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Quantum statistical mechanics in a closed system

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A closed quantum-mechanical system with a large number of degrees of freedom does not necessarily give time averages in agreement with the microcanonical distribution. For systems where the different degrees of freedom are uncoupled, situations are discussed that show a violation of the usual statistical-mechanical rules. By adding a finite but very small perturbation in the form of a random matrix, it is shown that the results of quantum statistical mechanics are recovered. Expectation values in energy eigenstates for this perturbed system are also discussed, and deviations from the microcanonical result are shown to become exponentially small in the number of degrees of freedom.

A question that normally occurs to anyone learning the basics of statistical mechanics is the following: Why does the Gibbs formula work? The crudest explanation appearing in many undergraduate textbooks relies on coupling the system to some much larger heat bath. This simply pushes back the problem one stage further, to understand the heat-bath-"plus" system. The more convincing explanation considers a classical system in isolation. From the assumption of ergodicity, the microcanonical distribution can be derived, and for a large number of degrees of freedom this can then be shown to give the Gibbs formula.[1]

The notion of ergodicity is easily seen to lead to statistical mechanics classically. Attempts at extending the notion of ergodicity to the quantum domain have not succeeded in leading to a similar conclusion. Attempts at a quantum-mechanical justification of statistical mechanics have taken several paths.[2] Criteria for quantum ergodicity[3] have either been too general to separate systems obeying statistical mechanics from those that do not,[4] or they have been too complex to allow one to find a system satisfying the criteria.[2] Much work has emphasized the need to couple to an external environment[2,5] such as a heat bath in order to obtain statistical mechanics. In this paper a new approach is presented to understand if, and why, the laws of quantum statistical mechanics work for a closed quantum-mechanical system.

When a system has a well-defined total energy e, quantum statistical mechanics assumes that the average over time $\langle \cdots \rangle_t$ of some observable quantity $\langle \Psi | A | \Psi \rangle$ is equal to an ensemble average of all states around energy e:

$$\langle \langle \Psi | A | \Psi \rangle \rangle_t = \sum_j \Delta(e,j) \langle j | A | j \rangle \equiv \langle A \rangle_{\text{micro}} , \quad (1)$$

where j labels an energy eigenstate of the entire system and $\Delta(e,j)$ is a normalized function of j that is sharply peaked at $\langle j|H|j\rangle = e$. For a system containing a large number of degrees of freedom and for a large class of operators A, this can be written with negligible error in terms of the usual canonical distribution at fixed temperature. The above formulas can be easily extended to take into account large fluctuations in the total energy, as will be done below. For the purposes of this paper, systems obeying the above equation will be called ergodic.

There are many examples of systems in classical mechanics with a few degrees of freedom that have time averages given by the microcanonical distribution. A quantized version of such a system cannot be expected to give the microcanonical distribution. It is easy to show by counterexample that one needs at least one more requirement—the number of degrees of the system must also be large. Having a large number of degrees of freedom, however, is not enough to ensure ergodicity. The distinction between an "ergodic" and an "integrable" quantum system is illustrated by the following *gedanken* experiments.

First, consider a perfect harmonic crystal. If the system is in an energy eigenstate that has been picked at random with equal probability from within some energy

range, the expectation of many observables, such as the mean-square displacement of one atom, are in agreement with the results obtained from the Gibbs formula. One can still find many states that do not agree; however, the vast majority of them do.

If we now shine a laser on this system, to bring it to a new energy, then, although the quantum-mechanical uncertainty in its energy is very small, time averages will not, in general, agree with Gibbs. This is because the external perturbation will couple most strongly to some phonon modes, giving rise to a distribution significantly different from the Bose distribution. In contrast, if the crystal were "ergodic," then after it was acted on by the external perturbation it should give the microcanonical distribution, but now at a higher energy.

