Non-Markovian Dynamics Impact on the Foundations of Statistical Mechanics

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(Dated: Oct. 15, 2013)

The foundations of statistical mechanics, namely how equilibrium hypothesis emerges microscopically from quantum theory, is explored through investigating the environment-induced quantum decoherence processes. Based on the recent results on non-Markovian dynamics [Phys. Rev. Lett. 109, 170402 (2012)], we find that decoherence of quantum states manifests unexpected complexities. Indeed, an arbitrary given initial quantum state, under the influence of different reservoirs, can evolve into four different steady states: thermal, thermal-like, quantum memory and oscillating quantum memory states. The first two steady states de facto provided a rigorous proof how the system relaxes to thermal equilibrium with its environment. The latter two steady states, with strong non-Markovian effects, will maintain the initial state information and not reach thermal equilibrium, which is beyond the conventional wisdom of statistical mechanics.

As it is well-known, any realistic quantum system inevitably interacts with its environment. When such interaction is not negligible, the system must be treated as an open system. Understanding the dynamics of open systems is one of the most challenging topics in physics, chemistry, and biology. The dynamical evolution of an open quantum system is determined by the master equation. The master equation plays the same role for open quantum systems as the Newtonian equation for macroscopic objects, the Maxwell equation for electromagnetic fields, and the Schrödinger equation for isolated quantum systems. In 1928, the first master equation was phenomenologically introduced by Pauli [24]. Since then, many progresses were made with various approaches in deriving the master equation for various different open quantum systems [9, 10], in particular, for quantum Brownian motions [25, 27]. However, there is still a lack of satisfactory answers. Indeed, not having a rigorous and solvable master equation remains a primary obstacle to understand the foundations of statistical mechanics.

Recently, we have derived microscopically the exact master equation [16, 29, 30] for noninteracting fermion (boson) systems coupled, via particle-particle exchanges, to various noninteracting fermion (boson) reservoirs, using the coherent state path-integral formulation [28] and the Feynman-Vernon influence functional method [10, 25]. The result is

\[
\dot{\rho}(t) = -i[H^S(t), \rho(t)] + \sum_{ij} \{\gamma_{ij}(t) [2a_i\rho(t)a_j^\dagger - a_j^\dagger a_j \rho(t) - \rho(t)a_i^\dagger a_j] \\
+ \tilde{\gamma}_{ij}(t) [a_i^\dagger \rho(t)a_j + a_j \rho(t)a_i^\dagger - a_j^\dagger a_j \rho(t) - \rho(t)a_j^\dagger a_i^\dagger]}. \tag{1}
\]

Here \(\rho(t)\) is the reduced density matrix describing the state of the system; \(H^S(t)\) is the renormalized system Hamiltonian after the environmental degrees of freedom are completely integrated out; \(a_i^\dagger, (a_i)\) is the particle creation (annihilation) operator; the up (down) sign of \(\pm\) in the third line, and also hereafter, corresponds to the system being bosonic (fermionic). The environment-induced energy dissipation (i.e., relaxation) coefficients \(\gamma_{ij}(t)\) and thermal fluctuations (i.e., noises)
coefficients $\gamma_{ij}(t)$ are determined microscopically and exactly from Keldysh’s nonequilibrium Green functions [29, 31]. These single-particle nonequilibrium Green functions obey Dyson equations that include nonperturbatively all environment-induced non-Markovian memory effects. Thus, the exact master equation showed that single-particle dynamics in an open system is intrinsically irreversible [4], so is the system. The remaining question for the foundations of statistical mechanics could be answered by solving the exact master equation. Solving this, one could monitor the evolution of an open quantum system, and its steady state, thus unambiguously unveiling the microscopic statistical process.

