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Action principle for nonequilibrium statistical dynamics based on the Lindblad density matrix evolution

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Abstract

A time-dependent variational principle is constructed which gives the Liouville–von Neumann–Lindblad equation governing the time evolution between pure and mixed states. This construction, besides providing an efficient approximation scheme, leads to an underlying physical principle of stationary "effective action" for nonequilibrium statistical dynamics. Implications of these to nonisoentropic processes are briefly discussed by examining the Gaussian ansatz. The results are contrasted with those for the Markovian model of dissipation. © 1997 Published by Elsevier Science B.V.

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Over the past few years a variety of considerations ranging from nonequilibrium statistical mechanics to quantum field theory, has led to suggestions for generalizing the conventional density matrix formalism of quantum theory. The fundamental reason underlying all of these is the desire to incorporate into the theory the feature of moving from pure to mixed quantum states, which is not contained in the traditional Liouville–von Neumann (referred to henceforth as LvN) framework of unitary quantum time evolution. Most recently Reznik [1] has reviewed some of these considerations and has proposed an alternate unitary evolution between pure and mixed states based on a wave operator, which is related to the usual density matrix. Both of these reformulations may be considered as versions of the Liouville–von Neumann–Lindblad (hereafter referred to as LvNL) form of the equation for the time evolution of the density matrix. The reader may supplement the review of the literature in Ref. [1] with additional references [2–4] to other approaches to this question. In this paper, we construct a time-dependent variational principle for the LvNL equation for the density matrix, as this exposes succinctly the physical content of a quantum theory for any field. This is done by a suitable modification of the time-dependent variational principle constructed for the LvN equation by Eboli et al. [2] who adopted the work of Balian and Veneroni [5,6] on the variational approach to the average value of an operator defined by taking the trace over the product of the operator and the density matrix. This variational principle implies an underlying physical principle of stationarity of an "effective action" even for dissipative systems. We illustrate our theory by reexamining the Gaussian ansatz in Ref. [2] but now generalized for the nonisoentropic case. We contrast the results obtained with those based on the Markovian model for dissipation.

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It may be worthwhile to point out that Umezawa [7] has summarized his Liouville space quantum field theory for a unified approach to the combined temperature and time-dependent problems that occur in both field theory and statistical mechanics. A variational theory of this Liouville space formalism was constructed only recently [8]. In a separate paper [9], this is used to develop the variational reformulation of the work of Reznik [1], as well as that developed here.

We may add that in the nonrelativistic, nonequilibrium statistical mechanical problems in condensed matter physics and in nanometric device physics [10] these considerations will play important roles, specifically when the systems considered are innately quantum mechanical, when semi-classical considerations do not suffice. The LvNL equation is extensively used in quantum optics (see Ref. [11] for references) and in studies of open nanostructures [11], and in discussions of dissipation in quantum systems [12], where this equation is derived from ordinary quantum mechanics for a subsystem interacting with an environment. From considerations of generators of quantum dynamical semigroups, Lindblad [13], and independently and almost simultaneously, from considerations of completely positive dynamical semigroups of N-level systems, Gorini, Kassakowski, and Sudarshan [14] derived what is now known as the LvNL equation. To the best of our knowledge, a variational approach such as the one derived here is not found in the literature. In this connection we may also mention that the nonequilibrium Green function methods of Keldysh and Schwinger which were based on unitary time evolution of the LvN framework ought to be modified by using the time-dependent density matrix solutions of the equations discussed in this paper. The effective action functionals obtained here will be useful in developing such a nonequilibrium Green function theory.

