y_k)\chi_k^*(y_k) - \chi_k^*(y_{-k})\chi_k(y_{-k})}{\chi_k(y_k)\chi_k^*(y_k) - \chi_k^*(y_{-k})\chi_k(y_{-k})},
\end{equation}
and $\sigma_k$ in $\alpha_k$ can be obtained in a similar way. But physically only the phase sum $\sigma_k + \theta_k$ could be measured.

Transforming (54) to the density matrix in quadrature amplitudes $Q_{\pm k}$ representation, one obtains
\begin{equation}
\rho[\cdots, Q_k, Q_{-k}, \cdots, Q'_k, Q'_{-k}, \cdots] = \Psi[\cdots, Q_k, Q_{-k}, \cdots]\Psi^*[\cdots, Q'_k, Q'_{-k}, \cdots],
\end{equation}
where $\Psi = \prod_k^+ \Psi_k$ and
\begin{equation}
\Psi_k = e^{-\frac{i}{2} \int_0^{\pi} dy_k^{\pm} \frac{d^4 e_k^{\pm}(y_k^{\pm})}{\sqrt{\pi^2 a_k^{\pm}}} \exp \left[ \frac{1}{2 g_{\pm k}} \left( 1 + 2 n_k + c_k^2 - e_k^2 \right) (Q_{\pm k}^2 + Q_{\pm k}^2) + 4 \left( c_k (n_k + 1) - e_k n_k \right) Q_{\pm k} \right]}
= e^{\frac{i}{2} \int_0^{\pi} dy_k^{\pm} \frac{d^4 e_k^{\pm}(y_k^{\pm})}{\sqrt{\pi^2 a_k^{\pm}}} \left[ \frac{1 + \sinh^2 r_k (1 - e^{2i(\sigma_k + \theta_k)})}{1 + \sinh^2 r_k (1 - e^{-2i(\sigma_k + \theta_k)})} \right] \sum_{n=0}^{\infty} \left( e^{i(\sigma_k + \theta_k)} \tanh r_k \right)^n \Phi_n (Q_k) \Phi_n (Q_{-k}),
\end{equation}
with $g \equiv (1 + 2n_k^2 - (c_k + e_k^2)^2$ and the number eigenstates in $Q$ representation,
\begin{equation}
\Phi_n (Q) \equiv \sqrt{\frac{1}{2\pi n!} H_n (Q)e^{-Q^2/2}}.
\end{equation}
So the density matrix (54) can be expressed as
\begin{equation}
\rho = \prod_k^+ \sum_{n,m} \rho_{nn,mm}^k \Phi_n (Q_k) \Phi_n (Q_{-k}) \Phi_m^* (Q'_k) \Phi_m^* (Q'_{-k}),
\end{equation}
with
\begin{equation}
\rho_{nn,mm}^k = \frac{\tanh^{n+m} r_k}{\cosh^{2n} r_k} e^{i(n-m)(\sigma_k + \theta_k)}.
\end{equation}
Equation (54) shows that $k$ and $-k$ particles associated with $Q_k$ are always created in pairs, because the outcome of the measurement on numbers of $k$ and $-k$ particles separately will always be the same. From (50) and according to (29), one can write down the probability distribution of the quantum phase-sum $\theta_+$,
\begin{equation}
P(\theta_+) = \left\{ 2\pi \left[ \cosh^2 r_k + \sinh^2 r_k - 2 \cosh r_k \sinh r_k \cos (\theta_+ - \sigma_k + \theta_k) \right] \right\}^{-1},
\end{equation}
which peaks at $\theta_+ - (\sigma_k + \theta_k) = 2n\pi$, $n \in \mathbb{Z}$, while the probability distribution of the quantum phase-difference $\theta_-$, $P(\theta_-) = 1/2\pi$, is constant through $0 \leq \theta_- < 2\pi$ so $\theta_-$ of the quantum state (54) is totally uncertain. This shows that
[(\sigma_k + \theta_k) \mod 2\pi] is the quantum phase complementary to the particle number, while \sigma_k and \theta_k cannot be observed separately.

The matrix elements Eq. (57) are proportional to \( e^{i \alpha - \beta} \). If the phase changes so fast that \( \sigma_k \) could not be measured precisely by any apparatus, then the information for quantum state tomography will never be complete. Most likely in this case the off-diagonal elements with \( m \neq n \) would be averaged out, then the quantum state of the field may appear like a classical state. This “fake decoherence” due to the technical limitation of measurement is different from environment-induced decoherence such as from intermode couplings.

