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Dynamics of open quantum systems: From the Rabi model to coupled qubits

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Summary. — Employing the worldline Monte Carlo technique, Matrix Product State simulations and a variational approach, we focused on the dissipative quantum Rabi model, revealing a Beretzinski-Kosterlitz-Thouless quantum phase transition under low bath coupling. Exploring the dynamics of a slow qubit coupled to a fast oscillator, we found functional relationships, analyzed couplings' effects, and evaluated the qubit Bloch vector. Weak to intermediate bath coupling simplifies qubit state evaluation, while the ultra-strong coupling regime exhibits non-Markovian effects and entanglement growth. Recent investigations include the impact of baths on two interacting qubits, showcasing a method for quasi-fully non-decoherent qubit encoding. This work provides insights into open quantum systems, emphasizing potential applications in quantum computing and communication.

1. – Introduction

In the realm of quantum physics, we deal with complex interconnected systems, where numerous individual components interact dynamically. Each element possesses distinct properties and collectively forms composite systems exhibiting intricate behavior. These systems are usually not isolated; instead, they exist in constant interaction with their environment, which can influence the systems within it, either ejecting a component, altering its trajectory or inducing novel interactions among systems. These phenomena lay the foundation for the concepts explored in this work, specifically, the dynamics of open quantum systems. We will start by examining the fundamental Rabi model and progress to scenarios involving two qubits. The modeling framework employed throughout the work for all the physical models under investigation refers to the established concept proposed by Caldeira and Leggett. Our focal subsystem is then linearly coupled to a set of N harmonic oscillators. As N tends to infinity, they collectively transform into a real reservoir. This transition from reversible to irreversible dynamics results in the exclusive flow of energy from the system to the reservoir, maintaining the reservoir's equilibrium state. We implement the Caldeira-Leggett model in its quantum formulation. This approach allows us to take the continuum limit and describe the bath's structure using a spectral density function.

2. – Models and techniques

First, we focus on the quantum Rabi model (QRM), which involves a two-level system coupled to an oscillator. The oscillator, in turn, interacts with a thermal bath at zero temperature (see fig. 1(a)). We set $\hbar = k_B = 1$. The qubit frequency is Δ , the oscillator one ω_0 , and the parameter g represents the coupling strength between them. The bath is represented as a collection of N oscillators coupled to the position operator of the oscillator x_0 . The definition of α , linking the oscillator to the bath, characterizes the bath spectral density $J(\omega) = \frac{\alpha}{2}\omega f(\frac{\omega}{\omega_c})$. Here $f(\frac{\omega}{\omega_c})$ is a function that depends on the cutoff frequency for the bath modes, ω_c , which governs the behavior of the spectral density at high frequencies.

We proceed by investigating the behavior of two interacting qubits in an Ohmic bath composed of harmonic oscillators, similar to our previous analysis (see fig. 1(b)). Δ is the frequency of the two qubits and ν the strength of the interaction between them. The bath is again made of N harmonic oscillators and α is defined such that the bath spectral density is given by the same expression as before. The only difference is that now the bath is directly connected to the two qubits.

We employed various techniques to investigate the equilibrium and non-equilibrium properties of the open quantum systems under study. We derive solutions for the Heisenberg equations of motion (HEM) for both the system and the degrees of freedom of the bath. These solutions involve complex coupled differential equations, and we use the time evolution of the qubit observables, assuming zero coupling to the oscillator to solve them. In the low coupling to the environment regimes, we utilize solutions of Lindblad master eq. (LME), adopting a global approach [1]. This entails diagonalizing the closed system and utilizing its eigenstates to formulate the Lindblad equation.

To analyze the equilibrium properties of the systems, we implement World-line Monte Carlo (WLMC), a path integral technique based on a Monte Carlo algorithm. We remove exactly all the phonon degrees of freedom of the thermal bath, obtaining the density matrix dependent only on the effective Euclidean action with the kernel depending on the bath spectral density [2-4].

Another approach to the thermodynamic equilibrium properties is a variational approach based on Feynman's work with the charge polaron problem (FM) [5]. He introduced a clever variational action, such that in the perturbation expansion the first order was sufficient to obtain an excellent description of the physics for arbitrary coupling strengths. This method, combined with the Mori formalism, enables us to investigate the non-equilibrium properties calculating the time-dependent relaxation functions.

The final method we employ is based on the Matrix Product State (MPS) ansatz for



Fig. 1. – (a) Quantum Rabi model: a qubit of energy gap Δ connected to an oscillator through g. The oscillator housing the qubit interacts with an Ohmic bath through α [9]. (b) Two coupled qubits: two qubits of energy gap Δ interacting one with another through ν and coupled to an Ohmic bath through α .

