

# Quantum cosmological entropy production and the asymmetry of thermodynamic time

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The Hamiltonian for the time-dependent Schrödinger equation for matter fields derived from the Wheeler-DeWitt equation for a quantum minisuperspace cosmological model minimally coupled to free massive minimal scalar fields consists of a set of parameter-dependent and implicitly cosmological time-dependent harmonic oscillators. By using the generalized invariant method we obtain the exact quantum states whose number states at an earlier gravitational configuration in an expanding stage get evolved unitarily by a squeeze operator into the same number states at the later identical gravitational configuration in the subsequent recollapsing stage. It is proposed that during an expansion and the subsequent recollapse of the Universe following a wide class of wave functions of the quantum minisuperspace cosmological model, the cosmological entropy production determined by the squeeze parameters may break the symmetry of the thermodynamic time.

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## I. INTRODUCTION

In recent years there have been various attempts to explain the asymmetry of the cosmological, thermodynamical, and psychological times in the context of quantum cosmology [1]. At the classical level, the first scientific study about the connection between the thermodynamic and cosmological times dates back to Gold [2], who argued the time-symmetric entropy increase and decrease with respect to the maximum expansion of the Universe. But this argument was refuted by Penrose [3] from the point of view of an observer falling into a black hole, which can be regarded as a recollapsing small universe. On the other hand, at the quantum level, the connection between the thermodynamic and cosmological times was proposed by Hawking [4] from the Hartle-Hawking no boundary wave function [5], in which the wave function of the Universe should be *CPT* invariant. This argument again was refuted immediately by Page [6], who pointed out that the *CPT* theorem does not exclude a time-asymmetric wave function in which entropy can increase monotonically throughout an expansion and the subsequent recollapse of the Universe. Quite recently, Hawking *et al.* [7] argued in support of the latter point of view that the thermodynamic arrow of time need not reverse even in the recollapsing stage of the Universe, due to the density perturbations which start small but grow larger and become nonlinear as the Universe, expands and recollapses. There have been many related and similar quantum cosmological arguments on the connection between the thermodynamic and cosmological times [8,9,1].

In a previous paper [9], we proposed that for any quantum cosmological model with many degrees of freedom for the gravitational and matter fields the symmetry of the cosmological time may be broken due to the geo-

metric phases during an expansion and the subsequent recollapse of the Universe. Such a quantum cosmological model has a spectrum of wave functions, in which the recollapsing wave function differs from the expanding wave function by the holonomy (Wilson loop operator) of the gauge potential coming from the matter fields or some other gravitational inhomogeneity and anisotropy if the Universe traces a closed loop in a projected minisuperspace. In this paper, we shall further propose that in the Universe following a wide class of wave functions, the symmetry of the thermodynamic time may be broken due to the cosmological particle creation and the entropy production by further elaborating the same quantum cosmological model. This, however, does not exclude some particular wave functions of the universe expanding from an asymptotic region and recollapsing to the same asymptotic region in which the entropy may decrease during the recollapse.

## II. DERIVATION OF TIME-DEPENDENT SCHRÖDINGER EQUATION

Let us consider the Wheeler-DeWitt equation (in units of  $\hbar = 1$ ) for a quantum minisuperspace cosmological model:

$$\left[ -\frac{1}{2m_P} F^{ab}(\zeta) \frac{\partial^2}{\partial \zeta^a \partial \zeta^b} + V_g(\zeta) - \frac{1}{2m_s} G^{kl}(\zeta) \frac{\partial^2}{\partial \phi^k \partial \phi^l} + V_s(\phi, \zeta) \right] \Psi(\zeta, \phi) = 0, \quad (1)$$

where  $F^{ab}$  and  $G^{kl}$  are the inverse supermetrics of the supermetrics  $F_{ab}$  and  $G_{kl}$  on the extended minisuperspace of the three-geometry plus scalar fields with the signatures  $\eta_{ab} = (-1, 1, \dots, 1)$  and  $\delta_{kl} = (1, \dots, 1)$ . Following

