Numerical and Analytical Approach to the Quantum Dynamics of Two Coupled Spins in Bosonic Baths

Alessandro Sergi
School of Physics, University of KwaZulu-Natal, Pietermaritzburg, Private Bag X01 Scottsville, 3209 Pietermaritzburg, South Africa

Ilya Sinayskiy
Quantum Research Group, School of Physics, University of KwaZulu-Natal, Durban, 4001, South Africa

Francesco Petruccione
Quantum Research Group, School of Physics and National Institute for Theoretical Physics, University of KwaZulu-Natal, Durban, 4001, South Africa

Abstract

The quantum dynamics of a spin chain interacting with multiple bosonic baths is described in a mixed Wigner-Heisenberg representation. The formalism is illustrated by simulating the time evolution of the reduced density matrix of two coupled spins, where each spin is also coupled to its own bath of harmonic oscillators. In order to prove the validity of the approach, an analytical solution in the Born-Markov approximation is found. The agreement between the two methods is shown.

*Electronic address: sergi@ukzn.ac.za
†Electronic address: ilsinay@gmail.com
‡Electronic address: petruccione@ukzn.ac.za
I. INTRODUCTION

For the sake of studying quantum information transport in solid state devices, the quantum dynamics of spin chains coupled to bosonic baths has attracted much attention in the recent scientific literature [1, 2, 3, 4, 5, 6, 7, 8]. Here, we show how a mixed Wigner-Heisenberg representation of quantum mechanics is particularly well-suited to the numerical simulation of such systems. This is illustrated by studying the time evolution of the reduced density matrix of a minimal chain, composed of two spins, each coupled to a bath of harmonic oscillators. The temperature of each bath can be defined independently, so that nonequilibrium situations can be addressed with no further theoretical or computational efforts. The dynamics of the total systems, spins plus harmonic oscillators, is unitary and numerically exact. No Markovian or rotating waves approximations need to be invoked. Reduced operators are obtained simply by integrating the coordinates of the oscillators in Wigner phase space. Our numerical solution is compared with an analytical solution of the Markovian master equation of the two spins and good agreement is found. It is very easy to extend the algorithm to study longer chains and multiple bosonic baths.

It is worth remarking that the mixed Wigner-Heisenberg representation that we adopt in this paper has been originally proposed for introducing a quantum-classical representation of systems immersed in gravitational fields and in plasma physics [9]. In particular it has been developed [10] and applied to a variety of models in chemical physics [11, 12], and it has already been noted [13] that such a representation is exact in the case of (bosonic) bath of harmonic oscillators.

This paper is organized as follows. Section II illustrates the Wigner-Heisenberg representation of quantum mechanics. Section III provides the details of the model we have studied. The numerical algorithms for the computer simulation is illustrated in Sec. IV. The Born-Markov approximation for the master equation and details of the analytical solution are given in Sec. V. Results of both our numerical and analytical studies are displayed in Sec. VI. Finally, our conclusions are reported in Sec. VII.
II. WIGNER-HEISENBERG REPRESENTATION OF QUANTUM MECHANICS

Let us consider a system defined by the total Hamiltonian operator

\[ \hat{H} = \hat{H}_S + \hat{H}_B + \hat{H}_{SB}, \]

where the subscripts \( S, B, \) and \( SB \) stand for subsystem, bath, and coupling, respectively. The Heisenberg equation of motion of the density matrix can be written as

\[ \frac{\partial}{\partial t} \hat{\rho} = -\frac{i}{\hbar} \left[ \hat{H}, \hat{\rho} \right] \cdot \mathcal{B} \cdot \left[ \hat{H} \hat{\rho} \right], \]

where \( \mathcal{B} \) is the antisymmetric constant matrix

\[ \mathcal{B} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}. \]

Assuming that the bath Hamiltonian depends on a pair of canonically conjugated operators \( \hat{X} = (\hat{R}, \hat{P}) \), and the coupling has the form \( \hat{H}_{SB} = \hat{H}_{SB}(\hat{R}) \), we can introduce a partial Wigner transform for the density matrix

\[ \hat{\rho}_W(X) = \frac{1}{(2\pi \hbar)^{3N}} \int dze^{iPz/\hbar} \langle R - \frac{z}{2} | \hat{\rho} | R + \frac{z}{2} \rangle, \]

and for the generic bath-dependent operator \( \hat{\chi}(\hat{R}, \hat{P}) \)

\[ \hat{\chi}_W(X) = \int dze^{iPz/\hbar} \langle R - \frac{z}{2} | \hat{\chi} | R + \frac{z}{2} \rangle, \]

where \( X = (R, P) \) are canonically conjugated classical variables in phase space. Taking the partial Wigner transform of Eq. (2)

\[ \frac{\partial}{\partial t} \hat{\rho}_W(X, t) = -\frac{i}{\hbar} \left[ \hat{H}_W(X), \hat{\rho}_W(X) \right] \cdot \mathcal{D} \cdot \left[ \hat{H}_W(X) \hat{\rho}_W(X, t) \right], \]

where

\[ \mathcal{D} = \begin{bmatrix} 1 & e^{i\Phi} \overline{\partial}_I b_{ij} \overline{\partial}_j \\ -e^{-i\Phi} \overline{\partial}_I b_{ij} \overline{\partial}_j & 0 \end{bmatrix}. \]

