Diffusion and entanglement in open quantum systems

**Ohad Shpielberg**

Collège de France - 11 place Marcelin Berthelot, 75231 Paris Cedex 05, France and Laboratoire de Physique Théorique de l’École Normale Supérieure de Paris, CNRS, ENS & PSL Research University, UPMC & Sorbonne Universités - 75005 Paris, France

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**Abstract** – The macroscopic fluctuation theory provides a complete hydrodynamic description of nonequilibrium classical diffusive systems. As a first step towards a diffusive theory of open quantum systems, we propose a microscopic open quantum system model —the selective dephasing model. It exhibits genuine quantum diffusive scaling. Namely, the dynamics is diffusive and the density matrix remains entangled at large length scales and long time scales.

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**Introduction.** – Recently, transport properties of nonequilibrium quantum systems have been extensively studied [1–3]. Of particular interest are dissipative quantum systems [4–12], which in many cases lead to diffusive transport —ubiquitous in both quantum and classical physics.

The macroscopic fluctuation theory (MFT) [13], a universal coarse grained theory, has been rigorously shown to completely encapsulate the dynamics of classical diffusive systems [14–16]. The MFT allows to calculate nonequilibrium long-range correlations [17], large deviations [18], fluctuation-induced forces [19], predict dynamical phase transitions [20–24], their associated critical exponents [16, 25, 26] and many more [27, 28]. The present study is motivated by a salient question: Does a universal description of quantum diffusive dynamics, comparable to the MFT, exist?

Let us briefly recap the MFT. Rather than describing a diffusive process at the mesoscopic scale through a master equation, the MFT takes a coarse grained approach where, away from criticality, only conserved fields survive. To make this more concrete, consider a 1D diffusive system of interacting particles with particle density \(n\). Conservation of particles in the bulk implies the continuity equation \(\partial_t n = -\partial_x j\). Then, the diffusion equation results from the combination of the continuity equation and Fick’s law \(j = -D\partial_x n + \sigma E\), where \(D, \sigma\) are the diffusivity and conductivity encapsulating the dynamics and \(E\) is an external field. To infer what the correlations in the system are, one must go beyond the mean description and include fluctuations. The MFT asserts that the fluctuations of the process at the coarse grained level are entirely described by supplementing the current in Fick’s law with a white noise term of magnitude proportional to the conductivity. Therefore, regardless of the microscopic description, the dynamics of the coarse grained mean behaviour as well as the fluctuations are entirely encapsulated by \(D, \sigma\). This is the universal structure of the MFT.

A universal coarse grained theory of quantum diffusion is required to go beyond the classical MFT, e.g., to exhibit entanglement. First, it is necessary to provide a microscopic model that exhibits entanglement and diffusive dynamics at the coarse grained level [29], expanding the MFT’s mean evolution structure. Then, one can verify whether the structure of the fluctuations remains universal.

In this letter we introduce a microscopic model described by a quantum master equation that demonstrates at the coarse grained level both diffusive dynamics and entanglement at the steady state. The mean evolution is a set of non-local diffusion equations. This example demonstrates that a general theory describing diffusive open quantum system goes beyond the MFT. Furthermore, it provides us with a working example that will allow in turn to develop such a diffusive theory of open quantum systems.

**Setup.** – Since simple diffusive systems are Markovian and dissipative, a convenient initial starting point would be to consider Markovian open quantum systems, given by the Gorini-Kossakowski-Sudarshan-Lindblad (GKSL)
Consider a quantum system, coupled to a large environment with fast relaxation times. The backaction of the system on the environment can thus be neglected on the relevant time scale of the system. The evolution of the system's density matrix follows \( \partial_t \rho = \mathcal{L}(\rho) \), where

\[
\mathcal{L}(\rho) = -i[H, \rho] + \sum_k L_{M_k}(\rho),
\]

\[
L(\rho) = \frac{1}{2} [M_x M_x, \rho].
\]

Here \([\cdot, \cdot]\) and \(\{\cdot, \cdot\}\) are correspondingly the commutation and anti-commutation relations. \(H\) is a Hermitian operator and may contain both the system's Hamiltonian and its interaction with the environment. The set of \(M_k\) operators, orthonormal under the trace norm \(\text{Tr} M^\dagger_k M_k = \delta_{k, k'}\), are related to the interaction with the environments. One can also follow the evolution of operators in the Heisenberg picture, given by the adjoint equation \(\partial_t \hat{O} = \mathcal{L}^\ast(\hat{O})\). If all the \(M_k\) are Hermitian, \(\mathcal{L}^\ast(\bullet) = -i[H, \bullet] + \sum_k L_{M_k}(\bullet)\).

