The decoherence criterion

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Abstract

The decoherence mechanism is an useful tool signaling the limits beyond which the use of quantum mechanics becomes meaningless from a physical point of view and then classical mechanics has to be applied. We show that decoherence also signals the limits beyond which quantum field theory must be used instead of quantum mechanics.

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The problem of the range of applicability of quantum mechanics (QM) has been the object of much attention and studies since the early days of its foundation. However, only at a later time it has been fully recognized and appreciated the purely quantum phenomenon of decoherence \cite{1, 2, 3, 4, 5}, which in many cases signals the \textit{appearance of a classical world in quantum theory} \cite{5}. Decoherence is normally triggered by the interaction of the system with the environment and formally consists in suppressing the off-diagonal elements of the reduced density matrix. Its effect is such that quantum superposition in the system wave function is destroyed and thus, provided the time-scale $\tau_{\text{dyn}}$ characteristic of the dynamics is much greater than the decoherence time-scale $\tau_{\text{dec}}$, $\tau_{\text{dyn}} \gg \tau_{\text{dec}}$, the classical behavior may be approached. It should be noted that sometimes the system under consideration, assumed to be a closed system, is viewed as composed of two subsystems and we are actually interested only in one of them. The other subsystem is then regarded to be the environment in which the former one is embedded. The reduced density matrix is

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the one obtained by tracing over the degrees of freedom of the environment (the rest of the Universe, whatever it is).

Decoherence provides an interesting explanation why we do not experience superpositions of objects in the macroscopic world. In fact interaction with the environment produces decoherence in the superposition of macroscopically separate positions so that the familiar classical behavior of non-superposing macroscopic objects is obtained. However, we also have experience (and sound theoretical understanding) of the existence of macroscopic quantum systems, such as superconductors, ferromagnets, crystals, and in general systems presenting ordered patterns, where coherence over macroscopically large distances appears to be particularly stable against environment perturbations. Any system is made by quantum components. It is, of course, not in such a trivial sense that macroscopic systems such as a superconductor or a crystal are quantum systems. These are quantum systems in the specific, non-trivial sense that their macroscopic (classical) behavior cannot be explained without recourse to quantum theory. It is then natural, and necessary, asking the question of the consistency between the decoherence phenomenon and the existence of macroscopic quantum systems. This is indeed the question we address in this paper.

Our result is that the decoherence mechanism is a powerful tool in signaling that macroscopic quantum systems cannot be in fact described by QM. This is consistent with the well known fact that one needs to use quantum field theory (QFT) in order to describe macroscopic quantum systems \(\text{[6, 7, 8]}\). Decoherence thus characterizes QM by designing its borderlines with classical mechanics, from one side, and with QFT, from the other side.

We arrive at our result by computing the decoherence time for a series of known crystal salts and we show that the decoherence mechanism in QM forbids the existence of such crystals, including the familiar crystal of NaCl salt. The same result is obtained by considering X-ray diffractometry data compared with decoherence mechanism.

There is a large body of literature on decoherence and for the sake of shortness we do not reproduce here the already published derivations of the formulas we are going to use. We refer for that to the quoted papers. We consider as our examples of macroscopic quantum systems the crystals listed in Tab.1. Our considerations apply in general to all of them; however to be specific, we focus our attention on the sodium chloride. The wave function of the \(Na^+\) ion, centered at the proper site in the \(NaCl\) crystal, must present spatial superposition over a length of the order of the \(Na - Cl\) separation distance. We consider two possible sources of decoherence: the ion-ion collisions and the interactions with distant ions. There are also other sources of decoherence such as, e.g., the interaction with the environment, or else with the crystal lattice as a whole (under the assumption that the crystal is already formed), or with dipole and higher moments of charge distribution. These interactions may be interfering with the crystal formation (or with its stability, if the crystal is already formed). However, the decoherence effect we compute from ion-ion collisions and distant ion interactions are so strong that we can neglect any other decoherence
The density matrix for the $Na^+$ ion may be shown to be proportional to a function $f(x, x', t)$ which does not depend on the ion state $|\Psi_i\rangle$. Here $x$ denotes the ion position. For scattering of environment particles with de Broglie wavelength $\lambda$, we have

$$f(x, x', t) = e^{-\Lambda t \left(1 - e^{-\frac{|x' - x|^2}{2\lambda^2}}\right)},$$

that is,

$$f(x, x', t) \sim \begin{cases} e^{-\Lambda t \frac{|x' - x|^2}{2\lambda^2}} & \text{for } |x' - x| \ll \lambda, \\ e^{-\Lambda t} & \text{for } |x' - x| \gg \lambda, \end{cases}$$

where $\Lambda \equiv n < \sigma v >$ is the scattering rate cross section. The product of the cross section by the velocity $v$ is averaged over the thermal velocity distribution at $T = 310$ K, $n$ is the density of the scatterer centers (ions). Since the de Broglie wavelength of the $Na^+$ ion (mass $m_{Na} = 22.990$ amu) or the $Cl^-$ ion (mass $m_{Cl} = 35.453$ amu) is