Ref. [9], one can expand the wave function

$$\Psi(\zeta, \phi) = \sum_{\lambda} \Psi_{\lambda}(\zeta) |u_{\lambda}(\phi, \zeta)\rangle = \vec{U}_u^T(\phi, \zeta) \vec{\Psi}(\zeta), \quad (2)$$

by the adiabatic or nonadiabatic basis of the eigenstates for the matter field Hamiltonian

$$H_{\text{matter}}(\phi, \zeta) = \frac{1}{2m_s} G^{kl}(\zeta) p_k p_l + V_s(\phi, \zeta). \quad (3)$$

In an intermediate step, one obtains a matrix effective gravitational Hamiltonian equation

$$\left[ -\frac{1}{2m_P} F^{ab}(\zeta) \left( \frac{\partial}{\partial \zeta^a} - iA_{u,a}(\zeta) \right) \left( \frac{\partial}{\partial \zeta^b} - iA_{u,b}(\zeta) \right) + V_g(\zeta) + H_{\text{matter},u}(\zeta) \right] \vec{\Psi}(\zeta) = 0, \quad (4)$$

where

$$A_{u,a}(\zeta) = i\vec{U}_u^* \frac{\partial}{\partial \zeta^a} \vec{U}_u^T(\phi, \zeta), \quad (5)$$

is a gauge potential (Berry connection) [10] and

$$H_{\text{matter},u}(\zeta) = \vec{U}_u^* \frac{\partial}{\partial \zeta^a} H_{\text{matter}}(\phi, \zeta) \vec{U}_u^T(\phi, \zeta) \quad (6)$$

is a back reaction of the matter fields to the gravitational fields. Depending on the choice of bases,  $H_{\text{matter},u}(\zeta)$  needs not to be a diagonal matrix.

In either of the bases, the wave function determined from the gravitational Hamiltonian equation (4) has the WKB approximation

$$\Psi_{\lambda}(\zeta) \approx \exp[iS_{\lambda}(\zeta)], \quad (7)$$

which is peaked along a classical trajectory in an oscillatory region. The classical trajectory is a solution of the Einstein equation with the matter fields [11]. One can define the cosmological time along each classical trajectory through a tangent vector [12] as

$$\frac{\partial}{\partial t_{\lambda}} = \frac{F^{ab}}{m_P} \frac{\partial}{\partial \zeta^a} S_{\lambda}(\zeta) \frac{\partial}{\partial \zeta^b}. \quad (8)$$

The cosmological time defined without the gauge potential is symmetric with respect to an expansion and the subsequent recollapse, whereas with the gauge potential it is asymmetric. So we may set the exact wave function of the form

$$\Psi_{\lambda}(\zeta, \phi) = \exp[iS_{\lambda}(\zeta)] \Phi_{\lambda}(\phi, \zeta), \quad (9)$$

and substitute Eq. (9) into the Wheeler-DeWitt equation (1) to derive the time-dependent Schrödinger equation for the matter fields in the curved Universe:

$$i \frac{\partial}{\partial t_{\lambda}} \Phi_{\lambda}(\phi, \zeta) = H_{\text{matter}}(\phi, \zeta) \Phi_{\lambda}(\phi, \zeta) + \left[ \frac{1}{2m_P} F^{ab}(\zeta) \left( \frac{\partial S_{\lambda}}{\partial \zeta^a} \frac{\partial S_{\lambda}}{\partial \zeta^b} - i \frac{\partial^2 S_{\lambda}}{\partial \zeta^a \partial \zeta^b} - \frac{\partial^2}{\partial \zeta^a \partial \zeta^b} \right) + V_g(\zeta) \right] \Phi_{\lambda}(\phi, \zeta). \quad (10)$$

It should be remarked that in defining the cosmological time the effects of the matter fields have already entered the matrix effective gravitational Hamiltonian equation (4) just as the back reaction and the gauge potential have. This procedure seems more systematic and correct than the ordinary WKB approximation given by

$$\Psi(\zeta, \phi) = \exp[iS(\zeta)] \Phi(\phi, \zeta), \quad (11)$$

where the action is expanded in a power series of  $\hbar/\sqrt{m_P}$ , and the lowest order action satisfies the Einstein-Hamilton-Jacobi equation [13]

$$\frac{1}{2m_P} F^{ab}(\zeta) \frac{\partial S_{(0)}}{\partial \zeta^a} \frac{\partial S_{(0)}}{\partial \zeta^b} + V_g(\zeta) = 0. \quad (12)$$

