On the nature of the quantum states of macroscopic systems

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It is assumed that the quantum state that may describe a macroscopic system at a given instant of time is one of the eigenstates of the reduced density matrix calculated from the wave function of the system plus its environment. This implies that the above quantum state is a member of a special orthonormed set of states. Using a suitable Monte-Carlo simulation, this property is shown to be consistent with the extremely small standard deviation for the coordinates and the momenta of macroscopic systems. Consequences for statistical mechanics and possible observable effects are discussed.

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Despite of the well known conceptual difficulties [1, 2, 3], there is no compelling reason to believe that quantum mechanics fails when applied to macroscopic systems. It is then reasonable to ask what are the properties of quantum states of macroscopic systems. In order to fit experience, such a quantum state should yield extremely small standard deviation for both the position and the momentum of the center of mass. On the other hand, due to the large number of particles contained in macroscopic bodies, they possess an extremely high energy level density, or an extremely small average level spacing. Correspondingly, a macroscopic system \( M \) cannot be isolated from its environment \( E \); hence, according to orthodox quantum mechanics, it cannot be characterized by a wave function, only by a suitable reduced density matrix \( \rho \), resulting from the wave function \( \Psi \) of the composite system \( M + E \) by taking the partial trace of \( |\Psi\rangle\rangle \) over the Hilbert space of the environment [4].

Nevertheless, it is still possible to assign a wave function to the system \( M \). To show this, let us consider a simplified description of a spin measurement on a spin-half particle. Suppose that the \( S_z \) spin component is measured, and initially the particle is in the state \(|\uparrow\rangle\rangle\), which is the eigenstate of the \( S_z \) operator corresponding to the eigenvalue \( +\frac{1}{2} \). Then the measurement process may be symbolically written as \(|\uparrow\rangle\rangle |m_0\rangle \rightarrow |\uparrow\rangle |m_\uparrow\rangle \), where \(|m_0\rangle \) stands for the initial state of the measuring device, and \(|m_\uparrow\rangle \) stands for the state of the measuring device when it shows the result \( +\frac{1}{2} \). The horizontal arrow denotes the (unitary) time evolution, satisfying the Schrödinger equation.

Similarly, if the initial state of the particle is \(|\downarrow\rangle\rangle\), corresponding to the eigenvalue \( -\frac{1}{2} \), the measurement process can be written as \(|\downarrow\rangle\rangle |m_0\rangle \rightarrow |\downarrow\rangle |m_\downarrow\rangle \).

If the initial state of the particle is the superposition \(|\alpha\rangle\rangle + |\beta\rangle\rangle \) (with \(|\alpha|^2 + |\beta|^2 = 1\)), then, owing to the linearity of the Schrödinger equation we may write \(|\alpha\rangle\rangle + |\beta\rangle\rangle |m_0\rangle \rightarrow \alpha |\uparrow\rangle |m_\uparrow\rangle \beta |\downarrow\rangle |m_\downarrow\rangle \).

Looking at the final state of the system, one can see that the measuring device has no own wave function, instead, it can be characterized by the density matrix \( \bar{\rho} = |m_\uparrow\rangle \langle m_\uparrow| + |m_\downarrow\rangle \langle m_\downarrow| \). Extrapolating the conclusion of this simple example, it is reasonable to assume that a macroscopic system is described by one of the eigenstates of its reduced density matrix \( \bar{\rho} \), calculated from the wave function of the Universe, and the probability that this particular eigenstate occurs is given by the corresponding eigenvalue. This has already been proposed by several authors [5, 6, 7]. A consistent theory involving this idea can be found in Ref. [8]. It is of worth mentioning that this latter theory is an explicit counterexample to Bell’s theorem [9].

The next question is how the reduced density matrix of a macroscopic system looks like if the interaction with the environment is taken into account. This is the central problem of the phenomenon ‘environment induced decoherence’ [7, 9], and as such, has been much studied in model systems. A typical model [10] contains a number of harmonic oscillators playing the role of a heat bath (this is the environment) and a macroscopic object coupled to it. As a result of the interaction, the reduced density matrix of the macroscopic object becomes nearly diagonal in both coordinate and momentum representation, so that the width along the diagonal is macroscopically small, while the distribution along the diagonal (this is the probability distribution of the coordinate in coordinate representation and the probability distribution of the momentum in momentum representation) extends to a macroscopic regime. Note that (up to the present author’s best knowledge) none of the decoherence models studied so far possesses the property that the eigenstates of the reduced density matrix are generically localized. The reason may well be that these models are oversimplified.