If the resolution of the apparatus gets higher, more phase information could then be observed. However, it is easy to verify that once \( \rho_{nm,mm}^k \propto e^{i \alpha - \beta} \) for all nonzero \( \sigma_k \in \mathbb{C} \), the vN entropy of \( \rho \) will be zero. So vN entropy cannot be generated by just replacing all the original \( \sigma_k \) by some outcomes of measurement with smaller absolute values. One simple way to produce vN entropy is to perform a truncation such as \( \rho_{nm,mm}^k \equiv 0 \) for all \( |n - m| > N \) with some positive integer \( N \), meaning that the off-diagonal elements oscillating quicker than \( \exp \pm iN(\sigma_k + \theta_k) \) are not resolvable and being averaged out. For this truncated effective density matrix, the purity will be

\[
\mathcal{P}_{\text{eff}} = \prod_k^+ \frac{1}{1 + 2n_k \eta} \left[ 1 + 2 \sum_{m=1}^N \left( \frac{n_k}{1 + n_k} \right)^m \right].
\]

For all \( n_k \geq 0 \), the larger \( \mathcal{P}_{\text{eff}} \) is, the closer it is to unity, so the effective density matrix is purer, and the vN entropy of it is closer to zero.

The RDM obtained by tracing out the \( Q_{-k} \) and \( Q'_{-k} \) components in Eq. (60) reads

\[
\rho^R = \prod_k^+ \sum_n \rho_{nm,nn}^k \Phi_n^* (Q_k) \Phi_n^* (Q'_k).
\]

One can immediately see that the vN entropy of Eq. (60), which is the entanglement entropy between the particles with \( k \) and \(-k\), has exactly the same value as the vN entropy of the effective density matrix of the vacuum with all off-diagonal elements averaged out, namely,

\[
\rho_{\text{eff}} = \prod_k^+ \sum_n \rho_{nm,nn}^k \Phi_n^* (Q_k) \Phi_n (Q_{-k}) \Phi_n^* (Q'_k) \Phi_n^* (Q'_{-k}).
\]

Thus one could say that the tracing-out process in obtaining the RDM Eq. (60) represents the “strongest” coarse graining, though the coincidence of the entropy values here does not occur for general quantum states.

One should be careful that simply ignoring fast-oscillating elements could create one more problem if our quantum state tomography is designed to reconstruct the Wigner function. The amplitude of \( c_k \) plays an important role in obtaining the correct entanglement entropy from the Wigner function. If one finds that \( c_k \) in Eq. (37) appears to be zero, then the factor in the exponent of the reduced Wigner function will become \( 2(2n_k + 1) \) rather than \( 2/(2n_k + 1) \), so that the effective reduced Wigner function cannot be transformed back to the correct effective RDM. This effective reduced Wigner function yields an incorrect vN entropy or purity for the \( k \) particles, though here the vN entropy is no longer a well-defined entanglement entropy since the density matrix of the \((k, -k)\) mode pairs (not the RDM of the \( k \) particles) effectively constitutes a mixed state.

Since the quantum phase is conjugate to the particle number of a squeezed state, one may expect that one could obtain the phase information from time derivatives of \( \eta_k \) or equivalently, from evolution of the entanglement entropy in time. Indeed, by noting that \( \partial_{\eta_k} \chi_k (\eta) = 0 \) and from Eq. (46), one has \( \chi_k^2 (\eta) = \alpha_k^2 (\eta) \chi_k (\eta) - \beta_k^2 (\eta) \chi_k^* (\eta) \). This implies that

\[
n_k^\prime = -2 \Im \left\{ c_k \left[ \chi_k^* (\eta) + \Omega^2 (\eta) \chi_k^* (\eta) \right] \right\},
\]

where \( c_k = \alpha_k \beta_k = e^{i(\sigma_k + \theta_k)} \cosh r_k \sinh r_k \) provides information of the phase \( \sigma_k + \theta_k \). Unfortunately, in the right hand side of Eq. (62), \( c_k \) is always multiplied by a term in the square bracket, which often cancels the oscillation of \( c_k \) so that one cannot read off the quantum phase from the behavior of \( n_k^\prime \).

