

Dynamics of quantum information and entanglement in two qubits coupled to a Bose-Einstein condensate of microwave-shielded polar molecules

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We theoretically investigate the dynamics of quantum information and entanglement of two distant qubits embedded in a thermal dephasing reservoir consisting of three-dimensional Bose-Einstein condensates of microwave-shielded polar molecules. We calculate the decoherence factors, the quantum Fisher information, and the decay rates in terms of the spatial separation between qubits, temperature, and Rabi frequency that tunes the shielding potential. The results show that the dynamics of decoherence factors and the quantum Fisher information are nonmonotonic with revival oscillations at larger separations due to interqubit and qubit-environment correlations. Within our proposed model we can significantly improve the estimation of the environment parameters such as the spectral density, which exhibits a super-Ohmic behavior, and temperature. We demonstrate that the shielding interaction may drive the system from the Markovian to the non-Markovian regime enabling us to well control the information flow dynamics and to reach higher values of entanglement.

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I. INTRODUCTION

The ability to produce ultracold polar molecules offers a wealth of opportunities in accelerating the development of advanced technologies and to understand quantum information due to their rovibrational degrees of freedom, controllable long-range dipole-dipole interactions (DDIs), and tunable microwave fields. Experimental and theoretical studies of ultracold molecules have progressed rapidly over the last two decades (see, e.g., Refs. [1–22]).

One of the latest breakthroughs in the ultracold polar molecules is the realization of degenerate gases formed by fermionic and bosonic microwave-shielded polar molecules (MSPMs) [23,24]. Microwave shielding, which can eliminate the collision loss between ultracold polar molecules, is also crucial for the creation of p -wave superfluidity [25], tetratomic (NaK)₂ molecules [26], and molecular quantum droplets [27,28]. Most recently, the nonequilibrium dynamics and coherence of Bose-Einstein condensates (BECs) of MSPMs have also been deeply studied by one of us [29]. These exotic ensembles constitute an ideal platform for quantum information processing owing to their rich internal structure. The long-lived character and the coherence of the MSPMs enable them to encode quantum information for longer times and in an exquisite manner.

The aim of the present work is then to investigate the dynamics of quantum information and entanglement in two qubits with two hyperfine spin states coupled to a reservoir consisting of three-dimensional (3D) BECs of MSPMs via a long-range intermolecular potential. In the context of atomic BECs, the collective dephasing, the non-Markovianity, and the entanglement of two spatial state qubits were discussed in Refs. [30–35] and references therein. It has also been demonstrated that using two qubits can drastically improve the estimation of environment parameters [36,37].

This study scrutinizes the impact of the spatial separation between qubits, and the interaction between MSPMs on the ohmicity, the non-Markovianity, and the entanglement of the system. Our numerical results show that for small Rabi frequencies and at relatively long times, the reservoir displays a transition from a Markovian to a non-Markovian effect, manifested by the negative values of collective decoherence rates. These decoherence rates which display super- and sub-decoherent two-qubit states, strongly rely on the spatial separation between qubits. By analyzing the quantum Fisher information (QFI), we estimate key reservoir parameters such as the spectral density, Rabi frequencies which adjust the shielding potential, and the temperature. In this regard, we also show that changes in the spatial separation between qubits and in DDIs have a crucial effect on the super-Ohmic spectral density in the whole range of frequencies and on the decoherence factors. Furthermore, we illuminate the entanglement dynamics of the two-qubit states. Using the concurrence as a standard quantifier of entanglement we calculate it in terms of the initial-state and reservoir parameters. The optimal conditions for entanglement generation are also determined.

The rest of this paper is structured as follows. In Sec. II, we describe the model of two-qubit states with two hyperfine

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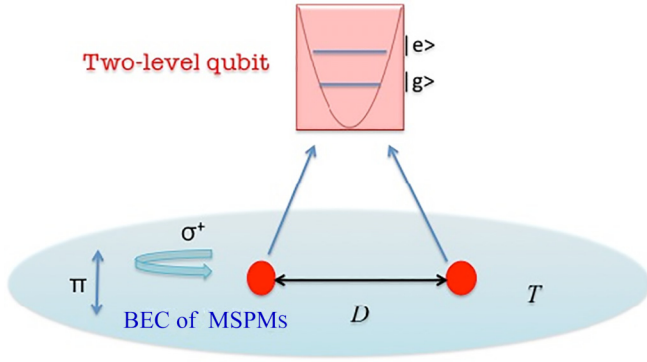


FIG. 1. Two impurity qubits separated by distance D are immersed in a thermally equilibrated 3D BEC of MSPMs at temperature T . The molecules are held in an optical dipole trap and dressed by circularly polarized (σ^+) and linearly polarized (π) microwave fields which have Rabi frequencies and detunings [24].

spin states embedded in a reservoir consisting of 3D BECs of MSPMs. Section III is devoted to the dynamics of two qubits. Analytical expressions are derived for the decoherence factor, the decay rate, and the QFI when the qubits are initially in a mixed Werner state. Sections IV and V present our numerical and analytical results obtained from the solution of the model described above. In Sec. VI, we report the dynamics of entanglement for different initial-state and reservoir parameters. Our conclusions are drawn in Sec. VII.

II. MODEL

We consider two identical impurity atomic qubits made of two-level atoms separated by a distance D embedded in a thermally equilibrated 3D BEC of MSPMs at temperature T (see Fig. 1). We take $\hbar = k_B = 1$ throughout.

