Modelling of quantum information processing with Ehrenfest guided trajectories: a case study

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We apply a numerical method based on multi-configurational Ehrenfest trajectories, and demonstrate converged results for the Choi fidelity of an entangling quantum gate between two two-level systems interacting through a set of bosonic modes. We consider both spin-boson and rotating wave Hamiltonians, for various numbers of mediating modes (from 1 to 100), and extend our treatment to include finite temperatures. Our results apply to two-level impurities interacting with the same band of a photonic crystal, or to two distant ions interacting with the same set of motional degrees of freedom.

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I. INTRODUCTION

The ability of tracking the evolution of complex quantum systems will be a crucial support to the design and development of future quantum technologies. A paradigm of particular interest for the latter is one where finite dimensional quantum systems, typically two-level systems (qubits), interact through a ‘bus’, made up of a set of bosonic field modes [1–33]. In this paper, we will consider the case of two qubits interacting with a common discrete set of modes in the non-perturbative regime. While the possibility of creating entanglement, even at steady state, by the interaction with a common bosonic bath has been highlighted repeatedly in the literature, the case of non-perturbative interactions with a bunch of 10 or 20 modes (as will be the case in our study) presents several major technical difficulties, essentially due to the impossibility of an analytic master equation approach – only possible in the continuum limit under the Born-Markov approximation – and to the huge size of the dynamically relevant part of the Hilbert space.

Various numerical approaches have been developed to emulate these dynamics on classical computers, such as the so called multi-configurational time dependent Hartree method [34, 35] and its “Gaussian” variation [36], various schemes based on path integral techniques [37, 38], and even the adaptation of time-adaptive density matrix renormalisation group techniques [39] borrowed from condensed matter theory. Here, we will tackle such difficulties by borrowing a method co-pioneered and developed by one of the authors in the arena of chemical physics [40, 41]. The method is based on the adoption of a set of tensor products of time-dependent coherent states as a discrete ‘basis grid’ on which to represent the field degrees of freedom (referred to as “coupled coherent states” in the literature [42]), and on letting the states of the co-moving grid evolve according to their Ehrenfest dynamics (whose application to a grid of coherent states goes under the name of “multi-configurational Ehrenfest” method). This approach has the advantage of being relatively light in terms of computational resources, easy to program, and yet of allowing one to follow coherent quantum dynamics in detail, as it will be shown.

In our study, we will focus on a specific, but very relevant, aspect of the quantum dynamics of the two qubits: we shall consider the realisation of an entangling quantum gate between them, namely of a controlled Z (CZ) gate. To estimate the quality of such a realisation we will consider the quantum fidelity between the pure state corresponding to the CZ gate by the standard channel-state duality (Choi isomorphism [43–45]) and the quantum state corresponding to the channel acting on the two qubits upon partial tracing over the field’s degrees of freedom.

Our main aim is demonstrating the capability of Ehrenfest guided trajectories in phase space to produce reliable and converged results for complex figures of merit, able to reveal detailed information about the quantum dynamics of the constituents. The ‘Choi fidelity’ of a two-qubit quantum gate is a property of the dynamics itself, and not of the initial state, and its evaluation requires, at any time, the evolution of ten initial states: it is, therefore, a rather cumbersome figure of merit to compute, let alone to optimise over a rather large range of values of the dynamical parameters, as we did. The advantages of the Ehrenfest guided trajectories over – arguably more precise but heavier – approaches based on full variational principles are manifest in such circumstances.

As for direct impact, let us remark that our study would apply on systems like two-level impurities trapped in a photonics crystal and interacting with the same band of allowed modes [46, 47, 48], or to the internal levels of two ions interacting with all the vibrational modes of an array of ions in a linear trap [49]. It is important to point out that our treatment can account for finite, although relatively small, temperatures as well.

Our paper is organised as follows. In section II we will review the basic theory behind methods of solution of the Schrödinger equation based on a set of time-dependent, Ehrenfest guided basis states. We will not dwell so much on the technical details, which are covered elsewhere, as
on the basic concepts, and will try to present them in
terms which will be friendly to an audience with no pre-
vious familiarity with the terminology of chemical physics
or molecular dynamics. In section [III] we will introduce
the physical Hamiltonian and define precisely our chosen
figure of merit. Section [IV] will contain the main results
of our numerical study. Finally, we will draw conclusions,
and discuss advantages and shortcomings of our method
of choice, in section [V].

II. EHRENFEST GUIDED TRAJECTORIES

The main difficulty in dealing with a system including
few two-level systems and a bunch of $M$ bosonic modes
is clearly how to handle the infinite dimensional bosonic
Hilbert space. The method we apply here, referred to
in the literature as ‘multi-configurational Ehrenfest’ and
first introduced in [41], tackles this difficulty on the shoul-
ders of two major assumptions:

i) the state space of the field modes is represented as a
superposition of $N$ time dependent coherent states;

ii) the time dependence of the coherent states is deter-
dined by a simplified variational principle (which,
in other words, dictates how the finite dimensional
subspace spanned by the set of coherent states changes
with time, trying to keep it in the dynam-
ically relevant region).