The LvNL equation for the density matrix, ρ, under the general requirements of linearity, locality in time, and conserving probability (traceclass nature of ρ) was derived by Banks et al. [15] and is written in the form

$$i\hbar\partial_t\rho = [H,\ \rho] - \frac{i}{2}\sum_{n,m} h_{nm}(Q_m Q_n \rho + \rho Q_m Q_n - 2Q_n \rho Q_m). \tag{1}$$

Since ρ is Hermitian, it suffices if Q_n are any Hermitian operators, and h_{nm} is a c-number Hermitian matrix, in Eq. (1). The traceclass property of the ρ operator (taken here with unit trace), then follows by a direct calculation of the trace of both sides of Eq. (1). From the property that ρ be positive, we find that the matrix h_{nm} be positive, by following the method given in Ref. [15]. This allows us to write Eq. (1) in an alternate, but equivalent form often found in the literature [16], because the c-number Hermitian matrix may be expressed in its diagonal form in terms of its eigenvalues, $h^{(\lambda)}$, and associated (complex) eigenvectors, $\{a_{n\lambda}\}$, and the introduction of new operators Q_λ and its Hermitian conjugate, $Q_\lambda^\dagger$, defined by

$$Q_\lambda = (h^{(\lambda)})^{-1/2}\sum_n a_{n\lambda}Q_n, \qquad Q_\lambda^\dagger = (h^{(\lambda)})^{-1/2}\sum_n a_{m\lambda}^* Q_m,$$

$$h_{nm} = \sum_\lambda a_{n\lambda}h^{(\lambda)}a_{m\lambda}^*, \qquad h^{(\lambda)} \text{ are real and positive.} \tag{2}$$

Thus

$$i\hbar\partial_t\rho = [H,\ \rho] - \frac{i}{2}\sum_\lambda \left(Q_\lambda^\dagger Q_\lambda \rho + \rho Q_\lambda^\dagger Q_\lambda - 2Q_\lambda \rho Q_\lambda^\dagger\right). \tag{3}$$

The von Neumann entropy, $S(t) = -\operatorname{tr}\rho(t)\ln\rho(t)$, is in general dependent on time, t. If we require that $dS(t)/dt \geqslant 0$, then we find that we must further restrict the matrix h_{nm} to be real and symmetric, implying that the operators Q_λ be Hermitian. This is proved by a direct calculation and the use of the inequality $(x-y)\log(x/y) \geqslant 0$, for positive x, y. All these are aspects of nonunitary evolution governing the LvNL formalism.

We will now construct a functional of $\rho(t)$ whose stationary property leads to Eq. (1) by adopting the method of Ref. [2]. (We could equally have used Eq. (3).) Consider the functional

$$\mathscr{L}[\rho, \Lambda] = -\int_{t_i}^{t_f} \mathrm{d}t \ \mathrm{tr}\ \rho\left(\frac{\mathrm{d}\Lambda}{\mathrm{d}t} + \frac{\mathrm{i}}{\hbar}[H, \Lambda] - \frac{1}{2\hbar}\sum_{n,m} h_{nm}(Q_m Q_n \Lambda + \Lambda Q_m Q_n - 2Q_m \Lambda Q_n)\right)$$
$$-\mathrm{tr}(\rho\Lambda)|_{t=t_i}. \tag{4}$$

Here Λ is an auxiliary time-dependent kernel and the time integral goes from an initial time t_i to a final time t_f. Λ obeys an equation which is adjoint to that obeyed by ρ, Eq. (1). This is derived by using the cyclic property of the trace and partial integration over time. Note that this adjoint equation is not the Hermitian adjoint of Eq. (1). At this juncture we have not assumed any special properties about the matrix h, except that it is Hermitian and positive, leaving open the sign of $\mathrm{d}S(t)/\mathrm{d}t$. As in Ref. [2], we consider the two variations of this functional, $\delta_\Lambda \mathscr{L}$, $\delta_\rho \mathscr{L}$, leading to

$$\Lambda|_{t=t_f} = \mathcal{I}, \tag{5}$$

implying that the Lagrange multiplier becomes the identity kernel at the final time and hence vanishes there. At initial time t_i, the boundary condition is set on the density matrix, which is at our disposal. We may leave it quite general or specify it by stating that it maximize some Lyapunov function such as von Neumann entropy at the initial time appropriate to some fixed constraints such as the average value of $H|_{t=t_i}$, etc. Requiring $\mathscr{L}$ to be stationary against both variations gives, along with the boundary conditions, the LvNL equation for $\rho(t)$ and a slightly different equation for Λ. Thus, Λ cannot be viewed as a density matrix. Moreover, the boundary condition (5) selects the static solution $\Lambda = \mathcal{I}$ for all time. With this development Λ disappears from the discussion, and we arrive at a variational formulation for the LvNL equation. As in Ref. [2], the condition (5) is needed in setting up the effective action formalism, which we develop next.