\[ \text{The environment itself is a physical system, consisting of air molecules, radiation field, other macroscopic systems etc.} \]
Considering now the mathematical consequences of the above idea, one finds that the quantum state of a macroscopic system is a member of an orthonormal set of states\[^2\]. The relevant eigenstates of the reduced density matrix (i.e., those which occur with non-negligible probability) must correspond to a macroscopic region of the classical phase space, therefore, their number is given by this phase space volume divided by Planck’s constant \( \hbar \) (in one dimension, in \( f \) dimension one must use \( \hbar^f \) instead). All the relevant eigenstates must possess the classical property that the standard deviation for both the coordinates and the momenta (\( \delta x \) and \( \delta p \), respectively) is microscopically small. The aim of the present paper is to answer the question whether it is possible mathematically at all.

It is natural to ask whether there exists such a complete, orthonormal basis that the standard deviations \( \delta x \), \( \delta p \) for all the basis functions lie below a common bound. The answer is known in the one-dimensional case when the basis functions are generated from the same function by translations along the \( x \) and \( p \) directions \[^3\]. It turns out that completeness, orthonormality and boundedness of \( \delta x \) and \( \delta p \) cannot be simultaneously fulfilled.

We made a numerical study to decide whether it is also true if the basis functions are not generated by translations. The method was the following. Initially one dimensional oscillator eigenstates \( |n> \) below a given energy \( E_0 = (N - 1/2)\hbar \omega \) were considered. Certainly, in this case \( \delta x_n \propto \delta p_n \propto \sqrt{n} \). Then new basis functions \( |\tilde{n}> \) were constructed by a unitary transformation \( |\tilde{n}> = \sum_{j=0}^{N-1} U_{nj}|j> \).

The transformation matrix was chosen so as to minimize the sum of \( \delta x^2 + \delta p^2 \) for all the \( N \) basis functions. (The units were chosen so that \( \hbar = 1 \), \( \omega = 1 \), \( m = 1 \).) As \( \delta x^2 = \langle \tilde{n}|\tilde{x}^2|\tilde{n}> - \langle \tilde{n}|\tilde{x}|\tilde{n}>^2 \), and \( \sum_{n=0}^{N-1} \langle \tilde{n}|\tilde{x}^2|\tilde{n}> = \sum_{j=0}^{N-1} \sum_{k=0}^{N-1} U_{nj}^* U_{nk} <j|\tilde{x}^2|k> \)

\( = \sum_{n=0}^{N-1} \sum_{j=0}^{N-1} \sum_{k=0}^{N-1} U_{nj}^* U_{nk} <j|\tilde{x}^2|k> \) (similarly for \( \delta p \)), it was enough to maximize the quantity \( S = \sum_{n=0}^{N-1} |\tilde{n}|\tilde{x}|\tilde{n}>^2 + |\tilde{n}|\tilde{p}|\tilde{n}>^2 \).

The transformation matrix was built up as a product of unitary matrices, each having only one nontrivial 2 by 2 block. The corresponding indices were randomly chosen. For the other indices the matrix was just the unit matrix. The most general 2 by 2 unitary transformation is the transformation matrix of the basic spinors which may be parametrized by three angles. For each matrix, these angles were chosen at random, and it was subsequently considered whether the result of this transformation gave rise to a larger sum \( S \) or not. If yes, then the transformation was kept, if not, it was discarded. The method was therefore a simple Monte-Carlo simulation. The procedure was continued until the quantity \( S \) saturated. The resulting average deviations (i.e., the sum of \( \delta x^2 + \delta p^2 \) for all the \( N \) states divided by \( N \)) as a function of various \( N \) values is plotted in Fig.1. The error of the data is less than \( 0.2^{-2} \). The measured values are surprisingly well fitted by the logarithmic function \( 1.0 + 0.6 \ln(N) \). This result supports the generalization of the statement of Ref. \[^1\], i.e., it shows that no complete, orthonormed basis with bounded standard deviations \( \delta x, \delta p \) exists.

\[\text{FIG. 1. Diamonds: the average of } \delta x^2 + \delta p^2 \text{ over all the } N \text{ states versus } N. \text{ Dashed line: the logarithmic fit } 1.0 + 0.6 \ln(N).\]