The finite dimensional systems involved are, on the other
hand, treated by representing their entire Hilbert space,
spanned by $d$ orthonormal basis states $|l\rangle$, for $l \in \{1,d\}$.
In agreement with i), the ansatz wave-function of the
whole system reads

$$|\psi\rangle = \sum_{l=1}^{d} \sum_{j=1}^{N} \alpha_{j,l}(t) (|l\rangle \otimes |\alpha_{j}(t)\rangle),$$

(1)

where $\alpha_{j} \in \mathbb{C}^{M} \forall j$ and each $|\alpha_{j}\rangle$ is a tensor product of coherent states: $|\alpha_{j}\rangle = \bigotimes_{m=1}^{M} |\alpha_{j,m}\rangle$, such that, if $a_{m}$ is
the annihilation operator of mode $m$, one has $a_{m}|\alpha_{j}\rangle = \alpha_{j,m}^{(m)}|\alpha_{j}\rangle$. Since we will be dealing with two qubits, it
will be $d = 4$ for us.

The evolution of the dynamical parameters is more
conveniently described by adopting a Lagrangian formu-
lation. For a Hamiltonian operator $\hat{H}$, let us define $\mathcal{L}$ as

$$\mathcal{L} = \langle \psi | \hat{H} - i\partial_{t}| \psi \rangle.$$

(2)

The time-derivative operator is defined as the differentia-
tion of the time dependent coefficients $c_{l,j}$ and by the
relationships $\partial_{t}|l\rangle = 0$ (the finite dimensional system’s
basis is time-independent) and $\partial_{t}|\alpha_{j}\rangle = \sum_{m=1}^{M} (\partial_{t}^{(m)}(a_{m}^{\dagger} - a_{m}^{(m)})/2 - a_{m}^{(m)}(a_{m}^{\dagger} - a_{m}^{(m)})/2)|\alpha_{j}\rangle$ (derived from the time-
dependence of a coherent state with varying phase space
position). The quantity $L$ is hence a function of the co-
efficients $c_{l,j}$, the complex parameters $\alpha_{j}$ and their time-
derivatives $\dot{\alpha}_{j}$ and $\ddot{\alpha}_{j}$. In fact, it can be shown that $L$
serves as a Lagrangian for the quantum system, in the
sense that the Euler-Lagrange equations

$$\frac{\partial L}{\partial \dot{\alpha}_{j}} = \frac{d}{dt} \frac{\partial L}{\partial \alpha_{j}},$$

(3)

are equivalent to Schrödinger equation \([68]\). See Ap-
pendix [B] for more details.

Besides determining the state evolution, the vari-
ational formalism also provides one with a recipe to update
the basis such that the expression $L$ of Eq. \((2)\), which
clearly always equals 0 in the exact dynamics, is min-
imised during the time-evolution. Such a minimisation,
which in essence keeps the basis in the ‘most relevant’
region of the Hilbert space within the constraints of the
adopted approximation, would be obtained by consid-
ering the full Euler-Lagrange equations for the $M \times N$
complex parameters $\alpha_{j}$ and their time-derivatives. This
would be a large nonlinear system of coupled equations,
requiring a substantial numerical effort to be solved. In-
stead, we introduce here assumption ii), and replace
the full variational equations for $\alpha_{j}$ with a simplified ver-
sion thereof. In particular, we will neglect all terms cou-
ing the different $\alpha_{j}$’s, on the grounds that the overlaps
$\langle \alpha_{j} | \alpha_{k}\rangle$ are typically very small if the number of modes
$M$ is large enough. For each $j$, let us then define the
vector $|\psi_{j}\rangle$ as

$$|\psi_{j}\rangle = \sum_{l=1}^{d} c_{j,l}(t) |l\rangle \otimes |\alpha_{j}(t)\rangle,$$

(4)

and the corresponding ‘approximated’ Lagrangian $\tilde{L}_{j}$ as

$$\tilde{L}_{j} = \langle \psi_{j} | (\hat{H} - i\partial_{l}) \psi_{j} \rangle.$$

(5)

The equation of motion for the parameter $\alpha_{j}^{(m)}$ (the $m$-th
component of the vector $\alpha_{j}$) is

$$\frac{\partial \tilde{L}_{j}}{\partial \alpha_{j}^{(m)}} = \frac{d}{dt} \frac{\partial \tilde{L}_{j}}{\partial \dot{\alpha}_{j}^{(m)}},$$

(6)

where we also neglect the time-dependence of the coeffi-
cients $c_{l,j}$, such that each Lagrangian $\tilde{L}_{j}$ only depends
on the four complex parameters $c_{l,j}$ and on the $M$ com-
plex parameters represented by the entries of $\alpha_{j}$ (and
on their time-derivatives $\dot{\alpha}_{j}$, see Appendix [A] for
further details). Eq. \((6)\) defines the “Multi-Configura-
tional Ehrenfest” (MCE) method we are using.

