Lindblad Formalism based on Fermion-to-Qubit mapping for Non-equilibrium Open-Quantum Systems

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We present an alternative form of master equation, applicable on the analysis of non-equilibrium dynamics of fermionic open quantum systems. The formalism considers a general scenario, composed by a multipartite quantum system in contact with several reservoirs, each one with a specific chemical potential and in thermal equilibrium. With the help of Jordan-Wigner transformation, we perform a fermion-to-qubit mapping to derive a set of Lindblad superoperators that can be straightforwardly used on a wide range of physical setups. To illustrate our approach, we explore the effect of a charge sensor, acting as a probe, over the dynamics of electrons on coupled quantum molecules. The probe consists on a quantum dot attached to source and drain leads, that allows a current flow. The dynamics of populations, entanglement degree and purity show how the probe is behind the sudden deaths and rebirths of entanglement, at short times. Then, the evolution leads the system to an asymptotic state being a statistical mixture. Those are signatures that the probe induces dephasing, a process that destroys the coherence of the quantum system.

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I. INTRODUCTION

The study of the boundary between quantum and classical mechanics raised as one of the most interesting and challenging issues for the last thirty years [1–3]. Motivated by the necessity of exploring problems like the measurement of quantum properties or the classical limit for a specific quantum model, different ways to treat the so-called open quantum systems has been proposed [2, 4]. In particular, the density matrix formalism [5] becomes an important theoretical frame to explore multipartite systems with mixed quantum and classical features. From the wide set of problems linked with open systems, the analysis of the dynamics of a quantum system in contact with reservoirs, larger physical systems, stands as a fundamental quest. Speaking specifically of the “know-how”, master equations become adequate to circumvent the task, being deduced by tracing out the variables of the reservoirs [2, 4]. The integro-differential equations obtained after the application of several approximations permits to summarize the effect of reservoirs via a Lindblad operator [6, 7]. Extensions has been made in order to include memory effects, known as non-markovian approaches [8, 9], which has been observed in carefully prepared experimental setups [10].

On the other hand, since the seminal work of Jauho, Wingreen and Meir [11] about non-equilibrium quantum transport, a wealth of theoretical and experimental works have investigated the transport phenomena under the action of time-vary fields [12–15]. Recently, open quantum systems out-of-equilibrium have been theoretically investigated in quantum dots attached to leads in the presence of photonic or phononic fields [16]. In this specific context, a method to deal with transport problems in semiconductor nanostructures has been developed by W.-M. Zhang and co-workers [17–19], mixing the density operator formalism with nonequilibrium Green functions. From the point of view of the treatment of time-memory effects, this method is powerful because its direct application on the description of non-markovian setups. Still, the approach requires some familiarity with Keldysh nonequilibrium Green function technique.

Here, we present a formalism that offers an alternative path with immediate application on the study of dynamics of a general configuration of open quantum systems far from equilibrium. Using the Fermion-to-Qubit (FTQ) mapping, we provide a straightforward recipe to construct both, multi-partite Hamiltonian and Lindbladians, as tensor products of Pauli matrices. The FTQ mapping also sets automatically the complete computational basis to analyze the dynamics, written in terms of occupied and non-occupied states. The formalism presented here opens the possibility of future applications in the context of fermionic quantum computation [20].

The paper is organized as follows: in Sec. II, we set the foundations of our formalism, starting with the definition of a general form for fermionic operators. It is deduced an expression for a generic reservoir-system coupling, which is the key behind the construction of super-operators for open quantum dynamics. Section III presents the deduction of Lindbladian super-operators, for the case of non-interacting reservoirs considering a markovian condition. Section IV is devoted to the discussion of an application of our formalism on the context of transport phenomena. We focus on the behavior of electrons on charged quantum molecules, being probed by a nearby narrow conduction channel describing the action of a charge sensor. The

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behavior of populations, the entanglement dynamics, and
the purity permits to conclude that the probe induces de-
phasing, a decoherence process which acts over the quan-
tum dynamics of the coupled molecules. In Sec. V we
summarize our results.

II. FERMION-TO-QUBIT MAPPING AND
THE GENERAL HAMILTONIAN

Consider the open multipartite system illustrated in
Fig. 1 with N subsystems in space \( \mathcal{S} \), in contact with
M reservoirs, each with \( K_n \) inner states, defined in a
space denoted as \( \mathcal{R} \). We use \( i \) as the index of the \( i \)-th
subsystem in \( \mathcal{S} \) so \( i = 1, 2 \ldots N \). In the reservoir space,
we use two indexes: \( n \), which labels the \( n \)-th reservoir,
with \( n = 1, \ldots, M \), and \( k \), indicating the \( k \)-th state with
\( k = 1, \ldots, K_n \). The dimension of the whole, system and
reservoirs, is given by \( D = N + \sum_{n=1}^{M} K_n \). The general
Hamiltonian can be written as \( H(t) = H_0 + V(t) \) where

