Thermodynamic Limit and Decoherence: Rigorous Results

Marco Frasca
Via Erasmo Gattamelata, 3
00176 Roma (Italy)
E-mail: marcofrasca@mclink.it

Abstract. Time evolution operator in quantum mechanics can be changed into a statistical operator by a Wick rotation. This strict relation between statistical mechanics and quantum evolution can reveal deep results when the thermodynamic limit is considered. These results translate in a set of theorems proving that these effects can be effectively at work producing an emerging classical world without recurring to any external entity that in some cases cannot be properly defined. In a many-body system has been recently shown that Gaussian decay of the coherence is the rule with a duration of recurrence more and more small as the number of particles increases. This effect has been observed experimentally. More generally, a theorem about coherence of bulk matter can be proved. All this takes us to the conclusion that a well definite boundary for the quantum to classical world does exist and that can be drawn by the thermodynamic limit, extending in this way the deep link between statistical mechanics and quantum evolution to a high degree.

1. Introduction

The problem of measurement in quantum mechanics is one of the greatest open questions hotly debated in physics being at the root of the way our common perceived reality is produced. Despite a longstanding analysis, after the introduction of a concept of environmental decoherence [1] with an external agent that eliminates quantum correlations, the idea of having some intrinsic effect producing the same results is still open. In the seventies Klaus Hepp proposed the thermodynamic limit as such a cause [2] but some others approaches were also put forward [3, 4, 5]. At the date the question is not settled yet.

It is important to point out that environmental decoherence poses some serious conceptual difficulties that motivated most of the approaches today considered. As an example, one should consider the rather strange situation of Hyperion, a Saturn’s moon, that was claimed by Zurek [6] to become quantum after the very short period of about ten years without environmental decoherence. This discussion is still open [7, 8].

In this paper we support the view that an instability is indeed at work in the thermodynamic limit [9] largely extending the initial proposal by Hepp. Indeed, both experimental and theoretical support today exists for this view and we present here some rigorous results about. It should be emphasized that this approach takes to completion the deep analogy between statistical and quantum mechanics.
2. A general theorem about bulk matter

All the low energy phenomenology is fully described by the Hamiltonian \[10\]

\[
H = -\sum_{j=1}^{N_e} \frac{\hbar^2}{2m} \nabla_j^2 - \sum_{\alpha=1}^{N_e} \frac{\hbar^2}{2M_\alpha} \nabla_\alpha^2 - \sum_{j=1}^{N_e} \sum_{\alpha=1}^{N_e} \frac{e^2}{|x_j - R_\alpha|} + \sum_{j<k} \frac{e^2}{|x_j - x_k|} + \sum_{\alpha<\beta} \frac{Z_\alpha Z_\beta e^2}{|R_\alpha - x_\beta|}
\]

that is able to describe all the properties of matter as far as we know. We have put \(N_e\) the number of electrons, \(N_t\) the number of positive ions, \(e\) the electron charge, \(Z_\alpha\) the number of positive charges for each ion.

Introducing the density and neglecting for our aims the repulsion between positive ions assumed to be pointlike and classical, the following energy functional is obtained

\[
\mathcal{E} = T - Ze^2 \int \frac{\rho(x')}{|x'|} d^3 x' + \frac{e^2}{2} \int \int \frac{\rho(x')\rho(x'')}{|x' - x'|} d^3 x' d^3 x''
\]

being \(T\) the kinetic energy given by

\[
T = \int d^3 x_1 d^3 x_2 d^3 x_3 \ldots d^3 x_N \Psi^*(x_1, x_2, \ldots, x_N) \left( -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \Delta_2i \right) \Psi(x_1, x_2, \ldots, x_N)
\]

being \(m\) the electron mass, \(\rho(x)\) the electronic density computed by the Slater determinant \(\Psi\), if the Hartree-Fock approximation is invoked, as \(\int d^3 x_1 d^3 x_2 d^3 x_3 \ldots d^3 x_N \Psi^*(x_1, x_2, \ldots, x_N) \Psi(x_1, x_2, \ldots, x_N)\), \(Z\) is the number of positive charges and \(e\) the electron charge. We assume neutrality, that is, the number of electrons, \(N = \int \rho(x) d^3 x\), is the same as the number of positive charges in the system. One could transform the functional \(\mathcal{E}\) into a density functional \(\mathcal{E}[\rho(x)]\), bypassing self-consistent Hartree-Fock equations for the Hartree-Fock approximation, if it would be possible to obtain the kinetic energy as a functional of \(\rho(x)\).

