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Nonlinear quantum evolution with maximal entropy production

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We derive a well-behaved nonlinear extension of the nonrelativistic Liouville–von Neumann dynamics driven by maximal entropy production with conservation of energy and probability. The pure-state limit reduces to the usual Schrödinger evolution, while mixtures evolve toward maximum entropy equilibrium states with canonical-like probability distributions on energy eigenstates. The linear, near-equilibrium limit is found to amount to an essentially exponential relaxation to thermal equilibrium; a few elementary examples are given. In addition, the modified dynamics is invariant under the time-independent symmetry group of the Hamiltonian, and also invariant under the special Galilei group provided the conservation of total momentum is accounted for as well. Similar extensions can be generated for, e.g., nonextensive systems better described by a Tsallis q entropy.

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I. INTRODUCTION

A number of recent, independent experiments [1] have provided impressive bounds on possible deviations from a linear and unitary propagation of pure quantum states, at least on a laboratory accessible space-time scale. The limits imposed in this way on potential generalizations of the standard unitary quantum equations of motions, as sought in relation to Hawking's blackhole evaporation process [2], are likewise severe. Certainly, there always remains the possibility of modified dynamical laws on the (inaccessible) Planck scale [3], as well as under the extreme physical environment characteristic of singular cosmological phenomena. Related models of open system dynamics due to alleged statistical perturbations, e.g., from the space-time foam, have enjoyed considerable attention lately [4]. But if the unitarity of pure-state propagation holds under universal conditions, one is necessarily led to a quest for genuine nonlinear extensions for isolated systems, possibly involving an explicit arrow of time. Indeed, it was pointed out in a fairly general ansatz [5,6] that if the pure states happen to be attractors of a nonlinear evolution, then testing the unitary propagation of pure states alone cannot rule out a nonlinear propagation of mixtures. This situation was noted recently in the context of certain nonlinear Lie-Poisson dynamics [6], wherein pure states still propagate in the usual Hamiltonian way, while density matrices evolve nonlinearly, but preserving a time-independent spectrum. Unfortunately, the underlying physics remains rather obscure in these theories, and the selection of particular realizations relevant to various experimental setups is, in general, a matter of guesswork.

In the following we show that a physically meaningful nonlinear extension emerges when the fundamental postulates of quantum mechanics are supplemented by the first and second principles of thermodynamics, at the sole expense of ignoring the constraint of a linear, unitary evolution in time. The result is a largely irreversible, highly nonlinear generalization of the nonrelativistic quantum Liouville equation, of a form closely related to the ansatz of Ref. [5] (but not in the Lie-Poisson class), which features a number of rather intriguing properties. In particular, pure states still propagate unitarily into pure states according to the usual (time-reversible) Hamiltonian dynamics. The same is true of mixed states characterized by an initial equiprobable distribution on a (finite) set of uncorrelated (orthogonal) states. Nonpure states evolve so as to maximize the entropy production at each moment in time, and to reach stationary states of maximum entropy (or minimum entropy production, according to Prigogine's nonequilibrium principle [7]) on the shortest path in the appropriate state space. Precisely, mixed states arbitrarily distributed on a finite set of uncorrelated states evolve into mixed states distributed on an equal number of uncorrelated states, have a time-dependent eigenspectrum, and eventually attain stationarity on a subset of energy eigenstates. A similar statement can be inferred, by extension, for mixtures of an infinite set of uncorrelated pure states. It follows as well that the probability distribution at equilibrium, on (a subset of) energy eigenstates, has a canonical-like dependence on the energy eigenvalues. For mixtures with an infinite energy range, the corresponding temperature is, of course, strictly positive, whereas for mixtures of a finite set of pure states the stationary state may display a ‘‘negative-temperature’’ distribution, in analogy to systems with a finite-dimensional state space. The above-mentioned properties are endorsed by the positivity of the underlying evolution equation, which ensues by construction despite the high degree of nonlinearity involved. The nature of this essentially irreversible propagation becomes evident in the close-to-equilibrium limit, when the matrix elements of the density operator between energy eigenstates are found to undergo simple exponential decays to the canonical equilibrium values. Finally, proper (nonrelativistic) invariance and conservation properties under the symmetry group of the Hamiltonian are also accounted for. However, in the absence of an explicit general law of entropy increase, the time scale for thermal relaxation is set by one multiplication factor, a scalar functional, which is yet to be given a specific expression.

Unlike the nonlinear Lie-Poisson dynamics [6], our framework apparently challenges the notion of separability

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of isolated, noninteracting systems, the lack of which has long been thought to be unacceptable [8]. We argue, nevertheless, that in a nonlinear theory it is necessary to refine the operational definition of isolation, and to acknowledge that the mutual isolation of two noninteracting systems prohibits entanglement, if individual time-translation invariance is to be preserved. When this restriction is properly taken into account in the formulation of the corresponding equation of motion, separability can be easily recovered. On the other hand, the case where noninteracting subsystems are allowed to develop correlations spontaneously and eventually exchange energy (heat) is shown to correspond in our ansatz to the phenomenon of ideal thermal contact. From a precise technical perspective, the effect has its origin in that the second principle applies, as usual, to the total entropy of a compound system and not to the entropies of individual subsystems. This necessarily results in such a redistribution of probabilities and energy as to maximize the overall entropy. In physical terms, an ideal gas is allowed to relax spontaneously to thermal equilibrium.

The formalism can be adapted straightforwardly to cover nonstandard forms for the entropy and energy functionals. As immediate examples, we construct a generalization of the Lie-Poisson dynamics with maximal entropy production and a nonlinear extension of the standard von Neumann evolution with maximal increase of the nonextensive Tsallis q entropy [9].

II. MODIFIED EQUATION OF MOTION

Following an earlier suggestion [10], the state of a quantum system will be represented by a generalized ''square root'' γ of the density matrix ρ, defined by

$$\rho = \gamma\gamma^{\dagger}. \tag{1}$$

In analogy to the common terminology, here the operator γ (not necessarily Hermitian) will be called a state operator. Note that the above decomposition is always well defined, although not unique, for any Hermitian and positive definite ρ. On the other hand, to any given γ there corresponds a unique Hermitian and positively defined ρ. We also adopt the standard inner product on the associated Hilbert space of operators,

$$(\beta|\gamma) = \mathrm{Tr}(\beta^{\dagger}\gamma), \tag{2}$$

such that for γ normalized, $(\gamma|\gamma) = \mathrm{Tr}(\gamma^{\dagger}\gamma) = 1$, the average of an observable O becomes the bilinear form

$$(\gamma|\mathbf{O}|\gamma) = (\gamma^{\dagger}O\gamma) = \mathrm{Tr}(O\rho), \tag{3}$$

with $\mathbf{O}$ the superoperator defined by O:

$$\mathbf{O}|\gamma) = |O\gamma). \tag{4}$$

It is further convenient to define the tilde conjugate $\tilde{\mathbf{A}}$ of an arbitrary, and not necessarily linear, superoperator $\mathbf{A}$ [11], by

$$(\mathbf{A}|\alpha))^{\dagger} = \tilde{\mathbf{A}}|\alpha^{\dagger}). \tag{5}$$

It can be immediately verified that the superoperator $\mathbf{A}$ maps Hermitian operators $\alpha = \alpha^{\dagger}$ into Hermitian operators $\beta = \beta^{\dagger} = \mathbf{A}|\alpha)$ if and only if it is tilde symmetric, $\mathbf{A} = \tilde{\mathbf{A}}$. For a superoperator generated by a linear operator, such as in Eq. (4) above, the tilde conjugate is given by

$$\tilde{\mathbf{A}}|\alpha) = |\alpha A^{\dagger}). \tag{6}$$

In particular, for the Hermitian observable O, it reads

$$\tilde{\mathbf{O}}|\alpha) = |\alpha O). \tag{7}$$

The tilde operation is distributive against the addition and multiplication of superoperators, $\widetilde{(\mathbf{A}+\mathbf{B})} = \tilde{\mathbf{A}} + \tilde{\mathbf{B}}$, $\widetilde{\mathbf{AB}} = \tilde{\mathbf{A}}\tilde{\mathbf{B}}$, and is antilinear against multiplication by scalars, $\widetilde{(a\mathbf{A})} = a^{*}\tilde{\mathbf{A}}$.

Let us now consider a massive isolated system characterized by an energy operator (Hamiltonian) H and a state operator γ (density matrix $\rho = \gamma\gamma^{\dagger}$), in an inertial reference system where its center of mass is at rest. We wish to find an equation of motion for this system which is first order differential in time and such that the following hold.

(1) Probability is conserved:

$$\frac{d}{dt}(\gamma|\gamma) = \frac{d}{dt}\mathrm{Tr}(\rho) = 0 \tag{8}$$

or

$$(\dot{\gamma}|\gamma) + (\gamma|\dot{\gamma}) = 0, \quad \dot{\gamma} = \frac{d}{dt}\gamma. \tag{8a}$$

(2) Energy is conserved (first principle of thermodynamics):

$$\frac{d}{dt}(\gamma|\mathbf{H}|\gamma) = \frac{d}{dt}\mathrm{Tr}(H\rho) = 0 \tag{9}$$

or

$$(\dot{\gamma}|\mathbf{H}|\gamma) + (\gamma|\mathbf{H}|\dot{\gamma}) = 0. \tag{9a}$$

(3) The entropy production is always positive (second principle of thermodynamics in nonequilibrium form),

$$\frac{d}{dt}S(\mathrm{t}) \geqslant 0. \tag{10}$$

or

$$\begin{aligned}\dot{S}(\mathrm{t}) &= -[\mathrm{Tr}(\dot{\rho}\ln\rho) + \mathrm{Tr}(\dot{\rho})]\\ &= -[(\dot{\gamma}|\ln(\gamma\gamma^{\dagger})|\gamma) + (\gamma|\ln(\gamma\gamma^{\dagger})|\dot{\gamma})\\ &\quad + (\dot{\gamma}|\gamma) + (\gamma|\dot{\gamma})]\\ &\geqslant 0.\end{aligned} \tag{10a}$$

where we adopt the standard entropy expression for a normalized state $[\mathrm{Tr}(\rho) = 1]$

$$\begin{aligned} S(t) &= -k_B \mathrm{Tr}[\rho(\mathrm{t}) \ln \rho(t)] \\ &= -k_B (\gamma(t)|\ln[\gamma(t)\gamma^\dagger(t)]|\gamma(t)), \end{aligned} \tag{11}$$

with k_B the Boltzmann constant.