In Equation (7) we have used the symbol \( \overline{\partial}_I = \frac{\partial}{\partial X_I} \) to denote an operator of derivation (with respect to the phase space point coordinates) which acts on whatever stands on its
right. Analogously, $\overleftarrow{\partial}_I$ acts on whatever stands on its left. Moreover, the summation over repeated indices must be performed in Eq. (7) and in the following. The mixed Wigner-Heisenberg form of the Hamiltonian operator, $\hat{H}_W$, is

$$\hat{H}_W(X) = \hat{H}_S + H_{W,B}(X) + \hat{H}_{W,SB}(R) . \tag{8}$$

Equation (6) provides a mixed Wigner-Heisenberg representation of quantum mechanics, where operators also depend on phase space (c-number) coordinates, which is completely equivalent to the usual Heisenberg representation. However, the difficulties associated to the solution of Eq. (6) are formidable. Yet, for quadratic bath Hamiltonians

$$\hat{H}_{W,B} = \sum_{I=1}^{N} \left( \frac{P_I^2}{2} + \frac{1}{2} \omega_I^2 R_I^2 \right) \tag{9},$$

where $(R_I, P_I)$, $I = 1, \ldots, N$, are the coordinates and momenta, respectively, of a system of $N$ independent harmonic oscillators with frequencies $\omega_I$, and for interaction Hamiltonians of the type

$$\hat{H}_{W,SB} = V_B(R) \otimes \hat{H}'_S \tag{10},$$

where $V_B(R)$ is at most a quadratic function of $R$ and $\hat{H}'_S$ acts only in the Hilbert space of the subsystem, Eq. (6) can be rewritten using the antisymmetric operator matrix

$$D_{\text{lin}} = \begin{bmatrix} \frac{1}{2} & \frac{i}{\hbar} \bar{\partial}_I B_{IJ} \bar{\partial}_J \\ -\frac{1}{2} - \frac{i}{\hbar} \bar{\partial}_I B_{IJ} \bar{\partial}_J & 0 \end{bmatrix}. \tag{11}$$

Actually, it can be shown that for the class of Hamiltonians specified by Eqs. (9) and (10)

$$D \rightarrow D_{\text{lin}} \tag{12}$$

holds exactly. For more general bath Hamiltonians and couplings, such a substitution amounts to performing a quantum-classical approximation [10]. What matters here is that for the class of systems we are interested in the Eq. (12) is exact and provides via Eq. (2) a Wigner-Heisenberg formulation of quantum mechanics which can be numerically simulated employing algorithms previously developed within a chemical-physical context [15].
III. MODEL SYSTEM

The system we are interested in this paper is defined by the following subsystem Hamiltonian

\[ \hat{H}_S = -j_x \hat{\sigma}_x^{(1)} \hat{\sigma}_x^{(2)} - j_y \hat{\sigma}_y^{(1)} \hat{\sigma}_y^{(2)} - j_z \hat{\sigma}_z^{(1)} \hat{\sigma}_z^{(2)} \]  

(13)

representing a chain of two quantum spins coupled to each other. The constants \( j_i \), with \( i = x, y, z \), dictate the strength of the coupling between the spins. The operators \( \hat{\sigma}_i^{(k_s)} \) with \( i = x, y, z \) are the Pauli matrix operators for spin \( k_s = 1, 2 \). The bath Hamiltonian is

\[ \hat{H}_{W,B} = \sum_{k_s=1}^{2} \sum_{I=1}^{N} \frac{P_{I,k_s}^2}{2} + \frac{\omega_I^2}{2} R_{I,k_s}^2. \]  

(14)

The above Hamiltonian represents two independent harmonic oscillator baths with coordinates and momenta \((R_{I,k_s}, P_{I,k_s})\), (where \( I = 1, N \) labels the oscillators and \( k_s = 1, 2 \) labels the bath). The harmonic oscillator frequencies \( \omega_I \) are taken to be bath-independent since we want to adopt two baths with identical spectral density. However, the baths can have different initial conditions (and eventually different temperature). The coupling is given by

\[ \hat{H}_{W,SB} = -\sum_{k_s=1}^{2} \sum_{I=1}^{N} c_I R_{I,k_s} \hat{\sigma}_z^{(k_s)}, \]  

(15)

showing that each spin is coupled to its own oscillator bath.

