Open Systems’ Density Matrix Properties in a
Time Coarsened Formalism

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Abstract

The concept of time-coarsened density matrix for open systems has frequently featured in equilibrium and non-equilibrium statistical mechanics, without being probed as to the detailed consequences of the time averaging procedure. In this work we introduce and prove the need for a selective and non-uniform time-sampling, whose form depends on the properties (whether thermalized or not) of the bath. It is also applicable when an open microscopic sub-system is coupled to another finite system. By use of a time-periodic minimal coupling model between these two systems, we present detailed quantitative consequences of time coarsening, which include initial state independence of equilibration, deviations from long term averages, their environment size dependence and the approach to classicality, as measured by a Leggett-Garg type inequality. An interacting multiple qubit model affords comparison between the time integrating procedure and the more conventional environment tracing method.

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1 Introduction

Though not usually presented as such, the density operator formalism provides at least a partial resolution of the quantum mechanical time-arrow conundrum (time inversion invariant equations \textit{versus} the expected and observed uni-directional trend towards equilibration), and does so by invoking some averaging procedure that spoils the unitary development of the pure
state density matrix (DM). The equilibration issue has been particularly acute for closed systems (the Universe or part of it hermetically segregated from the rest, such as trapped ultracold atoms) and has featured in many articles both much cited ones [1]-[4] and those quite recent [5]-[11]. The commonality among these appears to be the inclusion of a random process that is not implicit in the defining equation. There is no consensus on the dependence (or on its absence) on initial conditions of the equilibrating system and in what situation this (or that) occurs (e.g., [12]).

The time-arrow conundrum lends impetus to the present work which derives density matrices in arbitrary representation for open systems, such that a microscopic system is coupled to an ancilla (which can be another microscopic system or a finite or infinite "bath"), and does so by a method of time averaging of the microscopic system’s state function, in contrast to other, more frequently employed procedures, in which a stochastic process or tracing over the ancilla’s states is invoked [13]. It is a development arising from a previous work [14], in which justifications of the time averaging method were given based on the ergodic hypothesis (equating time- and state sampling-averages) [15, 16], and the "minimal coupling model" (shown in equation (1) below) was heuristically derived. [We note that this model, also known as the "monochromatic coupling model", has quite a history starting with laser coupling [17] and other topics, supported by detailed theoretical analysis of the model in the context of Floquet’s theorem by [18] and [19], and very recently in relation to Landau-Majorana-Stückelberg-Zener interferometry [20], also [21]]

After describing (for completeness and in a nutshell) our simplified employment of the time averaged DM method (in section 2), the present work makes the following advances requisite for the establishment and practice of the method: It shows first (in section 3) that the method satisfies the basic theoretical conditions on DM. It then identifies quantitatively the forgetting of initial conditions (section 4). In the short, but central section 5 (propped up by the formal proof in Appendix D) we delineate, apparently for the first time, how the "time coarsening" method for the DM is to be used for open systems coupled to finite-sized environments and, by a natural extension to infinite-sized environments, giving rise in general to non-uniform time weighting. Continuing, the paper develops an interacting N-qubit model (in section 6.1) in order to show how the standard deviation ("distance") of the open system DM vanishes with the size of the ancilla. This leads us (in section 6.2) to a quantitative comparison between the ancilla tracing and time averaging procedures regarding the ancilla’s size dependence of the DM standard deviation in each procedure. The formalism is then applied in sec-
tion 6 to a Leggett-Garg type inequality to investigate quantitatively how the inequality, violated by quantum systems, is reinstated as the ancilla size approaches macroscopics. To make the paper self contained we have briefly reiterated in Appendixes A and B the bare essentials of [14]. As already noted, the way time averaging is to be done for an open (microscopic) system coupled to a finite size environment is the subject of the (mathematical) Appendix D, with implications also for general macroscopic environments.