Consider now a field Φ such that the following subsidiary conditions are obeyed,

$$\mathrm{tr}\ \rho\tfrac{1}{2}\{\Lambda, \Phi\} = \left\langle \tfrac{1}{2}\{\Lambda, \Phi\}\right\rangle = \phi(r, t) \equiv \phi(x), \tag{6a}$$

$$\mathrm{tr}\ \rho\Lambda = \langle \Lambda \rangle = 1. \tag{6b}$$

We now define that the "effective action $\mathscr{A}(\phi)$" as the stationary value of $\mathscr{L}$ in (4) subject to the above boundary conditions and constraints. To this end, we introduce the Lagrange multipliers $J(x)$ (x denoting the space–time point) and $w(t)$, which ensure the constraints (6a), (6b), respectively,

$$\mathscr{L}' = \mathscr{L} + \int \mathrm{d}x\ J(x)\ \mathrm{tr}\ \rho\tfrac{1}{2}\{\Lambda, \Phi\} - \int \mathrm{d}t\ w(t)\ \mathrm{tr}(\rho\Lambda). \tag{7}$$

Variations with respect to Λ and ρ lead to, respectively, the equations

$$\partial_t \rho + \frac{\mathrm{i}}{\hbar}[H, \rho] + \frac{1}{2\hbar}\sum_{n,m} h_{nm}(Q_m Q_n \rho + \rho Q_m Q_n - 2Q_n \rho Q_m) + \int \mathrm{d}r\ J(x)\tfrac{1}{2}\{\rho, \Phi\} - w(t)\rho = 0, \tag{8}$$

$$\partial_t \Lambda + \frac{\mathrm{i}}{\hbar}[H, \Lambda] - \frac{1}{2\hbar}\sum_{n,m} h_{nm}(Q_m Q_n \Lambda + \Lambda Q_m Q_n - 2Q_m \Lambda Q_n) - \int \mathrm{d}r\ J(x)\tfrac{1}{2}\{\Lambda, \Phi\} + w(t)\Lambda = 0. \tag{9}$$

Eqs. (8), (9) are reminiscent of the time-path ordering – forward and backward – as in Refs. [5,6]. It should also be noted that Eq. (9) is the adjoint equation to Eq. (8), thus the time-path ordering interpretation mentioned above is evident. The $w(t)$ terms in these equations are removed by the substitutions

$$\tilde{\rho} = \rho \exp\left(- \int_{t_i}^{t} \mathrm{d}t' \; w(t') \right), \tag{10a}$$

$$\tilde{\Lambda} = \Lambda \exp\left(- \int_{t}^{t_f} \mathrm{d}t' \; w(t') \right). \tag{10b}$$

$\tilde{\rho}$ and $\tilde{\Lambda}$ then obey respectively Eqs. (8), (9) without the $w(t)$ terms.
We now observe that from (9), taking trace over the equation after multiplying it by ρ and using the defining relations, we obtain the result

$$\int_{t_i}^{t_f} \mathrm{d}t' \; w(t') = \mathscr{A}(\phi) + \int \mathrm{d}x \; J(x)\phi(x) \equiv \mathscr{W}(J),$$

$$\mathscr{A}(\phi) = - \int_{t_i}^{t_f} \mathrm{d}t \; \mathrm{tr} \; \rho \left(\frac{\mathrm{d}\Lambda}{\mathrm{d}t} + \frac{\mathrm{i}}{\hbar}[H, \Lambda] - \frac{1}{2\hbar} \sum_{n,m} h_{nm}(Q_m Q_n \Lambda + \Lambda Q_m Q_n - 2Q_m \Lambda Q_n) \right). \tag{11}$$

