Dynamics of Complex Quantum Systems: Dissipation and Kinetic Equations

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Abstract

We present a microscopic approach to quantum dissipation and sketch the derivation of the kinetic equation describing the evolution of a simple quantum system in interaction with a complex quantum system. A typical quantum complex system is modeled by means of parametric banded random matrices coupled to the subsystem of interest. We do not assume the weak coupling limit and allow for an independent dynamics of the “reservoir”. We discuss the reasons for having a new theoretical approach and the new elements introduced by us. The present approach incorporates known limits and previous results, but at the same time includes new cases, previously never derived on a microscopic level. We briefly discuss the kinetic equation and its solution for a particle in the absence of an external field.

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1. Introduction

The notion of a complex (quantum) system might not be an uniquely and universally accepted term, but it is certainly a very widely (over)used one. We shall call systems with a large number of degrees of freedom complex systems. One might reasonable ask: “Why a new term?”.

The real reason we believe, besides the temptation to add something “new” to the jargon, is to make a distinction with much simpler systems studied in the near past by the community contributing to this volume. Typically, in complex quantum systems a relatively small number of degrees of freedom (DoF) can be singled out in one way or another and one might be interested, or forced, to study the dynamics of this reduced set of DoF. Since these selected DoF are coupled, either weakly, but most likely strongly, to the rest of the DoF of the system and even to the rest of the Universe, one is faced with the problem of devising ways to predict and describe the dynamics of non-isolated quantum systems.

In a certain sense such systems can be also called open quantum systems. However, the term open quantum system has a slightly different connotation. In the case of an open system there is...
an “orifice” through which once in a while the system can “leak out”, or better put, “drop out”, and never come back. In an open system the role of the “rest of the Universe” is typically reduced to a simple “black hole” or a “drain” or a “sink”, which “swallows” matter out of the system as “been fed”, thus “stuff simply falls out of the system”, and the “rest of the Universe” does not really exert any real force on the system of interest. One can say that the “rest of the Universe” is “forced fed”, but with no “real effort”. The “rest of the Universe” can also serve as a “source” of matter, but again, this is done in the same somewhat “non–obtrusive way” as the time–reverse process of “swallowing”. The “rest of the Universe” can even play both roles, “sink” and “source”, at the same time. Thus an open system is nothing else, but a system with somehow modified boundary conditions. One might argue that a matter flux can influence dynamics. That would be correct if one would consider a system of interacting particles, whose number can vary in time. The folks typically involved with open quantum systems study physics at the independent particle level however.

A complex system in the sense we shall be using is however somewhat different. We shall not allow (yet) matter exchange, simply for the sake of simplicity, but allow only for energy exchange between the part of the system we have decided (or have been forced to) to focus our attention on and the “rest of the Universe”. Both parts of the system have their own dynamics, but at the same time, the interaction between them could be strong enough as to modify the dynamic evolution in a qualitative or quantitative manner. The qualifier “complex system” refers as a rule either to the “rest of the Universe” only or to the entire system. The dynamic evolution of the “rest of the Universe” is routinely assumed to fall in one or another universality class, described in Quantum Mechanics by some random Hamiltonian [1] or by some other Hamiltonian with “complex dynamics”. If the interaction between the two subsystems would have been weak, one would have dealt with a situation typically studied in Statistical Physics textbooks. The energy exchange between the two subsystems could be characterized as in Thermodynamics as either mechanical work (thus reversible) or heat exchange (consequently irreversible). If irreversible processes occur, one obviously has entropy production as well. Moreover, if one would have concentrated one’s attention only on the dynamics of the smaller system, the bigger one would most likely have been called a thermal bath, and one would have aimed at obtaining a kinetic description of the dynamics of the smaller/simpler system. If the “rest of the Universe” is huge, one might reasonable argue that the influence of the subsystem on it should be negligible and thus could be ignored. Besides the fact that that is not always the case of interest (when the “rest of the Universe” is not huge, like in the case of the interaction between the collective DoF in a nucleus and the rest), there is no need to influence all the “rest of the Universe”, but only the part lying nearby and if the heat conductivity of the “rest of the Universe” is low, energy will not be quickly transferred to the outskirts of the “rest of the Universe”.