The density matrix of the two-spin chains obeys the exact Wigner-Heisenberg equation

\[ \frac{\partial}{\partial t} \hat{\rho}_W = -\frac{i}{\hbar} \left[ \hat{H}_W, \hat{\rho}_W \right] \cdot \mathcal{D}_{\text{lin}} \cdot \left[ \hat{H}_W, \hat{\rho}_W \right], \]  

(16)

where \( \hat{H}_W = \hat{H}_S + \hat{H}_{W,B} + \hat{H}_{W,SB} \) is given by the sum of Eqs. (13)-15. The reduced density matrix of the spin subsystem is given at all times by

\[ \hat{\rho}_S(t) = \int \prod_{k_s=1}^{2} \prod_{I=1}^{N} dX_{I,k_s} \hat{\rho}_W(X, t). \]  

(17)

For the calculation presented in this paper, we assume an initially uncorrelated density matrix, which, once partially Wigner transformed, takes the form

\[ \hat{\rho}_W(t_0) = \hat{\rho}_S(t_0) \rho_{W,B}(X, t_0), \]  

(18)

where

\[ \rho_{W,B}(X, t_0) = \prod_{k_s=1}^{2} \prod_{I=1}^{N} \frac{\tanh(\beta_{k_s} \omega_I/2)}{\pi} \times \exp \left[ -2 \frac{\tanh(\beta_{k_s} \omega_I/2)}{\omega_I} H_{W,B} \right], \]  

(19)
and where $H_{W,B}$ is defined in Eq. (14) and $\beta_j = (k_B T_k)^{-1}$ is the inverse temperature of each oscillator bath ($k_B$ is the Boltzmann constant).

IV. NUMERICAL ALGORITHM

In cases in which the coupling Hamiltonian $\hat{H}_{W,SB}$ can be treated as a small perturbation (weak coupling), it is useful to represent the abstract Eq. (16) in the adiabatic basis. Such a basis is defined by the eigenvalue equation

$$ (\hat{H}_S + \hat{H}_{W,SB})|\alpha; R\rangle = E_\alpha(R)|\alpha; R\rangle. \quad (20) $$

Hence, Eq. (16) can be recast in propagator form

$$ \rho_{\alpha\alpha'}^{W}(X, t) = \sum_{\beta\beta'} (e^{-itL_{\alpha\alpha',\beta\beta'}} \rho_{\beta\beta'}^{W}(X)), \quad (21) $$

where

$$ iL_{\alpha\alpha',\beta\beta'} = iL^0_{\alpha\alpha'} \delta_{\alpha\alpha'} \delta_{\beta\beta'} + T_{\alpha\alpha',\beta\beta'} \cdot (22) $$

The operator $iL^0_{\alpha\alpha'}$ is defined as

$$ iL^0_{\alpha\alpha'} = i\omega_{\alpha\alpha'} + iL_{\alpha\alpha'}, \quad (23) $$

where $\omega_{\alpha\alpha'} = (E_{\alpha}(R) - E_{\alpha'}(R))/\hbar$ and

$$ iL_{\alpha\alpha'} = P \frac{\partial}{\partial R} + \frac{1}{2} (F_{\alpha}^0 + F_{\alpha'}^0) \cdot \frac{\partial}{\partial P} \cdot (24) $$

$F_{\alpha}^0 = -\langle \alpha; R | \partial \hat{H}_W / \partial R | \alpha; R \rangle$ is the Hellmann-Feynman force [16]. The transition operator $T_{\alpha\alpha',\beta\beta'}$ is purely off-diagonal and defined by

$$ T_{\alpha\alpha',\beta\beta'} = P \cdot d_{\alpha\beta} \left( 1 + \frac{1}{2} \frac{(E_{\alpha} - E_{\beta})d_{\alpha\beta}}{P \cdot d^*_{\alpha\beta} \cdot \frac{\partial}{\partial P}} \right) \delta_{\alpha'\beta'} + P \cdot d^*_{\alpha'\beta'} \left( 1 + \frac{1}{2} \frac{(E_{\alpha'} - E_{\beta'})d^*_{\alpha'\beta'}}{P \cdot d_{\alpha\beta} \cdot \frac{\partial}{\partial P}} \right) \delta_{\alpha\beta} \quad (25) $$

where $d_{\alpha\beta} = \langle \alpha; R | \partial / \partial R | \beta; R \rangle$ is the coupling vector between the adiabatic states $|\alpha; R\rangle$ defined in Eq. (20). Above and in the following, the quantities are defined adopting scaled coordinates, according to the definition of the Hamiltonians in Eqs. (13-15). The operator
FIG. 1: Time evolution trace of the reduced density matrix element vs time \((\beta_1 = \beta_2 = 0.005)\). Initial density matrix \(\hat{\rho}_s(0) = |1,0\rangle\langle 1,0|\). The error bars display the numerical error.