\[
H_0 = H_S \otimes I_{\mathcal{R}}^{\otimes(D-N)} + I_S^\otimes \otimes H_{\mathcal{R}},
\]

\[
V(t) = \sum_{n=1}^{N} \sum_{k=1}^{M} \sum_{l=1}^{K_n} u_n(t)V_{i(n,k)}d_{l(n,k)}^\dagger d_{l} + \text{h.c.} \tag{1}
\]

where \( H_{S(\mathcal{R})} \) is the Hamiltonian of the multipartite sys-
tem (reservoirs) without coupling and the term \( V(t) \) de-
scribes the coupling as a hopping process: a particle is
annihilated \( \langle d_l \rangle \) at \( \mathcal{S} \) at the same time that it is created
\( \langle d_{l(n,k)}^\dagger \rangle \) in \( \mathcal{R} \) and vice versa. Inside the coupling term,
the function \( u_n(t) \) is a time-dependent parameter [21],
and \( V_{i(n,k)} \) provides the coupling strength between sys-
tem and reservoirs.

Now we apply the FTQ mapping to this general sys-
tem. The operator \( d_m \) is defined by using the Jordan-Wigner transformation [22] as [23]

\[
d_m = \sigma_z^{\otimes(m-1)} \otimes \sigma_+^{(m)} \otimes I^{\otimes(D-m)}, \tag{2}
\]

where the index \( m \) now runs over both, \( \mathcal{S} \) and \( \mathcal{R} \) indexes.
\( \sigma_z \) is a Pauli matrix, \( I \) is the 2 \times 2 identity matrix, and \( O \) indicates a succession of \( L \) tensorial products of
operator \( O \). The creation operator \( d_m^\dagger \) is obtained by replac-
ing \( \sigma_-^{(m)} \) by \( \sigma_+^{(m)} \) with \( \sigma_{\pm} = (\sigma_x \pm i\sigma_y)/2 \). It is straightforward to prove that \( d_m \) and \( d_m^\dagger \) follows the anticommutation relations \( \{d_m, d_l\} = \delta_{m,l}, \{d_m, d_l^\dagger\} = \{d_m^\dagger, d_l\} = 0 \).

The explicit form for \( V(t) \) is now written as:

\[
V(t) = \sum_{i,n,k} u_n(t)V_{i(n,k)} \left( S_i \otimes \sigma_z^{\otimes K_1} \otimes \sigma_z^{\otimes K_2} \otimes \cdots \otimes (3)
\]

\[
\sigma_z^{\otimes K_{n-1}} \otimes R_{n,k}^\dagger \otimes I^{\otimes K_n+1} \cdots \otimes I^{\otimes M} \right) + \text{h.c.},
\]

where

\[
S_i = I^{\otimes(i-1)} \otimes \sigma_z^{(i)} \otimes \sigma_z^{\otimes(N-i)}, \tag{4}
\]

\[
R_{n,k}^\dagger = \sigma_z^{\otimes K_n-k} \otimes \sigma_z^{(k)} \otimes I^{\otimes K_n-k}.
\]

The \( S_i \) (\( R_{n,k}^\dagger \)) operators run only over the subspace \( \mathcal{S} \)
\((n\text{-th subspace of } \mathcal{R})\), and they preserve the fermionic
anticommutation relations.

In order to describe the quantum evolution of the en-
tire \( D \) dimensional system, we write the Von Neumann
equation in the interaction picture, \( \dot{\rho}(t) = \mathcal{L}(t)\rho_0 + \int_0^t dt_1 \mathcal{L}(t)\mathcal{L}(t_1)\rho(t_1) \) where \( \mathcal{L}(t) \) is the LIouville super-
operator, \( \mathcal{L}(t)\rho(t_1) = -i[V(t_1),\rho(t_1)] \) \((h = 1)\), and \( V(t) \)
is the coupling term defined as \( V(t) = e^{iH_0t}V(t)e^{-iH_0t} \) with
\( e^{iH_0t} = e^{iH_{\mathcal{S}}t} \otimes e^{iH_{\mathcal{R}}t} \). This transformation ap-
plies over the tensorial product inside Eq. (3) resulting
on a tensorial product between system operators \( S_i(t) = e^{iH_{\mathcal{S}}t}S_i e^{-iH_{\mathcal{S}}t} \) and similar terms for the re-
servoirs. Notice that, at the moment, we are treating the full
form of the system-reservoir interaction, using a mathema-
tical tool to distinguish the system from the reservoirs
without a loss of generality.