An open system is usually defined as a system consisting of only one or a few relevant dynamical variables in contact with a huge environment [10]. To be specific, here we consider a system with one dynamical variable coupled to a general environment having infinite dynamical variables. The environment is specified by the spectral density $J(\omega)$ and is initially in a thermal equilibrium state $\rho_E(t_0)$ at temperature $T$, with the particle distribution $\Pi(\epsilon, T) = 1/[e^{(\epsilon-\mu)/k_BT} + 1]$. The system initially is in an arbitrary pure quantum state: $|\psi(t_0)\rangle = \sum_{n=0}^{\infty} c_n |n\rangle$ (n only takes 0 and 1 for fermion systems), with density matrix

$$\rho(t_0) = \sum_{m,n} c_m^* c_n |m\rangle \langle n|.$$

Here the diagonal matrix element $|c_n|^2$ represents the probability for the system in the particle-number state $|n\rangle$ so that $\sum_{n} |c_n|^2 = 1$. The off-diagonal matrix element $c_m^* c_n (n \neq m)$ represents the quantum coherence between $|n\rangle$ and $|m\rangle$. The initial state of the total system, $\rho_{\text{tot}}(t_0) = \rho(t_0) \otimes \rho_E(t_0)$, will follow a unitary (reversible) evolution. However, the system and the environment are initially not in equilibrium, and the evolution of the system undergoes a nonequilibrium process, described by the reduced density matrix $\rho(t)$. Solving the master equation with the general initial state $|\psi(0)\rangle$, we find that

$$\rho(t) = \sum_{m,n} c_m^* c_n \sum_{k=0}^{\min(m,n)} d_k A_{mk}^{\ast}(t) \bar{\rho}(t) A_{mk}(t).$$

Here the kernel $\bar{\rho}(t) = \sum_{m'} \frac{|u(t, t_0)|^2}{[1 \pm \sqrt{\varepsilon(t)}]^{n+1}} |n\rangle \langle n'|$, the operator $A_{mk}(t) = \frac{\sqrt{m!}}{\sqrt{(m-k)!}} \frac{u(t, t_0)}{\sqrt{1 \pm \sqrt{\varepsilon(t)}}} a_k^{\ast} a_k^{\prime}$, and the coefficient $d_k = \left[ 1 - \frac{|u(t, t_0)|^2}{1 \pm \sqrt{\varepsilon(t)}} \right]^{k}$. The solution (3) shows that $\rho(t)$ is fully determined by the single-particle dissipative propagating function $u(t, t_0)$ and correlation function $v(t, t')$ with the relation $\langle a_\ell(t) a_\ell' \rangle = u(t, t_0) \Pi(t_0) u^\ast(t, t_0) + v(t, t')$, where $t' \leq t$, and $\Pi(t_0)$ is the initial average particle number in the system. As it has been shown [16, 29, 30], these two Green functions (corresponding to the retarded and correlation Green functions in Keldysh’s formalism [32]) are uniquely determined by the spectral density $J(\omega)$, which coincides with the conclusion reached by Leggett et al. [7] that for any problem in which a thermal equilibrium statistical average is taken over the initial states of the environment and a sum over the final states, complete information about the effect of the environment is encapsulated in the single spectral density.

The spectral density $J(\omega)$ is microscopically defined as a multiplication of the environmental density of states with the system-environment coupling strength. Due to different degrees of non-Markovian memory, different spectral densities can induce vastly different dissipations and fluctuations [4]. Indeed, this gives rise to four decoherence scenarios depicted in Fig. 1(a): A given arbitrary initial quantum state $\rho(t_0)$ of the system can decohere into one of four possible steady states $\rho(t_s)$: thermal state, thermal-like state, qumemory (quantum memory) state, and oscillating qumemory state, here $t_s$ denotes the time scale the system reaching its steady state. The former two provide indeed a rigorous foundation for statistical mechanics. They showed how a system is relaxed into equilibrium with its environment. The latter two go beyond standard statistical mechanics, namely the system would memorize its initial state information and not reach equilibrium. Which scenario will the system ultimately evolve into is determined by the dissipation dynamics. Thermal noise, given by fluctuating correlations, is naturally manifested through the fluctuation-dissipation relation. Below we shall detail these four decoherence scenarios.