The qubits are confined in a deep harmonic trap, $U_I(\mathbf{r}) = m_I \omega_I^2 r^2 / 2$, where m_I is the mass of the impurity and ω_I is the trap frequency, which is independent of the internal states. For $\omega_I \gg 1$, the spatial wave function of the qubit is given by $\psi_I = \pi^{-3/4} l_I^{-3/2} \exp(-r^2 / 2l_I^2)$, where $l_I = \sqrt{1/m_I \omega_I}$ is the impurity harmonic oscillator length. The Hamiltonian of the qubits is then given by

$$H_I = \frac{\Omega_I}{2} \sum_{j=1}^2 (|e_j\rangle\langle e_j| - |g_j\rangle\langle g_j|), \quad (1)$$

where Ω_I is the level splitting between the excited, $|e_j\rangle$, and the ground, $|g_j\rangle$, states of the j th qubit.

The Hamiltonian of a BEC of MSPMs of mass m produced in a box-shaped trap is given in the frame of the Bogoliubov theory as [29]

$$\hat{H}_{\text{PM}} = \sum_{\mathbf{k} \neq 0} \omega_{\mathbf{k}} \hat{b}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}}, \quad (2)$$

where $\hat{b}_{\mathbf{k}}^\dagger$ and $\hat{b}_{\mathbf{k}}$ are operators of elementary excitations obeying the usual Bose commutation relations, and the frequency of the Bogoliubov excitations is given by

$$\omega_{\mathbf{k}} = \sqrt{E_{\mathbf{k}}^2 + 2E_{\mathbf{k}} n V(\mathbf{k})}, \quad (3)$$

where $E_{\mathbf{k}} = k^2 / 2m$ is the kinetic energy, n denotes the density of the condensate, $V(\mathbf{k})$ is the Fourier transform of the effective intermolecular potential $V(\mathbf{r})$ which is defined as [25,27]

$$V(\mathbf{r}) = \frac{C_3}{r^3} (3 \cos^2 \theta - 1) + \frac{C_6}{r^6} \sin^2 \theta (\cos^2 \theta + 1), \quad (4)$$

where θ is the polar angle of $\mathbf{r}$, and $C_3 = d^2 / [48\pi\epsilon_0(1 + \delta_r^2)]$ and $C_6 = d^4 / [128\pi^2\epsilon_0^2\Omega(1 + \delta_r^3/2)]$ are interaction strengths tunable via the Rabi frequency Ω and detuning of the microwave field δ , with $\delta_r = |\delta|/\Omega$ being the relative detuning. Here d is the permanent dipole moment in the molecular frame and ϵ_0 is the vacuum permeability. The C_6 term represents the shielding potential.

For zero ellipticity, the long-range part of the interaction, $V(\mathbf{r})$, can be approximated by the standard DDI along the z axis [28,29] as

$$V(\mathbf{r}) = g\delta(\mathbf{r}) + \frac{d_{\text{eff}}^2}{4\pi\epsilon_0} \left(\frac{1 - 3 \cos^2 \theta}{r^3} \right), \quad (5)$$

where $g = 4\pi a/m$ corresponds to the short-range part of the interaction, with a being the scattering length, and $d_{\text{eff}} = d/\sqrt{12(1 + \delta_r^2)}$ is the effective dipole moment. The strength and the sign of the effective dipolar interaction can be adjusted by tuning the Rabi frequencies and detuning the microwave fields [25,27]. The approximation (5) is valid if the scattering lengths are unaffected by the anisotropy of the short-range potential for $l > 0$ and $a > 0$ [38].

Note that to calculate rigorously the short-range interaction potential which is characterized by the s -wave scattering length, a , and relate it to the parameters of the potential at hand, one should analyze the long-range behavior of the s -wave component of the wave function at low energy [28,29]. This is indeed not an easy task due to the contribution of the modes l , $l \pm 2$, and $l \pm 4$, originating from the repulsive term of the potential. Numerical values of a and the relative dipolar strength $\epsilon_{\text{dd}} = r_*/a$, where $r_* = md_{\text{eff}}^2/(4\pi\epsilon_0)$ is the effective characteristic dipole-dipole distance and $d_{\text{eff}} = d/\sqrt{12(1 + \delta_r^2)}$ is the effective dipole moment, for different parameters of the molecular interaction have been given in Ref. [28].

Let us now assume that the polar molecules in the reservoir are coupled to the excited state $|e\rangle$ of the qubits through a Raman transition. The qubit-bath interaction is governed by a contact pseudopotential, $V_{\text{IPM}}(\mathbf{r}) = g_{\text{IPM}}\delta(\mathbf{r})$, where $g_{\text{IPM}} = 2\pi a_{\text{IPM}}/m_{\text{IPM}}$, with a_{IPM} being the scattering length of the qubit-MSPM collisions and $m_{\text{PM}} = mm_I/(m + m_I)$ being the reduced mass. Then, the interaction of the molecular BEC with an impurity can be carried out using the standard Bogoliubov expansion and transformation. Keeping only linear terms in $\hat{b}_{\mathbf{k}}^\dagger$ and $\hat{b}_{\mathbf{k}}$, we obtain the following for the interaction Hamiltonian:

$$\hat{H}_{\text{IPM}} = \sum_j \left[g_{\text{IPM}} n |e_j\rangle\langle e_j| + |e_j\rangle\langle e_j| \sum_{\mathbf{k} \neq 0} (g_{\mathbf{k}}^j \hat{b}_{\mathbf{k}} + g_{\mathbf{k}}^{*j} \hat{b}_{-\mathbf{k}}^\dagger) \right], \quad (6)$$

where the qubit-reservoir coupling parameter is given by

$$g_{\mathbf{k}}^j = g_{\text{IPM}} \sqrt{n} \sqrt{\frac{E_{\mathbf{k}}}{\omega_{\mathbf{k}}}} e^{-(kl_I)^2/2} e^{i\mathbf{k} \cdot \mathbf{r}_j}, \quad (7)$$

where r_j is the spatial position of the j th qubit in the reservoir.