Although the asymptotic parameter for the Wheeler-DeWitt equation should be  $\sqrt{m_P}/\hbar$  rather than  $\sqrt{m_s}/\hbar$ , if the mass scale for the matter fields is lower by only a few orders than that of the Planck mass for the gravitational fields, one should include the matter fields into the action  $S(\zeta, \phi)$  for large quantum numbers and modify the Einstein-Hamilton-Jacobi equation as

$$\frac{1}{2m_P} F^{ab}(\zeta) \frac{\partial S_{(0)}}{\partial \zeta^a} \frac{\partial S_{(0)}}{\partial \zeta^b} + V_g(\zeta) + \frac{1}{2m_s} G^{kl}(\zeta) \frac{\partial S_{(0)}}{\partial \phi^k} \frac{\partial S_{(0)}}{\partial \phi^l} + V_s(\phi, \zeta) = 0. \quad (13)$$

Bearing Eq. (12) in mind, one is able to see that the terms in the square brackets of Eq. (10) are the quantum correction of the gravity to the matter fields. In the nonadiabatic basis of the generalized invariant, we may perform a new asymptotic expansion of the Wheeler-DeWitt equation, in which the lowest order solution of the time-dependent Schrödinger equation in curved space is the eigenstate itself of the generalized invariant, and the higher order corrections can be found analytically in the asymptotic parameter [14]. Hereafter, we shall confine ourselves to the time-dependent Schrödinger equation for the matter fields only.

### III. COSMOLOGICAL ENTROPY PRODUCTION

The time-dependent equation

$$i \frac{\partial}{\partial t_{\lambda}} \Phi_{\lambda}(\phi, \zeta) = H_{\text{matter}}(\phi, \zeta) \Phi_{\lambda}(\phi, \zeta) \quad (14)$$

is parametrized by the cosmological time  $t_{\lambda}$  defined along the classical trajectory of the  $\lambda$ th wave function. A change of the notation will be made hereafter: the subscript ‘‘matter’’ used to denote the matter fields and the  $\lambda$  for the modes will be omitted from the notation and carets will denote quantum operators. For the simple model, e.g., Eq. (30) of Ref. [9], the matter field Hamiltonian in some appropriate normal coordinates is the sum of harmonic oscillators with their own variable frequency squared:

$$\begin{aligned}\hat{H}(\phi, \zeta(t)) &= \sum_l \hat{H}_l(\phi, \zeta(t)) \\ &= \sum_l \frac{1}{2m_l} \hat{p}_l^2 + \frac{1}{2} m_l \omega_l^2(\zeta) \hat{\phi}_l^2.\end{aligned}\quad (15)$$

It is well known that the exact quantum states of a time-dependent harmonic oscillator are determined by the eigenstates of the Lewis-Riesenfeld invariant up to some time-dependent phases [15]. Of course, there are many methods [16] introduced to find the invariant for the time-dependent harmonic oscillator. The invariant is again the sum of the invariants for each  $\hat{H}_l(\phi, \zeta)$ :

$$\begin{aligned}\hat{I}(\phi, \zeta(t)) &= \sum_l \hat{I}_l(\phi, \zeta) \\ &= \sum_l \left[ g_{l,-}(\zeta) \frac{\hat{p}_l^2}{2} + g_{l,0}(\zeta) \frac{\hat{p}_l \hat{\phi}_l + \hat{\phi}_l \hat{p}_l}{2} \right. \\ &\quad \left. + g_{l,+}(\zeta) \frac{\hat{\phi}_l^2}{2} \right].\end{aligned}\quad (16)$$

The parameter-dependent harmonic oscillator has the Lie algebra of  $SU(2)^N$  ( $N$  being the number of normal modes) with the following Hermitian basis:

$$\hat{L}_{l,-} = \frac{\hat{p}_l^2}{2}, \quad \hat{L}_{l,0} = \frac{\hat{p}_l \hat{\phi}_l + \hat{\phi}_l \hat{p}_l}{2}, \quad \hat{L}_{l,+} = \frac{\hat{\phi}_l^2}{2}, \quad (17)$$

whose group structure is

$$\begin{aligned}\left[ i \frac{\hat{L}_{k,0}}{2}, \hat{L}_{l,\pm} \right] &= \pm \hat{L}_{k,\pm} \delta_{kl}, \\ \left[ \hat{L}_{k,+}, \hat{L}_{l,-} \right] &= 2 \left( i \frac{\hat{L}_{k,0}}{2} \right) \delta_{kl}.\end{aligned}\quad (18)$$