2 Time Averaging in the Minimal Coupling Model (MCM)

This model was introduced in [14], with motivations and heuristic justification given there, in the form of the Hamiltonian

\[ H(t) = E\sigma_z + k\sigma_x \sin(\omega t) \quad (\omega \to 1) \]  

and the (transposed) solution of the relevant time-dependent Schrödinger equation with pre-fixed initial conditions

\[ \psi(t)^T = [\psi_u(t), \psi_l(t)] \]  

\(\sigma_{z,x}\) are Pauli matrices, \(2E\) is the Zeeman splitting, \(k\) the coupling strength of the spin to the reservoir and the time \((t)\) dependent circular function represents the minimal effect of the latter on the former; \(u, l\) label the upper and lower component in the spinor solution. The DM \(\rho_{ij}\) in an \(ij\) representation is derived from the time averages over a time window \(2\Delta t\) of

\[ M_{ij}(t) \equiv \langle i|\psi(t)\rangle\langle \psi(t)|j > \]  

in the form

\[ \rho_{ij} = \frac{1}{2\Delta t} \int_{t-\Delta t}^{t+\Delta t} d\tau M_{ij}(\tau) \quad (i = u, l) \]  

3 Necessary Conditions for Density Matrices \(\rho_{ij}\)

These were formulated by Fano, as follows [22]:

1. Matrix is Hermitian. This is clearly the case in the above MCM.

2. Matrix trace is one. For the time averages this follows from the normalization to unity of the wave function at any time.
3. In any representation the diagonal elements $\rho_{ii} \geq 0$: this follows from the definition.

4. When diagonalized by a unitary transformation $Tr\rho^2 \leq 1$. This requires that for each diagonalized eigenvalue $(DM)_n(\rho)$ of the DM, $0 \leq (DM)_n(\rho) \leq 1$, in which the equalities hold for pure states. In the present spin-half formalism with two DM eigenvalues this translates to

$$0 \leq \frac{1}{2}(1 \pm \sqrt{G(t)}) \leq 1$$

where the unity in the parentheses comes from unit trace. Here, with a little manipulation,

$$G(t) \equiv \frac{1}{2\Delta t} \int_{t-\Delta t}^{t+\Delta t} (|\psi_u(t')|^2 - |\psi_l(t')|^2) dt' \quad (5)$$

and

$$G(t) \equiv \frac{1}{\Delta t} \int_{t-\Delta t}^{t+\Delta t} \psi_u(t')\psi_l(t') dt' \quad (6)$$

(involving the upper ($u$) and lower ($l$) components of the wave function) and this has to be numerically less than 1 for the last Fano requirement to hold. Now, $G(t)$ is clearly non-negative and is maximal when the two components are throughout real and positive, and limits for this quantity need to be sought. The derivation of a maximum of unity is given in Appendix C.

This completes the proof for the satisfaction of the Fano requirements for time averaged DM.

### 4 Equilibration

The first question that needs to be asked about the model is how it describes equilibration characteristics of the spin system. (The mode and time-duration of the evolution to the equilibrated state, discussed recently in e.g. [23], is outside the scope of the present time-integrated approach. Historically, the dependence of the rate of equilibration on the power-spectrum of the coupling seems to have been first given in [24].) Defining the equilibrated value of $\rho_{ij}(t)$ as that value which is only minimally dependent on time (an issue discussed further in the "Distance" section of this work), we ask how does this depend on the initial conditions and on the strength of the coupling $k$? Also, at what values of this coupling and of other parameters is "full equilibration" (= the maximal entropy stage) attained? Figures 2 and
Figure 1: Upper diagonal density matrix (DM) as function of the coupling strength $k$ for the half-Zeeman splitting $E = 1$, and the following starting values: 1, 0.75, 0.5.

Figure 2: Upper diagonal DM as function of the coupling strength $k$ for a different half-Zeeman splitting $E = \sqrt{2}$, and the following starting values: 1, 0.75, 0.5.
3 show the results. The curves show that the starting value is forgotten beyond $k = 2$ in figure 1 with $E = 1$ and beyond about $k = 3$ in figure 2 with $E = \sqrt{2}$.

Another important lesson from the figure is the strong fluctuations in the results, so that for physical interpretation only the rough averages and tendencies are meaningful. This strongly fluctuating property of the MCM and its analogues are well known from previous works [17]-[20], [25].