There was a significant interest over the years in quantum problems similar to the type we have just described. Caldeira and Leggett [2], using a technology outlined by Feynman and Vernon [3] have studied the motion a “heavy” particle interacting with a reservoir of harmonic oscillators. The reservoir of harmonic oscillators is assumed to mock a quantum “heat” reservoir. The quantum Hamiltonian describing the “Universe” according to Caldeira and Leggett has the form

$$H = \frac{p^2}{2M} + U(Q) + \sum_{k=1}^{\infty} \left[ \frac{p_k^2}{2m_k} + \frac{m_k\omega_k^2}{2}(q_k - c_kQ)^2 \right],$$

(1)

with the corresponding $p$’s and $q$’s and so forth and the coupling constants $c_k$. A continuous distribution of these harmonic oscillators leads to a dissipative dynamics of the “heavy” system described by momentum $P$ and coordinate $Q$ and in particular to a Langevin description in the classical limit. The fact that this particular classical limit should emerge in the high–temperature regime, was one of the requirements imposed on the structure of the model Hamiltonian in Eq.
This model Hamiltonian suffers however from one rather simple inadequacy, which is at least intellectually unsatisfactory. Let us assume that we would like to describe the dissipative motion of a particle in a homogeneous medium. There is no external potential $U(Q)$ then and it is completely unclear in this case how one can define a coupling to the reservoir, as there is obviously no special point with respect to which one can measure $Q$, since the medium is supposed to be homogeneous. One might consider instead a coupling through a derivative term, i.e. to the momentum of the “heavy” particle. Then one would have had to alter the time–reversal properties of the Hamiltonian for no other particular reason. A coupling to the momentum typically implies some gauge field. In particular, such a mechanism will not work in one dimension, as no magnetic field exists in 1D. Moreover, simply having to consider a gauge field for the sake of having dissipation looks like an overkill, at least from a theoretical point of view. Coupling to spin degrees of freedom for the same reason should be ruled out as generic. Thus we seem to find ourselves in a quandary. Even in the presence of an external field, the fictitious harmonic oscillators become more and more elongated as the “heavy” particle moves away from the “center” and thus the “reservoir” becomes “infinitely stretched” and consequently, due to the presence of an infinite number of DoF in the reservoir, “infinitely excited” too. Moreover, even though it is entirely reasonable to be guided by the “known” classical limit when “guessing” the structure of the model Hamiltonian, one can hardly accept this as a satisfactory recipe and a suitable solution for all cases. On one hand, the form of the friction force is not unique even in classical physics, classical friction force can be proportional to the velocity at various powers or even independent of velocity. On the other hand, atomic nuclei for example represent systems in which there is no classical limit and they are certainly not unique in this respect. Moreover, there very well could be a genuine quantum dissipative regime, which has no counterpart in the classical limit.

We would like to start from a model “typical Hamiltonian” of a “typical quantum complex system”, with a minimum and relevant amount of input and find out under what conditions a dissipative dynamics emerges, what is its character and how various properties of this dynamics depend on the particular properties of the initial Hamiltonian. It is not obvious that one will arrive at the same type of description as Caldeira and Leggett have obtained. As a matter of fact we find that choosing this alternative approach one sometimes arrives at a dissipative dynamics similar to that found by Caldeira and Leggett.

The surprise however is that dissipative dynamics with entirely new characteristics emerges as well. The particular example of quantum Lévy flights and fractional kinetics is one remarkable case [4].

There is another direction of inquiry in the theory of open quantum systems or quantum dissipative dynamics, which we shall mention only very superficially [5]. The main emphasis in these approaches is phenomenological, at the level of the von Neuman equation and its possible extensions, such as to accommodate a Markovian evolution, to preserve the positivity of the density matrix and to conserve the probability. As one might have expected from a pure phenomenological approach, there has been no effort to understand the nature and the origin of various terms added to the von Neuman equation from any underlying microscopic dynamics, as no such derivation has ever been attempted, except cases when perturbation theory could be implemented and one ends up with a textbook master equation.

This sketchy review of the literature is not meant to be exhaustive or comprehensive in any sense. The aim was merely to point the reader to some literature leads and to justify in some very limited way our approach and line of reasoning. We deeply apologize for not devoting more space and emphasis to so much fine work, not mentioned here mostly due to space limitations. The rest of the contributors to this volume will surely complement us.