Notice that the assumption ii) is not, per se, an ap-
proximation, but rather just a way of choosing the time-
dependence of the adopted basis. However, it should be
stressed that, in general, the exact Euler Lagrange equa-
tion for the full variation of the parameters $\alpha_{j}^{(m)}$ is likely
to provide one with a more accurate result in that it will
yield a smaller Lagrangian $L$ (which is zero in the exact
dynamics).
However, Eq. (6) is much easier to treat numerically, hence the advantage of our method, which can be easily programmed and applied with modest computational resources and often provides results in very good agreement with complete variational methods, like MCTDH or G-MCTDH [34–37].

Multi-configurational Ehrenfest guided trajectories have been thoroughly tested for spin-boson dynamics under different spectral densities, establishing the reliability of their converged results in several, diverse situations [11, 50]. Here, we will instead apply them to study a composite system including discrete sets of bosonic field modes, where coherent quantum information processing can be carried out.

III. MODEL AND FIGURE OF MERIT

We set out to study coherent quantum information processing for a system comprising two two-level systems (“qubits”) connected by $M$ bosonic modes through a spin-boson like coupling.

In principle, this represents the archetype of a quantum system where complex dynamics and information processing tasks can be carried out, and whose dynamics is impervious to non-approximated methods. In practice, our case study may be thought of as representing two two-level atoms (or impurities) interacting with the same photonic band of a photonic crystal [47], or a simulation of the same setting in a linear array of trapped ions (where the qubits are embodied by internal levels of the ions interacting with the same set of vibrational normal modes [61]).

For future convenience, let us re-label the four states of the computational basis of the two two-level systems as follows:

- $|1\rangle = |↓↓\rangle$, \hspace{1cm} (7)
- $|2\rangle = |↓↑\rangle$, \hspace{1cm} (8)
- $|3\rangle = |↑↓\rangle$, \hspace{1cm} (9)
- $|4\rangle = |↑↑\rangle$. \hspace{1cm} (10)

The operators $\hat{\sigma}_{z}^{(1)}$, $\hat{\sigma}_{z}^{(2)}$, $\hat{\sigma}_{x}^{(1)}$ and $\hat{\sigma}_{x}^{(2)}$, will stand for the customary Pauli operators in the Hilbert spaces of qubit 1 and 2. For instance, in the adopted basis, $\hat{\sigma}_{z}^{(1)}$ is defined by $\hat{\sigma}_{z}^{(1)}|1\rangle = |3\rangle$, $\hat{\sigma}_{z}^{(1)}|3\rangle = |1\rangle$, $\hat{\sigma}_{z}^{(1)}|2\rangle = |4\rangle$, $\hat{\sigma}_{z}^{(1)}|4\rangle = |2\rangle$.

In our study, we shall consider both an actual ‘spin-boson like’ Hamiltonian:

\[
\hat{H} = \sum_{j=1}^{2} \sum_{m=1}^{M} \left[ \varepsilon \hat{\sigma}_{z}^{(j)} + \Delta_j \hat{\sigma}_{z}^{(j)} + \omega_m a_{m}^{\dagger} a_{m} \right],
\]

and its rotating wave counterpart:

\[
\hat{H}_{rw} = \sum_{j=1}^{2} \sum_{m=1}^{M} \left[ \varepsilon \hat{\sigma}_{z}^{(j)} + \Delta_j \hat{\sigma}_{z}^{(j)} + \omega_m a_{m}^{\dagger} a_{m} \right],
\]

where $\sigma_{x}^{(j)} = \sigma_{z}^{(j)\dagger} = \sigma_{z}^{(j)} + i\sigma_{\hat{x}}^{(j)}$. As well known, the Hamiltonian $\hat{H}_{rw}$ is a good approximation of $\hat{H}$ in the almost resonant, high frequency case that is, in our notation, for $|2\varepsilon - \omega_m| \ll |2\varepsilon + \omega_m| \forall m$. In the following, we will consider systems with different numbers of bosonic modes $M$, various values of frequencies $\{\omega_m\}$ and spin-boson couplings $\{g_m^{(j)}\}$, and different parameters $\Delta_1$ and $\Delta_2$. Also, we will set $\hbar = 1$ throughout the paper.