One would like to find an example of a closed quantum-mechanical system that does "give back" the microcanonical distribution after it has been perturbed as described above. The approach taken here is similar to understanding the statistical mechanics of an "ideal gas." A genuine ideal gas has no interaction between different particles and therefore will not be ergodic. It can be made so, for example, by giving the particles hard cores of very small diameter. This will have a negligible effect on the statistical and thermodynamic properties as computed from the Gibbs distribution. However, after a long enough time, the system will explore all of its available phase space, enabling the rigorous application of these formulas. In the same spirit, it will be shown here that if one starts with a nonergodic system with a Hamiltonian that decouples into N separate subsystems,

$$H_0 = \sum_{i=1}^{N} h_0(x_i, p_i) , \tag{2}$$

it can be made ergodic for large N by the addition of a small perturbation. The perturbation added to the Hamiltonian is a real symmetric random matrix with certain physically sensible conditions on the statistics of the elements discussed below. Full details of the calculations are planned to be published elsewhere.[6]

This system provides a justification for statistical mechanics without invoking any coupling to the external world. This is interesting because, as mentioned above, external coupling has often been thought necessary in obtaining ergodicity.[2,5]

The choice of a random matrix as the perturbation added to H_0 appears to be a sensible choice for several reasons. As a model, it is analytically tractable and yet gives ergodicity. Analysis of experimental work on nuclei[7] supports the proposal of Wigner[8] that the spectrum of nuclei are well described by random matrices. Numerical and analytic work in the semiclassical regime also supports the choice of model used here.[9–11] Of course, this model should not be regarded as a universal description of an ergodic quantum-mechanical system. The relation between random-matrix models and specific quantum-mechanical Hamiltonians is still the subject of much research.

Before proceeding any further, it is useful to discuss how the microcanonical formula (1) should be modified to take into account fluctuations in the total energy. If we have an arbitrary initial state (Γ_i is a complex amplitude)

$$|\Psi\rangle = \sum_i \Gamma_i |i\rangle , \tag{3}$$

one could ask if it is possible to experimentally prepare a system having a very broad distribution for Γ_i—that is, large quantum-mechanical fluctuations in the total energy of the system. The answer appears to be that it is indeed possible.

One needs simply to superpose two wave functions of the system, one at a low energy and another at high energy, which can be done by a "Schrödinger's cat" apparatus.

For a macroscopic system, one would expect that the time average of an observable could be described by the weighted average of two microcanonical averages. The weights are the probability that the system was to be found in one or the other macroscopic state, and the microcanonical averages are taken at the appropriate energies. The assumption being made is that there is negligible interference between two macroscopically different states. If we denote $\langle A \rangle_e$ as the microcanonical average of an observable in a state with a well-defined total energy e, then, in general, we expect the time average of A for a wave function with a broad distribution of total energies to be

$$\langle A \rangle_t = \sum_e P(e) \langle A \rangle_e , \tag{4}$$

where $P(e)$ is the probability of finding that the system has an energy e. In terms of $|\Psi\rangle$, as defined by (3),

$$\langle \langle \Psi | A | \Psi \rangle \rangle_t = \sum_\nu |\Gamma_\nu|^2 \langle A \rangle_{e_\nu} . \tag{5}$$

In the "Schrödinger's cat" example a large uncertainty in the total energy was obtained by the addition of an external system, or potential, whose value is uncertain (e.g., radioactive decay). We can ask what happens if a known external potential is applied to the system and then switched off? For simplicity, consider the time evolution of the integrable case (2). Then, if the system starts out in an eigenstate of H_0, we can ask what is the spread ΔE of the total energy E after the external perturbation has been turned off. It can be easily shown that $\Delta E/E$ will decrease as $1/\sqrt{N}$. Therefore, applying an external potential to this system, which initially has a well-defined energy, will not create macroscopic fluctuations in its energy, so that Γ_ν remains localized around a small range of energies.

The model we will consider is the real symmetric Hamiltonian

$$H = H_0 + H_1 . \tag{6}$$

H_0 could represent, say, the Hamiltonian of a harmonic crystal, or describe an ideal gas. We are interested in the limit of a large number of degrees of freedom, and we shall see that considerable simplifications take place in this limit. H_1 is added in the hopes of making the system obey quantum-statistical mechanics. In the case of an ideal gas, for example, one may want to add two-body in-

teractions between the different particles. Instead of adding in these interactions explicitly, we model H_1 by a real symmetric matrix whose elements are chosen from a random Gaussian ensemble.