The recent investigation [4] show that the general non-Markovian dynamics of open quantum systems consists of...
nonexponential dissipative dampings and dissipationless oscillations. When the non-Markovian memory effects are negligible, non-exponential dampings are reduced to the exponential one. We consider first a system undergoing an exponential damping. Correspondingly, the dissipative propagation function \( u(t_s, t_0) \to 0 \), see Fig. 1(b1). Then the general solution (3) will evolve into a steady state of the form

\[
\rho(t_s) \to \begin{cases} 
\sum_{n=0}^{\infty} \frac{[v(t_s, t_s)]^n}{[1 - v(t_s, t_s)]} |n\rangle \langle n| & \text{for bosons} \\
[1 - v(t_s, t_s)] |0\rangle \langle 0| + v(t_s, t_s) |1\rangle \langle 1| & \text{for fermions}
\end{cases}
\]  

(4)

Here \( v(t_s, t_s) \) is the steady-state value of the single-particle correlation (fluctuation) function, which is found [13,31] in the exponential damping: \( v(t_s, t_s) = \tilde{\pi}(s, T) = 1/[e^{\epsilon_s} - n]) \), where \( \epsilon_s \) is the single particle energy in the system, and \( T \) is the environment temperature. This process usually occurs when system-environment couplings are sufficiently weak (compared with the characteristic energy scale of the system) and/or the spectral density has a rather wide distribution, see Fig. 1(c1). Consequently, particle correlations in the environment have nearly a delta-function profile in the time domain, and the system will lose all memory during its evolution. Ultimately, the initial quantum coherence is washed out and the steady state is independent of the initial state of the system. In other words, the system finally reaches thermal equilibrium with its environment. This is precisely given by the solution (4), which is the standard thermal state. It should be underscored that even if we had not made the assumption of large particle number in the system, this solution already provided the microscopic answer to the foundations of statistical mechanics: the system is eventually thermal equilibrium with its environment if there is no driving field acting on it.

For many real open systems, however, their dynamics do not follow an exponential damping. This is the case when the system-environment couplings become stronger or the reservoir has band structures. The corresponding dissipation dynamics usually manifests a nonexponential decay and sometimes even becomes dissipationless [3]. Therefore, the quantum state may not evolve into the expected thermal state. Specifically, we shall now consider the spectral density to be slightly different from a wide distribution (e.g. Fig. 1(c2)) or it may be very different from a wide distribution (e.g. Fig. 1(c3-c4)) but has a weak system-environment coupling. In these cases, in a short time scale the system retains partial memory on the information exchange with the environment. Consequently, the dissipation process exhibits a short-time oscillation over the exponential damping profile, although ultimately \( u(t_s, t_0) \to 0 \), see Fig. 1(b2). This manifests a weak (non-Markovian) memory effect. The system will reach a steady state with the same form as Eq. (4), but the particle correlation function \( v(t_s, t_s) = \int d\epsilon D(\epsilon) \tilde{\pi}(\epsilon, T) \neq \pi(\epsilon_s, T) \), where \( D(\epsilon) \) is the environment-modified density of states of the system. Since the steady-state particle distribution is different from the simple thermal particle distribution, the corresponding steady state shall be referred to as a thermal-like state. Notice that the memory effect in this scenario exists only in a quite short time, so that the steady-state solution is also independent of the initial state of the system. The quantum coherence at the end is also lost. The thermal equilibrium hypothesis of statistical mechanics remains intact. In other words, as long as the particle propagation in the system is a continuous damping under weak non-Markovian memory, the system and environment will eventually reach thermal equilibrium.