In reproducing the dynamics of the two qubits by treating the field through multi-configurational Ehrenfest trajectories, we will aim at obtaining converged results for a figure of merit of interest in the study of quantum information processing, namely the fidelity with which an entangling controlled Z (CZ) gate can be realised for the two qubits through the mediating bosonic modes. In terms of the basis states of Eqs. (7-10), a CZ gate is represented as a unitary $U_{CZ}$ leaving all the basis states invariant except for $|4\rangle$, which becomes $-|4\rangle$, that is

\[
U_{CZ}|j\rangle = f(j)|j\rangle \quad \text{for} \quad 1 \leq j \leq 4,
\]

where $f(j) = 1$ for $j \in \{1, 2, 3\}$ and $f(j) = -1$ for $j = 4$. The relevance of a CZ gate to quantum information processing stems from its being a maximally entangling gate which, combined with single-qubit unitaries, forms a universal quantum set for gate based quantum computation [51].

At zero temperature, the quantum operation $\Gamma_t$ we want to compare with the CZ unitary gate is defined as follows, in terms of a notional initial density matrix of the qubits $\varrho$:

\[
\Gamma_t(\varrho) = \text{Tr}_B \left[ e^{-i\hat{H}t} (\varrho \otimes |0\rangle \langle 0|) e^{i\hat{H}t} \right],
\]

where $\text{Tr}_B$ stands for partial tracing over the Hilbert space of the bosonic modes and $|0\rangle$ is the vacuum state of the modes. We will also extend our treatment to include a finite temperature $1/\beta$ of the bosonic modes (in natural units where $k_B = 1$), in which case the quantum operation $\Gamma_{t,\beta}$ will be given by

\[
\Gamma_{t,\beta}(\varrho) = \text{Tr}_B \left[ e^{-i\hat{H}t} \left( \varrho \otimes \int_{\mathbb{C}^{2M}} P_\beta(\alpha) |\alpha\rangle \langle \alpha| d^{2M} \alpha \right) e^{i\hat{H}t} \right],
\]

with

\[
P_\beta(\alpha) = \prod_{m=1}^{M} \left( \frac{e^{d\omega_m} - 1}{\pi} e^{-e^{(d\omega_m - 1)|\alpha_m|^2}} \right).
\]

The function $P_\beta(\alpha)$ is just the Glauber-Sudarshan P-representation of a thermal state of the bosonic modes (given by the product of individual P-representation for each of the modes). In our notation $\alpha \in \mathbb{C}^{2M}$, while each component of $\alpha$ is denoted by $\alpha_m$. Clearly, one has that $\lim_{\beta \to \infty} \Gamma_{t,\beta} = \Gamma_t$.

In our numerical study, we will reproduce the operations $\Gamma_t$ by adopting the method detailed in the previous section, which is defined for pure states, and also...
is bound to be pure:

\[ \varphi = \frac{1}{2} |1\rangle \otimes |1\rangle + |2\rangle \otimes |2\rangle + |3\rangle \otimes |3\rangle + |4\rangle \otimes |4\rangle . \]  

For a generic CP-map \( \Omega \), the corresponding quantum state \( \varrho_\Omega \) may be defined as

\[ \varrho_\Omega = (\Omega \otimes 1)(|\psi\rangle \langle \psi|) , \]  

where 1 is the identity map acting on \( \mathcal{H} \).

Since the CZ gate is unitary, the quantum state \( \varrho_{\text{CZ}} \) is bound to be pure: \( \varrho_{\text{CZ}} = |\varphi_{\text{CZ}}\rangle \langle \varphi_{\text{CZ}}| \), with

\[ |\varphi_{\text{CZ}}\rangle = \frac{1}{2} (|1\rangle \otimes |1\rangle + |2\rangle \otimes |2\rangle + |3\rangle \otimes |3\rangle - |4\rangle \otimes |4\rangle ) \]

\[ = \frac{1}{2} \sum_{j=1}^{4} f(j) (|j\rangle \otimes |j\rangle) . \]  

The state \( \varrho_{t,\beta} \) corresponding to \( \Gamma_{t,\beta} \) is instead given by

\[ \varrho_{t,\beta} = \frac{1}{4} \sum_{j,k=1}^{4} \Gamma_{t,\beta} (|j\rangle \langle k|) \otimes |j\rangle \langle k| . \]  

We can then naturally define the CZ operation fidelity \( F \) (which we shall informally refer to as ‘Choi fidelity’) as the overlap

\[ F = \langle \varphi_{\text{CZ}} | \varrho_{t,\beta} | \varphi_{\text{CZ}} \rangle = \frac{1}{16} \sum_{j,k=1}^{4} \langle j | \Gamma_{t,\beta} (|j\rangle \langle k|) |k\rangle . \]  

The quantity \( F \) captures, in one real number, a relevant facet of the quantum dynamics governing the two qubits. Its relationship to quantum coherence is manifest in that if the off-diagonal elements between the basis vectors of Eqs. (17) are set to zero, then one has \( F = 1/4 \). Any value of \( F \) larger than \( 1/4 \) is thus in a sense a signature of quantum coherence. More importantly, \( F \) is also a measure of how well a coherent quantum task can be performed and is also strictly related to the entanglement generated between the two qubits (in that entanglement a perfect CZ gate would get entanglement equal to 1 ebit for a properly chosen initial state). Moreover, \( F \), although partial to the chosen reference gate (CZ in this case) is completely independent of the initial state, and represents a property of the dynamics alone.