2. A generic quantum complex system

We shall describe here what we view as a generic quantum complex system and the rea-
sons why we have chosen this perspective. The Hamiltonian of the “entire Universe” we choose as follows [6]

\[ \mathcal{H} = \frac{p^2}{2M} + U(Q) + H(Q), \]  

(2)

where \( H(Q) \) is supposed to describe the “rest of the Universe” and the interaction with the selected DoF with canonical coordinates \((P, Q)\), which could stand for one or more pairs of canonical variables. The “rest of the Universe” is assumed typically to be a very large system, with a large heat capacity. It is convenient to choose an average level density of states of the “rest of the Universe” which is locally exponentially increasing,

\[ \rho(\varepsilon) = \text{Tr}\rho[H(Q) - \varepsilon] = \rho_0 \exp(\beta \varepsilon). \]  

(3)

The overline stands for averaging over some portion of the spectrum or for an ensemble averaging to be described shortly. Thus \( \beta = 1/T \) is nothing else but the inverse thermodynamic temperature of the “rest of the Universe”. So far we have always chosen an average level density which is independent of the coordinate \([4,6–8]\). In physical terms this means that only heat exchange is allowed so far between the selected subsystem and the “rest of the Universe”. We do not see any difficulties of any kind to incorporate the possibility for the system to perform work on the “rest of the Universe” as well (or vice versa). Allowing for the temperature \( T \) to vary apparently could require some further small technical developments of our formalism. The relevant “dependence” of the Hamiltonian \( H(Q) \) on the subsystem coordinate \( Q \) is implemented by modeling it with a random matrix \([1]\) and specifying the second cumulants of its matrix elements: \([9]\)

\[ \overline{[H(X)]_{kl}[H(Y)]_{mn}} - [H(X)]_{kl} [H(Y)]_{mn} = [\delta_{km} \delta_{ln} + \delta_{kn} \delta_{lm}] \frac{\Gamma^i}{2\pi \sqrt{\rho(\varepsilon_k)\rho(\varepsilon_l)}} \]

\[ \times \exp \left[ -\frac{(\varepsilon_k - \varepsilon_l)^2}{2\kappa_0^2} \right] G \left( \frac{X - Y}{X_0} \right). \]  

(4)

Here \( \Gamma^i \) is the so called spreading width, \( \kappa_0 \) defines the bandedness of the random matrix and it can be interpreted as the energy of a “single kick”. To \( X_0 \) we refer to as the correlation length. Even though we have used GOE-type of induced spectral fluctuations, similar results are obtained for the GUE or GSE case. This in a way could have been expected. It is natural to expect that most/many complex systems have universal spectral fluctuations at some small energy scales as both theory and experiment indicate. A GOE Hamiltonian is suitable for an even number of fermions, while a GSE Hamiltonian for an odd number of fermions \([1]\). A “reservoir” with an odd or even number of fermions could not influence in qualitatively different ways a given subsystem.

The correlation length \( X_0 \) is perhaps one of the most interesting parameters of the entire theory. The function \( G((X - Y)/X_0) \) \((G(0) = 1\) and \( G(x) = G(-x) = G^*(x) \leq 1\)) is assumed to have a bell shape with a characteristic width \( X_0 \). Thus \( X_0 \) specifies by how much one has to move the subsystem \((Q, P)\) in order to induce some noticeable changes in the “rest of the Universe”. Obviously, if the “rest of the Universe” does not react in any way and does not change its properties while the subsystem \((Q, P)\) evolves, there is no energy exchange and no change in entropy as well. (We trust that this is neither the place nor the time where one should discuss at any length why entropy can vary, even though one might claim that the entropy of the entire system is strictly conserved.) The restriction adopted here of “translation invariance” has no fundamental consequences and apparently can be lifted without much effort.

From the characterization given so far of the Hamiltonian \( H(Q) \) of the “rest of the Universe” and of the coupling to the subsystem \((Q, P)\) one can see the differences with other approaches mentioned in the introduction, in particular with the most “microscopic” theory of Caldeira and Leggett \([2]\). The “translation invariance” of the present approach includes the case of the motion of a subsystem \((Q, P)\) in a homogeneous medium.

From this point on the development of the theory follows Feynman and Vernon strategy \([3]\), one writes down a double path–integral for the density matrix of the entire system, one integrates out the “rest of the Universe” and in the end one
arrives at an evolution equation for the density matrix of the subsystem \((Q, P)\). It is surprising that in the limit of high temperatures and large bandwidth of the matrix \([H(Q)]_{kl}\) (namely, when \(\kappa_0\rho(\varepsilon) \gg 1\)) one arrives and an extremely simple looking evolution equation for the reduced density matrix of the subsystem \(\rho(X,Y,t)\), which reads:

\[
\frac{i\hbar}{\partial t} \rho (X,Y,t) = \left\{ \frac{P^2_X}{2M} - \frac{P^2_Y}{2M} + U(X) - U(Y) \right. \\
- \frac{\beta \Gamma_1 \hbar}{4X_0 M} G' \left( \frac{X - Y}{X_0} \right) (P_X - P_Y) \\
\left. + i\Gamma_1 \left[ G \left( \frac{X - Y}{X_0} \right) - 1 \right] \right\} \rho (X,Y,t). \tag{5}
\]

