Implications of the intrinsic decoherence in quantum mechanics to nonequilibrium statistical mechanics

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The discrete-time jump model for intrinsic decoherence in quantum mechanics proposed recently by Milburn is here generalized to explicitly time-dependent Hamiltonians. In this model, a time-dependent entropy is obtained and thus it admits of an interpretation that this is a model for an open system. Unlike in the Milburn model, we introduce a minimum uncertainty phase change dictated by the minimum ''time-energy uncertainty product'' to define the shortest time scale in the system. Implications of this model to quantum nanometric devices such as quantum dots or resonant tunneling devices are indicated. [S1050-2947(96)05308-5]

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The temporal behavior of intrinsically quantum systems such as nanometric devices involving quantum dots, quantum wells, etc [1]. will become an important issue as the times of operation, switching times, etc. become increasingly shorter and shorter, so that one may be approaching limitations due to the presence of the intrinsic quantum phases before the phase coherence is destroyed. This destruction of phase coherence may come about either because the physical properties of the device approach a ''macroscopic level'' of operation or due to the interactions with the other components in which this nanometric device is embedded. We call this ''intrinsic decoherence'' in a somewhat more general sense than Milburn [2]. The systems we have in mind are some future ultrafast, ultrasmall nanoelectronic devices based on, for example, quantum dots, quantum wells, etc. which are subjected to time-dependent bias or exposed to laser beams and the like and as such are nonequilibrium quantum statistical mechanical systems. We are thus focusing on the *high resolution in time* in contrast to the low resolution in phase space often associated with the classical limit. This should be contrasted with the recent discussion of the transition from quantum to classical behavior [3] due to decoherence. From such considerations, we are motivated in this paper to generalize the Milburn model to time-dependent Hamiltonians, and thus enlarge its scope.

Our description of the time-dependent phenomena described here is entirely within the nonrelativistic context. A general approach to this problem is in terms of a time-dependent density matrix $\hat{\rho}(t)$ whose trace is unity, $\hat{\rho}(t)^2 \leqslant \hat{\rho}(t)$, implying that the system need not be in a pure state, and obeying a Liouville–von Neumann equation with the dynamics determined by a time-dependent Hamiltonian operator $\hat{H}(t)$:

$$i\hbar \frac{d\hat{\rho}(t)}{dt} = i\hbar \frac{\partial \hat{\rho}(t)}{\partial t} + [\hat{H}(t), \hat{\rho}(t)]_- . \tag{1}$$

The first term on the right-hand side of this equation is due to intrinsic time dependence (arising from the possible time dependence of the occupation probabilities) and the second term represents the usual unitary time evolution of the Schrödinger wave function. The time dependence of the Hamiltonian, for example, may be because of the bias applied to the system. There are two important consequences of this equation.

(a) Time dependence of the von Neumann entropy associated with this density matrix becomes time dependent,

$$S(t) = -\mathrm{tr}\hat{\rho}(t)\ln\hat{\rho}(t), \tag{2}$$

because its time rate of change, using Eq. (1), is now

$$\frac{dS(t)}{dt} = -\mathrm{tr}\left\{ \left(\frac{\partial \hat{\rho}(t)}{\partial t} \right) \ln\hat{\rho}(t) \right\}, \tag{3}$$

which is nonzero because of the presence of the first term in Eq. (1). It is greater than or equal to zero, following from the properties of the density matrix listed above. Thus such time-dependent Hamiltonians describe open systems.

(b) The time rate of change of the average of any physical quantity represented by a Hermitian operator, $\hat{A}(t)$, which may have its own intrinsic time dependence, defined by

$$\langle \hat{A}(t) \rangle_t \equiv \mathrm{tr}\hat{A}(t)\hat{\rho}(t), \tag{4}$$

will acquire an additional contribution due to the intrinsic time dependence of the density matrix:

$$i\hbar \frac{d\langle \hat{A}(t) \rangle_t}{dt} = \left\langle \left\{ i\hbar \frac{\partial \hat{A}(t)}{\partial t} + [\hat{H}(t), \hat{A}(t)]_- \right\} \right\rangle_t + \left\langle \hat{A}(t) i\hbar \frac{\partial \ln\hat{\rho}(t)}{\partial t} \right\rangle_t . \tag{5}$$

The first term on the right-hand side is the usual term while the second term reflects the intrinsic time dependence of the system.

