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Statistical Behavior in Deterministic Quantum Systems with Few Degrees of Freedom

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Numerical studies of the dynamics of finite quantum spin chains are presented which show that quantum systems with few degrees of freedom ($N=7$) can be described by equilibrium statistical mechanics. The success of the statistical description is seen to depend on the interplay between the initial state, the observable, and the Hamiltonian. This work clarifies the impact of integrability and conservation laws on statistical behavior. The relation to quantum chaos is also discussed.

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Until recently it was believed that the laws of statistical mechanics were applicable only to systems with many degrees of freedom. This view has been revised by recent studies in classical nonlinear dynamics which show that classical mechanical systems with very few degrees of freedom can exhibit dynamical behavior which is indistinguishable from a random process.[1,2] Here we ask whether the deterministic evolution of quantum systems with a few degrees of freedom can also exhibit statistical behavior. Specifically, we ask whether the expectation values of observables approach equilibrium and whether the equilibrium values can be predicted by the methods of quantum statistical mechanics, namely the use of the microcanonical and canonical ensembles.[3] We emphasize that these predictions do not require full knowledge of the initial wave function but only the gross features (such as the mean energy) necessary to specify the ensemble. We will refer to deterministic systems which can be described with this limited information as statistical. By studying the quantum mechanisms which give rise to statistical behavior in small quantum systems, we hope to gain a better understanding of the foundations of quantum statistical mechanics. Finally, we comment on the relation of our work to quantum chaos.

We studied the deterministic dynamics of a finite, spin-$\frac{1}{2}$, quantum chain in a magnetic field described by the Hamiltonian

$$H=\alpha \sum_{n=1}^{N} \sigma_3(n)\sigma_3(n+1)+\lambda \sum_{n=1}^{N} \sigma_1(n) +\gamma \sum_{n=1}^{N} \sigma_3(n). \qquad (1)$$

Here $\sigma_1(n)$ and $\sigma_3(n)$ are Pauli matrices at the site n of a cyclic chain of N spins, α is the nearest-neighbor coupling, and λ and γ are components of an external magnetic field.

The use of such models for investigation of statistical behavior in quantum systems has several important advantages. First, since the Hilbert space has a finite dimension, $d=2^N$, numerical calculations of the energy spectra and the time evolution of arbitrary initial states can be performed to machine precision. Although much recent work has been devoted to the study of coupled nonlinear oscillators, numerical simulation of these systems must also restrict the Hilbert space to a finite dimensionality at the expense of introducing truncation errors. Second, by varying the parameters in H we can easily explore the effect of additional constants of motion as well as complete integrability on the statistical behavior. In particular, when $\gamma=0$, the Hamiltonian is integrable and can be diagonalized by the fermion method of Schultz, Mattis, and Lieb.[4]

To test for statistical behavior, we evolved various initial states with seven spins by numerically integrating the Schrödinger equation and plotted the expectation values of several observables as functions of time. We looked for an approach to equilibrium and compared the equilibrium values with the mean values computed on a microcanonical ensemble. Our main conclusion from these numerical studies is that both integrable and nonintegrable quantum systems with as few as seven degrees of freedom can exhibit statistical behavior for finite times.

Figure 1 shows typical results for the evolution of $M_1 = \sum_n \sigma_1(n)$ for a nonintegrable Hamiltonian with $\alpha = 0.5$, $\lambda = 1$, and $\gamma = 0.5$. M_1 exhibits an oscillatory decay to an equilibrium value around 2.5 from an initial value of 0. Of course a true equilibrium is never achieved since the system is quasiperiodic with a relatively long recurrence time.

The average value of M_1 over the corresponding microcanonical ensemble was determined by numerically computing the energy eigenvalues and eigenvectors and averaging the expectation values of M_1 over the eigenstates in the interval $E \pm \Delta E$ with equal weights, where E is the mean energy of the initial state and ΔE is a small interval in energy which must be large enough to span many energy levels of the system. (The results should not and did not depend on the precise value of ΔE.) In Fig. 2(a) the magnetization is plotted against energy for each of the energy eigenstates along with the microcanonical average computed with $\Delta E = 2.0$. For the state depicted in Fig. 1, which had a mean energy $E = 4.0$, this calculation predicts an equilibrium magnetization of $M_1 = 2.5$ which is in excellent agreement with the numerical experiment.

