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LETTER TO THE EDITOR

A comment on the 'fine-grained' quantum ergodic theorem

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Abstract. A sequence of measured values of a property of a quantum mechanical system is required to calculate the time average of that property. The implications of using the 'projection postulate' in elementary quantum mechanics during the process is discussed in relation to a simple example.

The rules of quantum mechanics have proved very successful in practice without undue attention being attracted to any underlying conceptual problems and work on the conceptual foundations of the subject has, if anything, provided support for the confidence shown in the applicability of the rules. Such work has, however, focused attention on the role of measurement in the theory and the dangers of discussing 'unobserved properties'. This letter considers some implications of the apparent neglect of the role of measurement in the derivation of the 'fine-grained' quantum ergodic theorem.

In classical mechanics the time average $\langle F \rangle$ of some time-dependent property F(t) of a system is defined by

$$\langle F \rangle = \lim_{T \to \infty} \frac{1}{T} \int_0^T F(t) \, \mathrm{d}t. \tag{1}$$

According to standard presentations of the foundations of quantum statistical mechanics [1-4] the time average $\langle F \rangle$ of an observable \hat{F} is, by analogy with the classical expression, to be calculated using an equation of the form

$$\langle F \rangle = \lim_{T \to \infty} \frac{1}{T} \int_0^T \left(\Psi(t), \, \hat{F} \Psi(t) \right) \, \mathrm{d}t \tag{2}$$

where the evolution of a wavefunction $\Psi(t)$ representing a quantum mechanical system with a Hamiltonian \hat{H} is determined by the time-dependent Schrödinger equation

$$i\hbar\partial\Psi/\partial t = \hat{H}\Psi.$$
(3)

If the wavefunction at some initial time is represented by $\Psi(0) = \sum_k a_k \phi_k$, where ϕ_k are the eigenfunctions of the Hamiltonian \hat{H} and E_k are the corresponding energy eigenvalues, then the wavefunction at a later time t is, according to equation (3), given by $\Psi(t) = \sum_k a_k \exp(-iE_k t/\hbar)\phi_k$. The expectation value of the observable \hat{F} at this later time is then given by

$$(\Psi(t), \hat{F}\Psi(t)) = \sum_{k,l} a_k^* a_l F_{kl} \exp[-i(E_l - E_k)t/\hbar].$$
(4)

The standard presentations then argue that two main conclusions follow.

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(a) The expectation value given by equation (4) is an almost periodic function of the time and as a consequence the time average (2) exists but, in general, this time average is not necessarily the same as the 'phase average' required by statistical mechanics [1-4].

(b) The almost periodic nature of expectation value implies that the system exhibits no irreversible behaviour or mixing in the sense of classical ergodic theory and is subject to an even stronger form of 'Poincaré recurrence' than in the classical case [3].

Two features should be noted.

(i) Equation (2) defines a time average of the expectation value of \hat{F} and the calculation must, accordingly, refer to an 'ensemble' of systems.

(ii) The time behaviour of a system is assumed to follow a continuous evolution as determined by the Schrödinger equation (3).

The significance of the latter point, with which this letter is mainly concerned, follows from realising that the classical definition (1) attempts to express in mathematical form the idea that a time average of some property of a system is determined by a sequence of measured (observed, recorded) values of that property. To calculate such a quantity in the case of classical mechanics it is assumed that the continuous evolution of a system (as determined by the equations of motion) is unaffected, in principle, by a sequence of measurements. This is sometimes referred to as macroscopic non-invasive measurability. (The expression does, of course, define a continuous time averaging process, but it will be expedient to consider the case of a sequence of discrete measurements.)

The rules of elementary quantum mechanics [5] state that the wavefunction $\psi(t)$ changes continuously according to equation (3) during intervals of time when no measurements are made. At the time of a measurement, however, the wavefunction changes discontinuously ('reduction postulate' or 'collapse of the wavefunction'). The state of the system immediately after the measurement process is then determined by the result obtained. The use of a continuously evolving solution obtained from equation (3) starting from some initial time is, accordingly, in conflict with a satisfactory interpretation of a time average since it fails to recognise the effect of the measurement process on the state of the system. During the time averaging procedure each measurement in the sequence exhibits a particular eigenvalue of the observable and there is a corresponding reduction of the wavefunction. The reduced wavefunction representing the system immediately after a measurement then evolves according to equation (3) and this evolved wavefunction determines the probabilities for the possible outcomes on the occasion of the next measurement.

The need to include the effects of the measurement process in the calculation of a time average is clear. Less apparent, perhaps, is the need to interpret the limiting time behaviour of a system as the limiting behaviour of a sequence of measured (recorded, observed) values, but this does correspond to 'recognising' such behaviour in practice.