III. NON-INTERACTING RESERVOIRS AND
THE MARKOV APPROXIMATION

Let us assume the Born approximation, \( \rho(t) = \rho_S(t) \otimes
\rho_{\mathcal{R}} \), where \( \rho_S(t) \) is the reduced density matrix of mul-
tipartite system and \( \rho_{\mathcal{R}} \) are the density matrices for
reservoirs, thus \( \rho_{\mathcal{R}} = \rho_1 \otimes \rho_2 \otimes \cdots \otimes \rho_M \). We now
consider the effect of non-interacting reservoirs, set in
thermodynamical equilibrium, each described by Hamil-
tonian \( H_{\mathcal{R}} = \bigoplus_{n=1}^M H^{(n)} \) with \( H^{(n)} = \bigoplus_{k=1}^{K_n} H^{(n,k)} = \bigoplus_{k=1}^{K_n} \epsilon_n^{(k)} (\sigma_+\sigma_-^{(k)})\) and \( \epsilon_n^{(k)} \)
being the energy of the \( k \)-th mode of reservoir \( n \). The density matrix for each reservoir is a mixed state described by \( \rho_n = \rho_{\mathcal{R}} = \rho_1 \otimes \rho_2 \otimes \cdots \otimes \rho_M \). We now
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being the energy of the \( k \)-th mode of reservoir \( n \). The density matrix for each reservoir is a mixed state described by \( \rho_n = \)
\[ \frac{1}{2} \text{Exp}[-\beta \sum_{k} \epsilon_{\alpha}^{(k)}(\sigma_{+})(\sigma_{-})(\sigma_{E})] \], where \( \beta = 1/(k_B T) \), \( \epsilon_{\alpha}^{(k)} \) is the free particle energy measured from the chemical potential \( \mu_n \), and \( Z \) is the partition function. After taking the partial trace over reservoirs degrees of freedom and ignoring the null terms, we find

\[
\rho_S(t) = -\frac{1}{2\pi} \int_0^\pi dt_1 \sum_{i,j,n,k} \{ \Gamma_{i,j}^{n,k}(t_1, t_1) S_i(t_1) S_j(t_1) \rho_S(t_1) \text{Tr}_R \left[ \rho \otimes \rho \otimes \cdots \otimes \rho_{n-1} \otimes R_{n,k}(t_1) \rho_{n,k}(t_1) \otimes \cdots \otimes \rho_M \right] \\
+ \Gamma_{i,j}^{n,k}(t_1, t_1) S_i(t_1) S_j(t_1) \rho_S(t_1) \text{Tr}_R \left[ \rho \otimes \rho \otimes \cdots \otimes \rho_{n-1} \otimes R_{n,k}(t_1) \rho_{n,k}(t_1) \otimes \cdots \otimes \rho_M \right] \\
- \Gamma_{i,j}^{n,k}(t_1, t_1) S_i(t_1) S_j(t_1) \rho_S(t_1) \text{Tr}_R \left[ \rho \otimes \rho \otimes \cdots \otimes \rho_{n-1} \otimes \rho_{n-1} \otimes \rho_{n-1} \otimes \rho_M \right] \\
- \Gamma_{i,j}^{n,k}(t_1, t_1) S_i(t_1) S_j(t_1) \rho_S(t_1) \text{Tr}_R \left[ \rho \otimes \rho \otimes \cdots \otimes \rho_{n-1} \otimes \rho_{n-1} \otimes \rho_{n-1} \otimes \rho_M \right] \\
+ \text{h.c.} \},
\]

where \( R_{n,k}(t_1) = e^{iH^{(n,k)}_{\xi}(t_1) - iH^{(n,k)^*}_{\xi}(t_1)} \) and \( \Gamma_{i,j}^{n,k}(t_1, t_1) = 2\pi V_{i,n}(k) V_{j,n}(k) u_n(t) u_n^*(t_1) \). The equation for the reduced density matrix of the system is written as

\[
\dot{\rho}_S(t) = -\frac{1}{2\pi} \sum_{i,j,n,k} \left\{ f_{n,k} \int_0^\pi dt_1 \Gamma_{i,j}^{n,k}(t_1, t_1) e^{i\epsilon_{n,k}(t_1-t_1)} \right. \\
\times \left[ S_i(t_1) S_j(t_1) \rho_S(t_1) - S_j(t_1) S_i(t_1) \rho_S(t_1) \right] \\
+ (1 - f_{n,k}) \int_0^\pi dt_1 \Gamma_{i,j}^{n,k}(t_1, t_1) e^{-i\epsilon_{n,k}(t_1-t_1)} \right. \\
\times \left[ S_i(t_1) S_j(t_1) \rho_S(t_1) - S_j(t_1) S_i(t_1) \rho_S(t_1) \right] + \text{h.c.} \},
\]