It possesses also the spectrum-generating algebra of  $SU(1,1)^N$  with the Hermitian basis

$$\hat{K}_{l,0} = \frac{1}{2}(\hat{L}_{l,-} + \hat{L}_{l,+}), \quad \hat{K}_{l,\pm} = \frac{1}{2}(\hat{L}_{l,+} - \hat{L}_{l,-} \mp i \hat{L}_{l,0}), \quad (19)$$

whose group structure is

$$\left[ \hat{K}_{k,0}, \hat{K}_{l,\pm} \right] = \pm \hat{K}_{k,\pm} \delta_{kl}, \quad \left[ \hat{K}_{k,+}, \hat{K}_{l,-} \right] = -2 \hat{K}_{k,0} \delta_{kl}.\quad (20)$$

Following [17], one can introduce the parameter-dependent basis of the spectrum-generating algebra

$$\begin{aligned}\hat{K}_{l,0}(\zeta) &= \frac{1}{4} \left( \frac{\omega_{l,0} \hat{\phi}_l^2}{g_{l,-}(\zeta)} + \frac{g_{l,-}(\zeta) \hat{p}_{c,l}^2}{\omega_{l,0}} \right), \\ \hat{K}_{l,\pm}(\zeta) &= \frac{1}{4} \left( \frac{\omega_{l,0} \hat{\phi}_l^2}{g_{l,-}(\zeta)} - \frac{g_{l,-}(\zeta) \hat{p}_{c,l}^2}{\omega_{l,0}} \mp i(\hat{p}_{c,l} \hat{\phi}_l + \hat{\phi}_l \hat{p}_{c,l}) \right),\end{aligned}\quad (21)$$

where  $\hat{p}_{c,l} = \hat{p}_l + g_{l,0}(\zeta) \hat{\phi}_l / g_{l,-}(\zeta)$  are the canonically transformed momentum operators. The basis preserves the same group structure as Eq. (20). Now, the generalized invariant can be rewritten as

$$\hat{I}(\phi, \zeta) = \sum_l^N 2\omega_{l,0} \hat{K}_{l,0}(\zeta), \quad (22)$$

where  $\omega_{l,0}$  is the invariant frequency of the  $l$ th generalized invariant, and it is usually fixed by the initially prepared quantum state. The number states of each invariant are

$$\hat{K}_{l,0}(\zeta) |n_l, k_{l,0}, \zeta\rangle = (n_l + k_{l,0}) |n_l, k_{l,0}, \zeta\rangle, \quad (23)$$

where  $k_{l,0}$  is the Bargmann index for the  $l$ th harmonic oscillator, which takes the values  $k_{l,0} = 1/4$  or  $3/4$  [18]. One can also obtain the number states by acting the raising operator on the ground state:

$$\begin{aligned}|n_l, k_{l,0}, \zeta\rangle &= \left( \frac{\Gamma(2k_{l,0})}{n_l! \Gamma(n_l + 2k_{l,0})} \right)^{1/2} \left( \hat{K}_{l,+}(\zeta) \right)^{n_l} \\ &\quad \times |0_l, k_{l,0}, \zeta\rangle.\end{aligned}\quad (24)$$