In order to construct the desired equation of motion, we find it convenient to consider a stronger form of the second principle, by requiring that the entropy, as a functional of γ, increase in time along a path of maximum ascent. In other words, let the entropy production [Eq. (10a)] be maximized, for any given state γ, against variations of the time derivative $\dot{\gamma}$, under constraints (8a) (of conservation of probability) and (9a) (of conservation of energy). Note that the variation of $\dot{\gamma}$ must avoid the simple multiplication by a positive scalar, i.e., a trivial norm increase, since $\dot{S}(t)$ increases then unconditionally. Hence the entropy production must be maximized against the ''direction'' of $\dot{\gamma}$, that is, against derivatives $\dot{\gamma}$ of equal, but otherwise arbitrary norm. This amounts to deriving the equation of motion from the following variational principle with constraints

$$\delta \Big\{ [\dot{\gamma}|\ln(\gamma\gamma^\dagger)|\gamma] + [\gamma|\ln(\gamma\gamma^\dagger)|\dot{\gamma}] + 2\zeta[\dot{\gamma}|\mathbf{H}|\gamma] + 2\zeta^*(\gamma|\mathbf{H}|\dot{\gamma}) + \xi[(\dot{\gamma}|\gamma) + (\gamma|\dot{\gamma})] + \frac{2}{\sigma}(\dot{\gamma}|\dot{\gamma}) \Big\} = 0. \tag{12}$$

The variation refers to $\dot{\gamma}$ and $\dot{\gamma}^\dagger$ only, and the form of the Lagrange multipliers ζ, ξ, and σ has been chosen for later convenience. σ and ξ are real scalars on account of their corresponding real functionals, while ζ is allowed to span complex values. Upon taking the variation of $\dot{\gamma}$ and $\dot{\gamma}^\dagger$, one is left with

$$|\dot{\gamma}) = -\sigma\left[\frac{1}{2}[\ln(\gamma\gamma^\dagger)]|\gamma) + \zeta\mathbf{H}|\gamma) + \frac{\xi}{2}|\gamma)\right] \tag{13}$$

and the Hermitian conjugate. Using Eq. (13) in conditions (8) and (9) immediately gives

$$\mathrm{Re}\,\zeta = -\frac{1}{2}\frac{(\gamma|\mathbf{H}\ln(\gamma\gamma^\dagger)|\gamma) + E(S/k_B)}{\overline{\Delta H^2}}, \tag{14a}$$

$$\xi = \frac{\mathrm{S}}{k_B(\gamma|\gamma)} - 2\,\mathrm{Re}\,\zeta E, \tag{14b}$$

with $(\gamma|\gamma)=1, E=(\gamma|\mathbf{H}|\gamma)/(\gamma|\gamma)$ the average energy of the system, $S \geqslant 0$ the entropy, and $\overline{\Delta H^2} = (\gamma|H^2|\gamma) - E^2$ the squared energy deviation. One can also check condition (10a) and find that

$$\frac{\dot{S}}{k_B} = \sigma(\theta|\theta), \tag{15}$$

$$|\theta) = \ln(\gamma\gamma^\dagger)|\gamma) + 2\zeta\mathbf{H}|\gamma) + \xi|\gamma); \tag{16}$$

hence inequality (10a) is satisfied provided

$$\sigma \geqslant 0. \tag{17}$$

In deriving expression (15) we used the fact that for $|\theta)$ as in Eq. (16), and $\mathrm{Re}\,\zeta$ and ξ given by Eqs. (14), it is also true that

$$(\gamma|\mathbf{H}|\theta) = 0, \quad (\gamma|\theta) = 0. \tag{18}$$

Let us stress at once that, unlike the usual stationary action principle, our variational principle [Eq. (17)] does not involve variations of functionals over an extended interval of time, but only variations against $\dot{\gamma}$ which are local in time, at each given instant *t*. As a result, the Lagrange parameters ζ, ξ, and σ need only be constants against these same variations of $\dot{\gamma}$ and *not* constants of time or γ itself. Likewise, condition (17) for σ only guarantees the positivity of the entropy production, but does *not* make $\dot{S}$ independent of time. Hence all parameters in the equation of motion (13) for γ, as well as the entropy production and the entropy itself, are time dependent through their dependence on γ. Furthermore, note that $\mathrm{Re}\,\zeta$ and ξ are really functionals of ρ and H only, and therefore are invariant under transformations of the form

$$\gamma \to \gamma U, \quad UU^\dagger = U^\dagger U = I, \tag{19}$$

which leave the density matrix unchanged:

$$\rho \to \rho = \gamma U U^\dagger \gamma^\dagger = \gamma\gamma^\dagger. \tag{20}$$

Equation (13) will be invariant in its entirety under transformation (20) provided σ and $\mathrm{Im}\,\zeta$ are likewise invariant as functionals of ρ and H . In this case the entropy production Eq. (15) will also be invariant under transformation (20), as should be expected on physical grounds.

Now let us introduce the equivalent equation of motion for the density matrix, starting from

$$\dot{\rho} = \dot{\gamma}\gamma^\dagger + \gamma\dot{\gamma}^\dagger. \tag{21}$$

It follows at once that

$$\begin{aligned} \dot{\rho} = &-\sigma[\rho \ln \rho + \mathrm{Re}\,\zeta\{H - E, \rho\} - \rho \mathrm{Tr}(\rho \ln \rho)] \\ &+ i\sigma(\mathrm{Im}\,\zeta)[\rho, H], \end{aligned} \tag{22}$$

where $\{,\}$ denotes the anticommutator, as usual. The commutator on the right-hand side of Eq. (22) obviously provides the unitary Hamiltonian limit, and the standard Liouville equation suggests

$$\sigma(\mathrm{Im}\,\zeta) = \frac{1}{\hbar}. \tag{23}$$

Setting now, for simplicity, $\mathrm{Re}\,\zeta \to \zeta$, the final form of our equation of motion for the density matrix is found to be, in common notation,

$$\dot{\rho} = -\sigma\left[\rho\ln\rho + \zeta(\rho,H-E)\{H-E,\rho\} - \rho\frac{\mathrm{Tr}(\rho\ln\rho)}{\mathrm{Tr}(\rho)}\right] + \frac{i}{\hbar}[\rho,H], \tag{24}$$

where

$$\zeta(\rho,H-E) = -\frac{1}{2}\frac{\mathrm{Tr}[(H-E)\rho\ln\rho]}{\mathrm{Tr}[(H-E)^2\rho]},$$

$$\sigma(\rho,H-E) \geqslant 0,$$

$$\mathrm{Tr}(\rho) = \mathrm{const} \quad (=1),$$

$$E = \frac{\mathrm{Tr}(H\rho)}{\mathrm{Tr}(\rho)} = \mathrm{const},$$

$$\dot{S} = -k_B\frac{d}{dt}\mathrm{Tr}(\rho\ln\rho) \geqslant 0.$$

The scale setting parameter σ remains unspecified so far, and will be regarded in the following as a functional of ρ and H. In order to secure that Eq. (24) is invariant under a scaling $\rho\rightarrow a\rho$, it must be assumed that $\sigma(a\rho,H)=\sigma(\rho,H)$, in which case scaling invariance is verified straightforwardly. Moreover, since Eq. (24) should not show a dependence on the zero point of the energy, it may also be assumed, as above, that $\sigma=\sigma(\rho,H-E)$. For simplicity, it will be understood throughout the following that $\mathrm{Tr}(\rho)=1$.

It is interesting to note that Eq. (24) can be recovered from a modified form of the nonlinear ansatz proposed in Ref. [5],

$$\dot{\rho} = \frac{i}{\hbar}[\rho,H] - \frac{a}{T}\left[f(\rho) - \rho\frac{\mathrm{Tr}(f(\rho))}{\mathrm{Tr}(\rho)}\right],$$

with the obvious substitutions

$$\frac{a}{T}\rightarrow\sigma, \qquad f(\rho)\rightarrow\rho\ln\rho + \zeta\{H,\rho\}.$$

III. FUNDAMENTAL PROPERTIES OF THE NONLINEAR EVOLUTION

Equation (24) secures the Hermiticity and positivity of the density matrix by construction, since it has been generated from an equation for the state operator γ. Conversely, Eq. (24) can be easily decomposed into the corresponding equations for γ and $\gamma^\dagger$ by using the substitution $\rho=\gamma\gamma^\dagger$; hence the equations of motion for ρ and γ are indeed equivalent.

Assuming again a well-behaved σ, Eq. (24) is seen to be covariant under time-independent unitary transformations,

$$\rho\rightarrow\tilde{\rho}=U^\dagger\rho U, \qquad H\rightarrow\tilde{H}=U^\dagger H U,$$

and, in particular, invariant under the (time-independent) symmetry group of the Hamiltonian, $[U,H]=0$. But an observable O which commutes with H, $[H,O]=0$, is not, in general, an integral of motion. More details on the problem follow in Sec. IV.

It is convenient to absorb the Hamiltonian commutator term by setting, in analogy to the usual Heisenberg representation,

$$\rho(t) = \exp\left[-\frac{i}{\hbar}Ht\right]\overline{\rho(t)}\exp\left[\frac{i}{\hbar}Ht\right]. \tag{25}$$

Upon substituting expression (25), Eq. (24) becomes

$$\dot{\overline{\rho}} = -\sigma[\overline{\rho}\ln\overline{\rho} + \zeta\{H-E,\overline{\rho}\} - \overline{\rho}\mathrm{Tr}(\overline{\rho}\ln\overline{\rho})]. \tag{26}$$

Now note that for $\overline{\rho}$ corresponding to a pure state, $\overline{\rho}=\overline{\rho}^2=|\Psi\rangle\langle\Psi|$, the entropy operator vanishes together with the coefficient ζ, i.e., $\overline{\rho}\ln\overline{\rho}\rightarrow 0,\zeta(H-E)\rightarrow 0$, such that $\dot{\overline{\rho}}(t)=0$ and $\overline{\rho}(t)=\overline{\rho}(0)=|\Psi\rangle\langle\Psi|$, if σ is also finite in this limit. From Eq. (25) it then follows that a pure state evolves into a pure state according to the usual Hamiltonian law:

$$\rho(t)=\rho^2(t)=\exp\left[-\frac{i}{\hbar}Ht\right]|\Psi\rangle\langle\Psi|\exp\left[\frac{i}{\hbar}Ht\right]. \tag{27}$$

Another situation where the nonlinear evolution reduces to the Hamiltonian law is found for uniform (equiprobable) distributions ρ_{unif}, when the eigenvalues of the density matrix are all identical. In this case one has the identity $\overline{\rho}_{unif}\ln\overline{\rho}_{unif}=\overline{\rho}_{unif}\mathrm{Tr}(\overline{\rho}_{unif}\ln\overline{\rho}_{unif})$ and $\zeta(\rho_{unif},H-E)\rightarrow 0$, from which $\dot{\overline{\rho}}_{unif}(t)=0,\overline{\rho}_{unif}(t)=\rho_{unif}(0)$, and

$$\rho_{unif}(t)=\exp\left[-\frac{i}{\hbar}Ht\right]\rho_{unif}(0)\exp\left[\frac{i}{\hbar}Ht\right]. \tag{28}$$

Recall that under unitary propagation the cardinality of the set of nonzero eigenvalues of the density matrix is preserved in time. The same holds true if the density matrix evolves according to Eq. (24). In order to see this, let $P_\nu=|\phi_\nu\rangle\langle\phi_\nu|$ be the projector on some eigenstate of $\overline{\rho}(t),\overline{\rho}\cdot P_\nu=\rho_\nu P_\nu$, where $\rho_\nu=\mathrm{Tr}(P_\nu\overline{\rho})$ denotes the corresponding eigenvalue. Since $\mathrm{Tr}(\dot{\overline{\rho}}\cdot P_\nu)=\dot{\rho}_\nu$, multiplying Eq. (26) by P_ν and taking the trace yields

$$\dot{\rho}_\nu = -\sigma[\rho_\nu\ln\rho_\nu + \alpha_\nu(\overline{\rho},H)\rho_\nu], \tag{29a}$$

$$\alpha_\nu(\overline{\rho},H) = 2\zeta(\overline{\rho},H)\mathrm{Tr}[P_\nu(t)(H-E)] + \frac{S(t)}{k_B}. \tag{29b}$$

Taking $\rho_\nu\ln\rho_\nu\rightarrow 0$ for $\rho_\nu=0$ gives $\dot{\rho}_\nu=0$ and $\rho_\nu(t)=0$, i.e., a zero eigenvalue evolves into a zero eigenvalue.