The total Hamiltonian of the system is given by the combination of three sub-Hamiltonians: $\hat{H} = \hat{H}_I + \hat{H}_{PM} + \hat{H}_{IPM}$. According to Eqs. (6) and (7), the coupling strength between the qubit and its bath depends on both the qubit's location and the relative dipolar strength ϵ_{dd} , which can be precisely controlled using the Feshbach resonance. Therefore, this enables us to analyze the effects of the molecular reservoir parameters on the qubit's information flow dynamics.

III. DYNAMICS OF TWO QUBITS

This section explores the dynamics of the two separated qubits interacting with one common thermal molecular reservoir. We derive analytical expressions for the time evolution of the decoherence factor, the decay rate, and the QFI for different initial states.

A. Decoherence factor

The time evolution operator $U(t) = e^{-i\hat{H}t}$ can be obtained using Magnus expansion [37]:

$$U(t) = \exp \left\{ -i \sum_{j=1}^2 [(\Omega t + \Delta(t)|e_j\rangle\langle e_j|)|e_j\rangle\langle e_j|] \right\} \\ \times \exp[-i\Theta(t, D)|e_1e_2\rangle\langle e_1e_2|] \\ \times \exp \left[\sum_{j=1}^2 |e_j\rangle\langle e_j| \sum_k (\alpha_k^j \hat{b}_k^\dagger - \alpha_k^{j*} \hat{b}_k) \right], \quad (8)$$

where $\alpha_k^j = \frac{g_k^j(1-e^{i\omega_k t})}{\omega_k}$, $\Delta(t) = \sum_k \frac{|g_k|^2}{\omega_k^2} [\sin(\omega_k t) - \omega_k t]$, and $\Theta(t, D) = \sum_k \frac{2|g_k|^2}{\omega_k^2} [\sin(\omega_k t) - \omega_k t] \cos(\mathbf{k}D)$ are phase parameters.

The reduced density operator of the two-qubit state is obtained through $\rho_{m_1 m_2, n_1 n_2} = \text{Tr}[\langle m_1, m_2 | U \rho^I(0) \otimes \rho^{\text{PM}} U^\dagger | n_1, n_2 \rangle]$, where $\rho^I(0)$ is the initial state of the qubit, and ρ^{PM} is the thermal equilibrium state of the molecular bath at temperature T . This yields [37]

$$\rho_{m_1 m_2, n_1 n_2}^I(t) = \exp \left[-i \Delta(t) \sum_{j=1}^2 (m_j - n_j) \right] \\ \times \exp[-i\Theta(t, D)(m_1 m_2 - n_1 n_2)] \\ \times \exp[-\Gamma^{\{n_j\}, \{m_j\}}(t, D)] \rho_{m_1 m_2, n_1 n_2}^I(0). \quad (9)$$

To find the decoherence exponent $\Gamma^{\{n_i\}, \{m_i\}}(t, D)$, we assume that the density matrix of the initial state is $\rho^T(0) = \rho(0) \otimes \rho^{\text{PM}}$, where the density matrix of the bath is $\rho^{\text{PM}} = \Pi_{\mathbf{k}}(1 - e^{-\omega_{\mathbf{k}}/T})e^{-(\omega_{\mathbf{k}}/T)\hat{b}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}}}$. Using the identity

$$\exp[-\Gamma^{\{n_i\}, \{m_i\}}(t, D, T)] \\ = \text{Tr} \left\{ \exp \left[\sum_j \sum_k (m_j - n_j) g_k^j \frac{1 - \omega_{\mathbf{k}}}{\omega_{\mathbf{k}}} \hat{b}_{\mathbf{k}}^\dagger + CC \right] \rho^{\text{PM}} \right\}, \quad (10)$$

we finally get for the decoherence exponent

$$\Gamma^{\{n_j\}, \{m_j\}}(t, D, T) \\ = \sum_{\mathbf{k}} \frac{2 \sin^2(\omega_{\mathbf{k}} t / 2)}{\omega_{\mathbf{k}}^2} \coth \left(\frac{\omega_{\mathbf{k}}}{2T} \right) \left| \sum_{j=1}^2 (m_j - n_j) g_{\mathbf{k}}^j \right|^2, \quad (11)$$

which encapsulates all the information concerning the time, the interaction, and the temperature dependence of the decoherence process.

The relevant decoherence functions are Γ^0 , Γ^+ , and Γ^- , which are related to the elements, such as $|\rho_{0,0;0,1}^I(t)\rangle = e^{-\Gamma^0(t)} \rho_{0,0;0,1}^I(0)$ or $|\rho_{0,1;1,1}^I(t)\rangle = e^{-\Gamma^0(t)} \rho_{0,1;1,1}^I(0)$, $|\rho_{0,0;1,1}^I(t)\rangle = e^{-\Gamma^+(t)} \rho_{0,0;1,1}^I(0)$, and $|\rho_{0,1;1,0}^I(t)\rangle = e^{-\Gamma^-(t)} \rho_{0,1;1,0}^I(0)$, respectively. They are expressed as

$$\Gamma^0(t, T) = \sum_{\mathbf{k}} \frac{2 \tilde{g}_{\mathbf{k}}^2}{\omega_{\mathbf{k}}^2} \sin^2 \left(\frac{\omega_{\mathbf{k}} t}{2} \right) \coth \left(\frac{\omega_{\mathbf{k}}}{2T} \right), \quad (12)$$

where the qubit-bath coupling parameter (7) simplifies to

$$\tilde{g}_{\mathbf{k}} = g_{\text{IPM}} \sqrt{n} \sqrt{\frac{E_{\mathbf{k}}}{\omega_{\mathbf{k}}}} e^{-(k l)^2 / 2}. \quad (13)$$

In addition, we have

$$\Gamma^\pm(t, D, T) = 2\Gamma^0(t, T) \pm \sum_{\mathbf{k}} \frac{2 \tilde{g}_{\mathbf{k}}^2}{\omega_{\mathbf{k}}^2} \sin^2 \left(\frac{\omega_{\mathbf{k}} t}{2} \right) \cos^2(\mathbf{k}D) \\ \times \coth \left(\frac{\omega_{\mathbf{k}}}{2T} \right), \quad (14)$$

which indicates the presence of sub- and super-decoherent states in Γ^+ and Γ^- , respectively, due to the superposition of the states $|0, 0\rangle$, $|1, 1\rangle$, $|0, 1\rangle$, and $|1, 0\rangle$. If the qubits are sufficiently far from each other, they interact independently with their environment, and hence $\Gamma^\pm(t) \approx 2\Gamma^0(t)$.