On the other hand, some simplification can be achieved by introducing the squeeze operators [19]. The basis of the spectrum-generating algebra at an arbitrary later gravitational configuration  $\zeta$  can be expressed by that at an earlier gravitational configuration  $\zeta_0$  as

$$\begin{aligned}\hat{K}_{l,0}(\zeta) &= \nu_{l,0}(\zeta) \hat{K}_{l,0}(\zeta_0) + \nu_{l,+}(\zeta) \hat{K}_{l,+}(\zeta_0) \\ &\quad + \nu_{l,+}^*(\zeta) \hat{K}_{l,-}(\zeta_0),\end{aligned}\quad (25)$$

where

$$\begin{aligned}\nu_{l,0}(\zeta) &= \frac{1}{2} \left( g_{l,-}(\zeta) + \frac{1}{g_{l,-}(\zeta)} + \frac{g_{l,0}^2(\zeta)}{\omega_{l,0}^2 g_{l,-}(\zeta)} \right), \\ \nu_{l,+}(\zeta) &= \frac{1}{4} \left( -g_{l,-}(\zeta) + \frac{1}{g_{l,-}(\zeta)} \pm 2i \frac{g_{l,0}(\zeta)}{\omega_{l,0}} \right. \\ &\quad \left. + \frac{g_{l,0}^2(\zeta)}{\omega_{l,0}^2 g_{l,-}(\zeta)} \right).\end{aligned}\quad (26)$$

The classical trajectory should pass through both of  $\zeta$  and  $\zeta_0$ . By introducing the squeeze operator

$$\hat{S}_l(\xi) = \exp \left( \xi \hat{K}_{l,+}(\zeta_0) - \xi^* \hat{K}_{l,-}(\zeta_0) \right), \quad (27)$$

one can show that the basis transforms unitarily as

$$\hat{K}_{l,0}(\zeta) = \hat{S}_l^\dagger(\xi) \hat{K}_{l,0}(\zeta_0) \hat{S}_l(\xi), \quad (28)$$

where the squeeze parameter [18] is

$$\begin{aligned}(\xi \xi^*)^{1/2} &= \frac{1}{2} \tanh^{-1} \left( \frac{2[\nu_{l,+}(\zeta) \nu_{l,+}^*(\zeta)]^{1/2}}{\nu_{l,0}(\zeta)} \right), \\ \frac{\xi^*}{\xi} &= \frac{\nu_{l,+}^*(\zeta)}{\nu_{l,+}(\zeta)}.\end{aligned}\quad (29)$$

Then it follows that a number state at the earlier gravitational configuration transforms unitarily into the same number state at the later gravitational configuration:

$$|n_l, k_{l,0}, \zeta\rangle = \hat{S}_l^\dagger(\zeta) |n_l k_{l,0}, \zeta_0\rangle. \quad (30)$$

Including the parameter-dependent phase factors the exact quantum states of the matter field Hamiltonian (14) are found to be [17]

$$\Phi(\phi, \zeta) = \prod_l^N \exp \left( -i \int_{\zeta_0}^{\zeta} [h_l(\zeta) - \varepsilon_l(\zeta)](n_l + k_{l,0}) \right) \times |n_l, k_{l,0}, \zeta\rangle, \quad (31)$$

where

$$h_l(\zeta) = \frac{\omega_{l,0}^2 + g_{l,0}^2 + \omega_l^2(\zeta)g_{l,-}^2(\zeta)}{\omega_{l,0}},$$

$$\varepsilon_l(\zeta) = \frac{g_{l,-}(\zeta)}{2\omega_{l,0}} \frac{\partial}{\partial \zeta^a} \left( \frac{g_{l,0}(\zeta)}{g_{l,-}(\zeta)} \right) \dot{\zeta}^a. \quad (32)$$

According to the standard (information-theoretic) definition of nonequilibrium entropy, the amount of entropy production for each normal mode is determined by the squeeze parameter [20] to be  $\Delta E_l = 2|\xi_l|$ , and the total amount of entropy production to be

$$\Delta E_{\text{total}} = \sum_l^N 2|\xi_l|. \quad (33)$$

The entropy is produced due to the cosmological particle creation of the matter fields which obey the time-dependent Schrödinger equation in the expanding and subsequently recollapsing Universe. It is a general feature of time-dependent harmonic oscillators that the generalized invariant does not evolve to be time symmetric even for the time-symmetric Hamiltonian and therefore the information-theoretic entropy increases according to Eq. (33). The generalized invariant is periodic even for a periodic frequency up to some factor determined from the Floquet theorem. Furthermore, even if the Universe returns to the same gravitational configuration in the recollapsing stage as the gravitational configuration in the expanding stage, it is the asymmetry of the cosmological time due to the gauge potential [9] that prevents the generalized invariant from evolving to the identical value. Thus there is always entropy production throughout an expansion and the subsequent recollapse.