1D tensor networks [6]. This representation is particularly effective when the entanglement entropy exhibits an area-law growth. In such cases, the numerical cost is no longer exponential with the system size but becomes polynomial. We utilize the Density-Matrix Renormalization Group technique to determine the ground states [7,8]. Furthermore, using the same MPS representation for the entire many-body open quantum system, we can compute its dynamical evolution. The two-site time-dependent variational principle proves to be a favorable technique, striking a balance between a small bond dimension and extended simulation times.

3. – Strategies and results

3¹. Quantum Rabi model. – In the first study [9], our focus lies in understanding the impact of dissipation on the qubit-oscillator interactions. To investigate the system's dynamics, we employ the HEM approach valid for low values of q and the LME which is applicable for low values of α . Furthermore, we employ MPS numerical simulations and compare the results obtained through these three methods. When examining the mean values of the oscillator quadratures and number, we perform a Bloch vector evaluation of the qubit state. This is because, upon computing the fast Fourier transform (FFT) of these quantities, we observe that the quadratures retain memory of the qubit dynamics, with a peak at the qubit frequency remaining unchanged even as dissipation increases. By focusing on the FFT of the cavity number, we detect two peaks at renormalized frequencies corresponding to "up" and "down," allowing for a qubit z-component evaluation that is more sensitive to the dissipation. We discovered that a Bloch vector evaluation is reliable for systems that are weakly to moderately coupled to their environment (see fig. 2(a)). However, when the coupling between the system and its environment is very strong, the system becomes entangled with its surroundings, that is its von Neumann entropy $S_q(t) = -\text{Tr}\{\rho \ln(\rho)\}$ grows towards its maximum value (ln(2)), making it harder to study the system in isolation (see fig. 2(b)).

In the same QRM we then look at the occurrence of a dissipative Beretzinski-Kosterlitz-Thouless quantum phase transition (QPT) [10]. The system transitions from a disordered phase to an ordered one by increasing the qubit-oscillator coupling g and



Fig. 2. – (a) Phase diagram of the QRM with $g/\Delta vs. \alpha$ in weak coupling (WC), strong coupling (SC) and ultra-strong coupling (USC) for z-component and Bloch vector evaluations [9]. (b) Qubit Von Neumann entropy S_q computed through MPS for weak coupling (WC), strong coupling (SC) and ultra-strong coupling (USC) [9].

crossing a quantum critical point. When considering the effective Euclidean action, which traces out the bath degrees of freedom, the system is mapped to a classical spin chain with long-range ferromagnetic interactions and a kernel behavior typical of a BKT transition. Therefore, the critical point corresponds to the transition to the ordered ferromagnetic phase under equilibrium conditions. Returning to our initial physical model of a qubit in contact with an Ohmic bath, this ordered phase manifests as the qubit always being in the state \uparrow or \downarrow , corresponding to the two degenerate ground states of the system due to the strong coupling to the bath. This occurs at zero temperature, where only quantum fluctuations are responsible for the ordering. At finite temperature, there is a region in which quantum fluctuations dominate over thermal ones, and the system still shows a quantum critical behaviour. We use the three independent methods introduced above to unveil the QPT: WLMC, FM, and MPS. The first two help us to understand when the system is at rest, while the latter two to bescribe how it behaves over time. At thermodynamic equilibrium, we compute the squared magnetization of the equivalent model undergoing the QPT as a function of q/Δ for three different values of $\beta\Delta$ (see fig. 3 (left)). This quantity jumps from zero to one at the critical q, steeper and steeper by increasing β , indicating that we are approaching the quantum critical point. The critical value of q can be approximated using an analytical formula [10], but it has also been determined through a numerical WLMC analysis. This analysis employs the approach suggested by Minnhagen *et al.* within the framework of the XY model [11,12]. The squared magnetization is then a measure of how ordered the system is, becoming non-zero after the critical q. In the time evolution of the system, we observe the effects of the QPT. Specifically, we adiabatically turn on a small magnetic field that we turn off at time zero, from which we start to observe the system relaxation. The plots in fig. 3 (right) show the relaxation function $\Sigma_z(t)$ for different g values. For low values, we observe Rabi oscillations between the two states of the qubit. By increasing q, the relaxation function shows exponential decay, and after the critical g, it no longer changes. This happens at the same critical q as before, and it means that the qubit cannot be in two states at once, as an evidence of the QPT.