As an immediate corollary, density matrices with a finite number of ''occupied'' state vectors (i.e., a finite number of nonzero eigenvalues) are necessarily driven toward a stationary state with a thermal-like distribution on a finite set of energy eigenstates. Indeed, in this case the entropy, as a functional of the eigenvalues ρ_ν and under the constraint of conserved energy and probability, has a finite absolute maximum. For this reason, and because $\dot{S}(t)\geqslant 0$ at all times, it can only evolve toward a stationary value less than or equal to that maximum. But, as will be shown, $\dot{S}(t)=0$ implies in fact $\dot{\overline{\rho}}=0$ and $[\overline{\rho},H]=0$, and the stationary version of Eq. (29) gives then the thermal-like distribution. Let us now prove that $\dot{S}(t)=0$ implies stationarity. We begin by making a change of variables, $\rho_\nu=e^{-\eta_\nu}$, with $\eta_\nu\geqslant 0$, such as to write

$$\frac{S}{k_B}=\sum_\nu \eta_\nu e^{-\eta_\nu} \tag{30}$$

and

$$\frac{\dot{S}}{k_B}=\sum_\nu (\dot{\eta}_\nu-\eta_\nu\dot{\eta}_\nu)e^{-\eta_\nu}=-\sum_\nu \eta_\nu\dot{\eta}_\nu e^{-\eta_\nu}, \tag{31}$$

since $\Sigma_\nu\dot{\eta}_\nu e^{-\eta_\nu}=\Sigma_\nu\dot{\rho}_\nu=0$. Also, Eqs. (29) give

$$\dot{\eta}_\nu=-\sigma[\eta_\nu-\alpha_\nu], \tag{32}$$

which taken into Eq. (31) produces

$$\begin{aligned}\frac{\dot{S}}{k_B}&=\sigma\sum_\nu [\eta_\nu^2-\alpha_\nu\eta_\nu]e^{-\eta_\nu}\\ &=\sigma\sum_\nu [\alpha_\nu\eta_\nu-\alpha_\nu^2]e^{-\eta_\nu}+\frac{1}{\sigma}\sum_\nu (\dot{\eta}_\nu^2)e^{-\eta_\nu}.\end{aligned} \tag{33}$$

Further, use of the explicit expression for α_ν [Eq. (29)], will show that

$$\begin{aligned}\sum_\nu [\alpha_\nu\eta_\nu-\alpha_\nu^2]e^{-\eta_\nu}={}&\sum_\nu\left[2\zeta\eta_\nu\mathrm{Tr}[P_\nu(H-E)]e^{-\eta_\nu}+\frac{S}{k_B}\eta_\nu e^{-\eta_\nu}\right]\\ &-\sum_\nu\left[4\zeta^2\{\mathrm{Tr}[P_\nu(H-E)]\}^2e^{-\eta_\nu}+4\zeta\frac{S}{k_B}\mathrm{Tr}[P_\nu(H-E)]e^{-\eta_\nu}+\left(\frac{S}{k_B}\right)^2e^{-\eta_\nu}\right]\\ ={}&-2\zeta\,\mathrm{Tr}[(H-E)\rho\ln\rho]+\left(\frac{S}{k_B}\right)^2-4\zeta^2\mathrm{Tr}[(H-E)^2\rho]-4\zeta\frac{S}{k_B}\mathrm{Tr}[(H-E)\rho]-\left(\frac{S}{k_B}\right)^2\\ ={}&0,\end{aligned} \tag{34}$$

where we have used the explicit expression of ζ [Eq. (14a)]. Accounting for Eq. (34) in Eq. (33) shows that

$$\frac{\dot{S}}{k_B}=\frac{1}{\sigma}\sum_\nu \dot{\eta}_\nu^2e^{-\eta_\nu}, \tag{35}$$

from which it follows that $\dot{S}=0$ if and only if $\dot{\eta}_\nu=0$ or, equivalently, $\dot{\rho}_\nu=0$. Now consider that the system is evolving in an asymptotic region where $\dot{S}(t)\rightarrow 0$ for all $t>0$. Since necessarily $\dot{\rho}_\nu\rightarrow 0$, $\dot{\overline{\rho}}$ must be driven by a unitary evolution, $\overline{\rho(t\geqslant t_0)}=U(t)\overline{\rho(t_0)}U^\dagger(t)$. But for $\dot{\rho}_\nu\rightarrow 0$, Eq. (31) gives $\ln\rho_\nu=-\alpha_\nu$, which in turn shows that

$$\begin{aligned}\overline{\rho}\ln\overline{\rho}&=-\sum_\nu \rho_\nu\alpha_\nu P_\nu\\ &=-2\zeta\sum_\nu \rho_\nu P_\nu\mathrm{Tr}[P_\nu(H-E)]-\sum_\nu \rho_\nu P_\nu\frac{S}{k_B}\\ &=-2\zeta\{H_D-E,\overline{\rho}\}-\frac{S}{k_B}\overline{\rho},\end{aligned} \tag{36}$$

where $H_D=\Sigma_\nu P_\nu\mathrm{Tr}(P_\nu H)$ is the diagonal part of H in the eigenbasis of $\overline{\rho}$, $[H_D,\overline{\rho}]=0$. Introducing the above result into Eq. (26), one is led to

$$\dot{\overline{\rho}}=-\sigma\zeta\{H_{ND},\overline{\rho}\}, \tag{37}$$

with $H_{ND}=H-H_D$ the nondiagonal part of H relative to $\overline{\rho}$. But Eq. (37) cannot generate a unitary evolution unless $H_{ND}=0$, which implies that stationary entropy over an extended period of time is equivalent to

$$H_D=H; \tag{38}$$

hence $[\overline{\rho},H]=0$ and $\dot{\overline{\rho}}=0$. In other words, the density matrix of the system [also see Eq. (25)] is stationary, and also diagonal over energy eigenstates. The explicit form of the occupation probability corresponding to an (occupied) energy state of energy E_ν follows from Eqs. (29),

$$\rho_\nu^{eq}=\exp\left[-2\zeta^{eq}(E_\nu-E)-\frac{S^{eq}}{k_B}\right], \tag{39}$$

and can be brought to the recognizable thermal form

$$\rho_\nu^{eq}=\frac{1}{Z}e^{-\beta E_\nu}, \tag{40}$$

with $\beta=2\zeta^{eq}$ and $Z=-\beta E+(S^{eq}/k_B)$. Surprisingly, the parameter ζ is seen to become at equilibrium, up to a factor of 2, the reciprocal temperature $\beta=1/k_BT$. It should be noted, nevertheless, that according to our initial assumptions Eq. (40) applies only to a finite number of energy eigenstates, and therefore does not refer to a canonical equilibrium distribution. More precisely, the sign of ζ^{eq}, and of the generalized temperature T, is not necessarily positive. For instance, let the occupied energy eigenstates be labeled by ν in order of their increasing energy E_ν, and let their total number be N. If the conserved average energy E is such that

$$E \geqslant \frac{1}{N} \sum_{\nu=1}^{N} E_\nu, \tag{41}$$

a simple calculation will verify that the entropy will have an (absolute) maximum, corresponding to the equilibrium state, on a distribution characterized by a negative ζ^{eq}, and hence a ''negative temperature.''

At this point, let us examine more closely the restrictive assumption of a finite number of nonvanishing eigenvalues for the density matrix. It can be noted that this entered the argument developed above solely by way of the related assumption of a finite absolute maximum for the entropy, at the given value E for the average energy. However, there is good reason to assume that such an absolute maximum exists, at least for a large class of distributions over infinite sets of (orthogonal) state vectors. If we can extend this ''finite absolute maximum'' conjecture to all distributions with a finite average energy, it becomes possible to generalize the results in Eqs. (38)–(40) and state that the nonlinear dynamics described by Eqs. (24) and (26) drives the system toward an equilibrium state on energy eigenstates, with thermal-like occupation probabilities. Of course, when the range of occupied energy eigenvalues extends to infinity, relation (41) can no longer be satisfied for any finite E, and the corresponding temperature can only be positive.

Finally, we wish to clarify the consistency of the present nonlinear dynamics, which follows a path of *maximal* entropy production, with Prigogine's celebrated principle of *minimum* entropy production. Let us recall that, according to the latter, physical systems evolve toward stationary states which have minimum entropy production compared to slightly displaced neighboring states. Given that the entropy is a convex functional on the state (configuration) space, bounded from above for any finite average energy, this implies that the physical evolution will take the system toward a local maximum of the entropy or at least toward a ridge. Indeed, in a small enough vicinity of a maximum of the entropy, or of a ridge, *any* evolution with positive entropy production will eventually enter a regime where $\dot{S}$ decreases in time until it vanishes in the equilibrium state or is minimized for the stationary states corresponding to a ridge. The variational principle [Eq. (12)] only complements this picture by stating that the evolution should follow the *shortest route* to a state of maximum entropy, i.e., the *direction* of the physical path is selected from among all directions satisfying $\dot{S} \geqslant 0$ by the requirement that the increase in entropy be maximized at each point in time. In this case it can be said that the entropy production evolves toward a minimum of the maximum, to be attained on a local maximum or a ridge of the entropy (hyper)surface in state space.

IV. LINEAR NEAR-EQUILIBRIUM LIMIT

It is natural to anticipate a linear limit for any nonlinear dynamics evolving sufficiently close to a canonical thermal equilibrium state, at least in the high-temperature limit. For the modified equation of motion proposed here, the linearization process essentially entails the approximation of the entropy operator $-\bar{\rho}\ln\bar{\rho}$ to first order in $\Delta(\bar{\rho}-\rho^{eq})$ around the target equilibrium state

$$\rho^{eq} = \frac{1}{Z} e^{-\beta H}, \quad \ln Z = -\beta E + \frac{S^{eq}}{k_B}, \tag{42}$$

with a given average energy E and reciprocal temperature β. We proceed from the exact expansion

$$-\ln\bar{\rho} = \sum_{n=1}^{\infty} \frac{1}{n} (I-\bar{\rho})^n, \tag{43}$$

which gives for $\bar{\rho} = \rho^{eq} + \Delta\bar{\rho}$, in symmetrized form,

$$\begin{aligned} &-(\rho^{eq}+\Delta\bar{\rho})\ln(\rho^{eq}+\Delta\bar{\rho}) \\ &\quad = \frac{1}{2}\left\{ (\rho^{eq}+\Delta\bar{\rho}), \quad \sum_{n=1}^{\infty} \frac{1}{n} (I-\rho^{eq}-\Delta\bar{\rho})^n \right\}. \end{aligned} \tag{44}$$

Separation of the zero- and first-order terms in $\Delta\bar{\rho}$ yields

$$\begin{aligned} -(\rho^{eq}+\Delta\bar{\rho})\ln(\rho^{eq}+\Delta\bar{\rho}) &= -\rho^{eq}\ln\rho^{eq} - \tfrac{1}{2}\{\Delta\bar{\rho}, \ln\rho^{eq}\} \\ &\quad + \tfrac{1}{2}\{\rho^{eq}, \Lambda(\Delta\bar{\rho})\}, \end{aligned} \tag{45}$$

where $\Lambda(\Delta\bar{\rho})$ represents the collection of all terms first order in $\Delta\bar{\rho}$ from the infinite sum on the right hand side of Eq. (44). In order to calculate $\Lambda(\Delta\bar{\rho})$, it is convenient to define the superoperator $\mathbf{R}$ and its tilde conjugate $\tilde{\mathbf{R}}$ by

$$\mathbf{R}\Delta\bar{\rho} = (I-\rho^{eq})\Delta\bar{\rho}, \tag{46a}$$

$$\tilde{\mathbf{R}}\Delta\bar{\rho} = \Delta\bar{\rho}(I-\rho^{eq}), \tag{46b}$$

$$[\mathbf{R}, \tilde{\mathbf{R}}] = 0.$$

The expression of $\Lambda(\Delta\bar{\rho})$ can now be obtained in the compact form

$$\Lambda(\Delta\bar{\rho}) = -\sum_{n=1}^{\infty} \frac{1}{n} \sum_{m=0}^{n-1} \mathbf{R}^m \tilde{\mathbf{R}}^{n-m-1} \Delta\bar{\rho}. \tag{47}$$