It should be remarked again that there is a geometric phase in Eq. (31):

$$\prod_l^N \exp \left( i \oint \varepsilon_l(\zeta)(n_l + k_{l,0}) \right) = \exp \left( i \sum_l^N \oint \varepsilon_l(\zeta)(n_l + k_{l,0}) \right) \quad (34)$$

for a closed trajectory in the projected minisuperspace. The geometric phase is identical to Eq. (36) of Ref. [9] in spite of a slight change of notation in Eq. (32).

#### IV. DISCUSSION

To summarize, we derived the time-dependent Schrödinger equations of Eq. (10) and Eq. (14) for the

matter fields from the Wheeler-DeWitt equation for a quantum cosmological model. As a simple model we considered the free massive minimal scalar fields and obtained the Hamiltonian (15) consisting of implicitly cosmological time-dependent and parameter-dependent harmonic oscillators and the Lewis-Riesenfeld invariant of Eq. (16). It is shown that the eigenstates of the generalized invariant are the number states of Eq. (23) and the exact quantum states of Eq. (31) for Eq. (15) are determined up to some time-dependent phase factors. The number states at an earlier gravitational configuration get evolved unitarily by the squeeze operator of Eq. (27) into the same number states of Eq. (30) at the later identical gravitational configuration. According to the information-theoretic entropy, the entropy increases by the squeeze parameters of Eq. (29). In the process of an expansion and the subsequent recollapse of the Universe, the entropy increases inevitably, because the generalized invariant starting at the earlier gravitational configuration does not evolve into the same value when returning to the identical gravitational configuration. It is proposed that the cosmological entropy production may break the symmetry of the thermodynamic time in an expansion and the subsequent recollapse.

The particle creation and entropy production has already been discussed in the context of quantum field theory in time-changing metrics [21], and quite recently it has been investigated using the squeeze state formalism in the expanding Universe [22]. The main difference of this paper from those is that, by studying the time-dependent Schrödinger equation in the functional Schrödinger picture, we obtained the exact quantum states and found the squeeze parameters explicitly using the generalized invariant method. With a suitable redefinition of imaginary time, the time-dependent Schrödinger equation can also be extended to the regimes of the tunneling universe, to which it is not possible to extend the field theory formalism. Moreover, quantum gravity should be taken into account in the early Universe, and our approach may provide a mechanism for the quantum gravity effect to the matter fields. For example, the perturbed quantum Friedmann-Robertson-Walker model [23] may provide us with a quantum cosmological model in which the entropy increase due to the gravitational wave modes as well as the scalar field modes from a small inhomogeneity can explain the present amount of entropy, whose quantitative study will be presented elsewhere [14].

After completing this paper, we were informed that there is one particular time-symmetric solution of the quantum cosmological model [24] in which the entropy defined by the squeeze parameter in Eq. (33) is time symmetric with respect to the time of the maximum expansion. In a sequel [25] to this paper, it is found that each mode of a free scalar field in the time-changing Friedmann-Robertson-Walker universe has a time-dependent harmonic oscillator of the form of Eq. (15) whose most general three-parameter-dependent invariant can be expressed analytically in terms of the solutions of the classical equation of motion. According to this result, for a toy model with a frequency squared

which is time symmetric around a particular time corresponding to the maximum expansion of the quantum cosmological model, the generalized invariant is in general not time symmetric. However, one particular situation with the same asymptotic frequency both in the far remote past and in the far remote future is observed in which the generalized invariant becomes time symmetric. For a quantum cosmological model with the same static gravitational configuration as asymptotic regions before and after the maximum expansion, there is no net entropy production at all when the Universe starts from the asymptotic region and returns to the same asymptotic region. During the expansion and the subsequent recollapse of the Universe, the amount of entropy production varies according to Eq. (33) but eventually vanishes

in returning to these asymptotic regions. From the investigation of a quantum cosmological model it can be inferred that the direction of the thermodynamic time is in general not time symmetric during an expansion and the subsequent recollapse of the Universe except for the particular case with the same asymptotic region. This does not imply necessarily that the arrow of thermodynamic time agrees with the arrow of the other times.

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