Origin of the Canonical Ensemble: Thermalization with Decoherence

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We solve the time-dependent Schrödinger equation for the combination of a spin system interacting with a spin bath environment. In particular, we focus on the time development of the reduced density matrix of the spin system. Under normal circumstances we show that the environment drives the reduced density matrix to a fully decoherent state, and furthermore the diagonal elements of the reduced density matrix approach those expected for the system in the canonical ensemble. We show one exception to the normal case is if the spin system cannot exchange energy with the spin bath. Our demonstration does not rely on time-averaging of observables nor does it assume that the coupling between system and bath is weak. Our findings show that the canonical ensemble is a state that may result from pure quantum dynamics, suggesting that quantum mechanics may be regarded as the foundation of quantum statistical mechanics.

1. Introduction

Statistical mechanics is one of cornerstones of modern physics but its foundations and basic postulates are still under debate.[1–21] There is a common believe that a generic "system" that interacts with a generic environment evolves into a state described by the canonical ensemble. Experience shows that this is true but a detailed understanding of this process, which is crucial for a rigorous justification of statistical physics and thermodynamics, is still lacking. In particular, in this context the meaning of "generic" is not clear. The key question is to what extent the evolution to the equilibrium state depends on the details of the dynamics of the whole system.

Earlier demonstrations that the system can be in the canonical ensemble state are based on showing that time-averages of the expectation dynamical variables of the system approach their values for the subsystem that is the thermal equilibrium state[2–5] or do not consider the dynamics of the system but assume that the state of the whole system has a special property called "canonical typicality"[6–12] in which case it is as yet unclear under which conditions the whole system will evolve to the region in Hilbert space where its subsystems are in the thermal equilibrium state. A very different setting to study nonequilibrium quantum dynamics is to start from an eigenstate of some initial Hamiltonian and push the system out of this state by a sudden change of the model parameters.[13–19] To the best of our knowledge, it has not yet been shown that this approach leads to the establishment of the canonical equilibrium distribution. Finally, we want to draw attention to the fact that a demonstration of relaxation to the canonical distribution requires a system with at least three different eigenenergies because a diagonal density matrix of a two-level system can always be represented as a canonical distribution.[20,21]

The main result of this paper is that we show, without any time-averaging procedure or any approximation, that systems embedded in a closed quantum system generally evolve to their canonical distribution states. This result complies with the fact that if we make a real measurement of a thermodynamic property, we observe its equilibrium value without having to perform time averaging. Furthermore, we show that the relaxation to the canonical distribution is not limited to the regime of weak coupling between system and environment, an assumption that is often used.[1,6–12]

2. General Theory

In general, the state of a closed quantum system is described by a density matrix.[22,23] The canonical ensemble is characterized by a density matrix that is diagonal with respect to the eigenstates of the system Hamiltonian, the diagonal elements taking the form $\exp(-\beta E_i)$ where $\beta = 1/k_B T$ is proportional to the inverse temperature (k_B is Boltzmann's constant) and the E_i's denote the eigenenergies. The time evolution of a closed quantum system is governed by the time-dependent Schrödinger equation (TDSE).[22,23] If the initial density matrix of an isolated quantum system is non-diagonal, then, according to the TDSE, its density matrix remains nondiagonal and never approaches the thermal equilibrium state with the canonical distribution. Therefore, in order to thermalize the system S, it is necessary to have the system S interact with an environment (E), also called heat bath. Thus, the Hamiltonian of the whole system ($S + E$) takes the form $H = H_S + H_E + H_{SE}$, where H_S and H_E are the system and environment Hamiltonian, respectively and H_{SE} describes the interaction between the system and environment.