But $\mathbf{R}$ has a well-defined inverse, and the superoperator sum in the above expression can be rewritten as

$$-\sum_{n=1}^{\infty}\frac{\tilde{\mathbf{R}}^{n-1}}{n}\sum_{m=0}^{n-1}(\mathbf{R}\tilde{\mathbf{R}}^{-1})^{m}$$
$$=(\mathbf{I}-\mathbf{R}\tilde{\mathbf{R}}^{-1})^{-1}\sum_{n=1}^{\infty}\frac{\tilde{\mathbf{R}}^{n-1}}{n}(\mathbf{I}-(\mathbf{R}\tilde{\mathbf{R}}^{-1})^{n})$$
$$=(\tilde{\mathbf{R}}-\mathbf{R})^{-1}\sum_{n=1}^{\infty}\left(\frac{\tilde{\mathbf{R}}^{n}}{n}-\frac{\mathbf{R}^{n}}{n}\right)$$
$$=(\tilde{\mathbf{R}}-\mathbf{R})^{-1}[\ln(\mathbf{I}-\mathbf{R})-\ln(\mathbf{I}-\tilde{\mathbf{R}})]. \tag{48}$$

Also taking into account that

$$\rho^{eq}\cdot\Delta\overline{\rho}=(\mathbf{I}-\mathbf{R})\Delta\overline{\rho},\quad \Delta\overline{\rho}\cdot\rho^{eq}=(\mathbf{I}-\tilde{\mathbf{R}})\Delta\overline{\rho} \tag{49}$$

and

$$\ln(\mathbf{I}-\mathbf{R})=-\beta\mathbf{H}-(\ln \mathrm{Z})\mathbf{I},\quad \ln(\mathbf{I}-\tilde{\mathbf{R}})=-\beta\tilde{\mathbf{H}}-(\ln \mathrm{Z})\mathbf{I}, \tag{50}$$

where

$$\mathbf{H}\Delta\overline{\rho}=H\cdot\Delta\overline{\rho},\quad \tilde{\mathbf{H}}\Delta\overline{\rho}=\Delta\overline{\rho}\cdot H, \tag{51}$$

we are led to

$$\tfrac{1}{2}\{\rho^{eq},\Lambda(\Delta\overline{\rho})\}=-\frac{\beta}{2}(\mathbf{H}-\tilde{\mathbf{H}})\coth\left[\frac{\beta}{2}(\mathbf{H}-\tilde{\mathbf{H}})\right]\Delta\overline{\rho}. \tag{52}$$

Returning to Eq. (45), the first-order in $\Delta\overline{\rho}$ approximation to the entropy operator now reads

$$-(\rho^{eq}+\Delta\overline{\rho})\ln(\rho^{eq}+\Delta\overline{\rho})$$
$$=-\rho^{eq}\ln\rho^{eq}-\frac{\beta}{2}\{\Delta\overline{\rho},H-E\}$$
$$-\frac{S^{eq}}{k_B}\Delta\overline{\rho}-\frac{\beta}{2}(\mathbf{H}-\tilde{\mathbf{H}})\coth\left[\frac{\beta}{2}(\mathbf{H}-\tilde{\mathbf{H}})\right]\Delta\overline{\rho}. \tag{53}$$

Note that taking the trace in Eq. (53) gives $S(t)\approx S^{eq}$ in this regime. Similarly, a simple calculation shows that $\zeta\approx\beta/2$. Assuming also that $\sigma\approx\sigma^{eq}=\mathrm{const}(E,\beta)$, and inserting everything into Eq. (26), yields the linearized equation of motion

$$\dot{\overline{\rho}}=-\sigma^{eq}\frac{\beta}{2}(\mathbf{H}-\tilde{\mathbf{H}})\coth\left[\frac{\beta}{2}(\mathbf{H}-\tilde{\mathbf{H}})\right]\Delta\overline{\rho} \tag{54}$$

or

$$\Delta\dot{\overline{\rho}}=-\sigma^{eq}\frac{\beta}{2}(\mathbf{H}-\tilde{\mathbf{H}})\coth\left[\frac{\beta}{2}(\mathbf{H}-\tilde{\mathbf{H}})\right]\Delta\overline{\rho}. \tag{55}$$

The general solution of Eq. (54) is given by

$$\overline{\rho}(t)=e^{-\sigma^{eq}(\beta)t}e^{-\mathbf{G}t}\overline{\rho}(0)+(1-e^{-\sigma^{eq}(\beta)t})\rho^{eq}, \tag{56}$$

where

$$\mathbf{G}=\sigma^{eq}(\beta)\frac{\beta}{2}(\mathbf{H}-\tilde{\mathbf{H}})\coth\left[\frac{\beta}{2}(\mathbf{H}-\tilde{\mathbf{H}})\right]-\mathbf{I}. \tag{57}$$

We observe immediately that $\mathbf{G}$ is tilde symmetric; hence it maps any Hermitian operator into a Hermitian operator, and that it preserves probability, since $\mathrm{Tr}[\mathbf{G}\overline{\rho}]=0$, $\mathrm{Tr}[e^{-\mathbf{G}t}\overline{\rho}(0)]=\mathrm{Tr}[\overline{\rho}(0)]=1$. This is entirely sufficient to secure the Hermiticity of $\overline{\rho}$ and the overall conservation of probability. Unfortunately, the action of $\mathbf{G}$ does not always preserve positivity, and $\mathbf{G}$ cannot be identified as a generator of Lindblad type [12]. But the positive domain of $\mathbf{G}$ does include the small neighborhood of ρ^{eq} identified as the near-equilibrium domain. Indeed, note first that in the diagonal representation of the Hamiltonian, the matrix elements of $\overline{\rho}^{0}(t)=e^{-\mathbf{G}t}\overline{\rho}(0)$ obey the simple damping law

$$\overline{\rho}^{0}_{\mu\nu}(t)=e^{-\gamma_{\mu\nu}(\beta)t}\overline{\rho}_{\mu\nu}(0), \tag{58}$$

where the (temperature-dependent) relaxation coefficient $\gamma_{\mu\nu}$ is given by

$$\gamma_{\mu\nu}(\beta)=\sigma^{eq}(\beta)\left[\frac{\beta}{2}(E_\mu-E_\nu)\coth\left[\frac{\beta}{2}(E_\mu-E_\nu)\right]-1\right], \tag{59}$$

$$\gamma_{\nu\nu}=0,\quad \gamma_{\nu\mu}=\gamma_{\mu\nu}.$$

If we now consider an arbitrary state vector $|\Psi\rangle=\Sigma_{\nu=0}^{\infty}\langle E_\nu|\Psi\rangle|E_\nu\rangle$ and the matrix element

$$\langle\Psi|\overline{\rho}^{0}(t)|\Psi\rangle=\sum_{\nu=0}^{\infty}\langle\Psi|E_\nu\rangle\overline{\rho}_{\nu\nu}(0)\langle E_\nu|\Psi\rangle$$
$$+\sum_{\substack{\mu,\nu=0\\ \mu>\nu}}^{\infty}\mathrm{Re}[\langle\Psi|E_\mu\rangle\overline{\rho}_{\mu\nu}(0)\langle E_\nu|\Psi\rangle]e^{-\gamma_{\mu\nu}t}, \tag{60}$$

it is easily seen that $\overline{\rho}(t)$ remains positive for $t>0$ if the initial off-diagonal matrix elements $\overline{\rho}_{\mu\nu}(0)$ $(\mu\neq\nu)$ are sufficiently small, as expected for the near-equilibrium regime. On the other hand, one can resort to the equation of motion for the state operator γ [Eq. (13)], and derive a linear approximation in $\Delta\gamma=\gamma-\gamma^{eq}$ and $\Delta\gamma^{\dagger}=\gamma^{\dagger}-(\gamma^{eq})^{\dagger}$ by the same procedure as above. The resulting expressions read

$$\Delta\dot{\gamma}=-\left[\left(\sigma\beta+\frac{i}{\hbar}\right)(\mathbf{H}-\tilde{\mathbf{H}})(\tilde{\mathbf{R}}-\mathbf{R})^{-1}\times(\gamma^{eq}\Delta\gamma^{\dagger}+\Delta\gamma(\gamma^{eq})^{\dagger})\right]\gamma^{eq}, \tag{61a}$$

$$\Delta\dot{\gamma}^{\dagger}=-\left(\sigma\beta-\frac{i}{\hbar}\right)(\gamma^{eq})^{\dagger}[(\mathbf{H}-\tilde{\mathbf{H}})(\tilde{\mathbf{R}}-\mathbf{R})^{-1}\times(\gamma^{eq}\Delta\gamma^{\dagger}+\Delta\gamma(\gamma^{eq})^{\dagger})], \tag{61b}$$

and show that, up to first-order terms in $\Delta\gamma$,

$$\rho(t)=\rho^{eq}+\Delta\rho\approx[\gamma^{eq}+\Delta\gamma][(\gamma^{eq})^{\dagger}+\Delta\gamma^{\dagger}], \qquad (62)$$

such that $\Delta\rho=\Delta\gamma(\gamma^{eq})^{\dagger}+\gamma^{eq}\Delta\gamma^{\dagger}$ evolves according to Eq. (55) derived above. Furthermore, the conservation of energy follows from

$$\mathrm{Tr}(H\Delta\overline{\dot{\rho}})=-\sigma^{eq}\mathrm{Tr}(H\Delta\overline{\rho}), \qquad (63)$$

upon recalling that, according to the original equation of motion, the initial state necessarily has the same average energy E as the asymptotic equilibrium state. The initial conditions for Eq. (56) are so restricted to $\mathrm{Tr}(H\Delta\overline{\rho}(0))=0$, which of course implies $\mathrm{Tr}(H\overline{\rho}(0))=E$.