Of course, we could have chosen more general quantifiers like, for instance, the largest eigenvalue of the operator \( \varrho_{t,\beta} \), which would equal 1 in the ideal case where the qubits undergo a unitary evolution and would quantify, in a sense, the overall coherence of the qubits’ evolution. However, we deem such choices to be less informative with regard to the applicative potential of a complex dynamics.

Given a potentially useful quantum dynamics, the knowledge of \( F \) is instead very desirable to possess. Demonstrating the use of a numerical technique capable of providing one with reliable estimates of \( F \) in relevant situations is, in a nutshell, the aim of the current analysis.

\section{IV. CHOI FIDELITY OF THE CZ GATE}

Here, we will slightly deviate from the previously adopted notation by setting \( g_j^{(i)} = g_j \) for all \( j \) and \( i \).

It is important to remark that assuming equal couplings...
between each qubit and all the modes is in no way essential to our numerical approach. Such an assumption can be – and will be, in the following – relaxed if needs be.

Let us then, to begin with, set the coupling between the first qubit and the field modes $g_1$ to 1, and essentially choose it as the unit of time. Let us also, until further notice, set $\varepsilon = \Delta = 0$, $\beta \to \infty$ (zero temperature) and consider the rotating wave Hamiltonian $\hat{H}_{rw}$. Note that the Hamiltonian $\hat{H}_{rw}$ with $\Delta = 0$ can be derived from the full Hamiltonian $\hat{H}$ with $\Delta = 0$ by switching to interaction picture and applying the rotating wave approximation: $\varepsilon$ can be thus be set to zero and each field frequency $\omega_m$ is shifted as per $\omega_m \rightarrow \omega_m - 2\varepsilon$.

By exploiting the conservation of the number of excitations, the dynamics governed by the Hamiltonian $\hat{H}_{rw}$ for $\Delta = 0$ can be easily solved analytically. The agreement between such analytical solutions and the MCE results has been tested for up to ten modes and is excellent. Figs. 1(a) and 1(b) show such an agreement in terms of CZ Choi fidelity $F$ for $g_2 = 1.9$ and, respectively, one mode with $\omega_1 = 0.1$ and three modes with $\omega_1 = 0.1$, $\omega_2 = 0.2$ and $\omega_3 = 0.3$. An initial peak with fidelity larger than 0.9 is immediately apparent: this peak will be the main object of our investigation, for larger numbers of modes too. For three modes, the peak appears at a time which is approximately reduced by a $\sqrt{3}$ factor with respect to the single mode case. This cooperative effect is confirmed for all number of modes up to 20, and is simply due to the fact that the qubits are coupled to the field through the mode $\sum_{m=1}^{M} a_m$, with an ef-
fidelity in the plots), in terms of the maximal converged Choi \( F \) versus rescaled time at zero temperature, for \( H_{rw} \) with \( \varepsilon = \Delta = 1, \ g_1 = 1, \ M = 10, \ \omega_m = 0.1m \) for \( 1 \leq m \leq 10 \) and different values of \( g_2 \). The line \( F = 0.25 \) is reported for reference.

Figs. 2-6 depict a detailed analysis of the Choi fidelity for \( M = 10 \) bosonic modes with frequencies \( \omega_m = 0.1m \) for \( 1 \leq m \leq 10 \), three different temperatures (\( \beta \to \infty \), \( \beta = 10 \) and \( \beta = 5 \)), and different values of the coupling \( g_2 \), scanned over the range \( 1.8 - 2.7 \). The zero temperature case (Fig. 2) shows how the dispersion of quantum coherence among the field’s degrees of freedom affects the gate’s fidelity (whose maximum is smaller than in the one- and three-modes cases), although in the considered region of dynamical parameters the effect is not as pronounced as one could imagine. The plots clearly show the detrimental effect of thermal fluctuations on coherent quantum effects, even at such relatively small temperatures. In practice, this suggests severe constraints on the temperature for the observation of coherent quantum effects mediated by discrete vibrational modes (typically much more susceptible to thermal excitations than optical modes due to their lower frequency), considering that the highest temperature accounted for is around 0.2\( g_1 \) in natural units. Most importantly, we were able to determine the optimal value of the coupling \( g_2 \) with respect to a vast range of values (much wider than what reported in the plots), in terms of the maximal converged Choi fidelity \( F \), and to establish that \( g_2 \approx 2.2 \) yields the closest results to an ideal CZ gate. Clearly, in practice, such couplings will not always be tunable at will, or possibly only within a given window of values: it is anyway remarkable to be able to identify optimal values given a specific dynamical figure of merit.