\(\mathcal{T}_{\alpha\alpha',\beta\beta'}\) realises the quantum transitions of the subsystem due to the coupling to the bath. Assuming weak coupling, and for the sake of comparison to a Markovian master equation, the action of the transition operator will be disregarded: This amounts to perform an adiabatic approximation of the dynamical evolution of the spin subsystem.

In the adiabatic approximation the evolution of the density matrix becomes simply

\[
\rho_W^{\alpha\alpha'}(X, t) = e^{-it\mathcal{L}_0^{\alpha\alpha'}} \rho_W^{\alpha\alpha'}(X) = e^{-i\int_0^t d\tau \omega_{\alpha\alpha'} e^{-it\mathcal{L}_{\alpha\alpha'}}} \rho_W^{\alpha\alpha'}(X). \tag{26}
\]

Equation (26) shows that using the adiabatic approximation, in the adiabatic basis, the evolution of the density matrix in the Wigner-Heisenberg representation can be calculated by propagating classical-like trajectories, under the action of the Liouville operator (24), and considering a phase factor integrated along the trajectory. The initial \(X\) coordinates, representing the quantum state of the bath in phase space, can be sampled from the initial density matrix (19).

Although in the adiabatic approximation the dynamics is easily calculated in the adiabatic basis, for quantum information problems it is more convenient to consider the reduced
density matrix
\[ \rho_W^\mu_\nu(t) = \int dX \sum_{\alpha \alpha'} U_\mu \alpha (R) \rho_W^{\alpha \alpha'}(X, t)(U^{-1})_{\alpha' \nu}(R) \] (27)
in the natural basis \(|1\rangle = |1, 1\rangle, |2\rangle = |1, 0\rangle, |3\rangle = |0, 1\rangle, |4\rangle = |0, 0\rangle\). The matrix \(U\) appearing in Eq. (27) is, of course, the rotation matrix from the adiabatic to the natural basis which can be constructed, as well known, by using the adiabatic eigenvectors as columns.

Everything seems quite straightforward so far. However, the definition of \(U\) is somewhat arbitrary, since the columns can be evenly permuted, and the adiabatic eigenvectors in the Wigner-Heisenberg representation of quantum mechanics depend on the configuration point \(R\). In addition, the LAPACK \[17\] numerical routines, which we have used to calculate the eigenvectors, return a matrix \(U\) with the columns ordered corresponding to the increasing value of the eigenvalues. It turns out that this configuration-dependent permutation of the columns of \(U\) introduces fictitious dynamics, as can be verified by propagating the density matrix \(\dot{\rho} = |1\rangle\langle 1|\), defined in terms of the natural state “spin-up spin-up” of the spin chain, which should be left invariant under the action of the Hamiltonian \(\hat{H}_S + \hat{H}_{W,SB}\), defined in Eqs. (13) and (15).

In order to solve this problem, it is sufficient to note that one would like to have a rotation matrix \(U\) as close as it could be to the matrix \(E\) formed by ordering the Cartesian basis vectors \(e^j\) (in the present case \(j = 1, \ldots, 4\)), with \(e^1 = [1 \, 0 \, 0 \, 0]\), \(e^2 = [0 \, 1 \, 0 \, 0]\) and so on. Upon writing \(u^\alpha\) for the adiabatic eigenvectors, \(\alpha = 1, \ldots, 4\), one can define a metric
\[ g^{\alpha j} = (u^\alpha - e^j) \cdot (u^\alpha - e^j). \] (28)
The definition of the metric in Eq. (28) allows us to solve the ordering problem in a unique way. As a matter of fact, for each \(j\), labelling the columns of the desired rotation matrix, we can look for the \(\alpha\) which minimizes the metric \(g^{\alpha j}\): This leads to the possibility of ordering the columns of \(U\) in such a way that this matrix is as close as it can be to \(E\), and it effectively solves the numerical problem with the fictitious dynamics arising from the permutations of the adiabatic eigenvectors along the phase space trajectory.