As a general feature of the underlying physics, it follows from Eqs. (56), (58), and (59) that the greater the energy gap between two energy eigenstates, the faster the quantum correlation between them is destroyed as the system evolves towards equilibrium. On the other hand, the relaxation of the occupation probabilities for each of the energy states proceeds at a common rate, independent of the corresponding energy level, since $\overline{\rho}_{\nu\nu}(t)=[e^{-\beta E_{\nu}}/Z](1-e^{-\sigma^{eq}(\beta)t})+e^{-\sigma^{eq}(\beta)t}\overline{\rho}_{\nu\nu}(0)$. As a corollary, the same holds true for the average of any observable O which commutes with the Hamiltonian, $[H,O]=0$, since $\langle O(t)\rangle=\mathrm{Tr}[O\rho(t)]=\mathrm{Tr}[Oe^{-(i/\hbar)Ht}\overline{\rho}(t)e^{(i/\hbar)Ht}]$ [see Eq. (26)] will involve only $\overline{\rho}_{\nu\nu}$'s. The same result can be obtained in a formal manner from a generalized Heisenberg representation for Eq. (54), in which the observables evolve in time according to

$$\dot{O}_{\Delta}(t)=-\left[\sigma^{eq}(\beta)\left(\mathbf{G}\left(\frac{\beta}{2}(\mathbf{H}-\tilde{\mathbf{H}})\right)+\mathbf{I}\right)-\frac{i}{\hbar}(\mathbf{H}-\tilde{\mathbf{H}})\right]O_{\Delta}(t), \qquad (64a)$$

$$O_{\Delta}(t)=\exp\left\{-\left[\sigma^{eq}(\beta)\left(\mathbf{G}\left(\frac{\beta}{2}(\mathbf{H}-\tilde{\mathbf{H}})\right)+\mathbf{I}\right)-\frac{i}{\hbar}(\mathbf{H}-\tilde{\mathbf{H}})\right]t\right\}O_{\Delta}(0). \qquad (64b)$$

Here $(\mathbf{H}-\tilde{\mathbf{H}})O=[H,O]$, and the lower label Δ means that all averages are to be calculated with $\Delta\rho(0)=\rho(0)-\rho^{eq}$. From Eq. (64) above, it is immediate that $[H,O]=(\mathbf{H}-\tilde{\mathbf{H}})O=0$ yields

$$\dot{O}_{\Delta}(t)=-\sigma^{eq}O_{\Delta}(t), \qquad (65a)$$

$$O_{\Delta}(t)=\exp[-\sigma^{eq}t]O_{\Delta}(0), \qquad (65b)$$

in agreement with the observation above. An unexpected outcome of this result is that the average of an observable which commutes with the Hamiltonian is conserved throughout the evolution, provided the initial average value is identical to the equilibrium average. In other words, $\langle O_{\Delta}(0)\rangle=0$ implies $\langle O\rangle(t)=\langle O\rangle^{eq}$. In fact the conservation of energy [Eq. (63)] is seen to be just a particular realization of this feature. Furthermore, for operators satisfying commutation relations of the form $[H,A]=\varepsilon A$, Eqs. (64) lead to

$$\dot{A}_{\Delta}(t)=-\left[\sigma^{eq}(\beta)\left(G\left(\frac{\beta\varepsilon}{2}\right)+1\right)-\frac{i}{\hbar}\varepsilon\right]A_{\Delta}(t), \qquad (66a)$$

$$A_{\Delta}(t)=\exp\left\{-\left[\sigma^{eq}(\beta)\left(G\left(\frac{\beta\varepsilon}{2}\right)+1\right)-\frac{i}{\hbar}\varepsilon\right]t\right\}A_{\Delta}(0), \qquad (66b)$$

where $\mathbf{G}(x)+1=x\coth(x)$.

Equations (65) and (66) allow us to provide a handful of instant examples.

(1) A two-level atom, with the Hamiltonian

$$H=E_1|1\rangle\langle 1|+E_2|2\rangle\langle 2|,$$

and the occupation numbers

$$n_1=\langle 1|\rho|1\rangle,\quad n_2=\langle 2|\rho|2\rangle,\quad n_1+n_2=1,$$

obeys a simple relaxation law which follows from Eq. (65):

$$\dot{n}_1=-\sigma^{eq}(\beta)(n_1-n_1^{eq}(\beta)), \qquad (67a)$$

$$\dot{n}_2=-\sigma^{eq}(\beta)(n_2-n_2^{eq}(\beta)). \qquad (67b)$$

If Eqs. (67) are rearranged into the kinetic form

$$\dot{n}_1=-k_{12}n_1+k_{21}n_2, \qquad (68a)$$

$$\dot{n}_2=k_{12}n_1-k_{21}n_2, \qquad (68b)$$

the corresponding (thermal) transition rates $k_{12}=\sigma^{eq}(\beta)n_2^{eq}(\beta)$ and $k_{21}=\sigma^{eq}(\beta)n_1^{eq}(\beta)$, are seen to have, up to the factor of σ^{eq}, an Arrhenius-like dependence on the temperature.

(2) For a harmonic oscillator of unit mass and frequency ω, described by

$$H=\frac{p^2}{2}+\frac{\omega^2q^2}{2},$$

$$\langle p\rangle_{eq}=0,\quad \langle q\rangle_{eq}=0,$$

one can apply Eq. (66) to the annihilation and creation operators

$$a=\sqrt{\frac{\omega}{2\hbar}}\left(q+i\frac{p}{\omega}\right),\quad a^{\dagger}=\sqrt{\frac{\omega}{2\hbar}}\left(q-i\frac{p}{\omega}\right),$$

to recover a coupled system of equations for the average momentum and the average coordinate,

$$\langle\dot{p}\rangle=-\gamma(\omega,\beta)\langle p\rangle-\omega^2\langle q\rangle, \qquad (69a)$$

$$\langle\dot{q}\rangle=\langle p\rangle-\gamma(\omega,\beta)\langle q\rangle, \qquad (69b)$$

where $\gamma(\omega,\beta)=\sigma^{eq}(\beta)[1+G(\beta\hbar\omega/2)]$. We recognize a typical damped motion, driven by the classical Langevin equation

$$\langle\ddot{q}\rangle+2\gamma(\omega,\beta)\langle\dot{q}\rangle+[\omega^2+\gamma^2(\omega,\beta)]\langle q\rangle=0, \tag{70}$$

which is obtained by elimination of the momentum variables from Eqs. (69).

(3) For the nonrelativistic free-particle Hamiltonian

$$H=\frac{p^2}{2m},$$

Eq. (65) gives the relaxation law

$$\langle\dot{p}\rangle=-\sigma^{eq}[\langle p\rangle-\langle p\rangle^{eq}], \tag{71}$$

which shows a (thermal) friction force linear in momentum. When the initial momentum average coincides with the final thermal average, one obviously obtains conservation of the average momentum. More details can be extracted from the Wigner function

$$f_\Delta(\vec{p},\vec{r},t)=\sum_{\vec{q}} e^{-(i/\hbar)\vec{q}\cdot\vec{r}}\left\langle\vec{p}-\frac{\vec{q}}{2}\right|\rho_\Delta(t)\left|\vec{p}+\frac{\vec{q}}{2}\right\rangle. \tag{72}$$

Differentiation of Eq. (71) on time and use of Eqs. (56), (58), and (59) yields

$$\dot{f}_\Delta(\vec{p},\vec{r},t)=\sum_{\vec{q}} e^{-(i/\hbar)\vec{q}\cdot\vec{r}}\left[-\sigma^{eq}(\beta)\left(G\left(\beta\frac{\vec{p}\cdot\vec{q}}{m}\right)+1\right)+\frac{i}{\hbar}\frac{\vec{p}\cdot\vec{q}}{m}\right]\left\langle\vec{p}-\frac{\vec{q}}{2}\right|\rho_\Delta(t)\left|\vec{p}+\frac{\vec{q}}{2}\right\rangle. \tag{73}$$

But note that

$$\frac{\vec{p}}{m}\cdot\nabla_{\vec{r}}f_\Delta(\vec{p},\vec{r},t)=\sum_{\vec{q}} e^{-(i/\hbar)\vec{q}\cdot\vec{r}}\left(-\frac{i}{\hbar}\frac{\vec{p}\cdot\vec{q}}{m}\right)\times\left\langle\vec{p}-\frac{\vec{q}}{2}\right|\rho_\Delta(t)\left|\vec{p}+\frac{\vec{q}}{2}\right\rangle, \tag{74}$$

and rewrite the right-hand side of Eq. (73) in differential form to obtain

$$\dot{f}_\Delta+\frac{\vec{p}}{m}\cdot\nabla_{\vec{r}}f_\Delta=-\sigma^{eq}(\beta)\left(G\left(i\frac{\hbar\beta}{m}\vec{p}\cdot\nabla_{\vec{r}}\right)+1\right)f_\Delta. \tag{75}$$

The operatorial expression on the right-hand side is to be understood in terms of the power expansion $G(x)+1=x\coth(x)=1+2\Sigma_{n=1}^{\infty}(-1)^{n-1}\zeta_R(2n)(x/\pi)^{2n}$ [13], where $\zeta_R(s)=\Sigma_{k=1}^{\infty}k^{-s}$ is the Riemann zeta function. Hence Eq. (75) reads, in explicit form,

$$\dot{f}_\Delta+\frac{\vec{p}}{m}\cdot\nabla_{\vec{r}}f_\Delta=\sigma^{eq}(\beta)\left[-1+2\sum_{n=1}^{\infty}\zeta_R(2n)\times\left(\frac{\hbar\beta}{\pi m}\vec{p}\cdot\nabla_{\vec{r}}\right)^{2n}\right]f_\Delta \tag{76}$$

and proves to be a Burnett-type (or generalized Fokker-Planck) equation. Note further that the dependence of f_Δ on momentum and coordinate variables can be separated in Eq. (76), and one can integrate over momentum to obtain an exact equation in coordinate space. It can also be safely assumed that the momentum distribution does not deviate significantly from equilibrium, such that one can write $f_\Delta(\vec{p},\vec{r},t)\approx n_\Delta(\vec{r},t)f^{eq}(|\vec{p}|)$, where $n_\Delta(\vec{r},t)=n(\vec{r},t)-n^{eq}(\vec{r},t)$ is the deviation from the equilibrium value of the localization probability, and $f^{eq}(|\vec{p}|)$ is the equilibrium momentum distribution. In this case, in the high-temperature limit, when only contributions to leading order in β survive, integration over momentum leads apparently to a diffusion-like equation,

$$\dot{n}_\Delta=D(\beta)\Delta n_\Delta-\sigma^{eq}(\beta)n_\Delta, \tag{77}$$

with the diffusion coefficient

$$D(\beta)=\sigma^{eq}(\beta)\frac{\hbar^2\beta}{3m}, \tag{78}$$

where it is taken into account that $\zeta_R(2)=\pi^2/6$. But let us recall that $\lambda_T=\sqrt{(\hbar^2\beta)/(3m)}$ is just the de Broglie wavelength corresponding to the root-mean-square momentum $\sqrt{\langle\vec{p}^{\,2}\rangle^{eq}}$, such that in fact $D(\beta)=\sigma^{eq}(\beta)(\lambda_T)^2$. It necessarily follows that the diffusion term in Eq. (77) can give significant contributions only if the localization probability varies substantially on the scale of the thermal de Broglie wavelength λ_T, regardless of the specific value of $\sigma^{eq}(\beta)$. But since states with such variations do not belong to the high-temperature, near-equilibrium regime, we are forced to recognize that Eq. (77) actually reduces to

$$\dot{n}_\Delta=-\sigma^{eq}(\beta)n_\Delta. \tag{79}$$

The linearization procedure developed in this section can be extended without significant modifications to equilibrium states other than the thermal canonical distribution. It can be shown that the relaxation laws for the elements of the density matrix in the diagonal representation of the Hamiltonian are similar to those found here for the canonical case. A detailed account of this issue will be given elsewhere.