Figure 2(a) also shows the equilibrium values of the magnetization calculated by evolving a number of different initial states.[5] The associated error bars indicate the level of fluctuations from the short-time average. *Not only does the magnetization for this system with seven degrees of freedom approach equilibrium but the equilibrium values are correctly predicted by the microcanonical ensemble. The fact that the short-time average of $M_1(t)$, which is computed using the full knowledge of the wave function, is accurately predicted by the ensemble calculation, based only on the knowledge of the mean energy, is what justifies our characterization of the dynamics as statistical.*

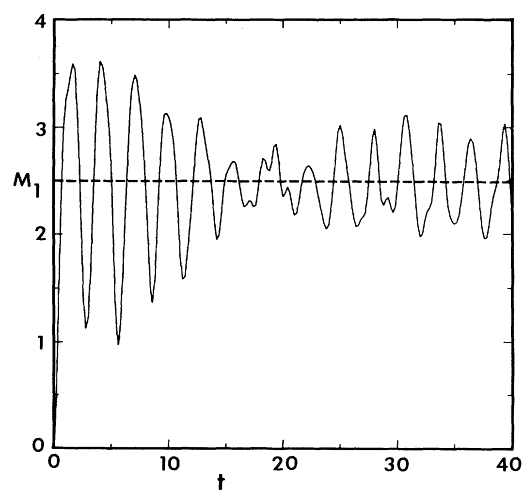

FIG. 1. The expectation value of the magnetization, M_1, as a function of time for a typical initial condition evolved by the spin Hamiltonian, Eq. (1). The dashed line shows the statistical prediction for the equilibrium magnetization.

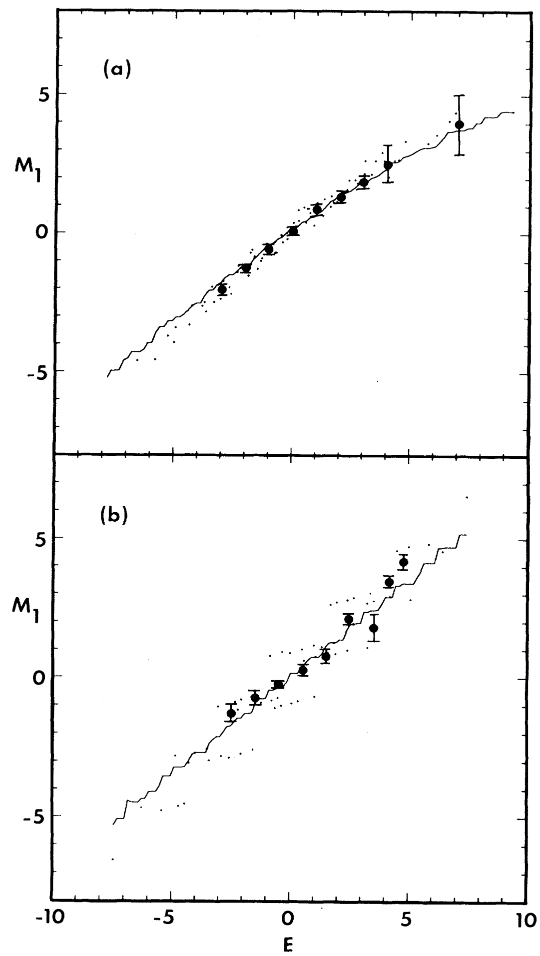

FIG. 2. The magnetization, M_1, plotted against energy for each of energy eigenstates (small dots) for (a) a nonintegrable Hamiltonian and (b) an integrable Hamiltonian; the solid curves represent the microcanonical average of the magnetization as functions of energy, and the large dots show the equilibrium values approached in numerical experiments performed with a variety of initial states. The associated error bars represent an estimate of the typical fluctuations from equilibrium.

Although lattice momentum was conserved because of the translational invariance of the Hamiltonian, it apparently had little influence on the dynamics of generic initial states. Only if the initial state were an eigenstate of momentum did we find a difference. In this case, the evolution of the initial state was restricted by selection rules and the appropriate ensemble was restricted to energy eigenstates with that momentum. Similarly, when the spin system was completely integrable the microcanonical ensemble was found to be applicable as long as the initial state was not an eigenstate of any of the conserved quantities. For generic initial states the constants of motion generally impose very mild constrains on the evolution of the wave function in the 2^N-dimensional Hilbert space. This is in contrast to the classical case where all dynamical variables are sharply defined in any initial state and the conserved quantities impose very severe restrictions on the dynamics.

In Fig. 2(b) the equilibrium values of M_1 for a number of different initial states evolved by an integrable Hamiltonian with $\alpha=0.5$, $\lambda=1.0$, and $\gamma=0$ are compared with the statistical predictions. Deviations from equilibrium tend to be larger than in the nonintegrable case partly because of degeneracies which reduce the number of distinct frequencies in the problem and partly because the observable, M_1, is not a function of the energy alone but also of the other conserved quantities that label the state. This latter consideration is apparent in Fig. 2(b) where the magnetization for each of the energy eigenstates increases in an oscillatory manner over a series of steps in contrast to the nonintegrable case shown in Fig. 2(a) where the magnetization is a fairly smooth and monotonic function of energy.