5 Non-Uniform Time-Weighting

5.1 Finite Bath: Discrete Energy Levels

For a finite, though large, environment (bath) its level scheme is strictly discrete and the density of states is singular. The coupled subsystem’s instantaneous energy $E(t)$ is continuous. The two systems form together a pure state with eigenenergy $E_{\text{total}}$ (6). Then the continuous (Lebesgue) time integration in equation (4) with uniform time weighting has to be replaced by a discrete sum. Alternatively, the integral has to weighted by the singular factor

$$\sum_i \delta(E_{\text{total}} - E(t) - E_i)/\langle \psi(t) | \delta(E_{\text{total}} - H_{\text{system}} - E_i) | \psi(t) \rangle > \quad (7)$$

where the sum runs over all energy values of the environment and $\delta(x)$ is the Dirac delta function. A proof of this formula is given in Appendix D and an application is provided in section 6.

5.2 Macroscopic Bath: (Quasi-) Continuous Energy Density

For this case, in a straightforward extension of the previous expression, the weighting factor for time coarsening is

$$D(E_{\text{total}} - E(t))/\langle \psi(t) | D(E_{\text{total}} - H_{\text{system}}) | \psi(t) \rangle > \quad (8)$$

in which $D(E_{\text{bath}})$ is the distribution of bath energies. This form was used in [14], there based on heuristic reasoning, for a bath distributed as in a canonical ensemble.

6 "Distance" from equilibrium state

Pursuing the environment-tracing formalism to derive the reduced density matrix of a small subsystem, and starting with an arbitrary but representative pure state of the subsystem plus the environment, in their above quoted
paper the Bristol group have shown that the long term time averaged deviation ("Distance") of the subsystem state (its truncated density matrix) from the equilibrated state is (or is upper-limited) proportional to the square root of the ratio between the subsystem’s dimension in its Hilbert space and that of environment (Equation 8 in [6], also [5]). Before establishing an analogous result for the time integration formalism we show that an interacting $N$ half-spin model verifies numerically the predicted inverse square root relationship for the "distance" [26].

6.1 $N$-spin model

Such systems with finite Hilbert state dimensions have been extensively studied for entanglement and other properties. A recently built processor consisting of eight interacting qubits and subject to time dependent interaction was investigated as a means to achieve feasible quantum computing [27].

In our model the total system of $N$ 1/2-spins (qubits), consisting of one subsystem (labelled 0) and $(N-1)$ bath 1/2-spins ($i = 1...N-1$), interact according to a Hamiltonian

$$H(N) = \sum_{i=0,...,N-1} E_i \sigma_i + \sum_{i,j=0,...,N-1; i \neq j} g_{ij} \sigma_i \sigma_j$$

(9)

with energy parameters, so chosen as to avoid any degeneracies in the eigenenergies, and two sets of coupling parameters for $g_{ij} = g_{ji}$, given by

$$E_0 = 1; E_j = 1.5 \sin^2 \frac{2\pi j}{10}; g_{0j} = 2.5, 3.5; g_{ij} = .75, 1.5; \quad 1 \leq i, j \leq N-1$$

(10)

The matrix of this Hamiltonian, that has to be diagonalized to obtain its eigenenergies and pure-state eigenfunctions, is of a square dimension of $2^N \times 2^N$. To formally write out in the spin’s representation the matrix for large $N$ and then let it be solved by a routine (e.g., Fortran or Mathematica), we have used the following trick, not used (to our knowledge) heretofore: We have replaced the ordinal, decimal number of the matrix rows (or columns) in the routine by its binary representation and have formalized the matrix elements in this representation. Thus, there is an entry at the decimal (13,25), or (25,13) matrix position with the value of $g_{3,5} = g_{5,3}$, because in the binary representation we have for $N = 8$ (with the spins labelled as 0,1,...,7, in which the last 7 digits label the bath spins)

$$13 = [00001\bar{1}01], \quad 25 = [000\bar{1}1001]$$

(11)
with the 3 and 5 spins that flip and counter-flip identified by a superbar.

The $2^N$ ordered energy values (labelled with the ordinal number index $r$) obtained by numerical diagonalization of the Hamiltonian equation (9) are shown in Figure 3. The figure shows sparseness in the lower range, uniform linear increase in the middle and some super linear increase towards the upper end.