Let us now move on to a case which is not analytically treatable, with \( \varepsilon = \Delta = 1 \) and \( \omega_m = 0.1m \) for \( 1 \leq m \leq 10 \). As usual, we set \( g_1 = 1 \) and consider different values of \( g_2 \) and different temperatures (zero temperature and \( \beta = 10 \)): the values of \( F \) for such a configuration are displayed in Figs. 7-10. The initial peak in \( F \) is still apparent, but the breaking of the phase invariance by the term \( \Delta \) clearly degrades the quality of the gate, with a maximum Choi fidelity which is now around 0.7, even at zero temperature.

We now turn to the full spin-boson like Hamiltonian \( \hat{H} \) (including the counter-rotating terms in the qubits-field coupling), and consider the case \( \varepsilon = \Delta = 1 \) and \( \omega_m = 0.1m \) for \( 1 \leq m \leq 10 \), \( \beta = 10 \) and different values of \( g_2 \). The line \( F = 0.25 \) is reported for reference.
are included. The time-dependent grid thus evolves much more rapidly in phase space and is likely to leave the dynamically relevant region and accumulate substantial errors earlier. We were however able to obtain well converged results by reducing the coupling $g_1$ to 0.5, which is still very far from the perturbative regime. Likewise, we scanned values of $g_2$ up to 0.5. Quite significantly – as confirmed by Figs. 11 and 12 respectively for zero temperature and $\beta = 10$ – we could not find any value of $g_2$ such that the Choi fidelity of the CZ gate reaches 0.25. In fact, strong enough couplings are necessary to entangle the two qubits on short enough time-scales but, with such strong couplings, the counter-rotating terms heat the qubits up too quickly for coherent effects to take place, at least in this region of parameters. This heating overshadows the effect of thermal fluctuations in the field, which are barely noticeable for $\beta = 10$ (and are instead manifest in the rotating wave regime at the same temperature).

In order to simulate the effect of a band of a 1-dimensional photonic band-gap medium, where modes are usually doubly degenerate in frequency (since they can propagate in either spatial direction), we have also considered a case with $M = 20$ modes, two for each equally spaced frequency. All the other parameters have been kept as above, with $\varepsilon = \Delta = 1$ and $g_1 = 1$ in the rotating wave case (Fig. 13), and $g_1 = 0.5$ in the full Hamiltonian (Fig. 14). Comparing Fig. 13 with Fig. 7 shows that the initial peak in Choi fidelity is still present: moreover, not only does it occur earlier by a factor $\sqrt{2}$ (as expected because of the cooperation between the modes due to the balanced coupling), but it is also higher. Con-
FIG. 14: MCE results for the Choi fidelity $F$ versus rescaled time at zero temperature, for $\hat{H}$ with $\varepsilon = \Delta = 1$, $g_1 = 0.5$, $M = 20$, $\omega_m = 0.1m$ for $1 \leq m \leq 10$, $\omega_m = 0.1(m - 10)$ for $11 \leq m \leq 20$ and different values of $g_2$. The line $F = 0.25$ is reported for reference.

FIG. 15: MCE results for the Choi fidelity $F$ versus rescaled time at zero temperature, for $\hat{H}$ with $\varepsilon = \Delta = 1$ and a common Ohmic bath with $\alpha = 0.09$, $\omega_c = 2.5$ and different numbers of total bath modes. The line $F = 0.25$ is reported for reference.

The notion of entangling separated systems and of distributing quantum coherence by interaction with common heat baths or other incoherent means is well established in the quantum information and condensed matter communities, and has been explored under a number of – either more specific and applied or more general and abstract – viewpoints [52–66]. However, the problem of studying the non-perturbative interaction of two qubits with a common bath is still in general a difficult one. Thus, to provide the reader with further evidence of the versatility and power of our approach, we also report the application of the MCE method to the controlled-Z Choi fidelity for the case of the spin boson Hamiltonian $\hat{H}$, with $\varepsilon = \Delta = 1$, and both qubits interacting with a common bath at zero temperature and with Ohmic spectral density $J(\omega)$ given by

$$J(\omega) = \frac{2}{\pi} \alpha \omega e^{-\frac{\omega}{\omega_c}},$$

where $\alpha$ is the Kondo parameter, which we fix at 0.09, and $\omega_c$ is a cutoff frequency.

We use a standard approach to discretise the bath, which has already been proven very reliable for single spin Ohmic spin-boson systems [41]. In particular, the frequencies and coupling strengths are chosen as follows:

$$\omega_m = -\omega_c \ln \left[ 1 - \frac{m \left( 1 - e^{-\frac{\omega_{\text{max}}}{\omega_c}} \right)}{M} \right],$$

$$g_m^1 = g_m^2 = \sqrt{\frac{\omega_m \omega_c \left( 1 - e^{-\frac{\omega_{\text{max}}}{\omega_c}} \right)}{2M}},$$

where $\omega_{\text{max}}$ is a free parameter of the numerics, which we will converge our results against (in that we choose it large enough to obtain converged results). In particular, we choose $\omega_{\text{max}} = 12.5$ for $\omega_c = 2.5$ and $\omega_{\text{max}} = 6$ for $\omega_c = 1$. Also, the coupling strengths $g_m^j$ are defined as in Eqs. [11] and [12].