To explore quantum diffusion, we introduce the "selective dephasing" model. Consider a periodic spin chain of \(\Omega \geq 2\) sites, with the Pauli matrices \(\sigma^x_{k, \Omega}, \sigma^y_{k, \Omega}, \sigma^z_{k, \Omega}\) operating at site \(k\). The selective dephasing model has the GKSL form (1). We set \(H\) to be the XX Hamiltonian \(H_{XX} = -\sum_{k=1}^{\Omega} \sigma^x_{k, \Omega} \sigma^x_{k+1, \Omega} + \sigma^y_{k, \Omega} \sigma^y_{k+1, \Omega}\) \(\Omega\). The operators \(M_k = \sqrt{\rho} \sigma^z_{k, \Omega}\) correspond to dephasing on the sites \(k \in \mathcal{A}\), where \(\nu_j\) has units of inverse time and \(\eta\) is a dimensionless parameter that controls the strength of the dephasing.

Three choices of \(\mathcal{A}\), which select the dephasing sites, are considered:

\[
\mathcal{A}_\Omega \equiv \{1, 2, \ldots, \Omega\}, \quad \mathcal{A}_{\xi} \equiv \{j \in \mathcal{A}_\Omega| j \neq \xi, \xi + 2\}, \quad \mathcal{A}_{\text{odd}} \equiv \{1, 3, 5, \ldots, \Omega - 1\},
\]

for which \(\mathcal{A}_{\text{odd}}\), \(\Omega\) is assumed to be even. Note that the exact value of \(\xi\) is irrelevant due to the periodic boundary conditions we consider. This GKSL model can be derived using the singular coupling limit for spins coupled to a set of thermalized bosonic baths [30] and for fermions in an optical lattice [31].

The \(A_{\Omega}\) model has been exhaustively studied [9,32–34] and even admits a Bethe ansatz solution [10]. First, we recap the derivation of the diffusive dynamics of the \(A_{\Omega}\) model. The dephasing leaves no quantum fingerprints at long times. Then, we show that protecting some of the sites from dephasing as in the \(A_{\xi}\), \(A_{\text{odd}}\) models may maintain the diffusive dynamics and exhibits quantum fingerprints at long times.

For the analysis, we define the operators

\[
P_{\pm}^k = \sigma^\pm_{k, k} \quad P_k = P^+_k \prod_{i \in \mathcal{A}_\Omega/\{k\}} P_i^-, \quad S_{M}^k = (\sigma^x_{k, k+m} \sigma^y_{k, k+m}) \prod_{i \in \mathcal{A}_\Omega/\{k,k+m\}} P_i^-
\]

In the following, the long time dynamics of the selective dephasing models will be shown to be governed by these operators. Furthermore, the \(S_{M}^k\) will be used as witnesses of entanglement.

\(A_{\Omega}\) dephasing. — The operator evolution for \(P_{\pm}^k\) is given by the discrete conservation equation \(\partial_t P_{\pm}^k = -J_{l} + J_{l-1}\), where \(J_{l} = 2i\epsilon(\sigma^+_l \sigma^-_{l+1} - \sigma^-_l \sigma^+_{l+1})\). Therefore, on a ring \(Q = \sum_{k \in \mathcal{A}_\Omega} \text{Tr} P_{\pm}^k \rho(s)\) is conserved for all \(\eta\). This is true for any \(\mathcal{A}\) dephasing model. Trying to evaluate \(\partial_t J_{l}\) reveals that the equations do not close [34], and so this naive approach fails. Fortunately, the dynamics simplifies as states not in the kernel of \(\sum_{k \in \mathcal{A}_\Omega} L_{M_k}\) are quickly filtered [9,34] (see the Supplementary Material Supplementary material.pdf (SM)). States in the kernel are called pointer states. The resulting long time dynamics, quickly attained for large \(\eta\) values, is governed by transitions between these pointer states. Hence, we derive a perturbative expression for the pointer states dynamics at large \(\eta\) for a general GKSL equation of the form

\[
\mathcal{L}(\rho) = \mathcal{L}_S(\rho) + \eta \mathcal{L}_b(\rho), \quad S(\rho) = -i[H, \rho] \quad \mathcal{L}_b(\rho) = \nu \sum_{k \in \mathcal{A}} L_{M_k}(\rho).
\]