after using the Baker-Hausdorff Lemma on the calculation of \( \text{Tr}_n \{ R_{n,k}(t_1) \rho_n R_{n,k}(t) \} = f_{n,k} e^{i\epsilon_{n,k}(t_1-t_1)} \) and \( \text{Tr}_n \{ R_{n,k}(t_1) \rho_n R_{n,k}(t) \} = (1 - f_{n,k}) e^{-i\epsilon_{n,k}(t_1-t_1)} \), where \( f_{n,k} = 1/[1 + e^{\beta \epsilon_{n,k}}] \) is the Fermi distribution function for reservoir \( n \) [24]. At this point, we consider the wideband limit [21]. We set \( V_{i,n}(k) = V_{i,n} \), meaning that all inner states on reservoir \( n \) have the same coupling with the system. The sum over \( k \) turns into an integral, \( \sum_k \rightarrow \int \cdots \text{D}_n(z) dz \), where the density of states is assumed constant, \( \text{D}_n(z) = \text{D}_n \). The bias voltage \( eV \) is given by \( \mu_n - \mu_m = eV \), where the source (drain) chemical potential is \( \mu_n (\mu_m) \). If \( eV \) is high and considering low values of temperature, we can assume that \( f_{n,(m),k} = f_{n(m),k} = 1(0) \) resulting in,

\[
\dot{\rho}_S(t) = -\frac{1}{2} \sum_{i,j,n} \Gamma_{i,j}^{n,n}(t) \left[ F_n(t,i,j) + G_n(t,i,j) \right],
\]

with

\[
F_n(t,i,j) = f_n \left[ S_i(t_1) S_j(t_1) \rho_S(t_1) - S_j(t_1) S_i(t_1) \rho_S(t_1) \right] \\
+ \rho_S(t) S_j(t_1) S_i(t_1) - S_j(t_1) \rho_S(t_1) S_i(t_1),
\]

\[
G_n(t,i,j) = (1 - f_n) \left[ S_i(t_1) S_j(t_1) \rho_S(t_1) - S_i(t_1) \rho_S(t_1) S_j(t_1) \right] \\
+ \rho_S(t) S_j(t_1) S_i(t_1) - S_i(t_1) \rho_S(t_1) S_j(t_1).
\]

and \( \Gamma_{i,j}^{n,n}(t) = 2\pi V_{i,n}(k) V_{j,n}(k) u_n(t) u_n^*(t_1) \). We apply the vec operation [25] to both sides of Eq. (7), obtaining

\[
\frac{d}{dt} \text{vec}[\rho_S](t) = -\frac{1}{2} \Gamma(t) \text{vec}[\rho_S](t),
\]

where \( \Gamma(t) \) is \( N^2 \times N^2 \) supermatrix defined as

\[
\Gamma(t) = \sum_{i,j,n} \Gamma_{i,j}^{n,n}(t) \left( f_n \left[ I_S \otimes S_i(t_1) S_j^T(t_1) - S_j^T(t_1) \otimes S_i(t_1) \right] \\
+ [S_i(t_1) S_j^T(t_1) \otimes I_S - S_j^T(t_1) \otimes S_i(t_1)] \\
+ [S_j^T(t_1) S_i(t_1) \otimes I_S - S_i^T(t_1) \otimes S_j(t_1)] \right).
\]

where the superscript \( T \) means matrix transposition.

Writing the reduced density matrix in the Schrödinger picture, \( \text{vec}[\rho_S^T](t) = [\text{Exp}(iH^T_{\xi} t) \otimes \text{Exp}(-iH_{\xi} t)] \text{vec}[\rho_S](t) \), and taking the time derivative we find the differential equation,

\[
\frac{d}{dt} \text{vec}[\rho_S^T](t) = \mathcal{L}(t) \text{vec}[\rho_S^T](t),
\]

where the superoperator \( \mathcal{L} \) is given by

\[
\mathcal{L}(t) = \mathcal{L}_0 - \frac{1}{2} \sum_{i,j,n} \Gamma_{i,j}^{n,n}(t) \left[ f_n \mathcal{L}_{i,j}^T + (1 - f_n) \mathcal{L}_{i,j}^T \right],
\]

with

\[
\mathcal{L}_0 = -i(I_S \otimes H_S - H^T_{\xi} \otimes I_S) \\
\mathcal{L}_{i,j}^T = I_S \otimes S_i S_j^T + S_i S_j^T \otimes I_S - S_j^T \otimes S_i - S_i \otimes S_j - S_j \otimes S_i.
\]