3[•]2. *Two coupled qubits*. – Finally, we delve into the scenario involving two qubits in an Ohmic bath and explore the potential of utilizing qubit-qubit interactions to safeguard



Fig. 3. – Left: squared magnetization of the mapped model vs. the coupling g/Δ at $\beta\Delta = 10$ and $\beta\Delta = 10^3$, comparing WLMC and FM. Right: qubit relaxation function $\Sigma_z(t)$ at different values of g/Δ comparing FM and MPS. In the inset of panel (d) the qubit no longer relaxes for $g \approx g_c$. Reprinted figures with permission from [10], copyright 2024 by the American Physical Society.

information against the effects of dissipation [13]. To gain a deeper understanding of how states affect the dynamic behavior of the system, we can look at the closed spectrum (only the two-qubit system). The four eigenstates depend on the interaction parameter ν . When it is positive, the qubit interaction is ferromagnetic; otherwise, it is antiferromagnetic. We find that the antiferromagnetic interaction tends to be more robust against the bath's tendency to ferromagnetize the two qubits. Additionally, it's worth noting that the ground state corresponds to the Ψ^- Bell state, which is the singlet state and represents a decoherence-free subspace (DFS). We have chosen to implement a tensor product structure within subspaces of the Bell basis $\{|\Phi^+\rangle, |\Phi^-\rangle, |\Psi^+\rangle, |\Psi^-\rangle\}$ to encode information in a single logical qubit. The four states are defined in the common eigenbasis of σ_z operator $\{|\uparrow\rangle, |\downarrow\rangle\}$ as follows: $\{|\Phi^+\rangle = (|\uparrow\rangle|\uparrow\rangle + |\downarrow\rangle|\downarrow\rangle)/\sqrt{2}, |\Phi^-\rangle = (|\uparrow\rangle|\uparrow\rangle - |\downarrow\rangle|\downarrow\rangle)/\sqrt{2}, |\Psi^+\rangle = (|\uparrow\rangle|\downarrow\rangle + |\downarrow\rangle|\downarrow\rangle / \sqrt{2}$.

Our investigation includes three encoding strategies:

- Single-Level Encoding (Antiferromagnetic Case AF): the singlet state represents the logical "up", and the Ψ^+ state serves as the logical "down".
- Multilevel Encoding (Symmetric Case SYMM): the two antiferromagnetic states $(\Psi^- \text{ and } \Psi^+)$ represent the logical "up", while the ferromagnetic states $(\Phi^- \text{ and } \Phi^+)$ correspond to the logical "down".
- Multilevel Encoding (Nonsymmetric Case NSYMM): the singlet state serves as the "up", while the "down" is a combination of the other three states within the triplet.



Fig. 4. – Left: fidelity F(t) of the free evolution with the open system evolution of encoded qubits AF, SYMM and NSYMM and one physical qubit as functions of time. We average the fidelity over many realizations of initial states, sampling the entire Hilbert space. Right: purity P(t) of encoded qubits for $\alpha = 0$ and $\alpha = 0.01$ as a function of time for the AF and NSYMM strategies. We average the purity over many realizations of the initial state in the new encoded subspace. Reprinted figures with permission from [13], copyright 2024 by the American Physical Society.

We optimize the two multilevel strategies by maximizing fidelity with respect to free evolution. Figure 4 (left) demonstrates that all the strategies outperform the physical qubit in terms of fidelity. Furthermore, fig. 4 (right) illustrates the purity of AF and NSYMM in the new logical subspace. The top plot represents the qubits without the bath. The purity oscillates, periodically returning to 1, indicating that the encoded qubit remains in a quantum state. On the other hand, the bottom plot shows the scenario with non-zero coupling to the bath. For NSYMM, all the peaks are shorter, and the purity no longer reaches 1 over time. In contrast, for AF, the amplitude of oscillations is reduced, but the purity remains consistently high, with a greater stationary value. Therefore, AF is an excellent choice for encoding information that is highly resilient to the effects of the bath over time.

4. – Discussion and conclusions

In conclusion, our research has deepened our understanding of qubit-oscillator interactions and revealed a QPT occurring when the qubit and oscillator are weakly coupled to their environment. Our findings suggest that the QPT in the Rabi model can be experimentally observed by adjusting the qubit-oscillator coupling. A suitable experimental platform to reproduce our model involves a flux qubit ultrastrongly coupled to its resonator, further coupled to an Ohmic bath [14, 15]. We have also developed an encoding strategy that demonstrates resilience to environmental factors, thanks to the antiferromagnetic interaction and the DFS. As we move forward, further study will include the addition of qubits or couplers and the implementation of a measurement process description. Indeed, our current research extends to studying the modifications in the QPT dynamics when an additional qubit is introduced into the quantum Rabi model. Specifically, we have investigated the behavior of entropy and entanglement among the components when the system is out of thermodynamic equilibrium and how these features can be related to dynamical and thermodynamic quantum phase transitions [16].

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