For large \(\eta\), the density matrix quickly converges into a mixture of pointer states —the states in the kernel of \(\mathcal{L}_b\). Then, the density matrix may only evolve on a long time scale [35–37]. A slow dynamics, where the density matrix spreads to other pointer states emerges if \(\Pi_0 \mathcal{L}_S \Pi_0 = 0\) and \(\mathcal{L}_b = \sum_{\nu > 0} \nu \Pi_\nu\). Here \(\Pi_\nu\) is the projector to the kernel \(\Pi_0\). To leading order \(\partial_t \rho = \nu \Pi_0\), where [9,34] (see the SM)

\[
u = -\Pi_0 \mathcal{L}_S (\mathcal{L}_b) \mathcal{L}_S^{-1} \mathcal{L}_S.
\]

with the rescaled time \(s = t/\eta\) at the limit of \(t, \eta \rightarrow \infty\). \(\mathcal{L}_b\) is the inverse to the restriction of \(\mathcal{L}_b\) outside of the kernel. The above assumptions are valid in all the variants of the selective dephasing model (see the SM). Finding the projector to the kernel \(\Pi_0\) may be easier than finding a basis for the pointer states as one needs to worry about positivity and unit trace. For Hermitian \(M_k\), the operator evolution is \(\partial_t \mathcal{O} = \nu \mathcal{O}\). Hence, dealing with pointer operators, i.e., \(\mathcal{O} = \Pi_0 \mathcal{O}\) may be easier than dealing with pointer states.

To analyze the effective dynamics, it is essential to identify the kernel of \(\mathcal{L}_b\). For \(A_{\Omega}\), this kernel is spanned by the \(2^\Omega\) pointer states \(\prod \sigma^\pm\). One can give a classical interpretation to the effective dynamics of (5) in this case. Interpreting the operators \(P_{\pm}\) as projectors into an occupied (empty) lattice site state implies that the pointer states span all the configurations of a lattice gas. Namely, each site is either occupied by a particle or not. The dynamics corresponds to the simple symmetric exclusion process (SSEP), where particles can jump to empty neighboring lattice sites with rate \(D = 2\epsilon^2/\nu\) [38,39]. The SSEP is diffusive and classical. So, we have gained no insight on the behaviour of diffusive open quantum systems.
By protecting some of the sites from the dephasing noise, one expects a larger kernel, which in turn could lead to richer dynamics. This is the reasoning behind the $A(t)$, $A_{dtd}$ models. We restrict the study here to the already interesting case $Q = 1$. For the analysis of the qualitatively similar $Q \neq 1$ see the SM.

$A(t)$ dephasing. – The kernel becomes larger than in the $A_{dtd}$ case as it contains, e.g., the pointer operator $S^2_k$ (see (3)), as well as the states $\mathbb{P}_k$. The effective dynamics for the $A(t)$ dephasing provides us with a closed set of pointer operator equations,

$$
\begin{align*}
\partial_t \mathbb{P}_k &= D \Delta \mathbb{P}_k, \quad k \neq \xi - 1, \xi, \xi + 1, \xi + 2, \\
\partial_t \mathbb{P}_\xi &= 2D \Delta \mathbb{P}_\xi + DS^2_\xi, \quad k = \xi, \xi + 2, \\
\partial_t \mathbb{P}_{\xi+1} &= 2D \Delta \mathbb{P}_{\xi+1} - 2D S^2_\xi, \\
\partial_t \mathbb{P}_{\xi-1} &= D \Delta \mathbb{P}_{\xi-1} + D(\mathbb{P}_\xi - \mathbb{P}_{\xi-1}), \\
\partial_t S^2_\xi &= -2D \Delta \mathbb{P}_{\xi+1} - 4DS^2_\xi,
\end{align*}
$$

(6)

where $\Delta$ is the discrete Laplacian operator.