Eq. (10) has the formal solution

\[
\text{vec}[\rho_S^T](t) = T e^{\mathcal{L}_0 t} \text{vec}[\rho_S^T](0),
\]

where \( T \) is the chronological time-ordering operator. Writing the superoperators above in terms of Pauli matrices, we arrive to
\[ \mathcal{L}^\pm_{i} = I^{\otimes (N+i-1)} \otimes (\sigma_+ \sigma_\pm^i)^{(i)} \otimes I^{\otimes (N-i)} + I^{\otimes (i-1)} \otimes (\sigma_+ \sigma_\pm^i)^{(i)} \otimes I^{\otimes (2N-i)} \]
\[ -2I^{\otimes (i-1)} \otimes \sigma_+^{(i)} \otimes \sigma_\pm^{(N-i)} \otimes I^{\otimes (i-1)} \otimes \sigma_+^{(i)} \otimes \sigma_\pm^{(N-i)} , \]
\[ \mathcal{L}^\pm_{i<j} = \pm I^{\otimes (N+i-1)} \otimes \sigma_+^{(i)} \otimes \sigma_\pm^{(j-i-1)} \otimes \sigma_\pm^{(j)} \otimes I^{\otimes (N-j)} \pm I^{\otimes (i-1)} \otimes \sigma_+^{(i)} \otimes \sigma_\pm^{(j-i-1)} \otimes \sigma_\pm^{(j)} \otimes I^{\otimes (2N-j)} \]
\[ - I^{\otimes (i-1)} \otimes \sigma_+^{(i)} \otimes \sigma_\pm^{(N-i)} \otimes I^{\otimes (j-1)} \otimes \sigma_+^{(j)} \otimes \sigma_\pm^{(N-j)} - I^{\otimes (j-1)} \otimes \sigma_+^{(j)} \otimes \sigma_\pm^{(N-j)} \otimes I^{\otimes (i-1)} \otimes \sigma_+^{(i)} \otimes \sigma_\pm^{(N-i)} , \]
\[ \mathcal{L}^\pm_{i>j} = \pm I^{\otimes (N+j-1)} \otimes \sigma_+^{(j)} \otimes \sigma_\pm^{(i-j-1)} \otimes \sigma_\pm^{(i)} \otimes I^{\otimes (N-i)} \pm I^{\otimes (j-1)} \otimes \sigma_+^{(j)} \otimes \sigma_\pm^{(i-j-1)} \otimes \sigma_\pm^{(i)} \otimes I^{\otimes (2N-i)} \]
\[ - I^{\otimes (i-1)} \otimes \sigma_+^{(i)} \otimes \sigma_\pm^{(N-i)} \otimes I^{\otimes (j-1)} \otimes \sigma_+^{(j)} \otimes \sigma_\pm^{(N-j)} - I^{\otimes (j-1)} \otimes \sigma_+^{(j)} \otimes \sigma_\pm^{(N-j)} \otimes I^{\otimes (i-1)} \otimes \sigma_+^{(i)} \otimes \sigma_\pm^{(N-i)} , \]

Eqs. (13) provide the recipe to construct Lindbladian operators for fermionic systems, based on fermion-to-qubit mapping. In order to apply Eqs. (13), it is enough to specify \( N \), the total number of sites or levels being considered in the system. Because the expressions are explicit tensorial products, they make numerical implementations very straightforward.

IV. QUANTUM DYNAMICS ON COUPLED QUANTUM MOLECULES

In this section, we proceed to apply the formalism in the context of charged quantum dots [26, 27]. In this physical setup, metallic gates are used to confine electrons within a small region of AlGaAs-GaAs [28]. Manipulating the chemical potential of sources and drains, both described as electronic reservoirs, charges can be introduced inside the nanostructure [29]. Coherent tunneling between two adjacent quantum dots, which form an artificial molecule, permits the codification of information in a qubit, once it is possible to define a two-level system [30]. From the point of view of quantum information processing, two-qubit operations are necessary for the implementation of a universal set of quantum gates. The Coulomb interaction between charges in two molecules [31, 32] provides a rich dynamics, enough to implement quantum gates [33], and the creation of maximally entangled states [34, 35].

We are interested in analyze the quantum dynamics of the coupled quantum molecules, under the effect of a small open quantum system. The last consists on an extra quantum dot with a source and a drain which can be used to charge or discharge the nanostructure. The configuration of the complete physical system is shown in Fig. 2. When a charge occupies the electronic level of this fifth dot, the electrostatic interaction between the charge and the electron in the molecule works as a capacitive probe. The tunneling between probe and molecules is forbidden, so there is no loss of electronic population of the molecule.

Using the formalism of Sec. II, it is straightforward to obtain the 16D complete computational basis for the two quantum molecules system, denoted as \( \mathcal{M} \). The basis is composed not only of the two-qubit subspace \( \mathcal{M}_{2QB} = \{(1100), (0101), (0011), (0110)\} \), but also of others like the one-particle subspace \( \mathcal{M}_1 = \{(1100), (0100), (0010), (0001)\} \), the two-particles per molecule subspace \( \mathcal{M}_2 \) \( \mathcal{M}_3 = \{(1110), (1101), (0111), (1011)\} \), the four-particle state \( 1111 \), and the vacuum \( 0000 \). The basis allows the description of closed and open quantum dynamics, as the effect of sources, which take an initial vacuum state to some occupied state (eventually the full-occupation state, \( 1111 \)), or drains, that take any occupied state to the vacuum state, \( 0000 \).