B. Decay rate and non-Markovianity

Given the decoherence factors, we can also examine the flow of the decay rates in order to characterize the non-Markovian dynamics of our two-level systems. They can be defined as [32,39]

$$\gamma^\pm(t) = \frac{d \Gamma^\pm(t)}{dt}. \quad (15)$$

When γ^+ and γ^- are positive, the dynamics is Markovian, while if at least one of these time-dependent decay rates takes negative values, then the dynamics is non-Markovian.

C. Quantum Fisher information

The QFI that quantifies the precision of the system parameters is defined as $\mathcal{F}_X = \text{Tr}[\rho_X L_X^2]$ [40], where ρ_X is the density matrix of the system depending on the estimable parameter X , and L_X is the symmetric logarithmic derivative given by $\partial \rho_X / \partial X = [\rho_X L_X + L_X \rho_X] / 2$. Using the spectrum decomposition $\rho_X = \sum_n \lambda_n |n\rangle\langle n|$, where λ_n are the eigenvalues of ρ_X , the QFI can be composed of two parts, namely,

$$\mathcal{F}_X = \mathcal{F}_X^C + \mathcal{F}_X^Q, \quad (16)$$

where

$$\mathcal{F}_X^C = \sum_n \frac{(\partial \lambda_n / \partial X)^2}{\lambda_n}$$

is the classical contribution to the QFI, and

$$\mathcal{F}_X^Q = 2 \sum_{n,m} \frac{(\lambda_n - \lambda_m)^2}{\lambda_n + \lambda_m} |\langle m | \partial_X n \rangle|^2$$

is the quantum part of the QFI. Note that the QFI is essential in entanglement detection and in the non-Markovianity characterization [39,41].

It is convenient to choose the Werner states as initial states: $\rho^\pm(0) = c|\psi^\pm\rangle\langle\psi^\pm| + (1-c)/4$, where $\psi^+ = (|00\rangle + |11\rangle)/\sqrt{2}$ and $\psi^- = (|01\rangle - |10\rangle)/\sqrt{2}$ are the maximally entangled Bell states and $c \in [0, 1]$. The explicit form of the density matrix operators can be obtained via Eq. (9):

$$\rho^+(t) = \frac{1}{4} \begin{pmatrix} 1+c & 0 & 0 & 2ce^{-i[2\Delta(t)+\Theta(t,D)]}e^{-\Gamma^+} \\ 0 & 1-c & 0 & 0 \\ 0 & 0 & 1-c & 0 \\ 2ce^{i[2\Delta(t)+\Theta(t,D)]}e^{-\Gamma^+} & 0 & 0 & 1+c \end{pmatrix}, \quad (17)$$

and

$$\rho^-(t) = \frac{1}{4} \begin{pmatrix} 1-c & 0 & 0 & 0 \\ 0 & 1+c & 2ce^{-\Gamma^-} & 0 \\ 0 & 2ce^{-\Gamma^-} & 1+c & 0 \\ 0 & 0 & 0 & 1-c \end{pmatrix}. \quad (18)$$

After diagonalizing the resulting density matrices and making use of Eq. (16), we obtain the following for the two components of the QFI [37]:

$$\mathcal{F}_X^+(D) = \frac{8c^2(1+c)[\partial_X \Gamma^+(D)]^2}{(1+c)^2 e^{2\Gamma^+(D)} - 4c^2} + \frac{c^2 e^{-2\Gamma^+(D)}}{1+c} [2\partial_X \Delta + \partial_X \Theta(t)], \quad (19a)$$

$$\mathcal{F}_X^-(D) = \frac{8c^2(1+c)[\partial_X \Gamma^-(D)]^2}{(1+c)^2 e^{2\Gamma^-(D)} - 4c^2}. \quad (19b)$$

Evidently, Eq. (19) show that the quantum contribution to $\mathcal{F}_X^\pm$ which incorporates phase parameters is crucial. However, in $\mathcal{F}_X^\pm$, the classical precision term is the dominant contribution. Both $\mathcal{F}_X^\pm$ are palpably sensitive to the interqubit distance and to the shielding potential, giving rise to an enhancement of the parameter precision estimation—the larger the QFI, the higher the precision of the estimate. By setting $c = 0$, $\mathcal{F}_X^\pm$ reduce to the standard expression for a single qubit.

To estimate the reservoir temperature as precisely as possible, we use Eq. (19). Keeping in mind that the phase parameters $\Delta(t)$ and $\Theta(t, D)$ are independent of temperature, we get immediately

$$\mathcal{F}_T^\pm(D) = \frac{8c^2(1+c)[\partial_T \Gamma^\pm(D)]^2}{(1+c)^2 e^{2\Gamma^\pm(D)} - 4c^2}, \quad (20)$$

where

$$\frac{\partial \Gamma^\pm(D)}{\partial T} = \frac{\tilde{g}_k^2 [\cos^2(kD) \pm 4] \sin^2(\omega_k t/2) \text{csch}^2(\omega_k/2T)}{T^2 \omega_k}.$$

If $c = 1$, $\mathcal{F}_T^\pm$ differ only by a factor 4 from the expression for a single-qubit state.