$$\lambda = \frac{2\pi \hbar}{\sqrt{3mkT}} \sim 0.3 \text{\AA},$$

while the inter-ionic distance ($|x - x'|$) in an elementary cell of the crystalline salt typically is of the order of few \text{\AA}, we are clearly in the $|x - x'| \gg \lambda$ limit of equation (2). In the case of two ion-ion collision with unit charge $q$ and with relative velocity $v$ the cross section is evaluated to be $\sigma$:

$$\sigma \sim \left(\frac{gq^2}{m^2}\right)^2,$$

where $g = 1/4\pi\varepsilon_0$ is the Coulomb constant. The decoherence time $\tau_1 \equiv (\Lambda N)^{-1}$, with $N$ the number of scatterers, is then given by

$$\tau_1 \sim \frac{\sqrt{m(kT)^3}}{N\rho g^2 q^4}.$$

We have used $v \sim \sqrt{\frac{kT}{m}}$ at thermal equilibrium. For a crystalline substance $N$ is of the order of $10^{23}$, and for $NaCl$ the density $n$ is $n = 2.163 \times 10^3 kg m^{-3}$ [11]. Then we have:

$$\tau_1 \sim \frac{\sqrt{m(kT)^3}}{10^{23} \frac{2.163}{m_{Na} + m_{Cl}} g^2 q^4} \sim 4.6 \times 10^{-10} \text{ s}.$$

For the other crystals see the $\tau_1$ values in Tab.1. In a similar way one can show that for the interaction with distant ions the decoherence time $\tau_2$ is given by $\tau_1$. 

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In this case $a = 5.64$ Å is the edge of the cubic elementary cell (distance between two $Na^+$ ions).

In the following table we report the decoherence time for a set of crystalline binary compounds, in the two cases of ion-ion collisions ($\tau_1$) and of interactions with distant ions ($\tau_2$), respectively.

Table I. Decoherence time for ion-ion collisions ($\tau_1$) and for interactions with distant ions ($\tau_2$)

<table>
<thead>
<tr>
<th>salts</th>
<th>$\tau_1/10^{-30}$s</th>
<th>$\tau_2/10^{-38}$s</th>
</tr>
</thead>
<tbody>
<tr>
<td>NaF</td>
<td>2.6</td>
<td>4.9</td>
</tr>
<tr>
<td>NaCl</td>
<td>4.6</td>
<td>4.4</td>
</tr>
<tr>
<td>NaBr</td>
<td>5.5</td>
<td>4.9</td>
</tr>
<tr>
<td>NaI</td>
<td>7.1</td>
<td>5.8</td>
</tr>
<tr>
<td>KF</td>
<td>5.1</td>
<td>5.2</td>
</tr>
<tr>
<td>KCl</td>
<td>8.3</td>
<td>7.1</td>
</tr>
<tr>
<td>KBr</td>
<td>9.6</td>
<td>7.9</td>
</tr>
<tr>
<td>CsF</td>
<td>13.4</td>
<td>12.0</td>
</tr>
<tr>
<td>CsCl</td>
<td>17.3</td>
<td>21.0</td>
</tr>
<tr>
<td>CsBr</td>
<td>19.6</td>
<td>25.6</td>
</tr>
<tr>
<td>CsI</td>
<td>23.6</td>
<td>27.8</td>
</tr>
<tr>
<td>AgCl</td>
<td>9.5</td>
<td>9.2</td>
</tr>
<tr>
<td>AgBr</td>
<td>10.7</td>
<td>10.0</td>
</tr>
<tr>
<td>AgI</td>
<td>15.3</td>
<td>12.7</td>
</tr>
<tr>
<td>ZnS</td>
<td>7.2</td>
<td>7.2</td>
</tr>
<tr>
<td>PbS</td>
<td>16.2</td>
<td>14.7</td>
</tr>
</tbody>
</table>

We stress that the results in Tab.1 are the output of the purely QM decoherence phenomenon. According to them, due to the very short decoherence time, the considered crystals are not QM systems: They do not exist as stable quantum systems. Then one could naively conclude that they are systems ruled by classical mechanics. Of course, such a conclusion is wrong: It contradicts the well known and experimentally well tested QFT description of the crystals. The correct conclusion from Tab.1 is then that in the case of the crystal system decoherence points to the border between QM and QFT. Indeed, it must be recalled that QFT is dramatically different from QM, in what QFT, on the contrary of QM, posseses infinitely many unitarily inequivalent representations of the canonical commutation relations. We will comment more on this crucial point in the following.
It is also interesting to observe that the wavelength used in the X-ray diffraction experiments with the crystals listed in Tab.1 is $\lambda \sim 1.5\text{Å}$, corresponding to oscillation time $\tau_X$ of the order of $0.5 \times 10^{-18}$ s, too long compared with $\tau_{1,2}$ in Tab.1. Again we see that the QM decoherence picture is not consistent with familiar experimental methodologies (which also, on the other hand, confirm the quantum dynamical nature of the system). Suppose, however, one wants to insist in using, e.g., eq. (5). Then, by putting $\tau_1 \equiv \tau_X$ and $n = n_X$, we have