The state of system S is described by the reduced density matrix

$$\widetilde{\rho}(t) \equiv \mathrm{Tr}_E \, \rho(t), \tag{1}$$

where $\rho(t)$ is the density matrix of the whole system at time t and Tr_E denotes the trace over the degrees of freedom of the environment. The system S is in its thermal equilibrium state if the reduced density matrix takes the form

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J. Phys. Soc. Jpn., Vol. 78, No. 9

S. YUAN *et al.*

$$\widehat{\rho} \equiv \frac{e^{-\beta H_S}}{\text{Tr}_S\, e^{-\beta H_S}}, \tag{2}$$

where Tr_S denotes the trace over the degrees of freedom of the system S. Therefore, in order to demonstrate that the system S, evolving in time according to the TDSE, relaxes to its thermal equilibrium state one has to show that $\widetilde{\rho}(t) \approx \widehat{\rho}$ for $t > t_0$ where t_0 is some finite time.

The difference between the state $\widetilde{\rho}(t)$ and the canonical distribution $\widehat{\rho}$ is most conveniently characterized by the two quantities $\delta(t)$ and $\sigma(t)$ defined by

$$\delta(t) = \sqrt{\sum_{i=1}^{N}\left(\widetilde{\rho}_{ii}(t) - e^{-b(t)E_i}\bigg/\sum_{i=1}^{N} e^{-b(t)E_i}\right)^2}, \tag{3}$$

with

$$b(t) = \frac{\displaystyle\sum_{i<j, E_i \neq E_j}[\ln\widetilde{\rho}_{ii}(t) - \ln\widetilde{\rho}_{jj}(t)]/(E_j - E_i)}{\displaystyle\sum_{i<j, E_i \neq E_j} 1}, \tag{4}$$

and

$$\sigma(t) = \sqrt{\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}|\widetilde{\rho}_{ij}(t)|^2}. \tag{5}$$

Here N denotes the dimension of the Hilbert space of system S and $\widetilde{\rho}_{ij}(t)$ is the matrix element (i, j) of the reduced density matrix $\widetilde{\rho}$ in the representation that diagonalizes H_S. As the system relaxes to its canonical distribution both $\delta(t)$ and $\sigma(t)$ vanish, $b(t)$ converging to β. As $\sigma(t)$ is a global measure for the size of the off-diagonal terms of the reduced density matrix, $\sigma(t)$ also characterizes the degree of coherence in the system: If $\sigma(t) = 0$ the system is in a state of full decoherence.

3. Model and Simulation Method

To study the evolution to the canonical ensemble state in detail, we consider a general quantum spin-1/2 model defined by the Hamiltonians

$$H_S = -\sum_{i=1}^{n_S-1}\sum_{j=i+1}^{n_S}\sum_{\alpha=x,y,z} J_{i,j}^{\alpha} S_i^{\alpha} S_j^{\alpha}, \tag{6}$$

$$H_E = -\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\sum_{\alpha=x,y,z} \Omega_{i,j}^{\alpha} I_i^{\alpha} I_j^{\alpha}, \tag{7}$$

$$H_{SE} = -\sum_{i=1}^{n_S}\sum_{j=1}^{n}\sum_{\alpha=x,y,z} \Delta_{i,j}^{\alpha} S_i^{\alpha} I_j^{\alpha}. \tag{8}$$

Here the S^{α}'s and I^{α}'s denote the spin-1/2 operators of the system and environment respectively (we use units such that $\hbar$ and k_B are one). Analytic expressions for $\rho(t)$ can only be obtained for very special choices of the exchange integrals $J_{i,j}^{\alpha}$, $\Omega_{i,j}^{\alpha}$, and $\Delta_{i,j}^{\alpha}$ but it is straightforward to solve the TDSE numerically for any choice of the model parameters. Here, we numerically solve the TDSE for $H = H_S + H_E + H_{SE}$ using the Chebyshev polynomial algorithm.[24–27] These *ab initio* simulations yield results that are very accurate (at least 10 digits), independent of the time step used.[28]