It is especially interesting when the spectral density does not cover the entire frequency regime, as shown in Fig. 1(c3), and also has a strong system-environment coupling. In this case, the strong system-environment coupling could induce a localized state at \( \omega_n \). The dissipation dynamics, shown in Fig. 1(b3), is significantly different from the previous two cases. In particular, the decay process even ceases after some time and the system becomes dissipationless with \( |u(t_s, t_0) \)

approaching a nonzero constant. This is due to strong non-Markovian memory [4]. The quantum state of the system will then evolve into a steady state that bears no resemblance to that of (4). It keeps the same form as the solution (4)

\[
\rho(t_s) = \sum_{m,n} c^*_m c_n \sum_{k=0}^{\min\{m,n\}} d_k A^k_{m,n} \rho(t_s) A_{nk}(t_s). 
\]  

(5)

with \( u(t_s, t_0) \to A \exp\{-i\omega_k(t_s - t_0)\} \), and \( A \) is the particle field amplitude arising from the localized state. The particle correlation function is given by \( v(t_s, t_s) = \int d\epsilon D(\epsilon, t_s) + D(\epsilon, T) \tilde{\pi}(\epsilon, T) \), where \( D(\epsilon, t_s) \) emerges from the localized state. The solution (5) is no longer a thermal or thermal-like state. The off-diagonal matrix elements in the state (5) do not vanish, thus signaling the maintenance of some quantum coherence. Furthermore, the average particle number in (5) is given by \( \tilde{\pi}(t_s) = |u(t_s, t_0)|^2 n(t_0) + v(t_s, t_s) \), which explicitly depends on the initial average particle number \( \tilde{\pi}(t_0) \) in the system. In this scenario, the system has a very long memory and does not reach the thermal equilibrium with its environment. This property remains valid when the system contains a macroscopically large particle number, and therefore is not expected from the conventional wisdom that thermal equilibrium can always be reached with its environment [11,13]. In this case, through non-Markovian memory processes, the system remains in a stationary but nonequilibrium state, which constantly keeps information (coherence) exchange with its environment. We call this state (5) a quantum memory state, or simply a memory state.

When the spectral density has a band structure, as shown in Fig. 1(c4), the system could involve more
than one localized state. These localized states produce dissipationless dynamics for the system with different oscillation frequencies. As a result, the system evolves into a steady state having the same form as \[ |4\rangle \] with vastly different dissipationless dynamics. It combines different localized states with \[ u(t_s, t_0) = \sum_j A_j \exp(-i\omega_j(t_s - t_0)) \], and forms an oscillating qumemory state. As a result, the average particle number, \[ \pi(t_s) = |u(t_s, t_0)|^2 \pi(t_0) + v(t_s, t_0) \], not only depends on its initial value but also oscillates in time. This oscillation is purely quantum in nature and can have interesting features for quantum device systems and also implications for quantum information processing against decoherence. It is noteworthy that the localized states have already incorporated all environmental back-action effects and are decoherence-free. In addition, the steady-state oscillations indicate that the system can maintain quantum coherence in a nonequilibrium manner with its environment. This is also unexpected.

We will now demonstrate how the above four decoherence scenarios can be realized in practice. Since the steady state of an open system depends closely on the spectral density structure, we consider a general environment with the Ohmic-type spectral density: \[ J(\omega) = 2\pi\sigma_\omega(\omega/\omega_c)^s \exp(-\omega/\omega_c) \], which was proposed by Leggett et al.\[7\] to simulate a large class of thermal reservoirs. Here \( \eta \) is a dimensionless system-environment coupling strength and \( \omega_c \) is a cutoff frequency. The spectral density can be classified into three regions: sub-Ohmic \((0 < s < 1)\), Ohmic \((s = 1)\), and super-Ohmic \((s > 1)\). Each region portrays a different environment. The Ohmic-type spectral density takes the structure shown by Fig. 1(c) with \( \omega_c \geq 0 \). In this case, there is a localized state with \( \omega_c < 0 \), when the coupling strength \( \eta \) exceeds the critical boundary \( \eta_c(\omega_c) = \omega_c / [\omega_c \Gamma(s)] \). As shown in Fig. 2, the boundary \( \eta_c(\omega_c) \) distinguishes the dissipation and dissipationless regimes (through the zero and nonzero values of the single-particle propagating field amplitude \( |u(t_s, t_0)| \)). This would indicate how and when a thermal-like state or a qumemory state emerges through varying the spectral density. Note that the thermal state \([4]\), with \( v(t_s, t_0) = \pi(\epsilon_\omega, T) \), corresponds to the limiting case that the height of the spectral distribution \( \eta_{\omega_c}/\omega_c \ll 1 \) and the spectral width \( \omega_c/\omega_S \gg 1 \), where the non-Markovian memory is negligible.