IV. NUMERICAL RESULTS

To be concrete, we consider two identical impurity qubits of ^{41}K atoms separated by a distance D with $a_I = 3.4 \times 10^{-9}$ m [42] embedded in NaCs molecules with $\epsilon_{\text{dd}} = 0.83$ [24]. In what follows, we employ the characteristic time $\tau = 1/E_*$, the energy $E_* = 1/(mr_*^2)$, and the characteristic dipolar length r_* as the units for time, energy, and length, respectively. Therefore, rescaling $t = t/\tau$, $E = E/E_*$, and $r = r/r_*$ casts our parameters as dimensionless. The results of our numerical simulations are shown in Fig. 2.

The dynamics of the decoherence factors $\Gamma^\pm$ is illustrated in Figs. 2(a) and 2(e) for three values of the interqubit separation. In the long time limit, i.e., when the qubits reach their stationary state ($t \gtrsim 3$), the decoherence factors for the super-Ohmic regime approach a constant value for all interqubit separations, indicating that the qubits preserve some of their coherence. The residual coherence in the two-qubit states is larger in Γ^- compared to that in Γ^+ . We also see that at short times, the two qubits decohere similarly regardless of the separation between them, whereas after some evolution time, quantum correlations induced by qubit-qubit and qubit-qubit-reservoir interactions cause oscillations in both Γ^- and Γ^+ for larger separations ($D \gtrsim 5$).

Figures 2(b), 2(f), 2(c), and 2(g) show a comparison of the time-dependent and temperature-dependent QFI in the sub- and super-decoherent states for different values of the spatial distance between qubits. It can be seen from Figs. 2(b) and 2(f) that, at fixed temperature and for small interqubit distance $D = 1$, the dynamics of both $\mathcal{F}^+(t)$ and $\mathcal{F}^-(t)$ monotonically increases and saturates at a specific time, and without the appearance of a local maximum. However, for larger distances, $D > 5$, the dynamics of QFI $\mathcal{F}^+(t)$ and $\mathcal{F}^-(t)$ is nonmonotonic with small oscillations and maxima at some optimal time. This latter depends on temperature and on distance between qubits. In Figs. 2(c) and 2(f), we present the QFI as a function of temperature at a given time $t = 10$. As

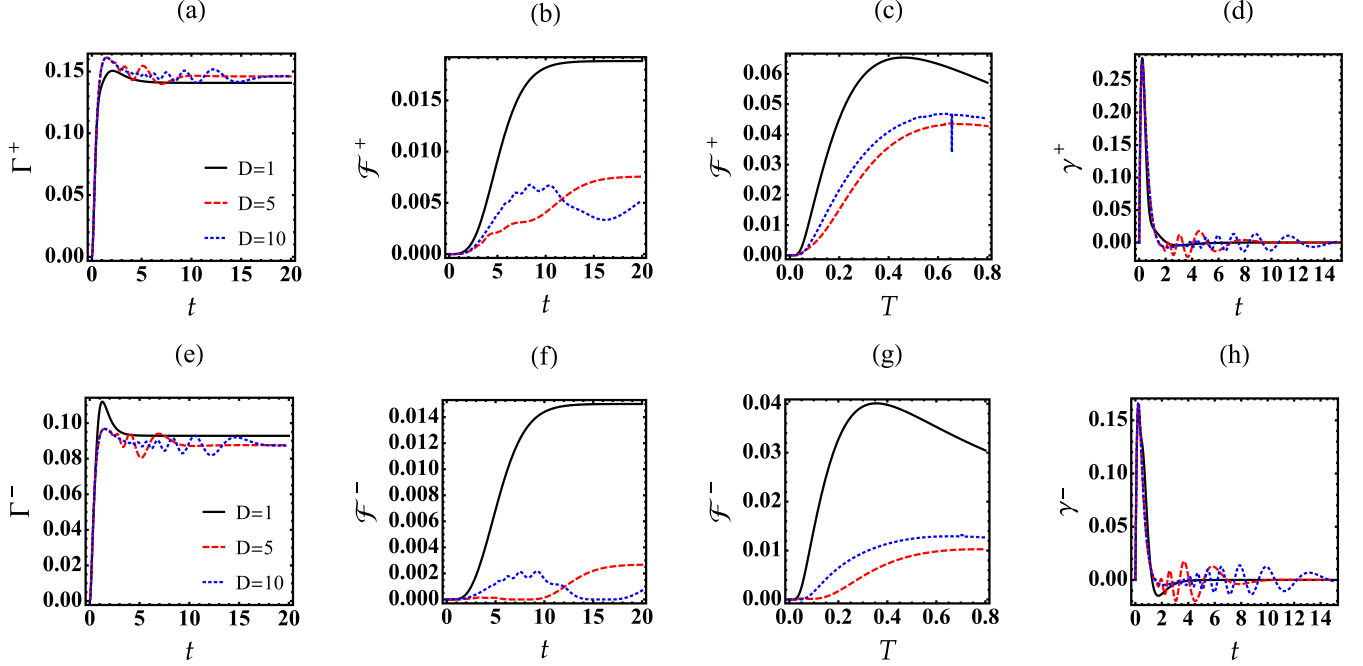


FIG. 2. (a) Time evolution of the decoherence factor $\Gamma^+(t)$, (b) dynamics of the QFI, $\mathcal{F}^+(t)$, (c) temperature-dependent QFI $\mathcal{F}^+(T)$ at time $t = 10$, and (d) time-dependent decay rates $\gamma^+(t)$, for different values of the interqubit distance D . Panels (e)–(h) are the same as panels (a)–(d) but for $\Gamma^-(t)$, $\mathcal{F}^-(t)$, $\mathcal{F}^-(T)$, and $\gamma^-(t)$, respectively. Parameters are as follows: $\sigma = 0.5$, $\epsilon_{dd} = 0.83$, $c = 1$, and $T = 0.1$.

it is apparent from the plots, QFI $\mathcal{F}^+(t)$ and $\mathcal{F}^-(t)$ have a maximum at a certain optimal temperature which strongly relies on separation between qubits. At higher temperatures where the decoherence is faster, the QFI is important in both states and for all distances most likely due to thermal fluctuations. We observe also in Figs. 2(b), 2(f), 2(c), and 2(g) that $\mathcal{F}^+(t) > \mathcal{F}^-(t)$ and $\mathcal{F}^+(T) > \mathcal{F}^-(T)$ for small spatial distances, leading to improved temperature sensing precision.