The state, that is the density matrix $\rho(t)$ of the whole system at time t is completely determined by the choice of

the initial state of the whole system and the numerical solution of the TDSE. In our work, the initial state of the whole system $(S + E)$ is a pure state. This state evolves in time according to

$$|\Psi(t)\rangle = e^{-iHt}|\Psi(0)\rangle = \sum_{i=1}^{2^{n_s}}\sum_{p=1}^{2^n} c(i, p, t)|i, p\rangle, \tag{9}$$

where the states $\{|i, p\rangle\}$ denote a complete set of orthonormal states. In terms of the expansion coefficients $c(i, p, t)$, the reduced density matrix reads

$$\widetilde{\rho}(t)_{i,j} = \text{Tr}_E \sum_{p=1}^{2^n}\sum_{q=1}^{2^n} c^*(i, q, t)c(j, p, t)|j, p\rangle\langle i, q|$$

$$= \sum_{p=1}^{2^n} c^*(i, p, t)c(j, p, t), \tag{10}$$

which is easy to compute from the solution of the TDSE. Another quantity of interest that can be extracted from the solution of the TDSE is the local density of states (LDOS)

$$\text{LDOS}(E) \equiv \frac{1}{2\pi}\int_{-\infty}^{+\infty} dt\, e^{-iEt}\langle\Psi(0)|e^{-iHt}|\Psi(0)\rangle$$

$$= \sum_{k=1}^{D} |\langle\Psi(0)|\varphi_k\rangle|^2 \delta(E - E_k)$$

$$= \sum_{i=1}^{2^{n_s}}\sum_{p=1}^{2^n} c^*(i, p, 0)c(i, p, t), \tag{11}$$

where $D = 2^{n+n_s}$, $\{|\varphi_k\rangle\}$, and $\{E_k\}$ denote the dimension of the Hilbert space, the eigenstates and eigenvalues of the whole system, respectively. The LDOS is "local" with respect to the initial state: It provides information about the overlap of the initial state and the eigenstates of H.

The notation to specify the initial state is as follows: $|GROUND\rangle_S$ is the ground state or a random superposition of all degenerated ground states of the system; $|RANDOM\rangle_S$ denotes a random superposition of all possible basis states; $|UU\rangle_S$ is a state in which all spins of the system are up meaning that in this state, the expectations value of each spin is one; $|UD\rangle_S$ is a state in which two nearest-neighbor spins of the system are antiparallel implying that in this state, the correlation of their z-components is minus one; and $|RR\rangle_S$ denotes the product state of random superpositions of the states of the individual spins of the system. The same notation is used for the spins in the environment, the subscript S being replaced by E.

As we report results for many different types of spin systems it is useful to introduce a simple terminology to classify them according to symmetry and connectivity. The terms "XY", "Heisenberg", "Heisenberg-type", and "Ising" system refer to the cases $J_{i,j}^x = J_{i,j}^y = J$ and $J_{i,j}^z = 0$, $J_{i,j}^x = J_{i,j}^y = J_{i,j}^z = J$, $J_{i,j}$ uniform random in the range $[-|J|, |J|]$, and $J_{i,j}^x = J_{i,j}^y = 0$ and $J_{i,j}^z = J$, respectively. The same terminology of symmetry is used for the Hamiltonian H_E of the environment and for the interaction Hamiltonian H_{SE}. In our model, all the spins of the system interact with each spin of the environment. To characterize the connectivity of spins within the system (environment), we use the term "ring" for spins forming a one-dimensional chain with nearest-neighbor interactions and periodic boundary conditions, "triangular-lattice" if the spins are located on a two-dimensional

triangular lattice with nearest-neighbor interactions, and "maximum-connectivity-system" when all the spins within the system (environment) interact with each other.

4. Results

In earlier work, it was found that a frustrated spin glass (Heisenberg-type maximum-connectivity-system) environment is very effective for creating full decoherence ($\sigma \to 0$) in a two-spin system.[29–31] As $\sigma \to 0$ is a necessary condition for the state of the system to converge to its canonical distribution, we have chosen spin glass environments, which have no obvious symmetries, for further exploration.