V. MASTER EQUATION FOR THE COUPLED SPINS

A system with total Hamiltonian (1), obeying the Liouville (Heisenberg) equation of motion (2), can be studied in the weak coupling limit by performing the Born-Markov
FIG. 2: Time evolution of the reduced density matrix element $\rho_{22}^S$ vs time ($\beta_1 = 1$, $\beta_2 = 0.3$). Initial density matrix $\hat{\rho}_0(0) = |\Psi_0\rangle\langle\Psi_0|$ with $|\Psi_0\rangle = (|1,1\rangle - |1,0\rangle)/\sqrt{2}$. The continuous line is the analytical solution. The filled circles display the results of the numerical calculation.

approximation [18]. In such a case, the equation for the reduced density matrix becomes

$$\frac{d}{dt} \hat{\rho}_S^{(I)}(t) =$$

$$-\int_0^\infty ds \text{tr} B \{ \hat{H}_{SB}^{(I)}(t), [\hat{H}_{SB}^{(I)}(t-s), \hat{\rho}_S^{(I)}(t) \otimes \hat{\rho}_B(0)] \}.$$  

(29)

where the index $I$ denotes the interaction picture with respect to the free Hamiltonians of the system and bath. The operator $\hat{\rho}_S$ denotes the reduced density matrix of the system $S$ and $\hat{\rho}_B$ is the density matrix of the reservoir $B$.

After performing the rotating wave approximation over the rapidly oscillating term in the master equation one gets:

$$\frac{d}{dt} \hat{\rho}_S(t) = -i[\hat{H}_S, \hat{\rho}_S(t)] +$$

$$\sum_\omega \sum_{\alpha,\beta} \gamma_{\alpha,\beta}(\omega) (\hat{V}_\beta(\omega)\hat{\rho}_S(t)\hat{V}_\alpha^\dagger(\omega) -$$

$$\frac{1}{2} [\hat{V}_\alpha^\dagger(\omega)\hat{V}_\beta(\omega), \hat{\rho}_S(t)]_+).$$  

(30)

To obtain Eq. (30) one assumes that the system-environment interaction has the form $\hat{H}_{SB} = \sum_i \hat{V}_i \otimes \hat{f}_i$; the operators $\hat{V}_i = \hat{V}_i^\dagger$ and $\hat{f}_i = \hat{f}_i^\dagger$ act on the system and the bath.
FIG. 3: Time evolution of the reduced density matrix element $\rho_{22}^{ss}$ vs time ($\beta_1 = \beta_2 = 0.005$). Initial density matrix $\hat{\rho}_s(0) = |1, 0\rangle \langle 1, 0|$. The continuous line is the analytical solution. The filled circles display the results of the numerical calculation. They are joined by a dashed line to help the eye.

degrees of freedom, respectively. In Eq. (30) a Lamb-type renormalization Hamiltonian was neglected and decay rates $\gamma_{\alpha,\beta}(\omega)$ are given by the Fourier image of the bath correlation functions:

$$\gamma_{\alpha,\beta}(\omega) = \int_{-\infty}^{+\infty} ds e^{i\omega s} \langle \hat{f}_\alpha^\dagger(s) \hat{f}_\beta(0) \rangle.$$ (31)

The transition operators $\hat{V}_\alpha(\omega)$ originates from the decomposition of the operator $\hat{V}_\alpha$ in the basis of the eigenoperators of the system Hamiltonian $\hat{H}_S$. If one denotes the eigenvalues of the Hamiltonian $\hat{H}_S$ by $\varepsilon$ and the corresponding projection operator as $\hat{\Pi}(\varepsilon)$ then:

$$\hat{V}_\alpha(\omega) = \sum_{\varepsilon' - \varepsilon = \omega} \hat{\Pi}(\varepsilon) \hat{V}_\alpha \hat{\Pi}(\varepsilon').$$ (32)

To obtain the master equation for the open system we rewrite the Hamiltonian of the whole system in the following way:

$$\hat{H} = \hat{H}_S + \hat{H}_{B1} + \hat{H}_{B2} + \hat{H}_{SB1} + \hat{H}_{SB2},$$ (33)

where $\hat{H}_S$ is defined in Eq. (13) and here we further assume that $j_x = j_y = j$, so that the constants $j \geq 0$ and $j_z \geq 0$ denote the strenght of XY and ZZ interaction, respectively.
As already stated in the previous section, in this article scaled units are chosen, so that $k_B = \hbar = 1$. We rewrite the Hamiltonians of the reservoirs $k_s = 1, 2$ as

$$
\hat{H}_{Bk_s} = \sum_n \omega_{n,k_s} \hat{b}_{n,k_s}^\dagger \hat{b}_{n,k_s}.
$$

(34)

The interaction between the spin subsystem and the bosonic baths is described by

$$
\hat{H}_{SBk_s} = -\hat{\sigma}_z^{(k_s)} \sum_n g_n^{(k_s)} (\hat{b}_{n,k_s} + \hat{b}_{n,k_s}^\dagger).
$$