These two new features introduce possibilities for device operations before the decoherence sets in, as well as complications not expected in the conventional density matrix approach.

In the present work we explore the implications of these features for the nonequilibrium systems mentioned earlier in some detail by applying a modified version of the model

proposed recently by Milburn [2] by identifying the cause for the presence of the intrinsic time-dependent term [the first term on the right-hand side of Eq. (1)] as due to the quantum nature of the system, which entails discrete-time phase changes [2]. The original model [2] has already been employed by Kuang, Chen, and Ge and others [4] to study its consequences in quantum optics based on the Jaynes-Cummings model. An alternate approach to decoherence based on diffusion processes [5] will not be addressed in the present paper.

It is not out of place here to mention that there is a vast literature on how to model, understand, and manipulate the intrinsic time dependence of the density matrix in Eq. (1) using semiclassical and stochastic notations (memory, Markov, Langevin, etc.), perturbation theoretic arguments (Pauli master equation), etc. In particular, the most successful among these is the model of Lindblad [6], who considered a subsystem interacting with an environment, and proposed a Markovian approach to describe this time-dependent problem by providing a nonunitary linear operator structure for the first term on the right-hand side of Eq. (1). More recently, Banks, Susskind, and Peskin [7] derived this nonunitary time evolution feature without invoking both the subsystem and the Markovian assumptions, but from general considerations of linearity, locality in time, and the requirement of conservation of probability, all of which are satisfied by the equation derived by Lindblad. In this development, one has, besides the Hamiltonian operator, other Hermitian operators which must be given at the outset. The Lindblad equation has only recently been employed to investigate problems in quantum optics and dynamics of open quantum nanostructure systems [8] and in discussing decoherence and dissipation in quantum systems [9]. The Milburn model is, however, very different from these, it should be stressed. It too has, besides the Hamiltonian operator, an extra parameter associated with the minimum phase change, and the phases obey a Poisson process.

Recent investigations of ideas based on ''decoherence'' to understand intrinsically quantum phenomena leading to ''classical'' behavior in macroscopic systems, which are entirely different from those mentioned above, open a new door to these questions again, particularly when one considers systems lying in the borderline of macroscopic and microscopic sizes. We here modify the model of Milburn [2] by generalizing it to include a time-dependent Hamiltonian that incorporates the basic features of quantum mechanics—phase changes generated by a unitary time-dependent Hamiltonian evolution. This generalization will make the system behave as if it is an open system. Our modification involves the change in the state of the system in a time interval $(t,t+\tau)$ when the system is evolving unitarily under the action of a time-dependent Hamiltonian, and is given by

$$\hat{\rho}(t+\tau)=\hat{U}_t(\tau)\hat{\rho}(t)\hat{U}_t^{\dagger}(\tau),$$
$$\hat{U}_t(\tau)=T\exp\left(-\frac{i}{\hbar}\int_t^{t+\tau}dt'\hat{H}(t')\right), \tag{6}$$

where † stands for Hermitian conjugate and T for positive time ordering. Our corresponding modification of Milburn's postulates essentially consists in the observation that for sufficiently small time scale τ, the probability that the system changes is $p(\tau)$, and that $\hat{U}_t(\tau)$ does not depend on t, being given by

$$\hat{U}_t(\tau)=\exp-\frac{i}{\hbar}\varphi(\tau)\overset{\frown}{H}\equiv\hat{U}(\tau), \tag{7}$$

where

$$\overset{\frown}{H}=\frac{1}{\varphi(\tau)}\int_t^{t+\tau}dt'\hat{H}(t').$$

Here $\varphi(\tau)$ is the phase change induced by the ''average'' Hamiltonian defined in Eq. (7). The change in the state of the system is thus given by

$$\hat{\rho}(t+\tau)=\hat{U}(\tau)\hat{\rho}(t)\hat{U}^{\dagger}(\tau)\equiv\hat{\mathcal{J}}(\tau)\hat{\rho}(t). \tag{8}$$