It is emphasized that no ensemble average is being taken. The elements of H_1 are precisely determined, but have correlations between them typical of a random matrix. The same philosophy has been adopted by others in studying the semiclassical limit of chaotic systems.[9-11]

It will be convenient to examine this model in the basis of the eigenvectors of H_0. In this basis the elements of H_1 are

$$h_{ij} \equiv \langle E_i | H_1 | E_j \rangle, \quad \langle h_{ij} h_{kl} \rangle = \varepsilon^2 \delta_{ik} \delta_{jl} , \tag{7}$$

keeping in mind that the elements are to be cut off—that is, set to zero—for $|E_1 - E_2| \gg T$. Here T is defined as the temperature associated with a total energy E for the system whose Hamiltonian is H_0. For finite T and large N this cutoff prevents an unphysical divergence in expectation values, and should be present on physical grounds. If, instead of a random matrix, H_1 represented two-body interactions between particles, then $\langle E_i | H_1 | E_j \rangle$ should also[6] become zero for $|E_1 - E_2| \gg T$. For small N, the width of the matrix H_1 has been discussed.[11] Properties of banded random matrices have recently received much attention.[12-14]

We now discuss what we intuitively expect this model to yield. For small enough ε, eigenvectors will differ only slightly from their $\varepsilon = 0$ value. However, for small but finite ε many neighboring levels ΔE will be coupled. This is because the distance between neighboring levels,[15] $D(E)$, is proportional to $\exp[-S(E)]$ [$S(E)$ is the total entropy at total energy E]. So, at fixed energy per particle, the separation between levels decreases exponentially with N and becomes arbitrarily small. Therefore there is a large range of values for ε which will couple a large number of levels; the number is proportional to $\Delta E \exp[S(E)]$. We would expect that, for large N, ε could be made much smaller than the energy per particle, and have a large effect on eigenvectors. The new eigenvectors should then mix in with random phases, the unperturbed eigenvectors within a window ΔE. It is this mixing that gives rise to ergodicity.

The distribution of eigenvectors for H is now discussed. With this information we will be able to examine physical properties of this model in eigenstates of the Hamiltonian, and also compute time averages of observables.

Given that we are in a basis where the noninteracting Hamiltonian (2) is diagonal, we would first like to compute the probability distribution of the normalized eigenvectors, c_{ij}, of H given that H_1 is drawn from a Gaussian random ensemble as described above. Here j labels the jth component of the ith eigenvector. It has not been possible to compute the distribution exactly, but an approximate method has been found that should work well in the limit of strong overlap between eigenvectors. We still require the overlap to be much less than the energy per particle.

One finds[6] that for one element of the matrix c, $P(c_{ij}) \propto \exp[-c_{ij}^2/\Lambda(i,j)]$, where

$$\Lambda(i,j) = \frac{A}{(i-j)^2 + \delta^2} , \tag{8}$$

and

$$A = \frac{\varepsilon^2}{2\Delta^2}, \quad \delta = \frac{\pi \varepsilon^2}{2\Delta^2} . \tag{9}$$

Here Δ is the average energy spacing between levels.

Before discussing time-averaged properties of observables, it is illustrative to consider the properties of observables in energy eigenstates. This will highlight the difference between a noninteracting system and one with very small but finite ε. We will see that fluctuations in results are exponentially reduced by the presence of a very small interaction of the form (7).

We denote the state vector of the interacting Hamiltonian in the ith energy eigenstate by $|i\rangle$. A noninteracting state vector in the jth energy eigenstate is labeled $|j\rangle_0$. They are related by

$$|i\rangle = \sum_j c_{ij} |j\rangle_0 . \tag{10}$$

We want to look at the variation in the expectation value of an operator A in an energy eigenstate,

$$\langle i | A | i \rangle = \sum_{k,l} c_{ik} c_{il0} \langle k | A | l \rangle_0 . \tag{11}$$

We will restrict our attention to real A. Since energy eigenstates for neighboring energy levels are different, $\langle i | A | i \rangle$ will vary from state to state. A good estimate of this variation[6] is to compute the variance in $\langle i | A | i \rangle$, keeping state i fixed, but averaging over different realizations of the random matrix H_1. We denote this kind of averaging by $\langle \cdots \rangle_{\text{rand}}$. The mean averaged over different H_1 is $\langle \langle i | A | i \rangle \rangle_{\text{rand}}$, which can be computed by substituting in (11), giving

$$\langle \langle i | A | i \rangle \rangle_{\text{rand}} = \sum_j \Lambda(i,j)_0 \langle j | A | j \rangle_0 . \tag{12}$$

This is just the microcanonical average of A, $\langle A \rangle_{\text{micro}}$, which is fortunate, since this gives a mean in agreement with the microcanonical distribution. The variance is

$$\Delta A^2 \equiv \langle \langle i | A | i \rangle^2 \rangle_{\text{rand}} - \langle \langle i | A | i \rangle \rangle_{\text{rand}}^2 . \tag{13}$$