(35)

To derive an equation of the form (30) for the Hamiltonian (33) one needs to find the eigenvalues and eigenvectors of the Hamiltonian $\hat{H}_S$ (13):

$$
\hat{H}_S = \sum_{i=1}^4 \lambda_i |\lambda_i\rangle\langle\lambda_i|,
$$

(36)

namely

$$
|\lambda_1\rangle = |1, 1\rangle, \quad \lambda_1 = -j_z, \quad (37)
$$

$$
|\lambda_2\rangle = |0, 0\rangle, \quad \lambda_2 = -j_z, \quad (38)
$$

$$
|\lambda_3\rangle = \frac{1}{\sqrt{2}} (|1, 0\rangle + |0, 1\rangle), \quad \lambda_3 = -2j + j_z, \quad (39)
$$

$$
|\lambda_4\rangle = \frac{1}{\sqrt{2}} (-|1, 0\rangle + |0, 1\rangle), \quad \lambda_4 = 2j + j_z. \quad (40)
$$

In this basis, the transition operators take the form:

$$
V^{(1)}_0 = V^{(2)}_0 = |\lambda_1\rangle\langle\lambda_1| - |\lambda_2\rangle\langle\lambda_2|, \quad (41)
$$

with $\omega_0 = 0$. The operators $V_0$ cause decoherence. The operators $V$

$$
V^{(1)} = -|\lambda_3\rangle\langle\lambda_4|, \quad (42)
$$

$$
V^{(2)} = |\lambda_3\rangle\langle\lambda_4|, \quad (43)
$$

describe the dissipation between the levels $\lambda_3$ and $\lambda_4$ with the transition frequency $\omega = 4j$. Finally, the master equation takes the form:

$$
\frac{d\hat{\rho}}{dt} = -i[\hat{H}_S, \hat{\rho}] + \sum_{i=1}^2 (\mathcal{L}_{Di}(\hat{\rho}) + \mathcal{L}_{Ci}(\hat{\rho})), \quad (44)
$$

where

$$
\mathcal{L}_{Di}(\hat{\rho}) = \gamma^{(i)}(-\omega) \left( \hat{V}^{(i)}_\dagger \hat{\rho} \hat{V}^{(i)}_\dagger - \frac{1}{2} \left[ \hat{V}^{(i)}_\dagger, \hat{V}^{(i)} \right]_+ \right) + \gamma^{(i)}(\omega) \left( \hat{V}^{(i)}_\dagger \hat{\rho} \hat{V}^{(i)}_\dagger - \frac{1}{2} \left[ \hat{V}^{(i)}_\dagger, \hat{V}^{(i)} \right]_+ \right), \quad (45)
$$

$$
\gamma^{(i)}(-\omega) \left( \hat{V}^{(i)}_\dagger \hat{\rho} \hat{V}^{(i)}_\dagger - \frac{1}{2} \left[ \hat{V}^{(i)}_\dagger, \hat{V}^{(i)} \right]_+ \right) + \gamma^{(i)}(\omega) \left( \hat{V}^{(i)}_\dagger \hat{\rho} \hat{V}^{(i)}_\dagger - \frac{1}{2} \left[ \hat{V}^{(i)}_\dagger, \hat{V}^{(i)} \right]_+ \right) \quad (46)
$$
\[ \mathcal{L}_{Ci}(\dot{\rho}) = \left( \gamma^{(i)}(0) + \gamma^{(i)}(0) \right) \times \left( \dot{\mathcal{V}}^{(i)}_0 \rho \mathcal{V}^{(i)}_0 - \frac{1}{2} \left[ \dot{\mathcal{V}}^{(i)}_0 \mathcal{V}^{(i)}_0, \dot{\rho} \right]_+ \right). \]  

(47)

(48)

In the basis of eigenvectors of the Hamiltonian \( \hat{H}_S \) the system of the corresponding differential equations can be solved. The exact solution of Eq. (44) is

\[ \dot{\rho}(t) = \sum_{i,j=1}^{4} f_{i,j}(t) |\lambda_i \rangle \langle \lambda_j|, \]  

(49)

where we have introduced the elements of the density matrix:

\[ f_{11}(t) = f_{11}(0), \]  

(50)

\[ f_{22}(t) = f_{22}(0), \]  

(51)

\[ f_{33}(t) = \left( \Omega_- + \Omega_+ e^{-\Omega t} \right) \frac{f_{33}(0)}{\Omega} + \left( 1 - e^{-\Omega t} \right) \Omega_- \frac{f_{44}(0)}{\Omega}, \]  