For this specific application, we consider that a previous process of initialization prepared the two-qubit system in one of the four state of subspace \( \mathcal{M}_{2QB} \). The Hamiltonian for the two qubits on the coupled quantum molecules is written as

\[ H_{\mathcal{M}} = H_0 + H_T + H_U \]
\[ = \bigoplus_{i=1}^{4} \xi_i^{(M)} P_i^{(i)} + H_T + H_U \]

where

\[ H_T = -\Delta_1^{\pm} \left[ \sigma_+^{(1)} \otimes \sigma_\pm^{(2)} + \sigma_+^{(1)} \otimes \sigma_\pm^{(2)} \otimes I^{\otimes 2} \right] \]
\[ - \Delta_4^{\pm} \left[ I^{\otimes 2} \otimes \sigma_\pm^{(3)} \otimes \sigma_\pm^{(4)} + I^{\otimes 2} \otimes \sigma_\pm^{(3)} \otimes \sigma_\pm^{(4)} \right], \]
\[ H_U = U_a \left[ P_+^{(1)} \otimes I \otimes P_+^{(3)} \otimes I + I \otimes P_+^{(2)} \otimes I \otimes P_+^{(4)} \right] \]
\[ + U_b \left[ P_+^{(1)} \otimes I \otimes P_+^{(4)} + I \otimes P_+^{(2)} \otimes P_+^{(3)} \otimes I \right], \]

with \( P_+ = \sigma_+ \sigma_- = |+\rangle \langle +| \) and the index 1 to 4 describes a specific dot on quantum molecules. The term \( H_0 \) is the uncoupled term with the electronic energies \( \xi_i^{(M)} \), while \( H_T \) and \( H_U \) terms describe electronic tunneling inside each molecule and the Coulomb interactions between electrons, respectively.

When the probe is introduced, the full Hamiltonian reads as

\[ H_{\text{full}} = H_S \otimes I + I^{\otimes 4} \otimes \varepsilon_5 P_+^{(5)} + U_p P_+^{(1)} \otimes I^{\otimes 3} \otimes P_+^{(5)}, \]

where the last term describes the capacitive coupling between system and the extra dot with parameter \( U_p \). To describe the action of both, source and drain of charge on the 5-th dot, we use Eq. (13) to obtain the Lindblad term

\[ \mathcal{L}^{\pm}_{55} = I^{\otimes 5} \otimes (\sigma_\pm \sigma_\pm)^{(5)} + I^{\otimes 5} \otimes (\sigma_\pm \sigma_\pm)^{(5)} \otimes I^{\otimes 5} \]
\[ - 2I^{\otimes 4} \otimes \sigma_\pm^{(5)} \otimes I^{\otimes 4} \otimes \sigma_\pm^{(5)}. \]
Our goal is to check the quantum dynamics at the specific condition for generation of maximally entangled states [35]. We start solving numerically Eq. (10), considering the terms of Eq. (16). The solution, \( \rho_{S_n}(t) \), describes the dynamics of system and probe. Then, by tracing out the 5-th dot, the behavior of the two-qubit system \( S \) (dots 1 to 4) is described by the reduced density matrix,

\[
\rho_{M}(t) = \text{Tr}_5[\rho_{S_n}(t)].
\]

The average occupation of \( i \)-th dot \((i = 1...4)\) is given by

\[
\langle \hat{N}_i \rangle = \text{Tr}\{\hat{N}_i \rho_{M}(t)\},
\]

where the operator \( \hat{N}_i \) is defined as

\[
\hat{N}_i = \mathbb{I}^{\otimes i-1} \otimes P_+^{(i)} \otimes \mathbb{I}^{\otimes 4-i}.
\]

To quantify the probabilities of occupation for each state on the two-qubit subspace \( \mathcal{M}_{2QB} \), we calculate the cross-population averages defined as,

\[
P_{[1001]} = \langle \hat{N}_1 (\mathbb{I}^{\otimes 4} - \hat{N}_2)(\mathbb{I}^{\otimes 4} - \hat{N}_3)\hat{N}_4 \rangle,
\]

\[
P_{[0110]} = \langle (\mathbb{I}^{\otimes 4} - \hat{N}_1)\hat{N}_2\hat{N}_3(\mathbb{I}^{\otimes 4} - \hat{N}_4) \rangle,
\]

\[
P_{[1010]} = \langle \hat{N}_1 (\mathbb{I}^{\otimes 4} - \hat{N}_2)\hat{N}_3(\mathbb{I}^{\otimes 4} - \hat{N}_4) \rangle,
\]

\[
P_{[0101]} = \langle (\mathbb{I}^{\otimes 4} - \hat{N}_1)\hat{N}_2(\mathbb{I}^{\otimes 4} - \hat{N}_3)\hat{N}_4 \rangle.
\]