$$\frac{\tau_1}{\tau_X} = \frac{n_X}{n},$$

i.e. the X-ray typical diffraction time $\tau_X$ would correspond, e.g. for NaCl, to a density $n_X$ of the scatterer centers of the unacceptable order of $10^{-18}$, and, from

$$n_X = 10^{-18} = \frac{(m_{Na} + m_{Cl}) \text{amu}}{a^3},$$

we have the equally absurd lattice cell length $a \sim 10^{-3}m = 10^7\text{Å}$. Equally unacceptable conclusions are reached by using eq. (7).

Let us now try to fit our result in the frame of the common knowledge of many body theory. We remark that our conclusions are nothing more than a confirmation of the fact that the crystal system is not a QM system. It is known that the crystal is a QFT system. It has infinitely many degrees of freedom. Let us recall that the von Neumann theorem states that in QM, since the number of the degrees of freedom is finite, all the representations of the canonical commutation relations are unitarily (and therefore physically) equivalent. In QFT there are infinitely many degrees of freedom and thus the von Neumann theorem does not hold and the space of the states splits into infinitely many unitarily inequivalent representations (foliation) \[11, 12, 13, 14, 7\]. Due to the von Neumann theorem, QM fails in describing degenerate phases such as the crystalline phase and other ordered phases occurring in the macroscopic quantum systems. Then one needs QFT. It is the existence of the state space foliation in QFT that makes the essential difference between QFT and QM. The novelty (and the interesting aspect) of the result we obtain is in the use of the decoherence mechanism as a criterion to scan the border QM/QFT. As far as we know, the existing literature has not paid attention to this side of the confining limits of QM by using the decoherence phenomenon.

According to our discussion, decoherence may be then promoted to the relevance of a criterion, able to discriminate between QM and QFT, from one side, and classical mechanics from the other side. Thus, generally speaking, decoherence does not necessarily signals the approaching of the classical mechanics regime; it may also signals the approaching of the QFT regime, indeed. One must carefully consider the physics of the system under study in order to correctly conclude on the implications of decoherence.

Thus, as shown above, the origin of the high stability of macroscopic quantum systems cannot be in the QM superposition mechanism. It is in the coherent condensation in the ground state of long range correlation modes (the Nambu-Goldstone
boson modes), which is implied by the mechanism of spontaneous breakdown of symmetry. In the crystal case, the continuous space translational symmetry is spontaneously broken and the Nambu-Goldstone boson modes are the phonons. Since in QFT there are many unitarily inequivalent representations of the canonical commutation relations, to each of them is associated a vacuum or ground state, and thus there is a large possibility of choice for the physical ground state of the system. Each of these ground states describes a different phase of the system and is therefore physically inequivalent to the other ones. One may select a physically relevant observable, called the order parameter (the magnetization in ferromagnets, the density in crystals, etc.), which, assuming different values in each of the vacua, fully characterizes the system ordering phase. Such an order parameter is a macroscopic observable since its value is not affected by quantum fluctuations. It is indeed a measure of the coherence (ordering) of the corresponding ground state. Because of the unitarily inequivalence one ground state (and the states of the corresponding phase) cannot be expressed as superposition of the other ground states (and of the states of the associated phases). Thus we have a non-perturbative scheme, in the sense that one cannot express, is some sort of perturbation series, the ground state with specified symmetry properties as superposition of other ground states: e.g. it is mathematically and physically meaningless trying to express the crystal ground state in terms of the gaseous (non-crystal) ground state or the superconducting ground state in terms of the "normal" (i.e. fully symmetric) ground state, and so on. Therefore one cannot expect that the crystal state may be expressed by spatial superposition of the crystal component wave functions: the crystal state is, on the contrary, the macroscopic quantum state dynamically generated by the coherent condensation of the phonons. These boson modes (the phonons) are responsible of the long range correlation among the system elementary components and thus they characterize the macroscopic properties of the system.

All of this is a well known story.

Of course, one might try less orthodox routes, such as theorizing the description of ferromagnets, superconductors, crystals and other ordered systems by using short range interactions (hooks) among the system components. However, presently the only available theory, experimentally well tested, is the QFT with spontaneous breakdown of symmetry depicted above.

In conclusion, the decoherence mechanism turns out to be an useful criterion to signal not only the approaching of the classical mechanics regime, but also the approaching of the QFT regime. Contrarily to current common belief, decoherence does not necessarily and uniquely implies the appearance of the classical world. It might as well imply the appearance of macroscopic quantum systems. Which one of these two dynamical regimes is realized can only be inferred from a further careful analysis of the system under study.

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Bibliography