(52)

\[ f_{44}(t) = \left( 1 - e^{-\Omega t} \right) \Omega_- \frac{f_{33}(0)}{\Omega} + \left( \Omega_+ + \Omega_- e^{-\Omega t} \right) \frac{f_{44}(0)}{\Omega}, \]  

(53)

\[ f_{12}(t) = f_{12}(0) \exp \left( -4g_c t + it(\lambda_2 - \lambda_1) \right), \]  

(54)

\[ f_{13}(t) = f_{13}(0) \exp \left( -g_c t - \Omega_+ t + it(\lambda_3 - \lambda_1) \right), \]  

(55)

\[ f_{14}(t) = f_{14}(0) \exp \left( -g_c t - \Omega_- t + it(\lambda_4 - \lambda_1) \right), \]  

(56)

\[ f_{23}(t) = f_{23}(0) \exp \left( -g_c t - \Omega_+ t + it(\lambda_3 - \lambda_2) \right), \]  

(57)

\[ f_{24}(t) = f_{24}(0) \exp \left( -g_c t - \Omega_- t + it(\lambda_4 - \lambda_2) \right), \]  

(58)

\[ f_{34}(t) = f_{34}(0) \exp \left( -\Omega t + it(\lambda_4 - \lambda_3) \right). \]  

(59)
In the above expressions we have defined the constants
\[ \Omega_\pm = \frac{1}{2} \left( \gamma^{(1)}(\pm \omega) + \gamma^{(2)}(\pm \omega) \right), \quad (60) \]
\[ \Omega = \Omega_+ + \Omega_- , \quad (61) \]
\[ g_c = \frac{1}{2} \sum_{i=1}^{2} \left( \gamma^{(i)}(0_+) + \gamma^{(i)}(0_-) \right) . \quad (62) \]

The above solution will be used in the following as a reference for the numerical simulation.

VI. CALCULATIONS AND RESULTS

We have performed various numerical calculations varying the temperatures of the oscillator baths and compared to the analytical solution given in Sec. V. The coupling constants in the Hamiltonian (13) have been taken as \( j_x = j_y = j = 1 \) and \( j_z = 1/2 \). The two baths, with \( N = 200 \) harmonic oscillators each, have been assigned an Ohmic spectral density. To this end we employed the form of the coupling constants \( c_I \) and frequencies \( \omega_I \) introduced in Ref. [19]:
\[ c_I = \left( \xi \omega_0 \omega_j \right)^{1/2} \quad (63) \]
\[ \omega_I = - \ln (1 - I \omega_0) \quad (64) \]

where \( \omega_0 = (1 - \exp(-\omega_{\text{max}}))/N \), with \( \xi = 0.007 \) and \( \omega_{\text{max}} = 3 \). In order to compare with the analytical solutions of the weak-coupling master equation of Sec. V, we have performed an adiabatic propagation in the mixed Wigner-Heisenberg representation of quantum mechanics and sampled 50000 initial conditions to calculate the reduced density matrix, \( \hat{\rho}_S \) of the two coupled spins. Figure 1 shows the numerical precision of our numerical scheme displaying the constancy of the trace of \( \hat{\rho}_S \) versus time in the case of \( \beta_1 = \beta_2 = 0.005 \).

In general, we have found a very good agreement between the results provided by both the numerical and the analytical approach for all the various temperatures investigated. Here, we discuss explicitly two calculations.

Calculation (i) has been performed with the baths in a nonequilibrium configuration, at the two different temperatures \( \beta_1 = 0.3 \) and \( \beta_2 = 1 \). The initial reduced density matrix \( \hat{\rho}_S(0) \) has been taken equal to \( \hat{\rho}_S(0) = |\Psi_0\rangle\langle\Psi_0| \), with \( |\Psi_0\rangle = \frac{1}{\sqrt{2}}(|1, 1\rangle - |1, 0\rangle) \). Figure 2 shows
the comparison between the numerical and the analytical dynamics of the matrix element \( \rho_{22}^S \). In this case, the analytical solution is

\[
\rho_{22}^S(t) = \frac{1}{4} \left[ 1 + \exp(-\Omega(\beta_1, \beta_2, \omega)t) \cos(\omega t) \right].
\]

(65)

Of course, in such a low-temperature case the Markovian approximation is expected to provide very good results and this is numerically confirmed.