A simple example illustrates the procedure (and at the same time clarifies the use of 'ensembles'—point (i) above). Consider a spin- $\frac{1}{2}$ particle in a *B* field directed along the *z* direction. Using standard notation the Hamiltonian \hat{H} is given by $\hat{H} = (e/mc)B\hat{S}_z$. Suppose that the system evolves from the eigenstate of \hat{S}_x corresponding to the eigenvalue $+\hbar/2$. The wavefunction at the end of an interval of time τ is given by

$$\frac{1}{\sqrt{2}} \left(\exp(-i\omega\tau/2) \\ \exp(+i\omega\tau/2) \right) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \cos(\omega\tau/2) + \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \sin(\omega\tau/2)$$

where the RHS expresses the result in terms of the eigenstates of the operator \hat{S}_x and

where $\omega = eB/mc$. The probability of measuring an x component of spin to be $+\hbar/2$ at the end of the interval of time τ is $\cos^2(\omega\tau/2)$ and that of $-\hbar/2$ is $\sin^2(\omega\tau/2)$. If, instead, the system evolves from an initial state corresponding to the eigenvalue $-\hbar/2$ then the corresponding probabilities are $\sin^2(\omega\tau/2)$ and $\cos^2(\omega\tau/2)$, respectively. Having made a measurement the spin- $\frac{1}{2}$ particle is in an eigenstate which then evolves according to equation (3) until the next measurement.

A sequence of observed values is a realisation of a random process and consists of a sequence of eigenvalues (in this case there are only two possibilities). By introducing an 'ensemble' the average behaviour of a large number of similar systems can be described. Consider an ensemble of spin- $\frac{1}{2}$ particles prepared such that the initial proportions with spins $+\hbar/2$ and $-\hbar/2$ at a time t = 0 are given by $n_+(0)$ and $n_-(0)$ respectively. After an interval of time τ the proportions $n_+(\tau)$ and $n_-(\tau)$ are given by

$$\binom{n_+(\tau)}{n_-(\tau)} = \binom{(1-p)}{p} \binom{n_+(0)}{n_-(0)}$$

where $p = \sin^2(\omega \tau/2)$.

The distribution after N such intervals, i.e. at the time $t = N\tau$, is then given by

$$\binom{n_+(N\tau)}{n_-(N\tau)} = \binom{(1-p)}{p} \binom{p}{(1-p)}^N \binom{n_+(0)}{n_-(0)}.$$

A sequence of measurements conducted with a constant time interval τ between measurements is, accordingly, represented by a simple Markov chain.

It is easy to verify (by induction) that

$$\binom{(1-p)}{p} \binom{p}{(1-p)}^{N} = \binom{\frac{1}{2} + (1-2p)^{N}/2 \quad \frac{1}{2} - (1-2p)^{N}/2}{\frac{1}{2} - (1-2p)^{N}/2 \quad \frac{1}{2} + (1-2p)^{N}/2}$$

so that as $N \to \infty$, there exists a limiting 'equilibrium state' of the ensemble with proportions $n_{+} = \frac{1}{2}$ and $n_{-} = \frac{1}{2}$ provided 0 .

This argument yields the following conclusions.

(a') The 'time average' is equal to the average corresponding to the final equilibrium state. The time average corresponds to the appropriate 'phase average' in this case.

(b') Any initial state of the collection, represented by the proportions $n_+(0)$ and $n_-(0)$, evolves during the sequence of measurements to the equilibrium state. This limiting time behaviour can be interpreted as an analogue of 'mixing'.

If the time interval τ is such that $p = \sin^2(\omega \tau/2)$ assumes the value 0 or 1 then the proportions remain constant or oscillate, respectively. A sequence of measurements made at random time intervals clearly yields the same results as for 0 above, although in this case the process is no longer a simple Markov chain. A random sequence of measurements has, however, the advantage of allowing the inclusion of intervals with <math>p = 0 and p = 1 without affecting the conclusions (a') and (b').

An analogue of the H theorem for the ensemble (being regarded as a collection of systems each of which can exist in one of two possible states) can easily be formulated by defining $H(N\tau) = \sum_{\sigma=+,-} [n_{\sigma}(N\tau)] \log[n_{\sigma}(N\tau)]$. $H(t = N\tau)$ is then a monotonically decreasing function of the time and attains its minimum value $H_{\min} = -\log 2$ in the equilibrium state.

The above time behaviour can be compared with that provided by the standard argument. This would clearly give oscillating values for the proportions as functions

of time. There would be no limiting 'equilibrium state' although, of course, the time average would exist.

This simple example illustrates that the interpretation of a time average in terms of observed properties has a considerable effect on the sequence of values required for its calculation. Furthermore, the operational interpretation of a time average exposes the inadequacy of a continuously evolving expectation value and reveals the need for observed values. This suggests that the 'behaviour of a system in time' might also be more appropriately described in terms of 'observed properties'. The resulting time behaviour of a system and, in particular, the limiting time behaviour of an ensemble of systems is likely to be very different from that obtained according to the standard treatments which simply consider the 'unobserved evolution' of the Schrödinger equation. This conclusion is not affected by attempts to render the projection postulate redundant by developing a 'theory of measurement' which basically tries to show that a macroscopic system evolves, according to the Schrödinger equation, to a well defined macroscopic state (macroscopic realism). Such attempts have not been particularly successful and quickly encounter the need to include ergodic properties or some aspect of irreversibility.

The continuous observation of a quantum mechanical system (in time) has been discussed in the literature and some difficulties in relation to decay processes noted (see, for example, 'Zeno's paradox' [6-9]). The problems do not appear to have attracted as much attention as the well known 'paradoxes' (for example, the EPR 'paradox', Schrödinger's cat or Wigner's friend [5,10,11]) which tend to emphasise spatial and macrosopic effects (separability, non-locality, macrosopic realism, etc) rather than temporal effects.

Perhaps the conclusion of this letter can be expressed in a provocative form by asking whether it is meaningful to discuss the growth of an unobserved tree in the quad if the unobserved tree is not there.

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