Even \( c_k \) per se are not always fast oscillating, though. Below we will give an example when the off-diagonal elements of \( \rho_{nm,mm}^k \) associated with the particle-number operators defined at the initial moment do not oscillate, namely, when the Universe undergoes inflationary expansion. But before we proceed, we want to make one more remark on an alternative oscillating "phase."
B. Quantum Vlasov equation

The $\eta$ time derivative of $c_k$ reads

$$c_k' = 2i\kappa \left[ |\chi_k(\eta)|^2 + \Omega^2(\eta) |\chi_k(\eta)|^2 \right] - i(2n_k + 1) \left[ (\chi_k(\eta))^2 + \Omega^2(\eta) (\chi_k(\eta))^2 \right]$$

(63)

Similar to [14], one can express $c_k$ in terms of $n_k$ by solving (63) then insert it into (62) to get

$$n_k'(\eta) = 2 \text{Re} \left\{ \left[ \chi_k^2(\eta) + \Omega^2_k(\eta) \chi_k^2(\eta) \right] \times \right.$$  

$$\left. \int_{\eta_0}^{\eta} d\eta \left( 2n_k(\eta) + 1 \right) \left[ \chi_k^2(\eta) + \Omega^2_k(\eta) \chi_k^2(\eta) \right] e^{-2i[\Theta_k(\eta) - \Theta_k(\eta_0)]} \right\},$$

(64)

where

$$\Theta_k(\eta) \equiv \int_{\eta_0}^{\eta} d\tau \left[ |\chi_k(\eta)|^2 + \Omega^2_k(\tau) |\chi_k(\eta)|^2 \right].$$

(65)

which demonstratively illustrates that the evolution of $n_k$ is in general non-Markovian. Only in the case that the phase $|\Theta_k(\eta) - \Theta_k(\eta_0)|$ grows rapidly in $\eta - \eta_0$, would the $\eta$ integration be effective only around $\eta_0 \approx \eta$, and the right-hand side of (63) becomes local in time.

Anyway, solving the quantum Vlasov equation (64), or (62) and (63), is equivalent to solving $\chi_k$ from (11) and then calculate $n_k$ and $c_k$, which is much simpler. We put (62) and (63) here simply to show the relation between the particle number and the phases. Often it is not economic to solve them directly.

We should emphasize that $\Theta_k$ in (64) and the counterpart in [14], which is the phase of the adiabatic mode function, are different from the quantum phase $\sigma_k + \theta_k$ in general.

V. ENTANGLEMENT IN COSMOLOGICAL PARTICLE CREATION

A. A real scalar field in the FRW universe

A real scalar field $\Phi$ with mass $m$ minimally coupled to a curved spacetime with metric $g_{\mu \nu}$ is described by the action,

$$S = \int d^4x \sqrt{-g} \left[ \frac{1}{2} \partial_\mu \Phi \partial^\mu \Phi - \frac{m^2}{2} \Phi^2 \right].$$

(66)

We are working with a test-field condition where the gravitational field $g_{\mu \nu}$ is a given background, in this case, the FRW spacetime, with line element

$$ds^2 = a(\eta)^2 \left[ -d\eta^2 + \frac{dr^2}{1 - \kappa r^2} + r^2 d\theta^2 + r^2 \sin^2 \theta d\phi^2 \right],$$

$$= a(\eta)^2 \left[ -d\eta^2 + h_{ij} dx^i dx^j \right],$$

(67)

where $\kappa = 1, 0, -1$ corresponds to closed, flat and open universes respectively. In terms of the conformal time $\eta$ and the conformal scalar field defined as

$$X(x) \equiv a(\eta) \Phi(x),$$

(68)

one can rewrite the field action $S$ as

$$S = \int d^3x \sqrt{h} \left[ \frac{1}{2} X'^2 - \frac{1}{2} \partial_i X^i X + \frac{1}{2} \left( \frac{a''}{a} - m^2 a^2 \right) X^2 \right]$$

(69)

plus a surface term $-\int d^3x X^2 a'/2a$. The field equation then reads

$$X'' + \left( m^2 a^2 - \frac{a''}{a} - \nabla^2 \right) X = 0.$$

(70)
To better handle the spatial derivatives in action $S$, we perform a transformation

$$X(x) = \sum_{k} \mathcal{Y}_k(x) \phi_k(\eta),$$

(71)

where $\sum_{k} \mathcal{Y}_k(x)$ for $\kappa = -1, 0, 1$ can be found in [8]. For $\kappa = 0$ (spatially flat), $\sum_{k} \mathcal{Y}_k(x)$ is simply $e^{ikx}$, and the action written in the Fourier $k$ space becomes [2] with time-varying squared frequencies

$$\Omega_k^2(\eta) \equiv k^2 + m^2 a^2 - n''/a.$$  

(72)

So the formulation in Sec. III can be directly applied.