First, we consider a system (H_S: Heisenberg-ring) interacting (H_{SE}: Heisenberg-type) with an environment (H_E: spin glass). The system has four distinct eigenvalues ($E_1 = -2$, $E_{2-4} = -1$, $E_{5-11} = 0$, and $E_{12-16} = 1$) and sixteen different eigenstates. The environment has 2^{18} eigenstates. During the time-integration of the TDSE, the reduced density matrix of the system is calculated every $\tau = \pi/10$. Following the general procedure described earlier, the values of the diagonal elements $\widehat{\rho}_{ii}$ yield an estimate for the effective inverse temperature $b(t)$, the error $\delta(t)$ for this estimate and the measure $\sigma(t)$ for the deviation from a non-diagonal matrix. We also monitor the energy $E_S(t) = \mathrm{Tr}_S \widehat{\rho}(t) H_S$, of the system.

From the simulation results, shown in Fig. 1, it is clear that for $t > 50\tau$, each diagonal element $\widehat{\rho}_{ii}$ of the reduced density matrix converges to one out of four stationary values, corresponding to the four non-degenerate energy levels of the system. This convergence is a two-step process. First the system looses all coherence, as indicated by the vanishing of $\sigma(t)$ for $t > 50\tau$. The time dependence of $\sigma(t)$ fits very well to an exponential law

$$\sigma(t) = \sigma_\infty + A\mathrm{e}^{-t/T_2}, \quad (12)$$

with $\sigma_\infty = 0.00128$, $A = 0.602$, and $T_2 = 8.01\tau$. Likewise, the vanishing of $\delta(t)$ on the same time-scale indicates that the density matrix of the system converges to the canonical distribution. The effective temperature $b(t)$ and the energy of the system $E_S(t)$ also fit very well to the exponential laws
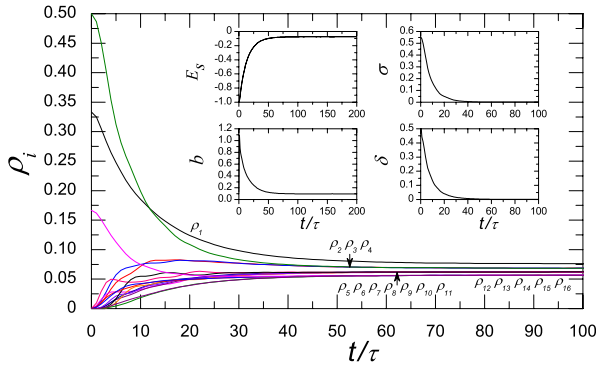
$$b(t) = \beta + B\mathrm{e}^{-t/T_1}, \quad (13)$$

$$E(t) = E_\infty + C\mathrm{e}^{-t/T_1}, \quad (14)$$

with $\beta = 0.0962$, $B = -0.900$, and $T_1 = 13.3\tau$ and $E_\infty = -0.0745$, $C = -0.952$. The estimated values for T_1 and T_2 change very little if we choose different random realizations for the initial state of the environment or for the model parameters $\Omega_{i,j}^\alpha$ and $\Delta_{i,j}^\alpha$ (data not shown) but if we change their range, T_1 and T_2 also change, as naively expected.

The simulation demonstrates that the system first looses all coherence and then, on a longer time-scale, relaxes to its thermal equilibrium state with a finite temperature. In terms of the theory of magnetic resonance,[32] T_1 and T_2 are the times of dissipation and dephasing, respectively. Note that in contrast to the cases considered in the theory of nuclear magnetic resonance, in most of our simulations, H_S, H_E, and H_{SE} are comparable so the standard perturbation derivation of σ and E does not work. In the case of very small H_E, one should expect, instead of an exponential decay of σ and E, a Gaussian decay, as observed in our earlier work.[29–31]