From (10a,b) we also have the relation

$$\mathrm{tr} \; \tilde{\rho}\tilde{\Lambda} = \exp\left(- \int_{t_i}^{t_f} \mathrm{d}t' \; w(t') \right) \equiv \mathrm{e}^{-\mathscr{W}(J)}. \tag{12}$$

By recasting the LvNL formalism in terms of the Liouvillean operator L defined below, we may express Eq. (12) in a more familiar form [2],

$$\mathrm{e}^{-\mathscr{W}(J)} = \mathrm{tr}\left[\rho(t_i) \mathrm{T}\left(\exp - \frac{\mathrm{i}}{\hbar} \int_{t_i}^{t_f} \mathrm{d}t' \; L \right) \mathrm{T}\left(\exp - \frac{\mathrm{i}}{\hbar} \int_{t_i}^{t_f} \mathrm{d}t' \int \mathrm{d}r \; \Phi_{\triangleleft}(r, t') J(r, t') \right) \right]. \tag{12'}$$

Here T is the time-ordering symbol, and

$$\Phi_{\triangleleft} = S(t_i, t)^{-1} \Phi S(t_i, t), \qquad S(t_i, t) = \mathrm{T} \exp - \frac{\mathrm{i}}{\hbar} \int_{t_i}^{t} \mathrm{d}t' \; L. \tag{13}$$

Here the operator and L is defined by its action on ρ as in Ref. [13],

$$L\rho \equiv [H, \rho] - \frac{\mathrm{i}}{2} \sum_{m,n} h_{nm}(Q_m Q_n \rho + \rho Q_m Q_n - 2Q_n \rho Q_m). \tag{14}$$

We note that Eq. (11) shares all the properties obtained in Ref. [2] and reduces to those for the LvN theory when L is just due to the Hamiltonian evolution. By a direct calculation, using Eqs. (8), (9), we establish the important Legendre transform properties,

$$\frac{\delta \mathscr{W}[J]}{\delta J(x)} = \phi(x), \qquad \frac{\delta \mathscr{A}[\phi]}{\delta \phi(x)} = -J(x). \tag{15}$$

We can thus interpret Eqs. (11), (12) as providing underlying stationary "effective action" principle for dissipative systems.

The time derivative of the average value of an arbitrary operator, $O(t)$, which may have its own intrinsic time dependence, defined as $\langle O(t)\rangle_t = \mathrm{tr}(O(t)\rho(t))$, is found to be

$$i\hbar\frac{d}{dt}\langle O(t)\rangle_t = \left\langle i\hbar\frac{\partial O(t)}{\partial t} + [O, H] - \frac{i}{2}\sum_{m,n} h_{nm}([O, Q_m]Q_n - Q_m[O, Q_n])\right\rangle_t . \tag{16}$$

This shows that the traditional definition of the "constant of motion" is modified by the appearance of the additional terms in Eq. (16). We will return to a discussion of this later.

As an important example [16], we here consider a special case of the time-dependent harmonic oscillator [2] along with the simplest choice of one Q-operator, in the framework of Eqs. (2), (3). This example provides a nonisoentropic generalization of that discussed in Ref. [2]. Thus, we have

$$H = \tfrac{1}{2}p^2 + \tfrac{1}{2}\omega^2(t)q^2, \qquad Q = \alpha q + \beta p,$$
$$\alpha, \beta \text{ complex}, \qquad \alpha^*\beta = |\alpha||\beta|e^{i\theta}, \qquad \alpha, \beta \text{ are in general time-dependent},$$
$$[q, p] = i\hbar, \text{ and others zero.} \tag{17}$$

The Gaussian ansatz for the density matrix is

$$\langle x_1|\rho(t)|x_2\rangle = N\exp -\frac{1}{4G}\left[(x_1 - q_c)^2 + (x_2 - q_c)^2 - 2\xi(x_1 - q_c)(x_1 - q_c)\right]$$
$$\times\exp i\mathscr{P}\left[(x_1 - q_c)^2 - (x_2 - q_c)^2\right]\exp ip_c(x_1 - x_2)/\hbar,$$
$$N = [(1-\xi)/2\pi G]^{1/2}. \tag{18}$$