The reduced density matrix of the small subsystem $\rho^S$ (of size 2 x 2) is obtained in the bath-tracing procedure by tracing over $2^{N-1}$ bath states the total system’s density matrix for any of its pure eigenstates (whose number is $2^N$). The ”distance” is taken as the root mean square deviation of $\rho^S$ over the different choices from the $2^{N-1}$ bath eigenstates.

### 6.1.1 N-spin distances

In Figure 4 we show our computed ”Distances”, plotted logarithmically ($\log_{10}$) against the dimension of the Hilbert space of the ($N-1$) half-spins with which the system (also: a half-spin) interacts. The full curve, the long broken line curve, the medium broken line curve and the short broken line curves are for different parameter sets in the Hamiltonian; the one (reaching up to $N = 9$) is for a parameter set in which all the $\sigma_x\sigma_x$ coupling strengths have the same value 2.5 for every (bath-spin) - (system-spin) coupling $g_{0i}$ and the value of 0.7 for all inter- bath couplings $g_{ij}$. The other curves are for varied coupling strength of the same order. The energy
6.2 DM through time summation with random partitioning

As noted in section 5 and Appendix D, for a finite-sized ancilla the time integration over a window of $2\Delta t$ needs to be replaced by a discrete time-summation. We have subdivided the window into P segments (partitions) having randomly chosen relative lengths and summed the DM eigenvalues at P points corresponding to the mid points of the segments. Figure 5 shows a characteristic set of results [28]. For finite P the discrete summation corresponds to a finite bath while for $P \to \infty$ the Standard Deviation (SD) should approach the time integration value, corresponding to an infinite bath environment. The computed curves appear to show initially a $P^{-\frac{1}{2}}$ relationship, similar to the inverse square root dependence for the environment tracing result in figure 4 followed for large P by one like $P^{-1}$.

The two figures, 4 and 5, show the congruity of the environment tracing and the time integration methods for a general result in [6] which is
Figure 5: Distance (or Standard Deviation SD of the density matrix upper eigenvalue over a large time interval) against the number $P$ of randomly partitioning the time integration interval $2\Delta t = 4\pi$ and summing the value of the upper eigenvalue of the density matrix at the midpoint of each partition. The curves are for parameter values of the Hamiltonian shown in equation (1) $\omega = 1, e = 0.5$. The solid lines are for $k \approx 1$ and the broken lines $k = 1.5$, with two different random partitioning in each case. The two dotted straight lines are, in the logarithmic plotting of the figure, slopes of $P^{-\frac{1}{2}}$ and $P^{-1}$, respectively.
7 A Leggett-Garg-Wrachtrup (LGW) Inequality

The Bell inequalities for correlations between measurements at different locations, famously potentially violated by quantum systems while observed by classical systems, were formulated for temporally subsequent measurements by Leggett and Garg [29]. A review of experimental and theoretical developments is found in [30]. A modification which tests the system for "reality" (meaning the characterization of the physical system, irrespective of whether it is measured or not) and "stability" ("the conditional probability $Pr(i, t|t, t_0)$ to find the system at times $t, t_0$ in the same state $i$, provided that this probability depends only on the time difference") was proposed in [31] by an inequality written, with $t_0 = 0$ being the starting time and $t$ a subsequent instance, as

$$Pr(i, 2t|i, 0) - Pr^2(i, t|i, 0) \geq 0 \quad (12)$$

We use this inequality to answer two questions:

1. Does the (reduced) density matrix arising from an open microscopic quantum system interacting with an ancilla have the property of a quantal or a classical system, in the sense of violating or observing the above inequality? (We recall that in a measurement of a quantal observable, after interaction with the measuring apparatus, the truncated DM has the status of classical probabilities.)

2. Assuming a classical status for the DM of an open system linked to an "infinite" environment and a quantum status for the same system when linked (entangled) to another microscopic system, is there a way to decide between the status of the combined systems in terms of the requirements of the above LGW inequality?