V. SYMMETRY INVARIANCE, CONSERVATION LAWS, AND SEPARABILITY

It was pointed out in Sec. III that Eq. (24) is invariant under any time-independent unitary transformations that leave the Hamiltonian unchanged. It is also obviously invariant against time translations, albeit this operation can no longer be associated with a unitary transformation. The same is not true, in this form, of time-dependent transformations relating different observers in relative motion. But at least in the nonrelativistic case, this deficiency can be easily corrected so that invariance under the complete dynamical group of the system is recovered. Indeed, let us rewrite Eq. (24) in the form

$$\dot{\rho} = -\sigma[\rho \ln \rho + \{D(\rho),\rho\} - \rho\,\mathrm{Tr}(\rho \ln \rho)] + \frac{i}{\hbar}[\rho,H], \tag{80}$$

where $D(\rho)$ replaces $\zeta(\rho,H-E)(H-E)$, and let us consider the invariance conditions for Eq. (80) under a time-dependent unitary transformation $U(t)$, $U(t)U^{\dagger}(t) = U^{\dagger}(t)U(t) = I$. As usual, the density matrix becomes $\rho'(t) = U(t)\rho(t)U^{\dagger}(t)$; hence

$$\dot{\rho}'(t) = U(t)\dot{\rho}(t)U^{\dagger}(t) - [\rho'(t),\dot{U}(t)U^{\dagger}(t)], \tag{81}$$

while multiplication of Eq. (80) by $U(t)$ on the left and $U^{\dagger}(t)$ on the right, followed by use of Eq. (81), gives

$$\dot{\rho}' = -\sigma[\rho' \ln \rho' + \{U(t)D(\rho)U^{\dagger}(t),\rho'\} - \rho'\,\mathrm{Tr}(\rho' \ln \rho')] + \frac{i}{\hbar}[\rho', U(t)HU^{\dagger}(t) + i\hbar \dot{U}(t)U^{\dagger}(t)]. \tag{82}$$

It is easily seen that Eq. (82) will regain the form of Eq. (80) provided H is invariant under $U(t)$ in the customary sense,

$$U(t)HU^{\dagger}(t) + i\hbar \dot{U}(t)U^{\dagger}(t) = H, \tag{83}$$

and if, in addition,

$$U(t)D(\rho)U^{\dagger}(t) = D(\rho'), \tag{84a}$$

$$\sigma(\rho,H-E) = \sigma(\rho',H-E'). \tag{84b}$$

In the absence of any evidence to the contrary, the functional σ will be assumed in the following to have all necessary invariance properties.

From Eq. (83) it follows in the customary way that if $U(t)$ spans a Lie group of order n, such that $U(t) = \exp[(i/\hbar)\lambda^j K_j(t)]$, with $\lambda^j, j = 1,2,\ldots,n$, the group parameters and summation over repeated indices being understood, then the corresponding infinitesimal, Hermitian generators $K_j(t), j = 1,2,\ldots,n$ satisfy the familiar commutation relations

$$\frac{i}{\hbar}[K_j(t),H] - \frac{\partial}{\partial t}K_j(t) = 0. \tag{85}$$

Note that a conservation law is not yet implied. But let us assume further that the transformations $U(t)$ are such that

$$\dot{U}(t)U^{\dagger}(t) = \frac{i}{\hbar}(a^j C_j(t) + b), \tag{86a}$$

$$U(t)C_j(t)U^{\dagger}(t) = c_j^l C_l(t) + f_j, \tag{86b}$$

where all parameters a^j, b, c_j^l, and f_j are real functions of the group parameters λ^j and time, and the C_j's are Hermitian operators (observables). In this case, if the conservation of energy is to be invariant under all transformations $U(t)$, it follows from the expression of the transformed average energy

$$\begin{aligned} E' &= \mathrm{Tr}[H\rho'(t)] = E + i\hbar\,\mathrm{Tr}[\dot{U}(t)U^{\dagger}(t)\rho'(t)] \\ &= E - a^j\langle C_j\rangle' - b \end{aligned} \tag{87}$$

that a conservation law is required for each C_j. Unfortunately, Eq. (24) does not account for such supplementary constants of motion, and simple algebra reveals that $D(\rho) = \zeta(\rho,H-E)(H-E)$ does not satisfy the first of Eqs. (84), despite an invariant Hamiltonian, since

$$\begin{aligned} U(t)[\zeta(\rho,H-E)(H-E)]U^{\dagger}(t) &= \zeta(\rho',H-i\hbar\dot{U}(t)U^{\dagger}(t)-E) \\ &\quad \times [H-i\hbar\dot{U}(t)U^{\dagger}(t)-E] \\ &\neq \zeta(\rho',H-E')(H-E'). \end{aligned} \tag{88}$$

Let us examine now whether modifying Eq. (80) to include conservation of the quantities C_j brings about the desired invariance under the transformations of the given Lie group. Let the conservation of each C_j be added to the set of constraints accounted for in the original variational principle, such that Eq. (12) is brought into the form

$$\begin{aligned} \delta\Big[&(\dot{\gamma}|\ln(\gamma\gamma^{\dagger})|\gamma) + (\gamma|\ln(\gamma\gamma^{\dagger})|\dot{\gamma}) + 2\zeta(\dot{\gamma}|\mathbf{H}|\gamma) \\ &+ 2\zeta^{*}(\gamma|\mathbf{H}|\dot{\gamma}) + \xi((\dot{\gamma}|\gamma) + (\gamma|\dot{\gamma})) + 2\eta^j((\dot{\gamma}|\mathbf{C}_j|\gamma) \\ &+ (\gamma|\mathbf{C}_j|\dot{\gamma})) + \frac{2}{\sigma}(\dot{\gamma}|\dot{\gamma})\Big] = 0, \end{aligned} \tag{89}$$

with the new parameters η^j assumed real, since the corresponding terms will not contribute to the Hamiltonian part of the equation of motion. Taking again the variation with respect to $\dot{\gamma}$ and $\dot{\gamma}^{\dagger}$ yields

$$|\dot{\gamma}) = -\sigma\left[\frac{1}{2}[\ln(\gamma\gamma^{\dagger})]|\gamma) + \zeta\mathbf{H}|\gamma) + \eta^j\mathbf{C}_j|\gamma) + \frac{\xi}{2}|\gamma)\right] \tag{90}$$

and the corresponding equation of motion for the density matrix,

$$\begin{aligned} \dot{\rho} = &-\sigma[\rho\ln\rho + \{\zeta(H-E) + \eta^j(C_j - \langle C_j\rangle),\rho\} \\ &- \rho\,\mathrm{Tr}(\rho\ln\rho)] + \frac{i}{\hbar}[\rho,H]. \end{aligned} \tag{91}$$

Here $\langle C_j\rangle = \mathrm{Tr}[C_j\rho]$ is the conserved average of C_j, ζ, and η^j are solutions of

$$\begin{aligned} &\mathrm{Tr}[(H-E)\rho\ln\rho] + 2\zeta\,\mathrm{Tr}[(H-E)^2\rho] \\ &\quad + \eta^j\mathrm{Tr}[\{H-E, C_j - \langle C_j\rangle\}\rho] = 0, \end{aligned} \tag{92a}$$

$$\begin{aligned} &\mathrm{Tr}[(C_j - \langle C_j\rangle)\rho\ln\rho] - (i/\hbar\sigma)\mathrm{Tr}[[C_j - \langle C_j\rangle, H-E]\rho] \\ &\quad + \zeta\,\mathrm{Tr}[\{C_j - \langle C_j\rangle, H-E\}\rho] + \eta^l\mathrm{Tr}[\{C_j - \langle C_j\rangle, C_l \\ &\quad - \langle C_l\rangle\}\rho] = 0, \quad j = 1,2,\ldots,n, \end{aligned} \tag{92b}$$

and we have identified $\sigma(\mathrm{Im}\,\zeta)=(1/\hbar)$, $\mathrm{Re}\,\zeta\rightarrow\zeta$, $\xi=-[\mathrm{Tr}(\rho\ln\rho)+2(\mathrm{Re}\,\zeta)E+2\eta^j\langle C_j\rangle]$. Equations (92) always have solution, as the matrix of coefficients for the unknowns ζ and η^j is recognized to be the positively defined covariance matrix for the Hamiltonian and the operators C_j. If we presume the invariance of the Hamiltonian as defined by Eq. (83), in accordance with the discussion above, it is now straightforward to verify that $\overline{D}=\zeta(H-E)+\eta^j(C_j-\langle C_j\rangle)$ is invariant as well in the sense of Eq. (84a), provided ζ and η^j change as

$$\zeta'=\zeta, \tag{93a}$$

$$\eta'^j=\eta^l c_l^j+\zeta a^j. \tag{93b}$$

In deriving Eqs. (93) use is made of Eqs. (86), and the following transformation of $\langle C_j\rangle$ under the action of $U(t)$:

$$\langle C_j\rangle\equiv\mathrm{Tr}[C_j\rho]=\mathrm{Tr}[U(t)C_jU^\dagger(t)\rho']=c_j^l\langle C_j\rangle'+f_j. \tag{94}$$

The complete invariance of Eq. (91) requires, of course, that ζ' and $\vec{\eta}'$ defined in Eqs. (93) be solutions of the transformed equations (92), obtained upon substituting ρ', E' and $\langle\vec{P}\rangle'$ for ρ, E, and $\langle\vec{P}\rangle$, respectively. But substitution of $\rho(t)=U(t)\rho'(t)U^\dagger(t)$, followed by rearrangement of U and $U^\dagger$ over observables, and use of the relations

$$U(t)HU^\dagger(t)-E=H-E'+a^j(C_j-\langle C_j\rangle'), \tag{95a}$$

$$U(t)C_jU^\dagger(t)-\langle C_j\rangle=c_j^l(C_l-\langle C_l\rangle),\quad j=1,2,\ldots,n, \tag{95b}$$

obtained from Eqs. (83), (86), (87), and (94), leads to

$$\begin{aligned}&\mathrm{Tr}[(H-E')\rho'\ln\rho']+2\zeta\,\mathrm{Tr}[(H-E')^2\rho']\\&\quad+(\eta^l c_l^j+\zeta a^j)\mathrm{Tr}[\{H-E',C_j-\langle C_j\rangle'\}\rho']\\&\quad+(i/\hbar\sigma)a^j\mathrm{Tr}[[C_j-\langle C_j\rangle',H-E']\rho']=0,\end{aligned} \tag{96a}$$

$$\begin{aligned}&\mathrm{Tr}[(C_j-\langle C_j\rangle')\rho'\ln\rho']-(i/\hbar\sigma)\mathrm{Tr}[[C_j-\langle C_j\rangle',\\&\quad\times H-E']\rho']+\zeta\,\mathrm{Tr}[\{C_j-\langle C_j\rangle',H-E'\}\rho']\\&\quad+(\eta^m c_m^l+\zeta a^l)\mathrm{Tr}[\{C_j-\langle C_j\rangle',C_l-\langle C_l\rangle'\}\rho']\\&\quad-(i/\hbar\sigma)a^l\mathrm{Tr}[[C_j-\langle C_j\rangle',C_l-\langle C_l\rangle']\rho']=0,\\&\qquad j=1,2,\ldots,n.\end{aligned} \tag{96b}$$

The first of these equations displays the required invariance only if the last term vanishes identically, which demands

$$[C_j(t),H]=0 \tag{97}$$

for $j=1,2,\ldots,n$, while the second equation is seen to be invariant provided

$$[C_j(t),C_l(t)]=0, \tag{98}$$

for $j=1,2,\ldots,n$, $l=1$, and $2,\ldots,n$. We conclude that Eq. (91) is invariant if and only if Eqs. (83), (97), and (98) are simultaneously verified, in which case the parameters ζ and η^j transform according to Eqs. (93). The generating variational principle, [Eq. (89)], is invariant, of course, under the same conditions.