An additional test of statistical behavior on the fact that if an isolated system is well described by the microcanonical ensemble, then a small subsystem should be described by the canonical ensemble.[3] We choose spin 7 to be our subsystem, weakly coupled to the reservoir composed of the remaining spins. Given the postulate of equal *a priori* probabilities for the eigenstates for the combined system, it follows that P_+/P_-, the ratio of the probablities that spin 7 is in its upper or lower energy eigenstate with energy $\pm\epsilon$, is

$$P_+/P_- = N(E-\epsilon)/N(E+\epsilon), \qquad (2)$$

where E is the energy of the combined system, $\pm\epsilon$ are the eigenvalues of the single spin Hamiltonian, $H_7=\lambda\sigma_1(7)+\gamma\sigma_3(7)$, and $N(E\pm\epsilon)$ is the density of energy eigenstates of the reservoir, determined by numerically diagonalizing the Hamiltonian for the reservoir and constructing a coarse-grained density of states by smoothing over an interval ΔE. Since the density of states for this system was too irregular to replace the right-hand side of Eq. (2) by a Boltzmann factor $e^{-2\beta\epsilon}$, Eq. (2) was used directly to test the postulate of equal *a priori* probabilities. Numerical solutions for the evolution of P_+ for both integrable and nonintegrable reservoirs once again showed an oscillatory approach to equilibrium which was accurately predicted by Eq. (2).

Numerous attempts have been made to extend the concept of chaos to quantum systems.[6–8] However, these efforts have led to much controversy because the linearity of the Schrödinger equation precludes the mixing behavior which characterizes chaos in classical systems.[1] Nevertheless, we find that the solutions of Schrödinger's equation are rich enough to exhibit statistical behavior. Moreover, we conclude that the applicability of statistical mechanics depends in the following way on the three interrelated factors: the initial state, the observable, and the Hamiltonian.[9]

The expectation of any observable, Ω, can be expressed as the sum of a time-independent and a time-dependent term:

$$\langle\Omega\rangle(t)=\sum_n |c_n(0)|^2\langle n|\Omega|n\rangle + \sum_{n\neq m}\sum c_n^*(0)c_m(0)\exp[i(E_n-E_m)t]\langle n|\Omega|m\rangle, \qquad (3)$$

where $c_n(0)$ are the coefficients of expansion of the initial state in terms of the energy eigenstates $|n\rangle$. The approach to equilibrium is a consequence of the phase-mixing decay of the time-dependent piece of $\langle\Omega\rangle(t)$. Although the initial state will recur as a large fluctuation, this recurrence time is long, $\tau_r\sim$ [minimum level spacing]$^{-1}$, compared with the decay time, $\tau_d\sim$ [energy spread of initial state]$^{-1}$, unless the initial state is an exact eigenstate or very close to one.

The equilibrium value of the observable is given by the time-independent part of $\langle\Omega\rangle$. For a generic initial state with given values of $c_n(0)$ the agreement with the equilibrium values predicted by the microcanonical average (with all c_n equal for eigenstates in the interval $E\pm\Delta E$) depends on the observable. If the expectation values are smooth functions of the energy as in Fig. 2(a), then the short-time average of the observable will be very close to the ensemble average. In fact, it is clear from Fig. 2(a) that the statistical behavior will be obtained for any initial state with a reasonably narrow spread in energy. Even an initial energy eigenstate will exhibit a constant value for the observable which is very close to that predicted by the statistical theory. An observable which exhibits this property for a particular system could be called a "good" statistical quantity for that system.[10]

If the expectation value of the observable is not principally determined by the energy, if other state labels exist and play an important role such that nearby energy eigenstates have very different expectation values, then the equilibrium approached in the dynamic evolution of a given initial state may not agree with statistical predictions based on the assumption of equal *a priori* probabilities. Nevertheless, although the expectation value of M_1 for the integrable system shown in Fig. 2(b) does not show the smooth dependence on energy that is required of "good" observables, the time average is in good agreement with the predictions of statistical mechanics. This can be attributed to the fact that the generic initial states were nearly uniformly distributed over all the eigenstates of H in the interval $E \pm \Delta E$.[11] As a result, the time-independent part of the expectation of the observable in Eq. (3) was very close to the equal weight average.

Finally, we come to the role of the spectrum of the Hamiltonian. A number of different criteria have been suggested to define quantum chaos by distinguishing between the regularity of the energy level spacing of integrable and nonintegrable Hamiltonians.[6–8,12,13] However, depsite the fact that our small quantum system had a distribution of energy levels which was peaked at zero separation (Poisson type) for integrable Hamiltonians and exhibited level repulsion for nonintegrable Hamiltonians (Wigner-Dyson type), we observed statistical behavior in both cases.

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