Returning to the original question, we show that the logarithmic dependence on \( N \) is consistent with the requirement that the relevant eigenstates (i.e., those with significant probability to occur) of the reduced density matrix must have small \( \delta x, \delta p \) values\[^4\]. Indeed, the relevant eigenstates of \( \tilde{\rho} \) are associated with a large but finite portion of the classical phase space. We choose the number \( N \) to be the ratio of this phase space volume and Planck’s constant \( \hbar \). The widths \( \delta x, \delta p \) of the relevant eigenstates are proportional to \( \sqrt{0.5 + 0.3 \ln(N)} \). This quantity remains moderate even for an astronomically large \( N \) value. As an example, consider the motion of the Earth. The linear size in coordinate space is \( 3 \times 10^{11} \) m, and that in momentum space is \( 3.6 \times 10^{29} \text{kg m}^2 \). Therefore,

\[^2\]The latter property is due to the hermiticity of the reduced density matrix \( \tilde{\rho} \).

\[^3\]The irrelevant eigenstates may be identified with the original oscillator eigenstates \( |n> \) with \( n \geq N \).

\[^4\]This is valid in one dimension. In dimension \( d \) we divide by \( \hbar^d \), and the number \( N \) is chosen to be the \( d \)-th root of the ratio, as the basis functions will be constructed as a \( d \)-fold direct product of the one-dimensional basis. For simplicity we shall consider only the one-dimensional case.
$N = 1.6 \times 10^{74}$ and $\sqrt{0.5 + 0.3 \ln (N)} = 7.2$. Thus the widths $\delta x, \delta p$ are only one order of magnitude larger than those of the minimal wave packet $|0\rangle$. As we see, the logarithmic dependence makes the above assumption about the wave functions of macroscopic systems physically acceptable. Nevertheless, the problem is left open whether these states actually occur in Nature and if so, what the origin of their 'localization' property is. Certainly, it should be due to the interaction between the macroscopic system and its environment (as this produces the mixed state described by $\hat{\rho}$), but that feature of the dynamics which is responsible for classical behavior is unknown. It should be emphasized that the 'nearly diagonal' shape of the density matrix is nearly diagonal in both coordinate and momentum representation, but its eigenstates are oscillator eigenstates with $\delta x_n \propto \delta p_n \propto \sqrt{n}$. Here we consider only some consequences if the above logarithmic localization of the macroscopic quantum states actually occurs.

Let us consider first a harmonic oscillator of unit mass and frequency (certainly, these units may be as large as 1 kg and 1 s$^{-1}$), and calculate the mean deviation of the energy in the above localized states. Certainly, the average of this quantity depends on the number of the states ($N$), as for larger $N$ the states are broader. The dependence of the average square deviation of the energy on the number of states is plotted in Fig.2.

![Graph](image)

**Fig. 2.** Diamonds: the average of $\delta E^2$ (the squared deviation of the energy) over all the $N$ states versus $N$. Dashed line: the fit $0.44N^{1.25}$.

Somewhat surprisingly, this dependence is not logarithmic, but power-like, with the exponent $\approx 1.25$. This means that

$$\delta E \propto N^{0.63}$$

(1)

The mean energy is proportional to $N$ (as $N$ is chosen according to the relevant classical phase space volume), therefore, the relative uncertainty of the energy, i.e., $\delta E/E$ goes to zero as $N^{-0.39} \propto (\frac{1}{N})^{-0.39}$. Certainly, in case of a macroscopic oscillator this is unobservable, although $\delta E$ itself can be quite large at the microscopic scale $\hbar\omega$.

In order to understand the behavior (1), let us consider the asymptotic behavior of the above localized states in coordinate representation. Beyond $\sqrt{N}$ they fall off as $\exp(-x^2/2)$, due to their construction. For smaller distances (down to some $x_0$) they decay like a power. The exponent is $\nu \approx -1.5$. This readily implies that

$$\delta^2 x = \int_{x_0}^{\sqrt{N}} dx |\psi(x)|^2 x^2 \approx \text{const.} \times \int_{x_0}^{\sqrt{N}} dx x^{-1} = a_1 + b_1 \ln (N)$$

where $a_1$ and $b_1$ are constants. The behavior in momentum space is the same. As for the square deviation of the energy, we have to consider the expectation value of $\hat{\delta}^2 x + \hat{\delta}^2 p + \hat{\delta}^2 p^2 + \hat{\delta}^2 x^2$. We may write e.g.

$$<\hat{\delta}^4 x> = \int_{-\infty}^{\infty} dx |\psi(x)|^2 x^4 \approx \text{const.} \times \int_{x_0}^{\sqrt{N}} dx x = a_2 + b_2 N$$

One can derive the same linear estimate for $<\hat{\delta}^4 x>$ as well. This implies that $\delta^2 E$ grows at least linearly with $N$, which is consistent with the numerically obtained $N^{1.25}$.