It is proposed that the time integrating formalism leads to answers in the following sense: The execution of the time integration is dependent on the coupled ancilla. For a macroscopic ancilla this has to be carried out over an effectively full temperature range (or over a full period, if there is a periodicity in the system), whereas for a finite ancilla the integration is to be restricted, either to a summation or to a limited range of the integration.
We then test the violation of the LGW inequality by increasing the time averaging range $2\Delta t$ from zero (the pure state case) to its effectively full averaging value $2\Delta t = 4\pi$, appropriate to a macroscopic bath.

We solve equation (2) with the initial condition $\psi_u(t = 0) = 1, \psi_l(0) = 0$. Then the inequality in equation (12), takes the simple form

$$|\psi_u(2t)|^2 - |\psi_u(t)|^4 \geq 0 \quad (13)$$

The results for some choices of the parameters in equation (1) are shown in Figure 6 for an infinitesimal averaging window, $2\Delta t \to 0$, corresponding to an instantaneous or pure state. It is seen that for a small range of time values [when the left hand side (LHS) of equation (13) takes negative values] the inequality is violated. Such violation may either indicate the quantal nature of the system or to the breakdown of the pre-conditions in [31]. We next select some time values where each curve is most negative and average the probabilities around these values, continuously increasing the extent of the integration window. As seen in Figure 7, above some finite size time windows the LGW inequality becomes satisfied, though it was violated for an infinitesimal time window (the pure state case). The transition from negative to positive values may indicate the transition from quantal to classical nature of the integrated DM in a continuous manner, though this is also contingent to the satisfaction of the ”stability” hypothesis in [31]. For the present purposes the results demonstrate the facility with which application of the time averaging procedure straddles the quantal-classical gap.

8 Conclusion

While the main result of this paper is the derivation of non-uniform weighting for the time coarsening process in section 6, a discussion of its application is appropriate. It may be argued that the Minimal Coupling Model MCM used in this work is too specific to represent the wide variety of real life interactions between a micro-system and its environment. (Extensions of the model, possible tasks for future work, are described in Appendix B.) However, it is almost axiomatic that, excluding the small proportion of integrable systems, in real life (exemplified in [5] by the Cooling Coffee Cup), thermal or equilibration processes depend only in a minor way on the details of the micro-system-environment coupling, and indeed most modelings of this coupling have hinged on their amenability to solution, rather than on their being a true description of real life situations. The strength of the
Figure 6: Pure sate results for the LHS of equation (13) obtained from solutions of the time dependent Schrödinger equation with a choice of parameters, each choice drawn with different lines. The curves are mainly positive, but there are some times at which they are negative, thereby violating the inequality in equation (13).
time-averaging approach in this paper is the ease with which it yields results (resolution of the time arrow problem being perhaps the most obvious one); it also opens the way to explore concrete physical situations by the selective, non-uniform time averaging, as set out in section 5.

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A Original outline of the three steps to construct the density matrix

In the quoted previous work [14] it was shown how the decohered-truncated phase of the full subsystem-environment state (their DM), leading into the reduced subsystem state, can be obtained by a time averaging approach. The abstract steps needed to achieve this and the main assumptions behind it were given by [14] in an "Outline", which is briefly reproduced in this Appendix. The Hamiltonians for which the system’s states were determined were (i) a Rabi-model (a single-spin in interaction with a single vibrator),
two mutually coupled spins, each coupled to a single vibrator. For completeness these Hamiltonians, formulated in a semi-classical, time-dependent language, are also shown in this article in Appendix B. While it is clear that a Hamiltonian in which a time dependent term appears represents an open system, what our results have shown is that even with the arguably simplest form of the time dependent term (namely, a single subsystem-environment harmonic interaction term), one obtains results equivalent to those in the standard environment-tracing formalism. The simplifying (and approximative) steps necessary to pass from the Leggett et al’s (spin-oscillatory ensemble) model [32] to ours were described in section 2.3 of the earlier article. The present text has extended the time-averaging formalism to issues not considered before, including second moments (fluctuations) of the DM (in section 6) and its approach through time averaging to classicality (section 7).

1. We adopt the von Neumann definition

\[
\rho_{ij}(t) = \frac{1}{(\sum_a 1)} \sum_a <i|\psi_a(t)> <\psi_a(t)|j> \quad (14)
\]

In this definition the summation index \(a\) represents the values of all coordinates, variables etc. external to the system (e.g., those of the environment affecting the system) and appearing also in the Hamiltonian. Thus the set \(\psi_a(t)\) for all \(a\)’s forms a time dependent ensemble of states. The variables of the system themselves are implicit (not written out) in \(\psi_a(t)\).