Hopefully no confusion with the notation used earlier for the average level density should arise. The derivation, which is somewhat lengthy and requires an extensive discussion of various steps, is described in our earlier works and shall not be repeated here. The “rest of the Universe” is allowed to have its own dynamic evolution and it is not assumed to be in thermal equilibrium or to have a prescribed evolution. Some rather innocent assumptions are also made about the nature of the initial conditions \([6,8,10]\). In the case when one simply drives the “rest of the Universe” one can show that the energy distribution has significant non-Maxwellian distortions \([8]\). The coupling between the subsystem \((Q, P)\) and the “rest of the Universe” is not assumed to be weak at any stage, even though the limit of weak coupling is obviously embodied as well in the evolution equation (5).

By means of a Wigner transform and in the case when for small arguments

\[
G(x) \approx 1 - x^2/2 + \ldots \tag{6}
\]

the evolution equation (5) reduces in the limit \(\hbar \to 0\) to the Kramers equation \([6]\), and thus the equivalent Langevin description is also obtained. The classical friction force in this case is proportional to the first power of the velocity, the friction and diffusion coefficients are given by

\[
\gamma = \frac{\beta \Gamma_1 \hbar}{2MX_0^2}, \quad D_{QQ} = \frac{2X_0^2}{\beta^2 \Gamma_1 \hbar} \tag{8}
\]

and the standard Einstein dissipation–fluctuation relation is satisfied.

One might have considered the fact that this classical limit is exactly reproduced under apparently correct conditions as a necessary self–consistency check of the entire approach. The power of the present approach is demonstrated however by being able to generate other distinct and consistent classical limits as well, which, as far as we can judge, was not shown to be possible within the framework of approaches previously known in the literature. In particular, a rather innocently looking change of the correlator \(G(x)\) for small arguments to

\[
G(x) = 1 - |x|^\alpha + \ldots \tag{9}
\]

with \(0 < \alpha \leq 2\) leads to apparently the first microscopic derivation of fractional kinetics with Lévy flights \([4]\), without assuming or introducing any kind of exotic noise. The only “noise” is of the usual rather boring Gaussian type. A completely different behavior, turbulent–like diffusion \([11]\]

\[
\langle Q^2 \rangle \propto t^\beta \tag{10}
\]

is also in the realm of this type of evolution equation (5). The double angle brackets stand for cumulants.

Surprisingly, in many cases the evolution equation can be solved in quadratures for arbitrary type of coupling between the two subsystems \([4,6,7]\). Time–dependent solutions of the Schrödinger equation are known for the case of free motion, linear potential, harmonic potential. Path–integrals also can be calculated in cases when the action is essentially quadratic in \(p\)'s and \(q\)'s. To our surprise the solution of Eq.(5) can be obtained easily if the classical trajectories in the absence of dissipation (i.e. no \(G((X - Y)/X_0)\)) are known. Several cases were discussed by us in Refs. \([6,7]\). Here we shall illustrate a few salient points of our approach on the example of motion in the absence of any external field \((U(Q) = 0)\), but for arbitrary type of coupling to the “rest of the Universe”. In 1D and representing the density matrix in the coordinates \(r = (X + Y)/2\),
s = X − Y one can show that for an arbitrary initial density matrix ρ0(X, Y), for t > 0 one has

\[ \rho(r, s, t) = \int \int \frac{dr' dk}{2\pi\hbar} \rho_0 \left( r', s - \frac{kt}{M} \right) \exp \left[ \frac{ik(r - r')}{\hbar} \right] + \frac{\Gamma M}{\hbar k} \int_{s - kt/M}^{s} ds' [G(s'/X_0) - 1]. \] (11)

This form of the density matrix is especially suited to evaluate the coordinate and momentum cumulants as functions of time.

In the long time limit the momentum distributions reaches an equilibrium, characterized by vanishing odd cumulants, while the even cumulants are given by \((n \geq 2)\)

\[ \langle \langle P^{2n} \rangle \rangle = (-1)^{n-1} \frac{(2n - 1)!!}{n} \frac{MX_0^2}{\hbar^2 \beta} \left( \frac{\hbar}{X_0} \right)^{2n}, \] (12)

for the particular case of a Gaussian correlator

\[ G(x) = \exp(-x^2/2). \] (13)

The second cumulant has the expected value

\[ \langle \langle P^2 \rangle \rangle = 2MT, \] (14)

if only for small arguments the correlator behaves as in Eq. (6). There is nothing special about the Gaussian form of the correlator \(G(x)\) used here, which was simply chosen for illustrative purposes.