Results for systems (H_S) with different symmetries and connectivities that interaction with the same type of environments (H_E) via the same type of couplings (H_{SE}) are shown in Fig. 2. The systems used are an XY-ring, a Heisenberg-ring, an Ising-ring, a Heisenberg-triangular-lattice, and a spin glass. From Fig. 2, it is clear that independent the internal symmetries and connectivity of the system and independent the initial state of the whole system [except for case (f) in which the environment is initially
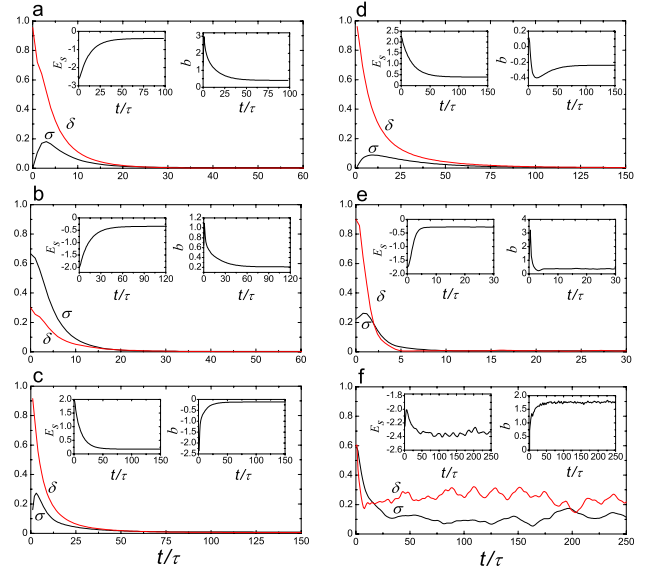

Fig. 1. (Color online) Simulation results for the diagonal elements $\rho_i \equiv \widehat{\rho}_{ii}(t)$ of the density matrix of S, the energy $E_S \equiv E_S(t)$, the effective inverse temperature $b \equiv b(t)$ and its variance $\delta \equiv \delta(t)$, and $\sigma \equiv \sigma(t)$ which is measure for the decoherence in S, as obtained by solving the TDSE for the whole system with Heisenberg-ring H_S ($J = -1$, $n_S = 4$), Heisenberg-type H_{SE} ($\Delta = 0.3$), spin glass H_E ($\Omega = 1$, $n = 18$), and $\tau = \pi/10$. The initial state of the whole system is a product state of $|UD\rangle_S$ and $|RANDOM\rangle_E$.

Fig. 2. (Color online) Simulation results for the energy $E_S \equiv E_S(t)$, the effective inverse temperature $b \equiv b(t)$, its variance $\delta \equiv \delta(t)$, and the deviation from a diagonal matrix $\sigma \equiv \sigma(t)$ as obtained by the solution of the TDSE for a variety of different systems S coupled to a spin glass H_E via a Heisenberg-type H_{SE}. The systems used are (a) XY-ring, (b and f) Heisenberg-ring, (c) Ising-ring, (d) Heisenberg-triangular-lattice, and (e) spin glass (Heisenberg-type maximum-connectivity-system). The initial states of the whole system are (a) $|GROUND\rangle_S \otimes |RANDOM\rangle_E$, (b) $|UD\rangle_S \otimes |RANDOM\rangle_E$, (c) $|UU\rangle_S \otimes |RR\rangle_E$, (d) $|UU\rangle_S \otimes |RANDOM\rangle_E$, (e) $|GROUND\rangle_S \otimes |UD\rangle_E$, and (f) $|UD\rangle_S \otimes |GROUND\rangle_E$. The numbers of spins in the system are $n_S = 8$ for cases (a)–(c) and $n_S = 6$ for cases (d)–(f). The numbers of spins in the environment is $n = 16$ for all cases. The model parameters are $J = -1$, $\Delta = 0.3$ and $\Omega = 1$, except for case (e) in which $\Delta = 1$.
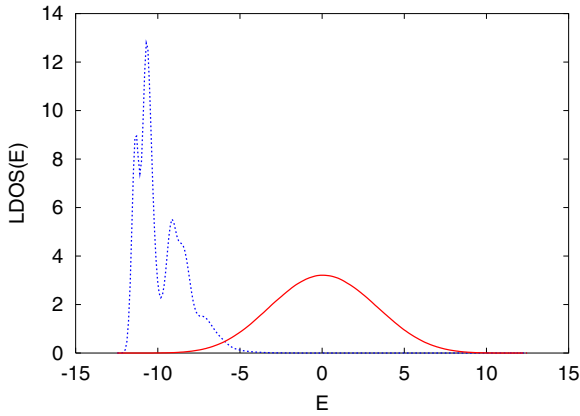
Fig. 3. (Color online) Simulation results for the local density of states as a function of the energy. Solid line: Case corresponding to Fig. 2(b). The initial state is $|UD\rangle_S \otimes |RANDOM\rangle_E$; Dashed line: Case corresponding to Fig. 2(f). The initial state is $|UD\rangle_S \otimes |GROUND\rangle_E$.