Note that in the slow dynamics regime, operators outside of the kernel have already decayed in the Heisenberg picture, i.e., $\partial_t \mathbb{P} = 0$ if $\Pi_0 \mathbb{P} = 0$. Therefore, more information on the slow dynamics can be recovered from the evolution equations of the (non-pointer operators) $S^2_k \neq \xi$. Since $\Pi_0 S^2_k \neq \xi = 0$, we obtain a set of identities

$$
\begin{align*}
\Delta \mathbb{P}_{k+1} &= 0, \quad |k - \xi| \geq 3, \\
\Delta \mathbb{P}_{\xi+1} &= \mathbb{P}_{\xi+1} - \mathbb{P}_{\xi+2}, \\
\Delta \mathbb{P}_{\xi-1} &= \mathbb{P}_{\xi-1} - \mathbb{P}_\xi, \\
S^2_\xi &= \Delta \mathbb{P}_\xi = \Delta \mathbb{P}_{\xi+2},
\end{align*}
$$

(7)

The effective dynamics identities (7) are at the operator level and hence do not depend on initial conditions. We denote by $S_\xi(s) = \text{Tr} S^2_k \rho(s)$ and $q_k(s) = \text{Tr} \mathbb{P}_k \rho(s)$ the expectation values associated with the pointer states. From the $\Omega - 1$ identities (7) and from the conserved $Q = 1 = \sum_k q_k$, we recover a single solution $q_k \neq \xi = 1/\Pi(1 - S^2_\xi)$ and $q_{\xi+1} = \frac{1}{1 + \Omega - 1} S^2_\xi$. The density matrix of the effective dynamics is a positive semidefinite, Hermitian and trace 1 combination of the operators $\mathbb{P}_k$ and $S^2_\xi$. The Peres-Horodecki criterion asserts that a two-two level system is entangled if and only if the partial transpose to the density matrix is not positive definite [40] (see the SM). We use the Peres-Horodecki criterion to probe for bipartite entanglement in our system. In the effective dynamics bipartite entanglement can occur in the $A(t)$ model only between the spins in $\xi, \xi + 2$ and only if $S^2_\xi \neq 0$ (see the SM). Hence, $S^2_\xi$ serves as a witness of entanglement in the system.

We evaluate the values $S^2_\xi$ and $q_k$ using the evolution equations (6). They correspond to the trivial solution $S^2_\xi = 0$ and $q_k = 1/\Omega$ in the effective dynamics. Hence, entanglement quickly decays. This suggests, as expected, that a microscopic protection from the environment is not enough to retain an interesting hydrodynamic quantum behaviour (see the SM for numerical verification).

$A_{odd}$ dephasing. – As before, we study the effective dynamics at large $\eta$ to obtain the evolution within the kernel. Notice that $\mathbb{P}_k$ for $k \in A_0$ and the operators $S^2_k$ are in the kernel for $k, m = 1, 2, \ldots, \Omega/2$. For $Q = 1$, we obtain a set of evolution equations and identities corresponding to the operators in the kernel. Here, we keep track also of $S^2_k$ for odd $k$, even though they are not in the kernel and thus have vanishing expectation values in the effective dynamics. This highlights the emerging diffusive picture, but does not change any expectation value (see fig. 1 and the SM). The (diffusive) evolution equations are

$$
\begin{align*}
\partial_t \mathbb{P}_k &= 2D \Delta \mathbb{P}_k - D \Delta S^2_k, \\
\partial_t S^2_k &= -2D \Delta \mathbb{P}_{k+1} + 2D \Delta S^2_k - D \Delta S^2_{k-1}, \\
\partial_t S^2_{k+2} &= -2D \Delta S^2_{k+1} + 2D \Delta S^2_k + 2D \Delta S^2_{k+2} - D \Delta S^2_{k-1},
\end{align*}
$$

(8)

for $2 \leq 2 + m \leq \Omega/2$. The periodicity of the system helps to truncate eq. (8) as $S^2_{\Omega/2} = S^2_{\Omega/2-2}$ for $\Omega/2$ even, and $S^2_{\Omega/2+1} = S^2_{\Omega/2+1}$ for $\Omega/2$ odd.