The first term on the right-hand side of (13) can be computed by substituting in (10), giving

$$\langle \langle i | A | i \rangle^2 \rangle_{\text{rand}} = \sum_{j,k,l,m} \langle c_{ij} c_{ik} c_{il} c_{im} \rangle_{\text{rand}} \times {}_0\langle j | A | k \rangle_{00} \langle l | A | m \rangle_0 . \tag{14}$$

We shall assume, as we did in the preceding section, that the c's are Gaussian. This can be shown explicitly when ε/Δ is infinite, and should be a good approximation when such a quantity is large. One can then show[6]

$$\Delta A^2 \leq 2\Lambda(i,i) \langle A^2 \rangle_{\text{micro}} . \tag{15}$$

From (8) and (9) we have $\Lambda(i,i) = 1/(\pi\delta)$. We will keep the spread in energy of the eigenvectors $\Delta\delta$ constant as the number of degrees of freedom N goes to infinity. However, because at a fixed energy the average energy

spacing $\Delta \propto \exp(-\text{const} \times N)$, then $\Lambda(i,i) \propto \exp(-\text{const} \times N)$. For a large class of operators, namely those related to extensive and intensive statistical quantities (e.g., total energy, correlation functions, and susceptibilities), $\langle A^2 \rangle_{\text{micro}}$ increases with no more than a power of N. Therefore we expect that ΔA^2 should decrease exponentially with N. This should be contrasted with the $\varepsilon = 0$ case, as is done below.

If one considers fluctuations in the expectation value of A with $\varepsilon = 0$, then the variance in such a system should be

$$\Delta A_0^2 = \langle {}_0\langle i | A | i \rangle_0^2 \rangle_{\text{micro}} - \langle {}_0\langle i | A | i \rangle_0 \rangle_{\text{micro}}^2 , \quad (16)$$

where $\langle \cdots \rangle_{\text{micro}}$ again denotes a microcanonical average, one that is done over a small width in energy. For the example of a harmonic crystal, ΔA_0^2 decreases[6] with a negative power of N. Thus for large N the fluctuations in the integratable case are dramatically larger than in the $\varepsilon \neq 0$ case.

The reason the interacting case shows much smaller fluctuations can be intuitively understood as the result of an additional averaging done over neighboring energy states, as given by (10). The fluctuations are then reduced by the square root of the number of states being averaged over, δ, which is exponential in N. It is this reduction in these fluctuations which makes the random-matrix model ergodic.

Now consider an arbitrary initial state

$$|\Psi\rangle = \sum_i \Gamma_i |i\rangle_0 , \quad (17)$$

evolving under the action of the interacting Hamiltonian (6). Here Γ_i is an arbitrary complex amplitude. Using the same procedure as above, one can obtain a simple formula for the time average of the expectation value of A in an arbitrary state. In terms of the interacting basis (where there should be no degeneracy), this is easily shown to be

$$\langle \langle \Psi | A | \Psi \rangle \rangle_t \equiv \lim_{T \to \infty} \frac{1}{T} \int_0^T \langle \Psi | A | \Psi \rangle dt = \sum_i |\langle i | \Psi \rangle|^2 \langle i | A | i \rangle . \quad (18)$$

This is known as the "fine-grained ergodic theorem."[2,3] Then, after substituting (10) for $|\Psi\rangle$ and averaging over H_1, one obtains two terms. One of these can be shown to vanish in the limit of large N,[6] and one recovers (5), so that this system is "ergodic." This is then an example of a system that we wanted to find. One that comes to the correct statistical equilibrium after being perturbed by an external perturbation, as was mentioned in connection with the *gedanken* experiments at the beginning of this paper.

Several predictions of this model could be tested. A Lorentzian distribution is predicted for the overlap between integrable eigenstates and those of the perturbed Hamiltonian. This could be tested for a system with a small number of degrees of freedom in the semiclassical limit, where these arguments should still be valid. For example, by comparing a free particle on a torus to the same situation but with a small billiard added, one could compare the overlap to these eigenstates. Numerically it is rather difficult to test predictions for large N, but this may be possible for spin systems of up to 10 spins. One eigenstate should give expectation values in accord with the microcanonical distribution.

The dynamics of this system are presently being investigated. These show dissipative effects and should give a new handle on the problem of how to introduce frictional forces into quantum mechanics.[16]

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