Let us now substitute for $U(t)$ the special Galilei boost of velocity $\vec{v}_0$,

$$U(t;\vec{v}_0)=\exp\left[\frac{i}{\hbar}(\vec{P}\cdot t-m\cdot\vec{X})\cdot\vec{v}_0\right], \tag{99}$$

where m is the total mass of the system, $\vec{X}$ is the position of the center of mass, and $\vec{P}$ denotes the total momentum. Expression (99) obviously prompts the identifications $C_j=P_j$, $a^j=1$, $b=(m\vec{v}_0)/2$, $c_j^l=\delta_{jl}$, and $f_j=m\vec{v}_0$, which, introduced into Eqs. (97) and (98), lead to the recognizable commutation relations

$$[H,P_j]=[P_j,P_l]=0. \tag{100}$$

Subsequent substitution in Eq. (91) gives the corresponding equation of motion in the form

$$\begin{aligned}\dot{\rho}=&-\sigma[\rho\ln\rho+\{\zeta(H-E)+\eta^j(P_j-\langle P_j\rangle),\rho\}\\&-\rho\,\mathrm{Tr}(\rho\ln\rho)]+\frac{i}{\hbar}[\rho,H].\end{aligned} \tag{101}$$

Remarkably, we recover the celebrated result that the Galilei invariance of the appropriate nonrelativistic equation of motion is equivalent to the corresponding invariance of the Hamiltonian, the conservation of total momentum, and the commutation of the Hamiltonian and the total momentum operators.

Equation (101) reduces to the original Eq. (24) in the center-of-mass referential, where only states corresponding to an eigenstate of zero total momentum for the center-of-mass coordinates need be considered, and the dissipative momentum terms vanish. It also retains the fundamental features previously outlined for Eq. (24). In particular, it can be checked that pure states evolve according to the usual Hamiltonian dynamics, the entropy of mixed states increases, and the nature of the asymptotic equilibrium states is preserved, up to a slight change of form which accounts for the conservation of momentum. It is also evident that Eq. (101) is invariant under time-independent symmetry transformations which leave the Hamiltonian and the dissipator $\overline{D}$ invariant, provided the time-scale parameter σ has the same property. In particular, if the Hamiltonian commutes with the total angular momentum, Eq. (101) is invariant under finite rotations. However, as for the linear momentum, rotational invariance alone does not imply, in general, a conservation law for the angular momentum. The latter can be brought into view by requiring that the equation of motion for the density matrix be covariant with respect to all reference frames where the conservation of energy is a valid physical law. In particular, we should consider translations to observers in uniform rotational motion around an axis at rest in some inertial frame. The rather cumbersome details of adding this supplementary constraint will be left aside, since nothing new will be gained for the formalism.

A more interesting lack of symmetry for Eq. (101), or better, the simpler Eq. (24), lies concealed in the apparent absence of separability. Indeed, let the system described by the Hamiltonian H be composed of two noninteracting subsystems, such that $H=H_1+H_2$ and $[H_1,H_2]=0$, and consider the situation of a separable initial state $\rho(0)=\rho_1(0)\rho_2(0)$, of energy $E=E_1+E_2$. Direct inspection of Eq. (24) shows that the energies of the two subsystems cannot be separately conserved, and a completely separable solution is thus prohibited. But we also observe that lifting the constraint of separate conservation of energy allows a pseudoseparable solution $\rho(t)=\rho_1(t)\rho_2(t)$ given by the coupled system

$$\dot{\rho}_1=-\sigma\left[\rho_1\ln\rho_1+\zeta\left\{H_1-\frac{\mathrm{Tr}(H_1\rho_1)}{\mathrm{Tr}(\rho_1)},\rho_1\right\}-\rho_1\frac{\mathrm{Tr}(\rho_1\ln\rho_1)}{\mathrm{Tr}(\rho_1)}\right]+\frac{i}{\hbar}[\rho_1,H_1], \tag{102a}$$

$$\dot{\rho}_2=-\sigma\left[\rho_2\ln\rho_2+\zeta\left\{H_2-\frac{\mathrm{Tr}(H_2\rho_2)}{\mathrm{Tr}(\rho_2)},\rho_2\right\}-\rho_2\frac{\mathrm{Tr}(\rho_2\ln\rho_2)}{\mathrm{Tr}(\rho_2)}\right]+\frac{i}{\hbar}[\rho_2,H_2]. \tag{102b}$$

In this case probability is independently conserved for each subsystem, since $\mathrm{Tr}(\dot{\rho}_i)=0$, while energy is only conserved globally,

$$\frac{\mathrm{Tr}(H_1\rho_1)}{\mathrm{Tr}(\rho_1)}+\frac{\mathrm{Tr}(H_2\rho_2)}{\mathrm{Tr}(\rho_2)}=E.$$

The coupling between the (noninteracting) subsystems appears to be as instantaneous and nonlocal as usual quantum entanglement, but, unlike the latter, it involves an unorthodox exchange of energy. The significance of this unusual outcome follows from the observation that, according to Eqs. (102), the equilibrium of the compound system is attained for values of σ and ζ common to both subsystems, hence for a common generalized temperature. Imagine now that the initial states for the two subsystems are chosen as individual equilibrium states with different corresponding temperatures. It follows that the dynamics given by Eq. (24) will drive the total system toward a new state of equilibrium, with a temperature common to both components. We cannot but concede the obvious similarity of this unconventional effect with the classical process of equilibration by thermal contact. Its origin lies in the very assumption of a maximal entropy increase on which Eq. (24) was derived. Indeed, even when the entropy of each subsystem is already maximal under individual isolation, if states of larger total entropy are available, probabilities and energy (heat) will be necessarily redistributed so as to enforce a further increase of the overall entropy. Whether this entropic entanglement, or ideal thermal contact, is or not an element of reality appears equivalent to accepting or rejecting the conjecture that an isolated, perfectly ideal gas can undergo relaxation toward equilibrium.

We can provide formal support toward the positive assumption by pointing out that the effect of entropic entanglement does not necessarily interfere with the concept of separable evolution for mutually isolated systems. First let us note that explicitly specifying an adiabatic separation (in the thermodynamic sense) of the noninteracting systems, and hence allowing for separate conservation of energy, removes most of the entropic entanglement. In this case the resulting equation of motion will display distinct ζ's for each of the systems, but a common time-scale parameter, i.e.,

$$\dot{\rho}=-\sigma[\rho\ln\rho+\zeta_1\{H_1-E_1,\rho\}+\zeta_2\{H_2-E_2,\rho\}-\rho\,\mathrm{Tr}(\rho\ln\rho)]+\frac{i}{\hbar}[\rho,H_1+H_2], \tag{103}$$

with

$$E_i=\frac{\mathrm{Tr}(H_i\rho)}{\mathrm{Tr}(\rho)}=\mathrm{const},\quad i=1,\ 2.$$

As before, it proves possible to extract a pseudoseparable solution $\rho(t)=\rho_1(t)\rho_2(t)$, but Eqs. (102) are replaced by

$$\dot{\rho}_1=-\sigma\left[\rho_1\ln\rho_1+\zeta_1\{H_1-E_1,\rho_1\}-\rho_1\frac{\mathrm{Tr}(\rho_1\ln\rho_1)}{\mathrm{Tr}(\rho_1)}\right]+\frac{i}{\hbar}[\rho_1,H_1], \tag{104a}$$

$$\dot{\rho}_2=-\sigma\left[\rho_2\ln\rho_2+\zeta_2\{H_2-E_2,\rho_2\}-\rho_2\frac{\mathrm{Tr}(\rho_2\ln\rho_2)}{\mathrm{Tr}(\rho_2)}\right]+\frac{i}{\hbar}[\rho_2,H_2]. \tag{104b}$$

where this time the ζ_i parameters, $i=1,\ 2$, will be found to depend only on the corresponding ρ_i and H_i, in exactly the manner obtained for a single isolated system. Yet the two evolutions remain tethered by the time-scale parameter σ, thus retaining a weaker form of entropic entanglement. The simple presence of other noninteracting, adiabatically separated systems appears to alter the time scale of dissipative relaxation for any given system. If σ is assumed variable in time, e.g., through a dependence on ρ, this influence will be time dependent unless all other systems have reached equilibrium. But since σ does not affect the nature of the asymptotic equilibrium state, the equilibrium of any one system will not be disturbed by other systems, and will display an individual temperature determined solely by the corresponding energy content.

A careful examination will trace the above type of nonseparability to the fact that the corresponding variational principle selects the direction of maximum entropy increase by referring to the time derivative of the total (entangled) state operator, and not to disentangled, individual state operators separately. However, this pitfall can be avoided if it is recognized that true mutual isolation precludes entanglement on invariance grounds. Indeed, regardless of the nature of the underlying dynamics, the evolution of two mutually isolated systems should remain invariant under *every* transformation pertaining to the individual symmetry groups. In particular, it should be invariant under individual time translations. Since entangled states certainly do not possess this invariance, they do not describe truly isolated systems. In other words, the restricted subspace of the state space that can be spanned by the dynamics of mutually isolated systems should contain only nonentangled states, and the evolution of each of the factor states should be driven independently. In our nonlinear setting, where this subspace is selected by means of the generating variational principle, this restriction has to be correctly built into the variational functional itself. Hence one has to account both for individual conservation laws, excluding thus any energy exchange, as well as for vanishing entanglement. The latter imposes a separable state operator $\gamma(t)=\gamma_1(t)\gamma_2(t)$, and also requires that the entropy production be maximized separately with respect to variations of $\dot{\gamma}_1$ and $\dot{\gamma}_2$, i.e., the σ term in the variational principle should be replaced according to

$$\frac{2}{\sigma}(\dot{\gamma}|\dot{\gamma})\rightarrow\frac{2}{\sigma_1}(\dot{\gamma}_1\gamma_2|\dot{\gamma}_1\gamma_2)+\frac{2}{\sigma_2}(\gamma_1\dot{\gamma}_2|\gamma_1\dot{\gamma}_2),$$

with each σ_i a functional only of γ_i and H_i. But then the variational principle takes the form

$$\delta\{(\gamma_2|\gamma_2)F_1+(\gamma_1|\gamma_1)F_2\}=0, \tag{105a}$$

$$\begin{aligned}F_i={}&(\dot{\gamma}_i|\ln(\gamma_i\gamma_i^{\dagger})|\gamma_i)+(\gamma_i|\ln(\gamma_i\gamma_i^{\dagger})|\dot{\gamma}_i)+2\zeta_i(\dot{\gamma}_i|\mathbf{H}_i|\gamma_i)\\&+2\zeta_i^{*}(\gamma_i|\mathbf{H}_i|\dot{\gamma}_i)+[\overline{\xi_i}(\dot{\gamma}_i|\gamma_i)+\overline{\xi_i^{*}}(\gamma_i|\dot{\gamma}_i)]\\&+\frac{2}{\sigma_i}(\dot{\gamma}_i|\dot{\gamma}_i),\quad i=1,\ 2,\end{aligned} \tag{105b}$$

where

$$\overline{\xi_1}=\xi_1+\left(\xi_2+\zeta_2E_2-\frac{S_2}{k_B(\gamma_2|\gamma_2)}\right),$$

$$\overline{\xi_2}=\xi_2+\left(\xi_1+\zeta_1E_1-\frac{S_1}{k_B(\gamma_1|\gamma_1)}\right).$$

Independent variation of $\dot{\gamma}_1$ and $\dot{\gamma}_2$, followed by extraction of the Lagrange parameters from the corresponding conservation conditions, now leads to the desired separate equations of motion for $\rho_i=\gamma_i\gamma_i^{\dagger}$,

$$\begin{aligned}\dot{\rho}_i={}&-\sigma_i\left[\rho_i\ln\rho_i+\zeta_i\{H_i-E_i,\rho_i\}-\rho_i\frac{\mathrm{Tr}(\rho_i\ln\rho_i)}{\mathrm{Tr}(\rho_i)}\right]\\&+\frac{i}{\hbar}[\rho_i,H_i],\quad i=1,2,\end{aligned} \tag{106}$$

with

$$\sigma_i=\sigma_i(\rho_i,H_i)\geqslant0,\quad \zeta_i=-\frac{1}{2}\frac{\mathrm{Tr}[(H_i-E_i)\rho_i\ln\rho_i]}{\mathrm{Tr}[(H_i-E_i)^2\rho_i]},$$

$$E_i=\frac{\mathrm{Tr}(H_i\rho_i)}{\mathrm{Tr}(\rho_i)}=\mathrm{const.}$$

Obviously, the invariance of the nonlinear dynamics under the symmetry group of each component subsystem is so restored, provided the σ_i's are also invariant.