### B. Entanglement of particle creation in a de Sitter spacetime

In the spatially flat FRW coordinatization of the de Sitter space, the scale factor is $a = -(H\eta)^{-1} = e^{Ht}$ with Hubble constant $H$ and cosmic time $t$, such that $\eta$ runs from $-\infty$ to 0 as $t$ goes from $-\infty$ to $\infty$ (see, for example, Sec. 5.4 in Ref. [8]). The squared time-varying natural frequency in (72) now reads

$$\Omega_k^2 = k^2 + \left( \frac{m^2}{H^2} - 2 \right) \frac{1}{\eta^2}.$$  

(73)

If $m^2 < 2H^2$, $\Omega_k^2$ will become negative at late times ($\eta \to 0$) for all finite $k$. The Bunch-Davies vacuum corresponds to taking the value [30]

$$\chi_k = \sqrt{\frac{\pi \eta}{4}} H_\nu^{(2)}(k\eta),$$

(74)

where $H_\nu^{(2)}$ is the Hankel function and $\nu \equiv [(9/4) - (m^2/H^2)]^{1/2}$.

The phase in the quantum Vlasov equation (74) of such a scalar field in this de Sitter spacetime

$$\Theta_k(\eta) - \Theta_k(\bar{\eta}) = (\eta - \bar{\eta}) \left\{ |\chi_k(\eta_0)|^2 + \left[ k^2 + \left( \frac{m^2}{H^2} - 2 \right) \frac{1}{\eta^2} \right] |\chi_k(\eta_0)|^2 \right\}_{\eta_0 \to -\infty},$$

(75)

varies quite rapidly in $\eta - \bar{\eta}$ time, so the integration in (74) is more pronounced around $\bar{\eta} \approx \eta$ and the behavior of $\sigma_k$ in an inflationary universe can be treated in a Markovian approximation. However, this does not imply that the quantumness of the field is lost in this epoch, as some authors working on the decoherence of quantum fields in inflationary cosmology are drawn to making such a claim.

Substituting (74) into (72) and the counterpart for $\sigma_k$, we find that $\sigma_k + \delta_k$ varies quite slowly except when $\eta^2 \approx |(m^2/H^2) - 2|/k^2|$, which is around the moment that $\Omega_k^2$ is crossing zero in the cases with $m^2 < 2H^2$. Far from this moment in cosmic time $t$, $c_k^{n-m}$ almost does not oscillate and could be identified correctly for very large $|n - m|$. Therefore perhaps contrary to common belief, in almost the whole inflation epoch, the off-diagonal elements of the density matrix corresponding to the quantum interference between the $k$ and $-k$ particles associated with $B_k$ corresponding to the in-vacuum manifest and the coarse-grained effective density matrix is extremely pure [38].

Alternatively, in the adiabatic number basis, the two concepts of phase in Sec. IV can coincide. For example, the (first-order) adiabatic mode function used by KME in [14] reads

$$\chi_k(\eta) = \sqrt{\frac{1}{2\Omega_k(\eta)}} \exp \left[ -i \int_{\eta_0}^{\eta} d\bar{\eta} \Omega_k(\bar{\eta}) \right].$$

(76)

Numerically we find that at early times when $\Omega_k$ is real and not very small, the adiabatic particle number [14]

$$N_k = |\chi_k(\eta)|^2$$

(77)

is indeed much less than $n_k$, and the counterpart of $c_k$ for the adiabatic mode function does oscillate, in exactly the same way as the oscillation in the phase $\Theta$ in their quantum Vlasov equation (which implies that it is still impossible to determine the quantum phase by observing the evolution of their $N_k$). This justifies the argument in [14]: The adiabatic particles look more classical since the off-diagonal elements of the density matrix of the vacuum
(the counterpart of (67) with \( r_k \) and \( \sigma_k + \theta_k \) obtained in the adiabatic number basis) oscillate too fast to be resolved. Then the vN entropy \( S_{\text{eff}} \) of the effective density matrix \( \rho_{\text{eff}} \) of the vacuum with all off-diagonal elements in the adiabatic number representation vanishing is \( (85) \) with \( n_k \) replaced by \( \mathcal{N}_k \) [cf. Eq.(3.23) in [14] for complex scalar fields],