As in Ref. [2], all the parameters introduced here are real and depend on time; ξ is the parameter that characterizes the mixed state of the system, $\xi = 0$ representing the pure state. We first note that by using the variational principle as in Ref. [2], gives us the dissipative dynamics of the mean position and momentum q_c, p_c and their dispersions of the oscillator,

$$\langle q(t)\rangle = q_c(t), \qquad \langle p(t)\rangle = p_c(t), \tag{19}$$

$$\Delta_q^2 = \mathrm{tr}(q^2\rho) - q_c^2, \qquad \Delta_p^2 = \mathrm{tr}(p^2\rho) - p_c^2, \qquad \Delta_{(qp)_s} = \mathrm{tr}\left(\frac{qp+pq}{2}\right)\rho - q_c p_c. \tag{20}$$

The details of the calculations are given elsewhere [17].

It is found that q_c, p_c obey homogeneous equations, and so it is reasonable to take them to be zero; in spite of this, we use the above form to keep the discussion general. We may then express the various mean values in Eq. (20) in terms of the parameters of the Gaussian ansatz, Eq. (18),

$$\Delta_q^2 = G/(1-\xi), \qquad \Delta_p^2 = \hbar^2\left(\frac{4\mathscr{P}^2G}{1-\xi} + \frac{1+\xi}{4G}\right), \qquad \Delta_{(qp)_s} = \hbar\frac{2\mathscr{P}G}{1-\xi}, \qquad 0 < \xi < 1. \tag{21}$$

Now consider the Heisenberg uncertainty product

$$\Omega(t) = \Delta_q^2(t)\Delta_p^2(t) - \Delta_{(qp)_s}^2(t) \geq \hbar^2/4, \qquad \text{for all } t. \tag{22}$$

and exhibit its time derivative using Eq. (20),

$$\dot{\Omega}(t) = -8|\alpha||\beta|\sin\theta\Omega(t) - 2\hbar\left(|\alpha|\Delta_q^2 + |\beta|\Delta_p^2 + 2|\alpha||\beta|\cos\theta\Delta_{(qp)_s}\right). \tag{23}$$

This shows that the dissipative terms give rise to a time dependence for this quantity arising from the non-unitary nature of the LvNL time evolution. This should be contrasted with the usual LvN unitary evolution where $\Omega(t)$ is independent of time, being invariant under unitary transformation.

If we invoke the Markov property [16], we have the condition

$$\mathrm{tr}(Q^{\dagger}\rho Q) \geqslant 0,$$

from which we obtain

$$|\alpha|^2\Delta_q^2 + |\beta|^2\Delta_p^2 + 2|\alpha||\beta|\cos\theta\Delta_{(qp)_s} + |\alpha q_c + \beta p_c|^2 \geqslant \hbar|\alpha||\beta|\sin\theta. \tag{24}$$

Combining with Eq. (23) which stands on its own, the Markov inequality may be expressed in the form

$$\dot{\Omega}(t)/2\hbar \leqslant |\alpha q_c + \beta p_c|^2 - \hbar|\alpha||\beta|\sin\theta\left[1 + 4\Omega(t)/\hbar^2\right]. \tag{25}$$

The Heisenberg uncertainty product is now expressed entirely in terms of ξ, the parameter designating the mixed state nature of the system. This should be contrasted with the pure state Gaussian dynamics discussed in Ref. [18]. We now have

$$\Omega(t) = \frac{\hbar^2}{4}\left(\frac{1+\xi(t)}{1-\xi(t)}\right) \geqslant \frac{\hbar^2}{4}. \tag{26}$$

Another feature of Eq. (21) is that the correlation between the position and momentum of the oscillator is related to the parameter $\mathscr{P}$.