To demonstrate the existence of oscillating qumemory states, a nanocavity subject to a structured reservoir consisting of coupled resonators is considered. By modeling the reservoir as a tight-binding 1D system, its dispersion takes the form \( \omega_k = \omega_c - 2\xi \cos(2k) \). This leads to the finite-band structure of the spectral density \( J(\omega) = \eta^2 \sqrt{4\xi^2 - (\omega - \omega_c)^2} \), with band \( |\omega - \omega_c| \leq 2\xi \), where \( \omega_c \) is the band center of the reservoir, \( \xi \) is the intercavity coupling in the reservoir, and \( \eta \) is a ratio between the cavity-reservoir coupling and intercavity coupling \( \xi \). It is easy to verify that when the coupling strength \( \eta > \eta_c = \sqrt{2 + |\Delta|/\xi} \), where \( \Delta = \omega_S - \omega_c \) is the detuning, there are two localized states \( \omega_{\pm} \) outside of the band \( [30] \). As shown in Fig. 1(c), these two simultaneously occurring modes will cause the dissipation dynamics to oscillate. In particular, in the zero detuning case the steady value of the single-particle propagating function oscillates as a cosine function: \( u(t_s, t_0) = n(\xi^2 - 2) e^{i\omega_S t_s} \cos \left( \frac{\pi\xi}{\sqrt{\eta^2 + 4}} \right) \). This gives rise to an oscillating qumemory state that could be easily discovered, since materials with band structures are common in nano-systems.

The possible observation of the above four decoherence scenarios can be achieved through the decoherence evolution of Schrödinger’s cat-like states. Schrödinger’s cat-like states, which is defined as a superposition of two opposite-moving coherent states \( |\pm c_0\rangle \), have been considered as an archetypical example to demonstrate quantum decoherence \([6, 33]\). Here we examine the dynamics of such a state in a general environment. In Fig. 3 we show the four decoherence scenarios through the time evolution of a cat-like state, in terms of Wigner function. It shows that in the Markov (memory-less) process, the initial cat-like state smoothly loses all its quantum coherence and becomes a thermal state, the corresponding Wigner function becomes a thermal Gaussian distribution located at the origin, see the last graph in Fig. 3(a). For other non-Markovian processes, the cat-like state takes on different decoherence behaviors. For a weak non-Markovian decay given in Fig. 3(b), although the steady state (reached at \( t = 10/\omega_S \)) is thermal-like, decoherence occurs much faster than the thermal state (it takes \( t = 500/\omega_S \) to reach the steady state as shown in Fig. 3(a)). Furthermore, when the strong non-Markovian effect is dominated by the localized mode(s), the Wigner function never becomes a thermal Gaussian distribution. It shows a non-thermal distribution or an oscillating non-
for the development of quantum information processing, but also advance the study of statistical mechanics for open systems when thermal equilibrium is not reachable. Acknowledgments We acknowledge the support from the National Science Council of ROC under Contract No. NSC-102-2112-M-006-016-MY3, and the National Center for Theoretical Science of ROC. 

Author Contributions W. M. Zhang proposed the ideas and methods; H. N. Xiong and P. Y. Lo performed the calculations; H. N. Xiong prepared an initial draft; W. M. Zhang and D. H. Feng interpreted the physics and wrote the manuscript; F. Nori participated in the discussions and contributed to the writing of the manuscript. 

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