Let us now analyze the flow of the decay rate and its sign in different states to understand the physical processes describing the dynamics. As shown in Figs. 2(d) and 2(h), at times $t \lesssim 1.6$, γ^+ and γ^- are always positive, meaning that information flows from the qubits to the reservoir; thus, the dynamics remains Markovian. This behavior holds true regardless of the interqubit distance. At long times, $t \gtrsim 1.6$, both decay rates take negative and positive values notably for larger separations. These oscillations and revivals of γ^+ and γ^- can be understood as the backflow of information from the molecular reservoir to the qubits giving rise to the occurrence of a transition from the Markovian to the non-Markovian regime.

Next, we focus on the effects of the Rabi frequency of the microwave field which can tune C_3 and C_6 interaction strengths on the QFI and on the non-Markovianity of the system. Comparison between Figs. 3(a) and 3(b) shows that both $\mathcal{F}^+$ and $\mathcal{F}^-$ increase continuously with Ω for small interqubit separation while they stabilize for larger separations. Note that $\mathcal{F}^-$ saturates more rapidly than $\mathcal{F}^+$. Such higher QFI $\mathcal{F}^+$ reveals the appearance of entangled states that are highly sensitive to parameter changes (see below).

In Figs. 3(c) and 3(d), we plot the decay rates γ^+ and γ^- for different values of Rabi frequency. The results show that high Ω leads to positive values of both decay rates,

signaling that the dynamics is almost Markovian. However, for small Rabi frequency, i.e., $\Omega < 10$, and at relatively long times, γ^+ and γ^- take negative values at certain critical times

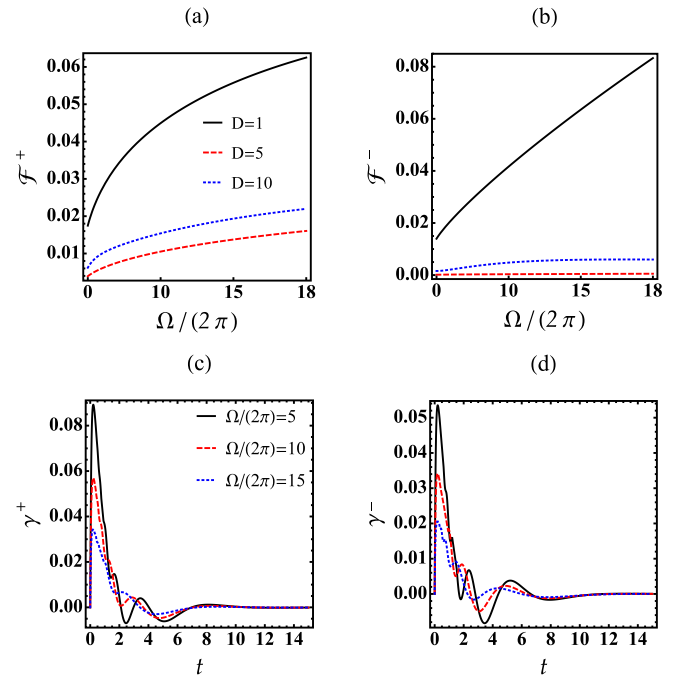


FIG. 3. (a) and (b) QFI $\mathcal{F}^+$ and $\mathcal{F}^-$ as a function of the Rabi frequency of the microwave field, Ω , for different values of interqubit distances and at time $t = 10$. (c) and (d) Time-dependent decay rates $\gamma^+(t)$ and $\gamma^-(t)$ for different values of Rabi frequency, Ω with $D = 5$. Parameters are as follows: $\sigma = 0.5$, $c = 1$, and $\epsilon_{dd} = 0.83$.

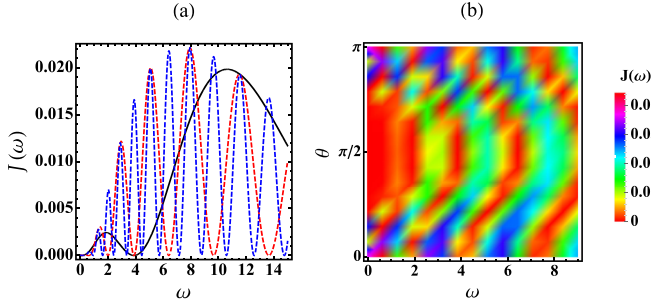


FIG. 4. (a) Spectral density function for different values of interqubit distance D with $\theta = \pi/2$. Black line: $D = 1$; red dashed line: $D = 5$; blue dotted line: $D = 10$. (b) Spectral density function as a function of polarization direction and the frequency with $D = 5$. Parameters are as follows: $\sigma = 0.5$, $c = 1$, and $\epsilon_{dd} = 0.83$.

showing the existence of a backflow effect. This behavior arises because the introduction of microwave shielding enables the continuous tuning of the dipolar length. Consequently, the shielding interaction plays a pivotal role in the information flow and provides deep insights into the limits of measurement precision.