As initial condition, we assume that the initialization process prepares the state \( |\Psi(0)\rangle = |1001\rangle \) so \( P_{[1001]}(0) = 1 \) \( \langle \hat{N}_1 \rangle = \langle \hat{N}_4 \rangle = 1 \). The effect of the probe over the evolution of cross-populations, Eqs. (20), is shown in Fig. 3, considering the physical parameters used to obtain maximally entangled states [35]. For the sake of comparison, we include in the inset the evolution of the same quantities when the probe is turned off, considering a shorter time scale. The periodic coherent dynamics from Ref. [35] is recovered from our approach, where a Bell state is dynamically generate at the times when \( P_{[1001]} = P_{[0110]} = 0.5 \), while \( P_{[1010]} = P_{[0101]} = 0 \).

When the probe is turned on, as a current passes through the narrow conduction channel in dot 5, the effect is to induce an attenuation of the coherent oscillations of populations \( P_{[1001]} \) and \( P_{[0110]} \), black and red lines on Fig. 3(a) respectively. Additionally, we note the increase of populations \( P_{[1010]} \) and \( P_{[0101]} \), as can be seen from green and blue lines on Fig. 3(b). Calculations of the value of population for states in subspaces of \( \mathcal{M} \) different from \( \mathcal{M}_{2QB} \) shows that the charges remains confined at the quantum molecules, as expected. At long times, the population for each state on subspace \( \mathcal{M}_{2QB} \) tend to 0.25 in the stationary regime.

To check the dynamics of population inside each molecule, we calculate the occupations for the single \( i \)-th quantum dot, \( \langle \hat{N}_i \rangle \). The results for the first molecule (dots 1 and 2) are shown in Fig. 4(a), for the same initial condition and physical parameters of Fig. 3. If probe
is turned off, the occupations $\langle \hat{N}_1 \rangle$ and $\langle \hat{N}_2 \rangle$, shown with dashed lines, develop periodic population inversions, which is a signature of the coherent tunneling between the dots inside the molecule. The same behavior, not shown here, is obtained for the second molecule (dots 3 and 4). Once the probe is turned on, the coherent dynamics of $\langle \hat{N}_1 \rangle$ is attenuated, as observed in Fig. 3 for cross-populations. It becomes clear that the second molecule is less affected by the probe, once the oscillations of $\langle \hat{N}_3 \rangle$ and $\langle \hat{N}_4 \rangle$ survive longer than those for the first molecule.

The exact nature of the asymptotic state is the question that rises from the analysis presented above. The occupations of the dots are not able to distinguish between quantum superpositions and mixed states, so it is convenient to analyze the quantum dynamics using the tools of quantum information. Because the physical conditions used for our calculations are the same for the dynamical generation of Bell states, it is interesting to check the behavior of the degree of entanglement in the system. In order to fulfill this task, we use the concurrence as defined by Wooters [36], which is a measurement of entanglement degree between two-qubits. Considering a generic density matrix in a two qubit space $\rho_{2QB}$, an auxiliary Hermitian operator $[37]$, $R$ is defined as
\begin{equation}
R = \sqrt{\rho_{2QB} \rho_{2QB}^* / \rho_{2QB}}.
\end{equation}
where $\rho_{2QB} = (\sigma_y \otimes \sigma_y) \rho_{2QB}^* (\sigma_y \otimes \sigma_y)$, is the spin-flipped matrix with $\rho_{2QB}$ being the complex conjugate of $\rho_{2QB}$. The concurrence is written as
\begin{equation}
C = \max(0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4),
\end{equation}
where $\lambda_i$ are the eigenvalues of the operator $R$ in decreasing order. For our application, we construct a $4 \times 4$ density operator using only the terms on $\rho_M$ related with states of subspace $M_{2QB}$. This can be done once the dynamics keeps the other state of the complete basis empty.

Because it is our interest to establish the purity of the coupled molecules, we calculate the linear entropy of the evolved density matrix $\rho_M$, which is defined as
\begin{equation}
S(t) = 1 - \Tr[\rho^2_M(t)].
\end{equation}
For bipartite quantum systems, the linear entropy works as an entanglement quantifier. Nevertheless, if the quantum system of interest is coupled with an open system, the linear entropy acts as a measurement of purity. If the state of the quantum system remains as a pure quantum state, the linear entropy value is $S = 0$. If the quantum system goes to any kind of mixed state $S \neq 0$ with a maximum value $S_{\text{max}}$ given by the expression
\begin{equation}
S_{\text{max}} = 1 - \frac{1}{d},
\end{equation}
where $d$ is the dimension of the Hilbert space of the quantum system. This value is associated with the statistical mixture of all elements of the basis.