We would like to accomplish such a task in the classical limit \(\hbar \to 0\). We can reach our aim by referring to standard results in nuclear physics [11] and Bose condensation [12] as also given in [13]: The density matrix can be developed into a \(\hbar \to 0\) series, derived from the Wigner-Kirkwood series for the Green function for a single particle moving in the Hartree-Fock potential \(V[13]\)

\[
G(x, x'; t) = G_{TF}(x, x'; t) \left[ 1 + \frac{\hbar^2}{12m} \left( \frac{t^2}{\hbar^2} \Delta V - i \frac{t^3}{\hbar^3} |\nabla V|^2 \right) + \ldots \right],
\]

whose leading order is just the Thomas-Fermi approximation

\[
G_{TF}(x, x'; t) = \left( \frac{m}{2\pi i \hbar} \right)^{\frac{3}{2}} \exp \left[ \frac{im(x - x')^2}{2\hbar t} - \frac{it}{\hbar} V \left( \frac{x + x'}{2} \right) \right]
\]

giving the density of kinetic energy as

\[
\tau_{TF} = \frac{3}{10} \frac{\hbar^2}{m} (3\pi^2)^{\frac{3}{2}} \rho(x)^{\frac{5}{2}}.
\]

So, we can conclude that the Thomas-Fermi approximation can represent classical objects being the leading order of a semiclassical approximation.

For our aims this is not enough as we are interested in the limit of a large number of particles in the energy functional we started with. Indeed, there is another theorem due to Lieb and Simon [15] [16] that gives an answer to this question: The limit of number of particles \(N\) going to infinity for energy functional \(\mathcal{E}\) is the Thomas-Fermi model. This means that in this limit
we recover again the leading order of a semiclassical approximation. So, classical objects can be obtained when the number of particles in a system increases without bound because the limit of a number of particles going to infinity coincides with the semiclassical limit \( \hbar \to 0 \).

This result can hold only if it is stable under perturbations. Indeed, the dynamical equations for the Thomas-Fermi approximation are given by [17]

\[
\frac{\partial W}{\partial t} + \mathbf{v} \cdot \nabla_x W - \frac{1}{m} \nabla_x (V + \mathcal{E}_F) \cdot \nabla_v W = 0
\]

(7)

\[
\Delta_2 V(x, t) = 4\pi e^2 [\rho(x, t) - Z \delta(x)]
\]

(8)

\[
\rho(x, t) = \int W(x, v, t) d^3 v
\]

(9)

being \( W(x, v, t) \) the Wigner function and \( \mathcal{E}_F = \frac{\hbar^2}{2m}(3\pi^2)^{\frac{3}{2}} \rho(x, t) \) the Fermi energy. This is just the classical limit of the Wigner-Poisson set of equations and the conclusion is that classicality holds only if the initial preparation of the system permits the effectiveness of Landau damping that damps out any perturbation. Otherwise, higher order quantum corrections come into play and the behavior is no more classical. This complete the proof.

3. Spin systems

Spin systems are crucial for an understanding of the way a decoherence mechanism does work. The reason for this relies on the fact that off-diagonal terms in the density matrix of such systems appears to oscillate without any apparent decay. Indeed, recently this opened up some discussion [18, 19]. The problem relies on the way numerical results should be considered reliable when a large number of spins is interacting. The point is that a sin function with a very large frequency, as happens when there are a large number of spins, is very difficult to sample and becomes just a random number generator [9]. Indeed the physics is quite different as recently proved by experiments with organic molecular crystals [20, 21, 22, 23]. They observe a Gaussian decay in time of quantum coherence that depends crucially on the number of spins of the system. So, we immediately see that numerical computations appear to be at odds with experiments.

An explanation to the experimental results comes from a recently proved theorem due to Hartmann, Mahler and Hess that can be stated in the following form (here and in the following \( \hbar = 1 \))

If the many-body Hamiltonian \( H = \sum_i H_i \) and the product state \( |\phi\rangle \) satisfy \( \sigma_\phi^2 \geq NC \) for all \( N \) and a constant \( C \) and if each \( H_i \) is bounded as \( \langle \chi | H_i | \chi \rangle \leq C' \) for all normalized states \( |\chi\rangle \) and some constant \( C' \), then, for fidelity, the following holds

\[
\lim_{N \to \infty} \langle \phi | e^{-iHt} | \phi \rangle^2 = e^{-\sigma_\phi^2 t^2}.
\]

(10)

and this is in perfect agreement with the experimental results as one has a Gaussian decay with a decaying time inversely proportional to the number of interacting spins. This is an intrinsic property of these systems.