\[
S_{\text{eff}} = -\text{Tr}\rho_{\text{eff}} \ln \rho_{\text{eff}} = \frac{1}{2} \sum_k ((\mathcal{N}_k + 1) \ln(\mathcal{N}_k + 1) - \mathcal{N}_k \ln \mathcal{N}_k),
\]

which is also valid for all values of \( \mathcal{N}_k \) and is much less than the vN entropy in \( n_k \). Again, as discussed in Sec. IV.A the value of the above \( S_{\text{eff}} \) is the same as the value of the entanglement entropy between the adiabatic particles with \( k \) and \(-k\), while \( S_{\text{eff}} \) will decrease as more and more phase information is resolved and the off-diagonal elements manifest.

Unfortunately \( (76) \) is not well defined if \( \Omega_k = 0 \), which occurs in the case \( m^2/H^2 < 2 \) when the physical wavelength of the mode crosses the horizon. At that very moment, \( \mathcal{N}_k \) diverges and the WKB approximation \( (76) \) fails. In this case, after \(|\eta| = (2 - (m^2/H^2))/k^2 \), when the wavelength of the field mode is longer than the size of the horizon (superhorizon), the notion of adiabatic particle is no longer viable until the inflation era ends and the universe becomes radiation dominated.

VI. SUMMARY REMARKS

We conclude with two remarks pointing to the main themes stated in the Introduction, namely, quantum entanglement depends on partition as well as the choice of physical variables or measurables. They pertain to 1) the conditions of separability of quantum states in particle creation processes and 2) the relation of entanglement dynamics and entropy generation both measured by the von Neumann entropy.

A. Conditions of separability of quantum states

For the model of a free scalar field theory in a dynamical background field or spacetime we see clearly that different quantities imply different separabilities of quantum states in different partition and different measurables. Using the vN entropy as a common currency for comparisons, we see that

1. The vN entropy of \( \rho = \prod_k \hat{\Psi}_k^\dagger \hat{\Psi}_k \) for \( (k, -k) \) mode pair, or of the Wigner functions \( (32) \) or \( (34) \), vanishes. This means that \( \rho \) is a pure state, and the quantum field here is a completely isolated system even in a classical dynamical background field or spacetime. The vanishing vN entropy of \( (15) \) and \( (17) \) is similar.

2. The vN entropy of \( \text{Tr}_{p\neq\pm k} \{\rho\} \) for some specific \( k \) with \( \rho = \prod_k \hat{\Psi}_k^\dagger \hat{\Psi}_k \), \( (32) \), or \( (34) \), is zero. This means that each \((k, -k)\) mode pair is separable from other mode pairs, and of course, each \( \hat{\Psi}_k \) is pure.

3. The vN entropy of the reduced Wigner function obtained by tracing out, say, the \( k^3 < 0 \) components of \( (32) \), is zero. This means that the quantum state of \( \hat{B}_k \hat{B}^*_k \) is separable from \( \hat{B}_{-k} \hat{B}^*_{-k} \) and all other field modes, while no particle with \( \pm k \) associated with the particle counter or the number operator defined by \( b_k(\eta) \) and \( b_k^\dagger(\eta) \) is created. The zero vN entropy of the reduced Wigner function from \( (15) \) is similar.

4. The vN entropy \( (39) \) of \( (37) \) is nonzero, meaning that the particles with \( k \) associated with the particle counter defined by \( b_k(\eta) \) and \( b_k^\dagger(\eta) \) are entangled with their \(-k\) partners. The nonzero vN entropy of \( (18) \) has a similar meaning.

5. The vN entropy of the exact density matrix of the vacuum \( \rho \) is zero, but the vN entropy of the effective density matrix in Fock representation with off-diagonal elements averaged out is not. The latter indicates that the phase information has been coarse grained.

6. The value of the vN entropy of the effective density matrix \( (61) \) with all off-diagonal elements averaged out [see statements above \( (59) \)] is the same as the value of the vN entropy of the reduced density matrix \( (60) \) after tracing out the particles with \(-k\). This suggests that the tracing-out process in obtaining the RDM represents the strongest coarse graining.