Fig. 4. (Color online) Simulation results for a Heisenberg-ring H_S ($J = -5$, $n_S = 4$, initial state $|UD\rangle_S$) coupled to a spin glass H_E ($\Omega = 0.15$, $n = 16$, initial state $|RANDOM\rangle_E$) via (a) Heisenberg H_{SE} ($\Delta = 0.075$) or (b) Heisenberg-type H_{SE} ($\Delta = 0.15$). Although full decoherence is observed in both cases, the the system S only relaxes to a state with equal probabilities within each energy subspace, that is to a "microcanonical" state per energy subspace.

in its ground state], all systems relax to a state with full decoherence. Notice that in case (b), σ vanishes exponentially with time, whereas in other cases (a, c, d, e), σ initially increases and then vanishes exponentially with time, due to the entanglement between the system and the environment. This observation is in concert with our earlier work.[29–31]

Furthermore, in all cases except (f), the system always relaxes to a canonical distribution ($\delta \to 0$) as soon as it is in the state with full decoherence ($\sigma \to 0$), indicating that the time of decoherence (T_2) and the thermalization is almost the same. In agreement with the results depicted in Fig. 1, the decoherence time T_2 is shorter than the typical time scale T_1 on which the system and environment exchange energy and the effective inverse temperature $b(t)$ reaches its stationary value.

The case (f) is easily understood in terms of the local density of states. In Fig. 3 we show the LDOS for the cases (b) and (f), the only difference between these two cases being the initial state of the environment. Up to a trivial normalization factor, the LDOS curve for case (b) is indistinghuisable from the density of states (data not shown) calculated from the solution of the TDSE using the technique described in ref. 33. This suggests that if the environment starts from the random superposition of all its states, all states of the whole system may participate in the decoherence/relaxation process. In contrast, the LDOS curve for case (f) has a very small overlap with the density of states (the curve of which coincides with the solid line in Fig. 3). Therefore, starting with an environment in the ground state, only a relatively small number states participates in the decoherence process, as confirmed by the results for $\sigma(t)$ shown in Fig. 2(f).