V. ANALYTICAL RESULTS: PHONON REGIME

The spectral density function, which encodes the relevant information characterizing the qubit-environment interaction, is defined as $J(\omega) = \sum_{\mathbf{k}} |g_{\mathbf{k}}|^2 \delta(\omega - \omega_{\mathbf{k}})$. In the phonon branch ($k \rightarrow 0$) and at $T = 0$, it turns out to be given as

$$J(\omega) = \frac{\gamma}{8\pi^2} f(\epsilon_{dd}, D) \omega^3 e^{-\omega^2/\omega_c^2}, \quad (21)$$

where $\omega_c = 2c_s/l_I$ is the cutoff frequency, $c_s = \sqrt{ng/m}$ is the sound velocity, $\gamma = g_I/g$, and $f(\epsilon_{dd}, D)$ describes the interplay of DDI and interqubit separation. For a nondipolar BEC ($\epsilon_{dd} = 0$), it reduces to $f(D) \approx \cos^2(2D\omega/\omega_c)$. For $D \rightarrow 0$, integration over θ yields

$$f(\epsilon_{dd}) = \frac{1}{6} e^{-2\epsilon_{dd}-1} \left(\frac{\sqrt{3\pi} e^{3\epsilon_{dd}} (3 - 2\epsilon_{dd}) \text{erf}(\sqrt{3\epsilon_{dd}})}{\sqrt{\epsilon_{dd}}} - 6 \right),$$

where $\text{erf}(x)$ is the error function. Clearly, Eq. (4) shows that the qubits are able to predict information transfer dynamics in super-Ohmic baths. For two impurity atomic qubits separated by a distance $D = 5$ immersed in NaCs molecules with $\epsilon_{dd} = 0.83$ [24], one has $f(\epsilon_{dd}) \simeq 0.25$, and thus the spectral density reduces to $J(\omega) \simeq 0.03 \gamma \omega^3 e^{-\omega^2/\omega_c^2}/\pi^2$.

The corresponding decoherence factors are, thus, given by

$$\Gamma^{\pm}(D, t) = 2\Gamma^0(\omega) \pm 2 \int d\omega J(\omega) \frac{\sin^2(\omega t/2) \cos^2(2\omega D/\omega_c)}{\omega^2}, \quad (22)$$

where

$$\Gamma^0(t) = \int d\omega J(\omega) \frac{\sin^2(\omega t/2)}{\omega^2}.$$

Upon substituting the function (4) into Eq. (22), we may arrive at

$$\begin{aligned} \Gamma^+(D) = & \frac{\gamma \omega_c^2}{64\pi^2} f(\epsilon_{dd}, D) \left[(4D - t\omega_c) F\left(2D - \frac{t\omega_c}{2}\right) \right. \\ & + (4D + t\omega_c) F\left(2D + \frac{t\omega_c}{2}\right) \\ & \left. - 8DF(2D) + 6t\omega_c F\left(\frac{t\omega_c}{2}\right) \right], \end{aligned} \quad (23a)$$

$$\begin{aligned} \Gamma^-(D) = & \frac{\gamma \omega_c^2}{64\pi^2} f(\epsilon_{dd}, D) \left[-(4D - t\omega_c) F\left(2D - \frac{t\omega_c}{2}\right) \right. \\ & - (4D + t\omega_c) F\left(2D + \frac{t\omega_c}{2}\right) \\ & \left. + 8DF(2D) + 2t\omega_c F\left(\frac{t\omega_c}{2}\right) \right], \end{aligned} \quad (23b)$$

where $F(x)$ is the Dawson function. It increases monotonically at short times and saturates in the long time limit. Equations (23) show that both $\Gamma^{\pm}$ in the phonon regime depend on the distance D and on the relative dipolar interaction ϵ_{dd} . Note that the coupling between the qubits and their environment may induce excitations of additional phonons, leading to qualitative difference in the steady state of $\Gamma^{\pm}$ notably for large separations.

Effects of the separation between qubits and polarization direction on the spectral density function are depicted in Fig. 4. We see that for small frequencies, $J(\omega)$ is super-Ohmic regardless of the value of the interqubit distance [see Fig. 4(a)], signaling the occurrence of non-Markovian dynamics of two qubits. However, at higher frequencies ($\omega > 1$), the spectral density exhibits an oscillatory behavior without any saturation. As the separation between qubits gets increased ($D = 10$), the function $J(\omega)$ oscillates rapidly. The spectral density vanishes for some critical values of ω , revealing that the qubits are dissociated from their bath even if they are close to each other.

Figure 4(b) shows that as the polarization direction varied from $\theta = 0$ to $\theta = \pi$, the spectral density changes its behavior progressively and oscillates with different amplitudes. For $\theta = 0$, $J(\omega)$ induces an anomalous behavior notably in the regime of low frequency. Importantly, the spectral density function is symmetric with respect to $\theta = \pi/2$; i.e., the properties of $J(\omega)$ are almost the same when the dipolar interaction is repulsive. We interpret this behavior as the distribution of entanglement (concurrence) across qubits, and the flow of information between the different partitions of the system are uniform. In contrast, $J(\omega)$ displays a somewhat different behavior when the dipoles were oriented along other directions, signaling an asymmetric information flow. One can infer that the variation in the polarization direction of the dipoles plays a crucial role in the spectral density and, thus, in the information flow.