A. Zero temperature Ohmic spin-boson bath

The notion of entangling separated systems and of distributing quantum coherence by interaction with common heat baths or other incoherent means is well established in the quantum information and condensed matter
Fig. 15 shows the convergence of our results for $\omega_c = 2.5$ and the full Hamiltonian $H$ in terms of the total number of modes in the bath ($M = 50$ and $M = 100$). Quite interestingly, if the counter-rotating terms are included we obtain larger gate fidelities when mimicking a bath than for a smaller set of discrete bus frequencies. Off resonant modes are more influential in the full Hamiltonian and seems to be captured faithfully by our method.

In Fig. 16, instead, we report results for the rotating wave Hamiltonian $\hat{H}_{\text{rw}}$ and different cutoff frequencies and number of bath modes. In this case, the effect of the counter-rotating terms is rather limited. Also, the influence of larger cutoff frequencies at longer times is clearly visible in the plot.

V. ENTANGLEMENT GENERATION

Typically, a large Choi fidelity for the (entangling) CZ gate corresponds to the generation of substantial entanglement between the two qubits. To support this statement, we report here a brief study on the entanglement generated between two qubits. As an entanglement quantifier, we adopt the concurrence, an entanglement monotone that can be easily calculated for a system of two qubits $|\psi\rangle = |\uparrow\downarrow\rangle$. Figs. 17(a), 17(b) and 17(c) show the concurrence versus rescaled time for the rotating wave Hamiltonian $\hat{H}_{\text{rw}}$ with different initial states, temperatures, dynamical parameters and number of modes. The degradation of quantum entanglement due to temperature is apparent (Figs. 17(a) and 17(b)), along with the speed up in the entanglement generation induced by a doubling of the modes (Fig. 17(c)).

It is also worth noticing that we did not find any region of parameters where entanglement between the two qubits is generated for the full Hamiltonian $H$ and $M = 10$, thus mirroring our failure in obtaining Cz fidelities larger than 0.25.

VI. CONCLUSIONS

We have presented an extensive numerical study, based on Multi-Configurational Ehrenfest trajectories, on the dynamics of two qubits interacting with a common set of bosonic field modes, obtaining converged results for the Choi fidelity of an entangling CZ gate between the qubits for a rather wide range of Hamiltonian parameters and field temperatures, which cannot be covered by perturbation theory or other approximate approaches. We thus demonstrated the capability of tracking, analysing in detail, and even optimising with respect of certain ranges of some parameters, specific aspects of the coherent quantum dynamics of the qubits.

We were able to properly take into account the effect of finite bath’s temperatures on the reduced dynamics of the qubits, and also to highlight some counterintuitive features related to the scaling of coherent signatures with the number of field modes (which we varied over the range $1 - 100$), showing that at times more mediating modes can actually be advantageous for the distribution of quantum coherence.

The main limitations of our approach lie in the difficulty of handling counter-rotating qubit-field coupling terms in the strong coupling regime (i.e., when the coupling strengths are comparable to the inherent dynamical frequencies of the qubits). Even in such instances, we could however reach convergence by somewhat limiting the range of the coupling strengths.

Within such limitations, the MCE approach has hence been established as a powerful tool for the detailed study of complex quantum dynamics even with relatively limited resources (desktop computers), typically for systems where discrete sets of up to 100 field modes are involved.
FIG. 18: Norm and expectation value of the energy for MCE results at zero temperature, for $\hat{H}_{tw}$ with $\varepsilon = \Delta = g_1 = 1$, $g_2 = 2.7$, $M = 10$ (with $\omega_m = 0.1m$ for $1 \leq m \leq 10$) and different values of $N$ and $\text{comp}$.

FIG. 19: Entries of the qubits’ density matrix $g_{11}$ and $g_{13}$ for MCE results at zero temperature, for $\hat{H}_{tw}$ with $\varepsilon = \Delta = g_1 = 1$, $g_2 = 2.7$, $M = 10$ (with $\omega_m = 0.1m$ for $1 \leq m \leq 10$) and different values of $N$ and $\text{comp}$.

FIG. 20: Norm and expectation value of the energy for MCE results at zero temperature, for $\hat{H}$ with $\varepsilon = \Delta = g_1 = 1$, $g_2 = 2.7$, $M = 10$ (with $\omega_m = 0.1m$ for $1 \leq m \leq 10$) and different values of $N$ and $\text{comp}$.