In standard quantum mechanics with time-independent Hamiltonian, $p(\tau)=1$ and $\varphi(\tau)=\tau$. We follow Milburn [2] and assume that there is a minimum unitary phase change, but unlike Milburn, we here suggest that it is dictated by the *minimum uncertainty product* [10], which in turn sets the minimum time scale. This involves the dispersion of the time-dependent Hamiltonian and thus a quantity arising entirely from quantum principles. The implication of this suggestion is that the time scales in the time-dependent Hamiltonian should not be smaller than τ. This relates to the statement in the introduction concerning the high-resolution time and ultrafast nature of the system we are envisaging in the system. But as discussed in [10], the minimum uncertainty product now depends on the definition of ''time'' and a corresponding definition of dispersion in ''energy'' in the problem. For example, in a resonant tunneling device, the ''time'' may be taken to be the ''dwell time'' of the electron in the quantum well, in which case the associated dispersion in energy that goes with the ''uncertainty principle'' is the dispersion of the Hamiltonian. For other definitions of ''time'' and associated energy, one may refer to [10].

Thus we assume $\lim_{\tau\to 0}\varphi(\tau)=\varphi_0$. With these modifications, dividing the time interval $(0,t)$ into K steps, each of length τ, following the rest of the arguments in [2], we find $\hat{\rho}(t)=\{1+p(\tau)[\mathcal{J}(\tau)-1]\}^{K=t/\tau}\hat{\rho}(0)$, from which we obtain finally the generalized evolution equation based on this ''Poisson model,''

$$i\hbar\frac{d\hat{\rho}(t)}{dt}=i\hbar\gamma\{\hat{\mathcal{U}}_t(\gamma^{-1})\hat{\rho}(t)\hat{\mathcal{U}}_t^{\dagger}(\gamma^{-1})-\hat{\rho}(t)\}, \tag{9}$$

where

$$\hat{\mathcal{U}}_t(\gamma^{-1})=T\exp-\frac{i}{\hbar}\int_t^{t+\gamma^{-1}}dt'\hat{H}(t').$$

Note that in this equation the short time jump feature has been made explicit. It may not be out of place here to mention that there is another approach [11] which incorporates the effects of stochastic fluctuations in the atom-field interactions of the Jaynes-Cummings model.

We may rewrite Eq. (9) in a deceptively simple form,

$$i\hbar\frac{d\hat{\rho}(t)}{dt}=i\hbar\gamma\{\hat{\rho}_{\mathcal{H}}(t;\gamma^{-1})-\hat{\rho}(t)\},\tag{9'}$$

where

$$\hat{\rho}_{\mathcal{H}}(t;\gamma^{-1})=\hat{\mathcal{U}}_t(\gamma^{-1})\hat{\rho}(t)\hat{\mathcal{U}}_t^{\dagger}(\gamma^{-1}).$$

Here the parameter γ^{-1} has the same meaning as in [2], and this equation is equivalent to the assumption that on a sufficiently short time scale the probability the system evolves is $\gamma\tau$. We should point out that this equation has the same form as that obtained by Milburn [2] for the time-independent Hamiltonian, to which it reduces, as it must. This then is the proposed generalized Milburn evolution equation for time-dependent Hamiltonians. In view of the observations (a) and (b) above, we will now employ this equation to be applicable to nonequilibrium time-dependent situations and thus be on par with Eq. (1).

The distinguishability of states differing by unitary transformations that cause the phase changes leading to inferring the time parameter—from which we here identify the first term in Eq. (1)—is thus explicitly found to be

$$\begin{aligned}i\hbar\frac{\partial\hat{\rho}(t)}{\partial t}&=i\hbar\gamma\{\hat{\mathcal{U}}_t(\gamma^{-1})\hat{\rho}(t)\hat{\mathcal{U}}_t^{\dagger}(\gamma^{-1})-\hat{\rho}(t)\}\\&\quad-[\hat{H}(t),\hat{\rho}(t)]_-\\&=i\hbar\gamma\{\hat{\rho}_{\mathcal{H}}(t;\gamma^{-1})-\hat{\rho}(t)\}-[\hat{H}(t),\hat{\rho}(t)]_-.\end{aligned}\tag{10}$$