To find the steady state solution, we use the translational invariance of the system (in discrete jumps of 2). Define $q_0 = \text{Tr} \rho(s) S^2_{k=1}$, $q_\Omega = \text{Tr} \rho(s) S^2_{k=\Omega/2}$ and $S^2_m = \text{Tr} \rho(s) S^2_{k=m}$. From (8) and for $\Omega/2$ even, we find the steady state values $S^2_m = -S^2_{m+2}$ as well as $q_0 - q_\Omega = \frac{1}{2} S^2$. This is numerically confirmed in the SM.

Similarly to the $A(t)$ dephasing, the expectation value of $S^2_m$ is a witness of entanglement in the steady state. Note that the steady state density matrix is constructed using the pointer operators $\mathbb{P}_k, S^2_{2k'}$. Then, using the Peres-Horodecki criterion shows that any two even sites $2k', 2k''$ are bipartite entangled if the expectation of $S^2_{(k' - k'')}^2$ is non-vanishing (see the SM).

For $\Omega/2$ odd, periodicity implies that $S^2_{\Omega/2+1} = S^2_{\Omega/2-1}$. Then, the steady state equations result in $S^2_m = 0, q_0 = q_\Omega = 1/\Omega$ and thus the system will not be entangled at the steady state. In what follows, we only study $\Omega/2$ even, where the entanglement can survive at the steady state. The effective evolution equations (8) suggest that the expectation values of $\sum_{k \in A_0} S^2_k$ are conserved quantities in the effective dynamics. However, this is not the case for the $t$ time evolution. It implies that only beyond a transient period $t \gtrsim \eta \tau^2/\epsilon^2$, $\sum_{k \in A_0} S^2_k$ is conserved.

Using the effective conservation, we define a witness of entanglement in the system $B(t) = \sum_{k \in A_0} \text{Tr} \rho(t) S^2_k$. Using this witness, fig. 1 and the SM numerically demonstrate that entanglement survives the long time limit for generic initial conditions, provided the initial conditions have some nonzero entanglement value (other initial conditions were tested with similar results). Notice that the entanglement survives on all length scales of the system. That is, the bipartite entanglement spreads to all length scales even if it is initially restricted to a local region. Hence, we have successfully found a model where long-range entanglement can be observed for diffusive transport.
Contrary to the classical diffusion equation description, the hydrodynamic equations for the quantum diffusion of the $A_{\mathrm{odd}}$ dephasing model can be expected to be non-local due to the long-ranged entanglement. For $\Omega/2$ even, we define the coarse grained length scale $x = j/\Omega$, and time $\tau = sD/\Omega^2$ scales as well as the coarse grained operators $\mathbb{P}(x,t), \mathbb{S}^{2m}(x,\tau)$. Using the vector representation $v = (\mathbb{P}, \mathbb{S}^2, \mathbb{S}^4, \ldots, \mathbb{S}^{\Omega/2})$, the non-local hydrodynamic diffusion equation stemming from (8) is

$$\partial_\tau v(x) = \partial_x \mathcal{D}_0 v(x) + \partial_x \mathcal{D}_1 v(x + \Omega/2),$$

where

$$\mathcal{D}_1 = \begin{pmatrix}
0 & \ldots & 0 \\
\vdots & \ddots & \vdots \\
0 & 0 & 0 \\
-1 & 0 & 0
\end{pmatrix},$$

$$\mathcal{D}_0 = \begin{pmatrix}
2 & -1 & 0 & 0 & 0 & \ldots & 0 \\
-2 & 2 & -1 & 0 & 0 & \ldots & 0 \\
0 & -1 & 2 & -1 & 0 & \ldots & 0 \\
0 & 0 & -1 & 2 & -1 & \ldots & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\
0 & 0 & \ldots & 0 & -1 & 2
\end{pmatrix}.$$
an important step towards a nonequilibrium theory of diffusive open quantum systems.

Recall that the selective dephasing model can be derived from a Hamiltonian dynamics through the singular coupling limit. Therefore, it is of interest to implement the selective dephasing model derived from a Hamiltonian dynamics through the singular cutting-edge experimental techniques [44–47]. How to take advantage of the entanglement propagation to all scales of the selective dephasing model is yet another open challenge.

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