Two points are relevant for this result. First of all there is a problem with recurrence. This means that coherence can be recovered after some time. The above experiments did not check this. We will see below for the Dicke spin-boson model how this fact is harmless for the appearance of a classical world in the thermodynamic limit. The second question is linked to the Gaussian evolution of the system. This result is well-known since the work of Misra and Sudarshan about quantum time evolution [25, 26]. One has that at very short times a quantum system display Gaussian time evolution. This means that in the thermodynamic limit just the short time evolution is meaningful for spin systems. We will support also this view with the discussion of the Dicke model.
4. Dicke model

A point that is generally neglected is that to realize a measurement on a quantum system, the only means we have is electromagnetic interaction. The question that naturally comes out in view of this simple consideration is if QED can manifest decoherence in the thermodynamic limit in the low energy limit. We showed recently that in the low energy limit several approximations hold for QED reducing the model to the well-known Dicke model [27, 28]. This model has Hamiltonian for a single radiation mode

\[ H = \omega a^\dagger a + \frac{\Delta}{2} \sum_{i=1}^{N} \sigma_{3i} + g \sum_{i=1}^{N} \sigma_{1i}(a^\dagger + a) \]  

(11)

being \( a, a^\dagger \) the annihilation and creation operators, \( \omega \) the frequency of the mode, \( \Delta \) the separation between the levels of each two-level atom in the ensemble we are considering, \( g \) the coupling and \( \sigma_{1i}, \sigma_{3i} \) the Pauli spin matrices of the i-th atom. We are interested on the effect of the limit \( N \to \infty \) on the radiation mode.

One can show [28] that when the limit \( N \to \infty \) is taken, the Hamiltonian ruling the dynamics of the model is

\[ H_F = \omega a^\dagger a + g \sum_{n=1}^{N} \sigma_{1i}(a^\dagger + a) \]  

(12)

that is, the model is integrable and the unitary evolution operator is straightforwardly written down as

\[ U_F(t) = e^{-iH_Ft} = e^{i\xi(t)} e^{-i\omega a^\dagger at} \exp[\hat{\alpha}(t) a^\dagger - \hat{\alpha}^*(t) a] \]  

(13)

being

\[ \hat{\xi}(t) = \left( \sum_{i=1}^{N} \sigma_{1i} \right) \frac{2}{\omega} g^2 (\omega t - \sin(\omega t)) \]  

(14)

and

\[ \hat{\alpha}(t) = \left( \sum_{i=1}^{N} \sigma_{1i} \right) \frac{g}{\omega} (1 - e^{i\omega t}) \]  

(15)

When the ensemble of two-level atoms is largely polarized (for the sake of simplicity we take a fully polarization), for a generic radiation state \( \sum c_n |n\rangle \) being \( |n\rangle \) number states, one has

\[ \langle U_F(t) \rangle = e^{i\xi(t)} e^{-\frac{N^2 g^2}{\omega^2} (1 - \cos(\omega t))} \sum_{m,n} c_m^* c_n e^{-im\omega t} \frac{1}{m!} \left[ \frac{Ng}{\omega} (1 - e^{i\omega t}) \right]^{m-n} L_n^{m-n} \left[ \frac{2N^2 g^2}{\omega^2} (1 - \cos(\omega t)) \right]^{n-m} \]  

(16)

The real significant term in this solution is given by \( e^{-\frac{N^2 g^2}{\omega^2} (1 - \cos(\omega t))} \) that for \( N \to \infty \) goes to zero except for very small times near the zeros of \( 1 - \cos(\omega t) \) where it reproduces a Gaussian. We have shown our main assertion that only short times are meaningful for time evolution in the Dicke model in the thermodynamic limit [9]. This describes a collapsing Gaussian evolution in agreement to Misra and Sudarshan analysis.

As the zeros of the function \( 1 - \cos(\omega t) \) are recurring with a period \( 2\pi/\omega \) we face here the problem of recurrence. The crucial point for this case is the width of the recurring Gaussian. This is given by a time \( 1/Ng \) that becomes decreasingly small with \( N \) becoming increasingly large reaching unphysical values for a macroscopic ensemble of atoms. This warrants that no recurrence is ever observed and a truly classical state is reached and maintained as also happens for spin systems. Numerical evidence exists for these results [29, 30].

Finally, we point out that the opposite limit of a large number of photons has been discussed by Gea-Banacloche [31, 32] and experimentally proved by Haroche’s group [33, 34].
5. Conclusions
We have presented a lot of theoretical, mostly theorems, and some experimental evidence supporting our view that the thermodynamic limit has a deep meaning also in quantum mechanics. A lot of experimental activity could be accomplished to understand how relevant is such an approach to real systems. E.g. Haroche’s group tested QED for a large number of photons but nobody has done the same for a large number of atoms so far. On the other side, the situation of spin systems appears more promising in the short term as also happens in interference of large molecules \[35\]. In this latter cases possible interesting news can be expected. The success of this view will prove more striking than ever the link between such different approaches as quantum and statistical mechanics.

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