For completeness, we discuss a two other situations in which, for fairly obvious reasons, the system cannot relax to its canonical distribution. Obviously, if the energy of the system is conserved ($[H_S, H] = 0$), the system cannot exchange energy with the environment and we should not expect relaxation to the canonical distribution. In this case, as shown in Fig. 4, after the system S has reached a state with full decoherence, its density matrix does not converge to the canonical state. Likewise, if the range of energies of the environment E is too small compared to that of the
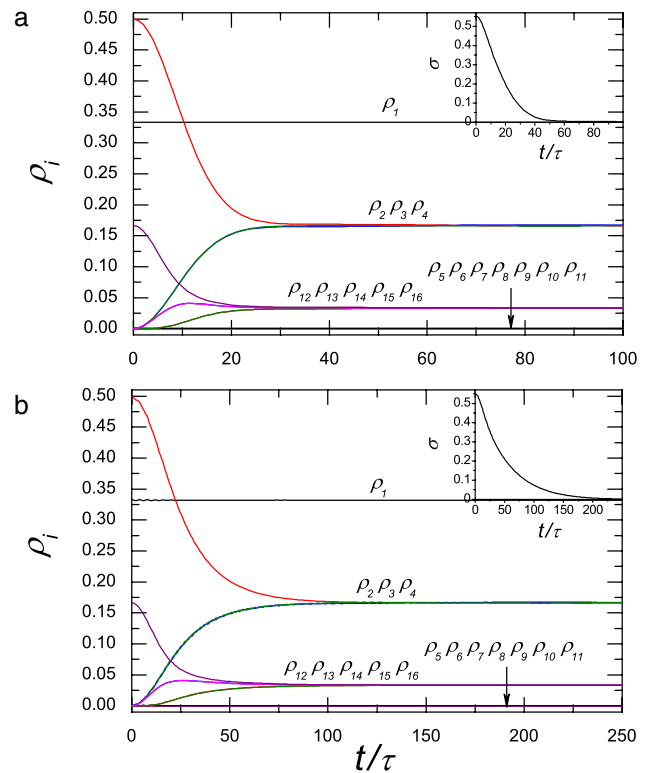
system ($|\Omega| \ll |J|$) as in the example shown in Fig. 4(b), there is no convergence to the canonical state either. It is to be noted that in both cases, the interaction with the environment leads to perfect decoherence ($\sigma(t) \approx 0$, see insets) such that the reduced density matrix converges to a diagonal matrix. However, from Fig. 4, it follows that S relaxes to a kind of microcanical state in which the states in each energy subspace have equal probability, the probabilities to end up in a subspace depending on the initial state.

Disregarding the three cases mentioned earlier, the simulation results presented in Figs. 1 and 2 suggest that the state of a system generally relaxes to the canonical distribution when the system is coupled to an environment of which the dynamics is sufficiently complex also in the case that the interaction between system and environment cannot be regarded as a perturbation. There are exceptions but these are easily understood: Either there are not enough states available for the decoherence [Fig. 2(f)] to yield a diagonal reduced density matrix or the energy relaxation (Fig. 4) is not effective in letting the diagonal reduced density matrix relax to the canonical distribution.

Although we have only presented results for a spin glass environment H_E, our results (not shown) for any of the choices for H_S and H_E mentioned earlier, in combination a Heisenberg-type H_{SE} interaction between system and environment, or for H_S and H_{SE} in combination Heisenberg-type H_E leads to the same conclusion, namely that the state of a system relaxes the canonical distribution.

J. Phys. Soc. Jpn., Vol. 78, No. 9

S. YUAN *et al.*

5. Discussion

The results presented here have been obtained from an *ab initio* numerical solution of the TDSE in the absence of, for instance, dissipative mechanisms, and demonstrate that the existence of the canonical distribution, a basic postulate of statistical mechanics, is a direct consequence of quantum dynamics.

We have shown that if we have a system S that interacts with an environment E and the whole system $S + E$ forms a closed quantum system that evolves in time according to the TDSE, S and E can exchange energy, the range of energies of E is large compared to the range of energies of S, and the interaction between S and E leads to full decoherence of S, then the state of S relaxes to the canonical distribution. Note that only the condition of full decoherence is a nontrivial requirement.

We emphasize that our conclusion does not rely on time averaging of observables, in concert with the fact that real measurements of thermodynamic properties yield instantaneous, not time-averaged, values. Furthermore and perhaps a little counter intuitive, our results show that relatively small environments (≈ 20 spins) are sufficient to drive the system S to thermal equilibrium and that there is no need to assume that the interaction between the system and environment is weak, as is usually done in kinetic theory.

In conclusion: The work presented here strongly suggests that the canonical ensemble, being one of the basic postulates of statistical mechanics, is a natural consequence of the dynamical evolution of a quantum system. This conclusion may be exciting but as quantum mechanics describes the dynamics of a system and statistical mechanics gives us the distribution when the system is in the equilibrium state, these two successful theories should not be in conflict once the conditions for the system to relax to its thermal equilibrium are satisfied.

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