2. We solve only for a single external condition thus dispensing with the \(a\) index in the wave function, but obtain \(\rho(t)\) as the average over an adequate set of adjacent times:

\[
\rho_{ij}(t) = \frac{1}{2\Delta t} \int_{t-\Delta t}^{t+\Delta t} d\tau <i|\psi(\tau)> <\psi(\tau)|j> \quad (15)
\]

This should be equivalent to equation (14) if the ergodic hypothesis holds for the duration \(2\Delta t\). While for several cases the off-diagonal matrix elements are small or vanishing, \(\rho_{ij}(t)\), as defined above, represents in general a mixed state whose diagonalized form \(\rho_{ij}(t) \to \rho_{ii}^d(t)\delta_{ij}\) satisfies \(\sum_i (\rho_{ii}^d(t))^2 < 1\) (section 5 in this paper).
B Minimal Coupling Hamiltonians

(a) Single spin:

\[ H(t) = e\sigma_z + k\sigma_x \sin(\omega t) \]  

(b) Interacting spins:

\[ H_{\text{total}}(t) = h(t) + H_{\text{int}} \]  

\[ h(t) = \sum_i [E_i\sigma_{zi} + k_i\sigma_{zi} \cos(\omega_i t + \alpha'_i) + k'_i\sigma_{xi} \sin(\omega_i t + \alpha'_i)] \]  

\[ H_{\text{int}} = \sum_{ij} [\gamma_{ij}(\sigma_{zi} \cdot \sigma_{zj}) + \gamma'_{ij}(\sigma_{xi} \cdot \sigma_{xj} + \sigma_{yi} \cdot \sigma_{yj})] \]

having written in the first line the total Hamiltonian, comprising the parts in the next two lines. First, the spin energy terms in which \( E_i \) are energies of the spin systems, the \( \sigma \)'s are Pauli matrices operating in the respective spin spaces; \( k, \alpha \), together with their tagged partners, are parameters of the spin-boson couplings and \( \omega \) is the frequency of the external source. This external, boson source is classical and for it the Hamiltonian need not be written out. The Hamiltonian does not include back-reaction on the source, which can at least approximately be justified for periodic coupling and energies. The last line is the spin-spin interaction term. A two-spin version of this interacting-spin Hamiltonian was treated in \[14\].

C Extremization of \( G(t) \) in equation (6)

We now prove that the maximum of \( G(t) \) is unity when the wave function components \( \psi_u(t) \) and \( \psi_l(t) \) are constant during the \( 2\Delta t \) integration range \[33\]. By implication, \( G(t) \) is less than unity (mixed state case) when the components are genuinely time dependent. The method of proof is a calculation of variations.

It has been stated in text that a maximum of \( G(t) \) occurs when the wave function components are throughout real and positive. We further simplify by writing

\[ \psi_u(t) \equiv f(t), \quad \psi_l(t) \equiv \sqrt{1 - f^2(t)} \]  

Written as

\[ G[f(t)] = \left[ \frac{1}{2\Delta t} \int_{t-\Delta t}^{t+\Delta t} (2f^2(t') - 1)dt' \right]^2 + \left[ \frac{1}{\Delta t} \int_{t-\Delta t}^{t+\Delta t} f(t') \sqrt{(1 - f^2(t'))} dt' \right]^2 \]  

(21)
a variation gives

\[
\delta G[f(t)] = \left[ \frac{1}{\Delta t} \int_{t-\Delta t}^{t+\Delta t} (2f'(t') - 1)dt' \right] \left[ \frac{1}{2\Delta t} \int_{t-\Delta t}^{t+\Delta t} 4f(t')\delta f(t')dt' \right] 
+ \left[ \frac{2}{\Delta t} \int_{t-\Delta t}^{t+\Delta t} f(t')\sqrt{1 - f^2(t')}dt' \right] \left[ \frac{1}{\Delta t} \int_{t-\Delta t}^{t+\Delta t} (\sqrt{1 - f^2(t')}) \delta f(t')dt' \right]
\]