VI. GENERALIZATION TO ARBITRARY ENTROPY AND ENERGY FUNCTIONAL FORMS

The framework developed in the previous sections can be easily expanded to accommodate nonstandard entropy functionals and/or energy forms with a nonlinear dependence on the density matrix ρ. This generalized formalism can then provide nonlinear extensions for, e.g., the Lie-Poisson dynamics or a standard Hamiltonian evolution supplemented by a nonextensive Tsallis entropy [9], appropriate for systems with fractal properties. Here we sketch only the derivation of the generalized equation of motion, since a detailed analysis exceeds the purpose of the present work.

To this end, let us recall a Lie-Poisson equation of motion of the form

$$\dot{\rho}=-\frac{i}{\hbar}[\rho,\hat{H}(\rho)], \tag{107}$$

where $\hat{H}(\rho)$ is in general a Hermitian, nonlinear functional of ρ. The energy conservation law is now replaced by

$$\mathrm{Tr}[\hat{H}(\rho)\dot{\rho}]=0,$$

or, in terms of the state operator γ,

$$(\dot{\gamma}|\hat{\mathbf{H}}(\rho)|\gamma)+(\gamma|\hat{\mathbf{H}}(\rho)|\dot{\gamma})=0. \tag{108}$$

The law of probability conservation, on the other hand, remains unchanged since $\mathrm{Tr}(\dot{\rho})=0$ or

$$(\dot{\gamma}|\gamma)+(\gamma|\dot{\gamma})=0. \tag{109}$$

Let us search now for a nonlinear evolution that observes the above conservation constraints [Eqs. (108) and (109)], and is also subject to a second principle based on some unspecified, positive definite entropy functional $S/k_B=\mathrm{Tr}[\hat{S}(\rho)]$, such that $\dot{S}=\mathrm{Tr}[(\delta\hat{S}/\delta\rho)\dot{\rho}]\geqslant0$ or

$$\left(\dot{\gamma}\left|\frac{\delta\hat{\mathbf{S}}}{\delta\rho}\right|\gamma\right)+\left(\gamma\left|\frac{\delta\hat{\mathbf{S}}}{\delta\rho}\right|\dot{\gamma}\right)\geqslant0. \tag{110}$$

Here the operator $\hat{S}(\rho)$ is assumed to be Hermitian, and $(\delta\hat{S}/\delta\rho)$ denotes its Hermitian functional derivative with respect to ρ. The corresponding variational principle is now written

$$\begin{aligned}\delta\Bigg\{ &-\left(\dot{\gamma}\left|\frac{\delta\hat{\mathbf{S}}}{\delta\rho}\right|\gamma\right)-\left(\gamma\left|\frac{\delta\hat{\mathbf{S}}}{\delta\rho}\right|\dot{\gamma}\right)+2\zeta(\dot{\gamma}|\hat{\mathbf{H}}(\rho)|\gamma)\\ &+2\zeta^*(\gamma|\hat{\mathbf{H}}(\rho)|\dot{\gamma})+\xi[(\dot{\gamma}|\gamma)+(\gamma|\dot{\gamma})]\\ &+\frac{2}{\sigma}(\dot{\gamma}|\dot{\gamma})\Bigg\}=0,\end{aligned} \tag{111}$$

and can be verified to generate the equation of motion

$$\begin{aligned}\dot{\rho}=-\sigma\left[-\frac{\delta\hat{S}}{\delta\rho}\rho+\zeta\{\hat{H}(\rho)-\langle\hat{H}(\rho)\rangle,\rho\}+\left\langle\frac{\delta\hat{S}}{\delta\rho}\right\rangle\rho\right]\\ +\frac{i}{\hbar}[\rho,\hat{H}(\rho)],\end{aligned} \tag{112}$$

where

$$\langle A\rangle=\frac{\mathrm{Tr}(A\rho)}{\mathrm{Tr}(\rho)}$$

and

$$\zeta=\frac{1}{2}\frac{\langle(\hat{H}(\rho)-\langle\hat{H}(\rho)\rangle)(\delta\hat{S}/\delta\rho)\rangle}{\langle(\hat{H}(\rho)-\langle\hat{H}(\rho)\rangle)^2\rangle},$$

$$\sigma=\sigma(\rho,\hat{H}(\rho)-\langle\hat{H}(\rho)\rangle)\geqslant 0.$$

We note that if $(\delta\hat{S}/\delta\rho)\rho=0$ for pure states, $\rho=\rho^2$, then $\langle\delta\hat{S}/\delta\rho\rangle=0$ and $\zeta=0$, and the pure-state dynamics reduces to that prescribed by Eq. (107).

When the energy functional reduces to the Hamiltonian, $\hat{H}(\rho)=H$, and the entropy is given the standard von Neumann expression, such that $\hat{S}(\rho)=-\rho\ln\rho,(\delta\hat{S}/\delta\rho)\rho=-\rho\ln\rho-\rho$, we recover the basic equation (24). A ρ-dependent $\hat{H}(\rho)$, complemented by the standard entropy, leads to a nonlinear extension of the Lie-Poisson dynamics,

$$\begin{aligned}\dot{\rho}=-\sigma\left[\rho\ln\rho+\zeta\{\hat{H}(\rho)-\langle\hat{H}(\rho)\rangle,\rho\}-\frac{\mathrm{Tr}(\rho\ln\rho)}{\mathrm{Tr}(\rho)}\rho\right]\\ +\frac{i}{\hbar}[\rho,\hat{H}(\rho)],\end{aligned} \tag{113}$$

with

$$\zeta=-\frac{1}{2}\frac{\mathrm{Tr}[(\hat{H}-\langle\hat{H}(\rho)\rangle)\rho\ln\rho]}{\mathrm{Tr}[(\hat{H}(\rho)-\langle\hat{H}(\rho)\rangle)^2\rho]}.$$

If $\hat{H}(\rho)$ is reduced to the standard Hamiltonian H, but the entropy is given a Tsallis form, with

$$\hat{S}(\rho)=-\frac{\rho-\rho^q}{q-1},$$

$$\frac{\delta\hat{S}}{\delta\rho}\rho=\frac{\rho-q\rho^q}{q-1}$$

for given real q, the result will be a nonlinear extension of the von Neumann dynamics under Tsallis q thermostatistics, which reads, after a few elementary manipulations,

$$\dot{\rho}=-\sigma\left[\frac{q}{q-1}\rho^q+\zeta\{H-E,\rho\}-\frac{q}{q-1}\frac{\mathrm{Tr}(\rho^q)}{\mathrm{Tr}(\rho)}\rho\right]+\frac{i}{\hbar}[\rho,H], \tag{114}$$

where

$$\zeta=-\frac{1}{2}\frac{q}{q-1}\frac{\mathrm{Tr}[(H-E)\rho^q]}{\mathrm{Tr}[(H-E)^2\rho]}.$$

Situations where the standard averages have to be replaced by q averages can be approached in the same fashion, by appropriately redefining the conserved functionals.

VII. CONCLUSION

We have constructed and analyzed a nonrelativistic nonlinear extension of the quantum law of evolution, which accounts for the second principle of thermodynamics *and* is not at odds with the factual linearity of pure-state propagation. The theoretical existence of such an extension confirms that the linear and unitary evolution of pure states is not in itself sufficient proof for the general linearity of quantum mechanics [5,6]. One must conclude that the linear propagation of mixed states also has to be corroborated experimentally, to a comparable precision, before a definitive conclusion can be drawn. It is hoped that the formal study developed here provides a meaningful benchmark in this sense.

Our main result is Eq. (24), which defines the modified time evolution of the density matrix. The equation of motion was extracted from a variational principle on the space of state operators, rather than the space of density matrices, as a trajectory of maximal entropy production under the constraint of energy and probability conservation, augmented eventually by the requirement of Galilei invariance [see Eq. (101)]. Should we drop the requirement of entropy increase, the parameters Re ζ and ξ vanish, and the equation of motion reduces automatically to the common Hamiltonian form. The outlined procedure may not be unique, but is encouraging in its consistency. In addition, it also applies to alternate theories which use nonstandard energy or entropy forms. It is notable that the variational principle has sense only in terms of state operators, whereas the equation of motion can be stated simply in terms of the conventional density matrix.

A peculiar and unexpected idea brought forth in our ansatz is that a maximal increase of entropy does not necessarily result in maximal decoherence, to the effect that a pure state of a perfectly isolated system is not allowed to evolve into a mixed state. Conversely, the proposed quantum equivalent of the second principle of thermodynamics is seen to introduce only a limited degree of decoherence, in the sense that the cardinality of the set of nonzero eigenvalues of the density matrix is preserved. As already mentioned, for the particular case of a pure initial state this leads to the usual unitary evolution. The same property also supports, aside from canonical equilibrium states, a rich class of ''negative-temperature'' equilibrium states, which bring to mind the notion of thermal coherence. Furthermore, the ideal thermal contact phenomenon discussed in Sec. V abides by the same rule and, according to Eqs. (102), a system in an initially pure state will remain in a pure state even if it is in contact with, but not necessarily interacting with, other systems. However, in that case the pure state undergoes relaxation according to a dynamics of Gisin type [14], as seen by taking, e.g., $\rho_1 = \rho_1^2, \rho_1 \ln \rho_1 = 0$, in Eq. (102a):

$$\dot{\rho}_1 = -\sigma\zeta\left\{H_1 - \frac{\mathrm{Tr}(H_1\rho_1)}{\mathrm{Tr}(\rho_1)}, \rho_1\right\} + \frac{i}{\hbar}[\rho_1, H_1]. \tag{115}$$

Depending on the sign of ζ, the asymptotic stationary state is an energy eigenstate for the lowest (if $\zeta > 0$) or highest (if $\zeta < 0$) energy level contributing to the initial state $\rho_1(0)$. As detailed in Sec. V, the state of thermal contact is not to be mistaken for a state of mutual isolation, despite the absence of explicit interactions.

We find it promising that bending quantum dynamics to account for classical phenomenological irreversibility suggests a rather unified picture of both reversibility and irreversibility, as well as coherence and decoherence, while preserving such fundamental features as symmetry invariance. However, the self-consistency of the theory is limited at this point by the need for an explicit expression for the entropy production, which means that the equation of motion remains determined up to the scale setting functional σ. We leave the resolution of this problem for future consideration, although a definite expression for σ certainly conditions the consistency of our results. For instance, Eq. (62) for the near-equilibrium damping constants of the density-matrix elements between energy eigenstates shows an acceptable dependence on the energy gap between the states, but the wrong temperature dependence ($\gamma_{\mu\nu} \to 0$ as $\beta \to 0$ and $\gamma_{\mu\nu} \to \infty$ as $\beta \to \infty$) if σ is assumed to be temperature independent. At least, this observation serves to hint that σ should behave like $\beta^{-(2+\delta)}, \delta > 0$, in the vicinity of canonical equilibrium, which in turn can be used, of course, as a theoretical benchmark.

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