Both quantities are shown in Fig. 5. Dashed lines in Fig. 5 illustrate the case when the probe is turned off ($U_p = 0$). The concurrence, Fig. 5(a), shows its periodic evolution from a separable ($C = 0$) to an entangled Bell state ($C = 1$), as discussed in Ref. [35]. For all evolution, the linear entropy in Fig. 5(b) has a value $S = 0$ (dashed line over the $Jt$ axis) which is consistent with the fact that the coupled molecules are a closed system.

This situation changes drastically when the probe is turned on. Red line on Fig. 5 shows a case when the capacitive coupling is comparable with the electrostatic interaction between the electrons inside the molecules so $U_p = J$. The probe changes the concurrence dynamics, Fig. 5(a), being the main features the lack of periodicity together with the decreasing of the entanglement degree. Around $Jt \sim 90$, occurs a sudden death of entanglement [38, 39], which were demonstrate experimentally in optical setups [40] through indirect measurements of concurrence. This phenomenon is an abrupt fall of entanglement to zero, which could be recovered (rebirth) after some time. The purity, red line in Fig. 5(b), increases smoothly with time, showing that the quantum
FIG. 5. Dynamics of (a) concurrence \( (C) \) and (b) linear entropy \( (S) \) for several values of coupling \( U_p \), for the same choice of physical parameters used on Fig.3: \( U_p = 0 \) (black dashed lines), \( U_p = J \) (red lines), \( U_p = 2J \) (green lines) and \( U_p = 3J \) (blue lines).

state inside the molecules becomes a mixed state as times evolves.

As we increase \( U_p \), the behavior of concurrence basically shares the same characteristics discussed above with some slight differences. The first is the decrease of temporal scale for the first sudden death and rebirth in Fig. 5(a). The second is the definitive suppression of the entanglement degree, meaning the asymptotic state has \( C = 0 \). Concerning the purity evolution, green and blue lines in Fig. 5(b), the time scale to attain the asymptotic mixed state decreases as the coupling parameter \( U_p \) increases, revealing the irreversible loss of quantum information on the coupled molecules due to the action of the probe. The results obtained for \( U_p = 3J \), blue line, confirms the nature of the asymptotical behavior: the value of \( S \) is \( S_{\text{max}} = 1 - 1/4 = 0.75 \) \( (d = 4) \) which means the system goes to a statistical mixture of all states on \( M_{2QB} \).

The results presented above characterize a process of decoherence, induced by the action of the probe on the dynamics of the charges inside the coupled quantum molecules. All these aspects together become signatures that the probe induces dephasing on the quantum system without the loss of particles. Additionally, the behavior of both, concurrence and linear entropy, shows that the initial pure system evolves to a statistical mixture when the system is probed.

V. SUMMARY

In this work, we present a formalism for the treatment of the interaction between quantum systems in contact with reservoirs based on a fermion-to-qubit map. The formalism has a flexibility which permits the analysis of general configurations of multipartite systems coupled with multiple reservoirs. We focus on the obtaining of a master equation, where Lindbladian operators keep the structure of fermion-to-qubit mapping. The success on the demonstration of such a form of master equation brings all the advantages of Jordan-Wigner transformation to problems of quantum information processing, as used for strong-correlated systems. Specifically, it is possible to treat problem where reservoirs can act as sources and drains of particles. In the particular case of non-interacting reservoirs prepared as thermal states, the method provides expressions for Lindblad super-operators that can be straightforwardly use on numerical implementations of non-equilibrium problems.

To illustrate, we apply our formalism to the problem of dynamics of two electrons inside quantum molecules in contact with a probe, the last being an open system. The probe is a narrow transmission channel, being an open quantum dot attached to source and drain leads. By using the general equation for Lindblad super-operators, we obtain a reduced density matrix for the coupled quantum molecules. Our calculations of populations, concurrence and linear entropy let us to conclude that the probe induces dephasing, which makes the system lose the ability to generate entangled Bell states as time evolves. It is worth to remark an interesting feature induced by the probe: the apparition of sudden deaths and rebirths of entanglement. This sudden death is usually explained as caused by the action of quantum noise over the composite entangled bipartite system. Additionally, the system evolves to an asymptotic state, being a statistical mixture of the four elements of the subspace \( M_{2QB} = \{ |1010\rangle, |0101\rangle, |1001\rangle, |0110\rangle \} \), indicated by a linear entropy compatible to the number of states in a reduced Hilbert space.

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