It is worth writing the equations for all the parameters in the Gaussian, and compare them with those obtained in Ref. [2]. A straightforward calculation gives the following equations,

$$\dot{G} + \left(\frac{G}{1-\xi}\right)\dot{\xi} = 4\hbar G\mathscr{P} - 4|\alpha||\beta|\sin\theta G - 2\hbar|\beta|^2(1-\xi), \tag{27a}$$

$$\dot{\mathscr{P}} = -2\hbar\mathscr{P}^2 + \hbar\frac{(1-\xi^2)}{8G^2} - \frac{\omega_s^2(t)}{2\hbar} + |\alpha||\beta|\cos\theta\frac{(1-\xi)}{G} + 2\hbar|\beta|^2\frac{(1-\xi)\mathscr{P}}{G} \times \tag{27b}$$

$$\times\frac{\dot{\xi}}{1-\xi} + 4|\alpha||\beta|\sin\theta(1+\xi) + \hbar|\beta|^2\frac{1-\xi^2}{G} + 16|\alpha||\beta|\cos\theta G\mathscr{P} + 16\hbar|\beta|^2 G\mathscr{P}^2 + \frac{4}{\hbar}|\alpha|^2 G = 0. \tag{27c}$$

These equations reduce to those derived in Ref. [2] when we set the dissipative terms α, β to zero. The striking result is Eq. (27c) in contrast to that in Ref. [2], where it was found that the character of the mixture does not change in the unitary time evolution. Thus the LvNL scheme leads to the possibility of the change in the nature of the mixture and even to a pure state in course of time. This is what Jackiw [2] was seeking.

As in Ref. [2], we write $R(t) = G^{1/2}(1-\xi)^{-1/2} = \Delta_q(t)$. It may be worth pointing out that this same parameter was used in Ref. [18] to establish the relation of the position dispersion to the constant of the motion for the time dependent harmonic oscillator first found by Lewis [19] long ago within the unitary evolution theory. After some algebra, one finds that it obeys the following equation,

$$\ddot{R}(t) + 4|\alpha||\beta|\sin\theta\dot{R}(t) + \left(\omega_s^2(t) + 4|\alpha|^2|\beta|^2\sin^2\theta + 2\frac{\mathrm{d}}{\mathrm{d}t}(|\alpha||\beta|\sin\theta)\right)R(t) = \left(\frac{1}{4}\frac{1+\xi}{1-\xi} - \hbar^2|\beta|^4\right)\frac{1}{R^3(t)} + \frac{2\hbar|\beta|}{R(t)}\left(|\alpha|\cos\theta - 2|\alpha||\beta|^2\sin\theta - \left(\frac{\mathrm{d}}{\mathrm{d}t}|\beta|\right) + 2|\beta|\mathscr{P}\right). \tag{28}$$

As in Eq. (19) for the mean position of the oscillator, its dispersion also has the same characteristic dissipation and renormalization of the oscillator frequency; the nonlinear term in the right hand side, besides containing the result obtained in Ref. [2], couples to the correlation term between coordinate and momentum of the oscillator.

Thus this equation is much more complicated now that we have allowed for dissipation in the theory. Also, when there is no dissipation in the pure state case, this result goes over to the Lewis constraint equation [18,19], if we scale R by $1/\sqrt{2}$.

It may be of interest to point out here the differences between the approach used here and the similar work on the quantum Brownian motion [20,21], where the model for dissipation is from the interaction of an open quantum system with environment. In the present work, the arbitrariness in the choice of the operators Q and their associated coefficients have their parallels in the choice of the coupling of the system to the environment (e.g. linear) and its subsequent approximate treatment in obtaining the kernels. Thus we have here a more general framework for exploring a wider class of models for studying dissipation including those discussed in Refs. [20,21]. The environment coupling model is not applicable in systems with long range interactions where we cannot separate out the subsystem, for example, in nanometric systems where the size of the system is smaller than the range of correlations, or as in gravitational systems.

While both of the LvNL and R schemes have a variational underpinning, the R-scheme does not seem to give the exponentially decaying/increasing solutions as was noted in Ref. [1], it remains to be seen what modifications are needed to lead to such solutions.

In conclusion, we have here developed a variational approach to the LvNL equation. Besides providing a method of approximate solutions, this leads us to a stationary "effective action" principle even for dissipative processes. We have discussed briefly an application of this to the Gaussian model and compared it with previous results based on pure state, isoentropic mixed state, and Markovian model.

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