The parameter which governs the deviation of the equilibrium distribution from the one expected in the weak coupling limit Maxwellian distribution is \(\hbar/X_0\) and not as one would have naively guessed the “strength” of the coupling \(\Gamma\). \(\hbar/X_0\) could be interpreted as the characteristic momentum exchanged between the system and the “rest of the Universe” in “one completed interaction act”. The equilibrium momentum distribution is narrower than a pure Maxwellian distribution at the same temperature.

Some information about the coordinate distribution has been inferred as well [6]. The second cumulant reveals what one would have expected, namely that for \(t \to \infty\)

\[ \langle \langle Q^2 \rangle \rangle \propto 2D_{QQ}t, \] (15)

again, if only for small arguments the correlator behaves as in Eq. (6). A qualitative analysis of the coordinate distribution seem to indicate the presence of “longer tails” than one would have obtained in the case of a simple Brownian particle. That does not seem so surprising now when we have learned that under very mild circumstances one easily obtains Lévy flights behavior and fractional kinetics [4] or turbulent–like diffusion [11]. However, a comprehensive analysis of the entire coordinate distribution is not achieved yet.

Analytical results can also be obtained for a particle in a linear potential or in a quadratic potential (both harmonic oscillator and parabolic barrier) and qualitatively similar deviations from the textbook cases of the weak coupling regime are found. The very interesting case of tunneling in a double well potential has been studied only numerically so far [6,7], along with other cases which have some resemblance to under the Coulomb barrier collision and tunneling of two atomic nuclei. Evidently, our approach is not limited to 1D as one might have concluded, simply because we did not explicitly display spatial subscripts.

3. Concluding remarks

On a closer analysis and in retrospective the fact that we have used a random matrix ensemble, with various adds-on, does not seem to have played a fundamental role. If that would have been the case we would have seen some distinction between GOE, GUE and GSE cases, which we did not confirm [10], even though at one time that was expected [12], but later on apparently not confirmed as well [13]. The fact that a random matrix approach is not critical to obtaining the final answer was confirmed as expected in Ref. [14] in the weak coupling limit. As we have mentioned in the Introduction, it would have been indeed very strange if a GOE–reservoir would lead to a different kinetic equation than a GUE– or GSE–reservoir.

However, the particular approach based on the use of parametric banded random matrices allowed us significantly more freedom in choosing various forms of coupling between the “rest of the Universe” and the subsystem of interest. In the wide band limit of a random matrix we find
that the kinetic equation is determined essentially completely by the correlator \( G(X - Y) \), which defines correlation between properties of the Hamiltonian describing the “rest of the Universe” at two different locations of the simple subsystem. Besides the thermodynamic temperature of the “rest of the Universe” one needs essentially only two more quantities to define the character of the dissipative dynamics, the “intensity” of the coupling controlled by the spreading width \( \Gamma \downarrow \) (we avoid using the term strength of the coupling for reasons discussed in Section 2) and by the so called correlation length \( X_0 \), which defines the typical momentum exchanged between the two subsystems. In the usual \( \hbar \to 0 \) limit, the friction and diffusion coefficients depend explicitly on \( \hbar \), see Eqs. (7,8), which seems inconsistent. The resolution of this apparent puzzle is simple, one cannot simply consider the limit \( \hbar \to 0 \), while keeping \( X_0 \) and \( \Gamma \downarrow \) fixed; the corresponding combinations entering in these relations could be held fixed, in particular \( \Gamma \downarrow \hbar / X_0^2 \).

As we have seen, the freedom of choice our approach gives us by allowing various shapes for the correlator \( G(X - Y) \), leads to new interesting cases, such of those of Lévy flights dynamics and turbulent diffusion, and perhaps some other cases, which at the moment we do not suspect yet.

Even though the limit of a wide band \( (\kappa \rho(\varepsilon) \gg 1) \) could prove more then adequate for many practical applications, it would be satisfying to attempt the calculation of the influence functional using alternative techniques, like the super–symmetry method [15], which do not rely on the \( 1/N \)–expansion. We did mention in previous publications that the present approach seems amenable to describe localization as well, when the finite bandwidth of the random matrix is explicitly taken into account. In that case the influence functional emerging from this model has the structure discussed in Ref. [16].

It would also be interesting to determine under what general requirements one can derive such kinetic equations, in particular by not using random matrix models at all. In spite of the fact that random matrix models have proved by now to be “universal”, we have seen that to some extent even they seem to be too specific.

REFERENCES

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