Calculation (ii) has been performed with \( \beta_1 = \beta_2 = 0.005 \) and an initial \( \hat{\rho}_s \) equal to \( \hat{\rho}_s = |1, 0\rangle \langle 1, 0| \). Figure 3 shows the comparison between the numerical and the analytical dynamics of the matrix element \( \rho_{22}^S \). The theoretical solution is in this case

\[
\rho_{22}^S(t) = \frac{1}{2} \left[ 1 + \exp(-\Omega(\beta_1, \beta_2, \omega)t) \cos(\omega t) \right].
\]

(66)

At higher bath temperature, the Markovian approximation (used in the analytical solution) can describe the numerical results in a good but qualitative way. The difference in the oscillation frequencies of the analytical and the numerical solutions arises from neglecting the Lamb-type renormalization of the Hamiltonian \( \hat{H}_S \) in the derivation of the master equation in the Born-Markov approximation. The discrepancy in the long time decay of the analytical and numerical results arises from the fact that \( \Omega(\beta_1, \beta_2, \omega) \) in the analytical expression of \( \rho_{22}^S(t) \) should contain some memory effects on the time-interval on which the evolution is considered.

VII. CONCLUSIONS

Upon adopting a mixed Wigner-Heisenberg representation, we have shown how the quantum dynamics of two coupled spins interacting with multiple bosonic baths can be numerically simulated. An analytical solution in the Born-Markov approximation has also been found and we have shown agreement between these two approaches.

Both the analytical and the numerical method can be generalized in order to study additional coupled spins, in order to build longer spin chains immersed in independent bosonic baths. Equilibrium and nonequilibrium situation can be addressed on an equal basis.

The numerical algorithm is suited to include nonadiabatic correction in the unitary evolution of the density matrix of the total systems. As such, it can also be used to assess novel approaches to non-Markovian dynamics of open quantum systems.
Acknowledgments

This work is based upon research supported by the South African Research Chair Initiative of the Department of Science and Technology and National Research Foundation.

[1] I. Sinaysky, F. Petruccione, and D. Burgarth, Phys. Rev. A 78 062301 (2008).
[2] L. Quiroga, F. J. Rodriguez, M. E. Ramirez, R. Paris, Phys. Rev. A 75 032308 (2007).
[3] D. Burgarth and V. Giovannetti, Phys. Rev. A 76 062307 (2007).
[4] D. Braun, F. Haake, and W. T. Strunz, Phys. Rev. Lett. 86 2913 (2001); D. Braun, Phys. Rev. Lett. 89 277901 (2002).
[5] P. Zanardi, Phys. Rev. A 57 3276 (1998); P. Zanardi, Phys. Rev. A 56 4445 (1997).
[6] M. J. Storcz and F. K. Wilhelm, Phys. Rev. A 67 042319 (2003); M. J. Storcz, F. Hellmann, C. Hrelescu, and F. K. Wilhelm, Phys. Rev. A 72 052314 (2005).
[7] M. Dubé and P. C. Stamp, Int. Journ. Mod. Phys. B 12 1191 (1998).
[8] P. Nagele, G. Campagnano, and U. Weiss, New J. Phys. 10 115010 (2008); G. Campagnano, A. Hamma, U. Weiss, e-print arXiv:0807.1987v1.
[9] I. V. Aleksandrov, Z. Naturforsch A 36 902 (1981); V. I. Gerasimenko, Teor. Mat. Fiz. 150 7 (1982); W. Boucher and J. Traschen, Phys. Rev. D 37 3522 (1988); W. Y. Zhang and R. Balescu, J. Plasma Phys. 40 199 (1988); W. Y. Zhang and R. Balescu, J. Plasma Phys. 40 215 (1988).
[10] R. Kapral and G. Ciccotti, J. Chem. Phys. 110 8919 (1999).
[11] A. Sergi and R. Kapral, J. Chem. Phys. 118 8566 (2003).
[12] G. Hanna and R. Kapral, J. Chem. Phys. 122 244505 (2005).
[13] D. Mac Kernan, G. Ciccotti and R. Kapral, J. Chem. Phys. 116 2346 (2002).
[14] A. Sergi, Phys. Rev. E 72 066125 (2005).
[15] A. Sergi, D. Mac Kernan, G. Ciccotti, and R. Kapral, Theor. Chem. Acc. 110 49 (2003).
[16] H. Hellmann, Einführung in die Quantenchemie (Deuticke, Leipzig, 1937); R. P. Feynman, Phys. Rev. 56 340 (1939).
[17] E. Anderson, Z. Bai, C. Bischof, S. Blackford, J. Demmel, J. Dongarra, J. Du Croz, A. Greenbaum, S. Hammarling, A. McKenney, and D. Sorensen, LAPACK Users’ Guide, (Society
[18] H.-P. Breuer and F. Petruccione, The Theory of Open Quantum Systems (Oxford University Press, Oxford, 2002).

[19] N. Makri and K. Thompson, J. Phys. Chem. 291 101 (1998); K. Thompson and N. Makri, J. Chem. Phys. 110 1343 (1999); N. Makri, J. Phys. Chem. 103 2823 (1999).