7. In the adiabatic number basis, the vN entropy \( (78) \) describing the entanglement between the adiabatic particles with \( k \) and their \(-k\) partners has a different value from \( (59) \), due to a different choice of physical measurables.
B. Entanglement entropy and entropy in statistical mechanics

As we saw in the above the von Neumann entropy has also been used as a measure of the entropy generation in particle creation processes. In [14] KME argued that the effective density matrix $\rho_{\text{eff}}$ would appear as a mixed state when the off-diagonal elements oscillate too rapidly to be resolved. We see close similarity between the vN entropy of a bosonic field used in this context of nonequilibrium mechanics and that measuring the quantum entanglement between the $(k, -k)$ particles in a single mode pair. Indeed, from our result [39] we see that the correlation between each particle pair seems to be equal, so that the entanglement entropy between $k$ and $-k$ particles seems to be counting the number of the degrees of freedom that are integrated out. Although the entropy of the former has the same value as the latter in the cases considered in this paper, the differences between these two forms of entropy are perhaps more revealing, especially when viewed from their respective theoretical structures.

Let us compare the difference between the vN entropy $S = -\text{Tr}\rho \log \rho$ [31] of a closed quantum system with the Boltzmann’s entropy in a microcanonical ensemble $S = -k_B \log \Omega$ where $\Omega$ is the number of accessible states. Note that both describes an isolated quantum system. The enumeration of accessible states is independent of the representation and can contain both entangled states and separable states. When one assumes that $\Omega = \text{Tr}\rho$ is given by the probability $\text{Tr}\rho$ of finding an isolated system in a particular quantum state, one has already ignored all physical information contained in the off-diagonal components of the density matrix such as quantum phase of quantum states. This is accomplished under the random phase approximation whereby one can use the concepts of probabilities exclusively to describe all statistical mechanical properties of the system. When a system can occupy all of its accessible states with equal $a \text{ priori}$ probability, then the system is in equilibrium. These are, as we know, the two fundamental postulates of equilibrium statistical mechanics, namely, (1) equal $a \text{ priori}$ probability, and (2) random phase [32]. (For a depiction of how a quantum system in contact with a thermal bath turn from a quantum fluctuation dominated phase to a thermal fluctuation dominated phase at increasing temperature, and under what conditions will these two postulates be satisfied in an open quantum system, see [33].) Finally it is when the particle number $n_k \gg 1$ that one can begin to use thermodynamic arguments.

Thus we see the three stages distinctly: vN and Boltzmann entropy (in its original form) both describe fully isolated quantum systems. When one begins to use probability for the description of the system, quantum phase information is lost. When one imposes in addition the equal $a \text{ priori}$ probability assumption one reaches an equilibrium condition. Thermodynamic description requires an additional assumption that both the number of particles and the volume of the system remain fixed while their ratio is kept a constant. As is known and shown in some of our earlier work [34] the thermodynamic entropy is different from the (equilibrium) statistical mechanical entropy and the quantum (nonequilibrium) vN entropy, in increasing order of specificity.

In contrast, it is clear that the von Neumann entropy of one of the two parties of an isolated, bipartite system is a well-defined measure of entanglement [16] and (39) is a good entanglement entropy for all $n_k$ for all time.

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[37] In [35], Berger suggested an alternative choice of the initial state $\Psi_B$ which satisfies $(1/2)\Omega_k(\eta_0)\Psi_B = \hat{H}(\eta_0)\Psi_B$ [which is stronger than (6)] at the initial moment $\eta_0$. She found that $\Psi_B = \sum_n a_{2n}\Psi_n$ with nonzero factors $a_{2n}$ for $n = 0, 1, 2, 3, \ldots$. However, in her setup (Kasner universe), $\Psi_B$ will become $\Psi_0$ as $\eta_0 \to -\infty$.

From here one can trace out $Q^{-k}$ and $Q^{-k}$ to get the RDM $\rho_{n,m} = \delta_{nm} \tanh^{2n} r_k / \cosh^{2n} r_k \equiv \delta_{nm} \rho_{0,0} e^{-n\Omega/k_B T_{\text{eff}}}$. One could presumably identify an “effective temperature” $T_{\text{eff}} = h\Omega/[k_B \ln(1 + n_k^{-1})]$ depending only on $n_k$ and valid for all values of $n_k$, just like the vN entropy (39). Since such an effective temperature can vary quickly in time, it is very remote from the usual concept of temperature defined in statistical mechanics (see the discussion in Section VI B).

[38] Campo and Parentani have come to a similar conclusion in [23] for a single interacting field, rather than the free field in this paper, in inflationary universe.