VI. ENTANGLEMENT

Here we compute the concurrence $\mathcal{C}$ for two-qubit X states, which is often used to quantify the entanglement of mixed

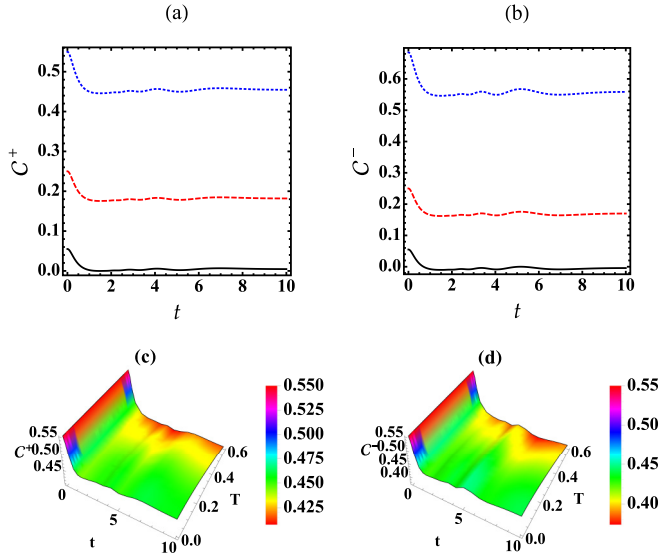


FIG. 5. (a) and (b) Time evolution of the concurrence $C^\pm(t)$ for different values of the initial-state parameter c . Black lines: $c = 0.37$; red dashed lines: $c = 0.5$; blue dotted lines: $c = 0.7$. (c) and (d) The concurrences $C^\pm$ as a function of the time and temperature for $c = 0.7$. Parameters are as follows: $\sigma = 0.5$, $D = 5$, and $\epsilon_{dd} = 0.83$. For $C_\pm \leq 0.37$, the state is separable. The color represents the magnitude of concurrence, showing that entanglement decays more rapidly at higher temperatures.

states. Using the results obtained in Eqs. (17) and (18), the density matrices turn out to be given as

$$\rho^\pm = \begin{pmatrix} \frac{1 \pm c}{4} & 0 & 0 & w^{\pm} \\ 0 & \frac{1 \mp c}{4} & z^{\pm} & 0 \\ 0 & z^\pm & \frac{1 \mp c}{4} & 0 \\ w^\pm & 0 & 0 & \frac{1 \pm c}{4} \end{pmatrix},$$

where $w^+ = ce^{i[2\Delta(t) + \Theta(t)]}e^{-\Gamma_+}/2$, $w^- = 0$, $z^+ = 0$, and $z^- = ce^{-\Gamma_-}/2$.

The concurrence for the above states is then written as

$$C^\pm = 2 \max\{|w^\pm| - (1 \mp c)/4, |z^\pm| - (1 \pm c)/4\}. \quad (24)$$

For $C^\pm > 0$, the qubits are entangled.

Effects of the initial-state parameter c and the temperature T on the dynamics of the concurrences $C^\pm(t)$ are reported in Fig. 5. As shown in Figs. 5(a) and 5(b), as the initial parameter increases, $C^\pm(t)$ shift from 0 to a finite value, revealing the existence of a steady-state concurrence for any initial state. Remarkably, the entanglement exhibits an oscillatory behavior in time arising from qubit-qubit interaction. For $c \lesssim 0.37$, the concurrence is vanishing and hence the state is separable. Figures 5(c) and 5(d) depict a slight decrease in the concurrence with increasing temperature, suggesting a decay of the entanglement between qubits. We also see that the reservoir temperature does not change the maximal value of $C^\pm(t)$. The revival of entanglement appearing after some times during which the concurrence vanishes, apparent in Figs. 5(c) and 5(d), more evident in $C^-(t)$, could be induced by the memory effects of the molecular reservoir. Such a revival of entanglement

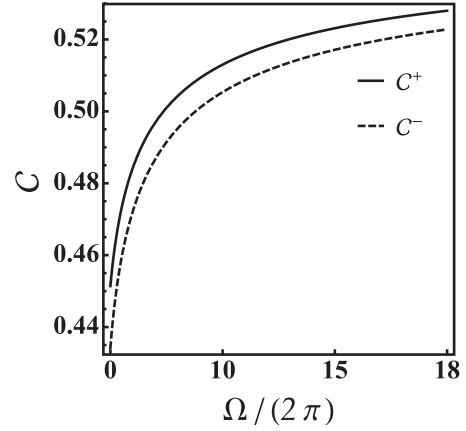


FIG. 6. Stationary concurrences $C^\pm$ as a function of the Rabi frequency of the microwave field, Ω , at time $t = 10$. Parameters are as follows: $c = 0.7$, $\sigma = 0.5$, $D = 5$, and $\epsilon_{dd} = 0.83$.

seems then to be connected to the non-Markovian dynamics observed above (see also, e.g., Ref. [43]).

Paying attention to the effect of the Rabi frequency of the microwave field, Ω , it is observed that an increase of this parameter may augment the stationary concurrences, $C^\pm$, for both sub-decoherent and super-decoherent states (see Fig. 6). Consequently, BECs of MSPMs are good candidates for enhancing the overall amount of entanglement.

VII. CONCLUSIONS

In this paper we studied the dynamics of quantum information and entanglement of two spatially separated qubits with two hyperfine spin states interacting with a thermal dephasing reservoir consisting of MSPMs. To address this issue, we calculated the decoherence factor, the QFI, the decay rate, and the concurrence associated with both sub-decoherent and super-decoherent states as a function of the spatial separation between qubits, the temperature, and the Rabi frequency.

Our findings revealed that the evolution of the decoherence factors and the QFI is nonmonotonic with revival oscillations at larger separations. We showed that the intricate interplay of the qubit-qubit correlation and the shielding interaction can improve the estimation of our super-Ohmic reservoir parameters, including the temperature and the spectral density. The latter is found to be affected by the polarization direction of the dipoles and the Rabi frequency. We also observed a transition from Markovian to non-Markovian dynamics by adjusting the interqubit separation and the shielding interaction. Moreover, a finite steady-state concurrence for two qubits initially prepared in the X state is obtained for any initial-state parameter with periodic oscillations. We demonstrated that, for certain values of Rabi frequency, the molecular BEC induces an extra interaction that can enhance entanglement between the two distant qubits.

The emerging results open new avenues not only for controlling quantum information flow but also for generating large quantum entanglement between qubits, offering a tantalizing framework for future advancements in quantum computing and sensing.

DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not

technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

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