In order to get further consequences, let us consider a macroscopic system being in thermal equilibrium with a heat bath at temperature $T$. What is the density matrix of that system at a given instant of time? One would guess that it is

$$\frac{1}{Z} \exp (-\beta H) ,$$

(2)

where $\beta = \frac{1}{k_BT}$ and $Z$ stands for the canonical partition function. This expression, however, substitutes a long time average, therefore, one cannot expect that it is strictly valid at a given instant of time. According to the previous considerations, it is more realistic to assume that (2) gives only the long time average of the density matrix, which is actually given by $\rho = \sum_\nu |\varphi_\nu> p_\nu <\varphi_\nu|$, where $|\varphi_\nu>$ is narrow in both coordinate and in momentum space if $p_\nu$ is not negligible small. As energy eigenstates are generically not localized, the $|\varphi_\nu>$-s are not eigenstates of the Hamiltonian $H$, therefore, $\hat{\rho}$ will have non-diagonal matrix elements in energy representation. Explicitly, these matrix elements are $\rho_{jk} = <\xi_j|\hat{\rho}|\xi_k> = \sum_\nu p_\nu <\xi_j|\varphi_\nu><\varphi_\nu|\xi_k>$, where $|\xi_k>$-s stand for the energy eigenstates. The states $|\varphi_\nu>$ are also localized in energy representation.
(i.e., for a given $n < \xi_j | \varphi_n >$) takes on significant values only for a narrow range of the energy eigenvalues $E_j$, thus $\rho_{j,k}$ is a narrow band matrix.

The existence of nondiagonal matrix elements in energy representation can in principle lead to experimentally observable effects. Suppose one isolates the macroscopic system in question so that the interaction energy $\Delta E_I$ with the environment becomes much less than the effective width $\delta E$ of the density matrix in energy representation. Under such circumstances consider the linear response of the system. For a time $t$ which is much less than $\hbar/\Delta E_I$ but much larger than $\hbar/\delta E$ the deviation in the expectation value of an operator $\hat{A}$ is

$$\delta < \hat{A} > (t) = -\frac{i}{\hbar} \int_0^t dt' \text{Tr} \left( \left[ \hat{A}(t), \hat{H}_1(t') \right] \hat{\rho}(0) \right),$$

where $\hat{H}_1$ is the perturbation, and the operators are Heisenberg operators calculated with the unperturbed Hamiltonian $\hat{H}_0$. Choosing $\hat{A} = \hat{H}_0$, the response can be cast to the form

$$\delta < \hat{H}_0 > (t) = \sum_{j,k} (\rho_{j,k}(t) - \rho_{j,k}(0)) < \xi_k | \hat{H}_1(0) | \xi_j >,$$

where $\rho_{j,k}(t) = \exp \left(-\frac{i}{\hbar}(E_k - E_j)t\right) \rho_{j,k}(0)$. If the density matrix were strictly diagonal in energy representation, the response $\delta < \hat{H}_0 > (t)$ would vanish. Actually, as noted above, $\rho_{j,k}(0)$ is a narrow band matrix, hence the Fourier transform of the response vanishes at high frequencies but becomes significant at low frequencies. Therefore, the localization property of the eigenstates shows up in a suitable linear response which increases at low frequencies. It is a challenging question whether this behavior may be related to the celebrated $1/f$ noise [12]. It is also of worth noting that the deviation of the density matrix from the canonical expression [12] implies the breakdown of the fluctuation-dissipation theorem.

In conclusion, we have seen that

i, in one dimension there is no localized basis in the strict sense

ii, the numerically found 'logarithmically localized' basis demonstrates that the idea that macroscopic systems are described by the eigenstates of their reduced density matrix is consistent with experience

iii, this idea implies that the density matrix of a macroscopic system being in thermal equilibrium is not diagonal in energy representation, that may be observed in the spectrum of a suitable linear response function as an enhancement at low frequencies.

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