FIG. 21: Entries of the qubits’ density matrix $g_{11}$ and $g_{13}$ for MCE results at zero temperature, for $\hat{H}$ with $\varepsilon = \Delta = g_1 = 1$, $g_2 = 2.7$, $M = 10$ (with $\omega_m = 0.1m$ for $1 \leq m \leq 10$) and different values of $N$ and $\text{comp}$.

Appendix A: Ehrenfest dynamics of the coherent states

Here, we elaborate on Eq. (10) and derive explicitly the equation of motion of each complex parameter $\alpha_j^{(m)}$. The approximated Lagrangian $L_j$ reads

$$
L_j = \sum_{l,n=1}^{d} c_{l,j}^* c_{n,j} \langle \alpha_j, l | \hat{H} | \alpha_j, n \rangle - i \sum_{l=1}^{d} c_{l,j}^* \partial_l \langle \alpha_j, l | \hat{H} | \alpha_j, n \rangle - i \sum_{l=1}^{d} |c_{l,j}|^2 \left( \frac{\hat{\alpha}_j \cdot \alpha_j^*}{2} - \frac{\hat{\alpha}_j^* \cdot \alpha_j}{2} \right),
$$

(A1)

where $|l, \alpha_j\rangle = |l \rangle \otimes |\alpha_j\rangle$. Note that $\langle \alpha_j, l | \hat{H} | \alpha_j, n \rangle$ is just a function of the vector $\alpha_j$ and the integers $l$ and $n$, promptly evaluated by normal ordering $\hat{H}$.

The Euler-Lagrange equation for $\alpha_j^{(m)}$ then is:

$$
\frac{\partial L_j}{\partial \dot{\alpha}_j^{(m)}} = \sum_{l,n=1}^{d} c_{l,j}^* c_{n,j} \frac{\partial}{\partial \dot{\alpha}_j^{(m)}} \langle \alpha_j, l | \hat{H} | \alpha_j, n \rangle + i \sum_{l=1}^{d} |c_{l,j}|^2 \left( \frac{\dot{\alpha}_j^{(m)} \cdot \alpha_j^*}{2} - \frac{\dot{\alpha}_j^{(m)*} \cdot \alpha_j}{2} \right) = \frac{d}{dt} \frac{\partial L_j}{\partial \dot{\alpha}_j^{(m)}}
$$

(A2)

which, by neglecting the time dependence of $c_{l,j}$ (setting $\frac{d}{dt} \sum_{l=1}^{d} |c_{l,j}|^2 = 0$), can be rearranged to obtain

$$
\dot{\alpha}_j^{(m)} = i \frac{\sum_{l,n=1}^{d} c_{l,j}^* c_{n,j} \frac{\partial}{\partial \dot{\alpha}_j^{(m)}} \langle \alpha_j, l | \hat{H} | \alpha_j, n \rangle}{\sum_{l=1}^{d} |c_{l,j}|^2}.
$$

(A3)

This equation governs the evolution of the vectors $\alpha_j$ in our numerics.

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FIG. 22: Choi fidelity and concurrence for two different separable initial states versus rescaled time, for $\hat{g}$ subspace spanned by the basis grid) for the parameters where $\Omega_{jk}$ is essentially a semi-classical action).

Throughout our study, the centres of the initial set of coherent states are distributed in phase space with a Gaussian distribution with standard deviation $1/\text{comp}$. The parameter $\text{comp}$ is a free parameter of the study, which is tuned to optimise convergence. As indicators of the quality of the numerics we will observe the convergence of specific entries of the density matrix of the two qubits $\rho$, as well as the ‘norm’ $\text{Tr}(\rho)$ and the expectation value of the energy $\text{Tr}(\hat{H}\rho)$, which are obviously conserved in the exact dynamics. Notice that our method does not have any in-built routine guaranteeing the conservation of the state vector’s norm, so that $\text{Tr}(\rho)$ is a relevant figure of merit to assess its reliability.

Figs. 18(a) and 18(b) display the norm and expectation value of the energy for a case of non-number-conserving rotating wave Hamiltonian, while in Figs. 19(a) and 19(b) the entries $\rho_{11}$ and $\rho_{13}$ are plotted. The reliability of the numerics over the whole timeframe considered is apparent (for large enough compression parameter $\text{comp}$), in terms of both convergence with increasing number $N$ of coherent states and of conservation of invariant quantities. As anticipated, the situation is much more dire for the full Hamiltonian $\hat{H}$. In this case, Figs. 20(a) and 20(b) show that our numerics are only reliable up to rescaled times around 2.5, after which both convergence, and norm and energy conservation are lost, even at smaller coupling strengths (in that $g_2 = 1$ rather than $g_2 = 2.7$ as before). Finally, we show three examples of convergence of our results at finite temperature (here, $\beta = 0.5$) with respect to the increase in the number of states $N_T$ over which the thermal distribution of Eq. (16) is sampled (Figs. 22(a) and 22(b) and 22(c)).

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