γ here is a parameter that is a measure of the minimum unitary phase change allowed by quantum mechanics. When this parameter is taken to be infinity, observing first that to leading order in γ^{-1} we have the result

$$\hat{\mathcal{U}}_t(\gamma^{-1})=T\exp-\frac{i}{\hbar}\int_t^{t+\gamma^{-1}}dt'\hat{H}(t')\approx\exp-\frac{i}{\hbar}\gamma^{-1}\hat{H}(t),$$

we recover the usual unitary Schrödinger description for the time-dependent Hamiltonian dynamics. As in [2], the decoherence or the rapid decay of coherence between states that are widely separated in energy compared to Planck's constant is obtained when we compute the first-order correction on the right-hand side of Eq. (10).

Also, we can show that the time rate of change of entropy in this model is now given by

$$\frac{dS(t)}{dt}=\gamma\mathrm{tr}\{(\hat{\rho}(t)-\hat{\rho}_{\mathcal{H}}(t;\gamma^{-1}))\ln\hat{\rho}(t)\}.\tag{11}$$

For short times compared to those determined by γ^{-1}, one obtains a change in entropy on that time scale due to intrinsically quantum phase fluctuations before decoherence occurs, exhibiting the possible transition from a mixed to a pure state and vice versa. Thus in this Poisson model we have a description of an open system different from the ones described earlier, including that of Lindblad, even though to leading order in γ^{-1} this equation takes superficially a similar form [2]. This is also an important aspect of the nonequilibrium phenomena.

In this model, the time rate of change of an operator given in Eq. (5) takes the form

$$\begin{aligned}i\hbar\frac{d\langle\hat{A}(t)\rangle_t}{dt}&=\left\langle\left\{i\hbar\frac{\partial\hat{A}(t)}{\partial t}+[\hat{H}(t),\hat{A}(t)]_-\right\}\right\rangle_t\\&\quad+\gamma\left\langle i\hbar(\hat{A}_{\mathcal{H}}(t;-\gamma^{-1})-\hat{A}(t))\right.\\&\quad\left.-\frac{1}{\gamma}[\hat{H}(t),\hat{A}(t)]_-\right\rangle_t.\end{aligned}\tag{12}$$

Here we have written $\hat{A}_{\mathcal{H}}(t;-\gamma^{-1})\equiv\hat{\mathcal{U}}_t^{\dagger}(\gamma^{-1})\hat{A}(t)\hat{\mathcal{U}}_t(\gamma^{-1})$.

It should be of interest to point out that Lewis [12] introduced a class of exact constants of motion for classical and time-dependent Hamiltonians and showed how they can be used to solve time-dependent problems in terms of these, either exactly or in a more accurate way. In this work we observe that there is an additional contribution to the time dependence through the intrinsic property of the density matrix on time scales of γ^{-1}. This may be interpreted as implying that there is breakdown of a dynamical constant of motion due to nonequilibrium processes in the system, a type of spontaneous symmetry breakdown, arising from the time-dependent ensemble.

The main point of this paper is to draw attention to the implications of the ideas of intrinsic decoherence in quantum mechanics in the discussion of nonequilibrium phenomena, by generalization Milburn's work to time-dependent Hamiltonians. In this process, we also give a different significance to his minimum phase by relating it to the minimum time-energy uncertainty product, as propounded in [10]. We believe that this may be a way to understand the performance of quantum nanometric devices before decoherence effects wash out the innate quantum processes in the system. This seems to indicate that the shortest time scale of quantum operation of such systems may be of the order of the decoherence time. Thus the observable effects of decoherence may be found in the nanometric quantum devices. In this connection we may cite Ref. [1], in which Gammon *et al.* describe their fabrication and spectroscopic analysis of well-separated single GaAs quantum dots and found than they possess unique finite structure splittings in their optical spectra, with energy splittings of the order of a few meV. These structures are precursors to future fast electronic devices. More generally, this effect may be found in determining the time scale of a phase transition where the buildup of ''anomalous'' correlations over a period of time leads to the transition of the normal state towards the new state. As noted above, the decoherence ideas naturally lead to temporal changes in the entropy and ''constant of motion'' of the system under consideration which are thus temporal markers of phase change in the system.

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