Remarkably, the cofactor of \( \delta f(t') \) vanishes when \( f(t) = f \), a constant throughout the range of integration, so that \( G[f(t) = f] \) is then an extremum. Its value is unity, independent of \( f \). That it is also a maximum can be shown by evaluating \( G(t) \) for the case that the function \( f(t) \) takes two values \( f_1, f_2 \neq f_1 \) in fractions \( F, (1 - F) \) (respectively) of the integration interval and showing that the leading term in \( G[f_1, f_2] \) is negative for \( |f_1|, |f_2| \leq 1 \), namely

\[
- \frac{F(1 - F)}{8} (f_1 - f_2)^2 [4 + (f_1 + f_2)^2] [1 + \frac{4 + (f_1 + f_2)^2}{(4 - (f_1 + f_2)^2)^2}] \] (23)

D Proof of Sum Formula in equation (7) for a Finite Bath.

It is assumed that the subsystem and the large, but finite sized bath form together a microcanonical ensemble with mean energy of \( E_{total} \) and small energy uncertainty \( \nu \). The range of the subsystem’s energies \( E(t) \), that vary in time, is divided up into \( N \) segments, numbered \( n(= 1, ..., N) \) each of spread \( \nu \). The segments contain \( r_{n+1} - r_n \) discrete (supposed non-degenerate) energy levels \( E_r \) of the bath, such that these bath state energy levels satisfy

\[
E_{total} = E(t) + E_r \] (24)

for some value of \( E(t)[\approx E(t_n)] \) situated within the segment spread \( \nu \). The corresponding time spread over the segment is \( t_{n+1} - t_n \), having assumed that for the short passage time over the narrow segment spread the subsystem energy is a monotonic, single-valued function of time. This time spread is of the order of the bath’s relaxation time.

The subsystem’s density operator ("the reduced" density operator) \( \rho^S(t) \) is obtained in the bath tracing formalism by weighting the system’s proper
density operator \( \rho_n(t) \) in each segment by the above number of bath states, giving

\[
\rho_n(t)(r_{n+1} - r_n) = \rho_n(t) \sum_{r_n}^{r_{n+1}} \int_{E(t_n)}^{E(t_{n+1})} dE' \delta(E_{total} - E' - E_b)
\]

\[
= \sum_{r_n}^{r_{n+1}} \rho_n(t) \int_{t_n}^{t_{n+1}} dt' \frac{dE(t')}{dt'} \delta(E_{total} - E(t') - E_b)
\]

\[
= \sum_{r_n}^{r_{n+1}} \rho_n(t_r)
\]

having in the last line interchanged the order of the summation and the time integration and taken heed of the property of the Dirac delta function. We thus obtain for the weighted density operator in the time segment a discrete sum with the time sum going over all such times that the system energy is complemented to \( E_{total} \) by a bath state’s energy. In the time-integrated formalism the system’s density matrix is obtained by integrating over time windows \( t_w \) that are much wider than the time spread of a segment. Then the resultant matrix element is

\[
\rho_{ij}(t) \propto \sum_{r_r \in t_w} \rho_{ij}(t_r)
\]

where the time sum goes over all such times \( t_r \) within the time window that the instantaneous subsystem energy \( E(t) \) is complemented by a bath level to add up to \( E_{total} \). The proportionality constant is fixed, by the requirement that the trace of density matrix is unity. In the case of an infinite bath with a continuous energy spectrum, the above sum is replaced by a time integral including the energy density of the bath levels \( D^b(E_b) \):

\[
\rho_{ij}(t) \propto \int_{t}^{t+tw} dt' D^b(E_b) \rho_{ij}(t')
\]

This formula is also applicable for the case that the bath is in thermal equilibrium at a temperature \( T \), so that the bath energy density is proportional to

\[
e^{\frac{E_b}{k_B T}} = e^{\frac{E_{total} - E(t)}{k_B T}}
\]

by virtue of the expression in equation (24) for the bath energy. This result, originally due to [34], has already been used in [14], with the time independent factor \( e^{\frac{E_{total}}{k_B T}} \) having been absorbed in the proportionality factor.
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