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Universal anomaly of dynamics at phase transition points induced by Pancharatnam-Berry phase

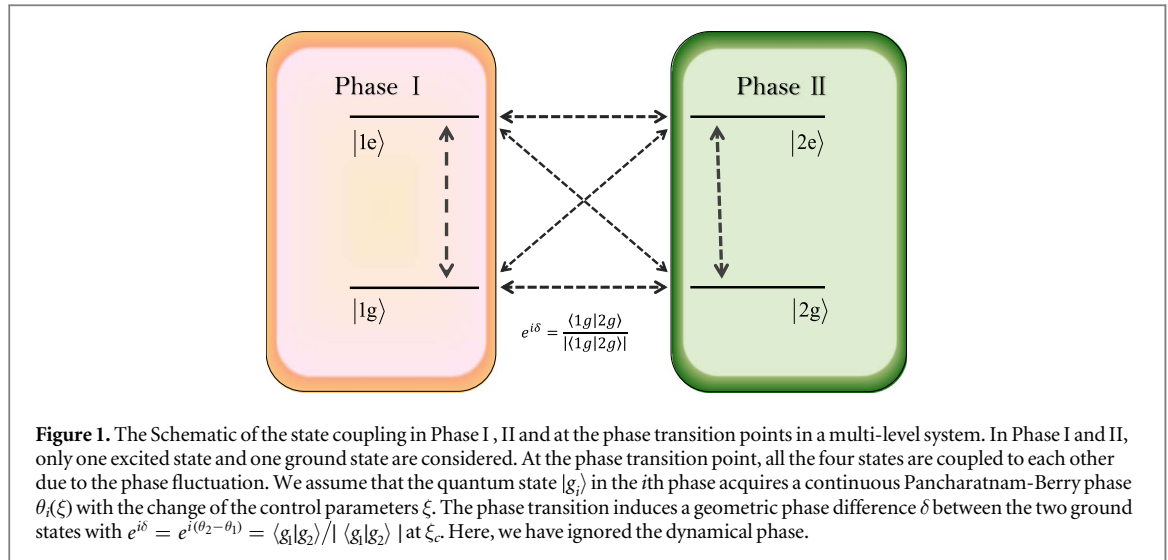
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14 April 2023Jia-Yuan Zhang¹, Xia Yin², Ming-Yu Liu¹, Jize Zhao^{3,4}, Yang Ding² and Jun Chang^{1,4} ¹ College of Physics and Information Technology, Shaanxi Normal University, Xi'an 710119, People's Republic of China² Center for High-Pressure Science and Technology Advanced Research, Beijing 100094, People's Republic of China³ School of Physical Science and Technology & Key Laboratory for Magnetism and Magnetic Materials of the MoE, Lanzhou University, Lanzhou 730000, People's Republic of China⁴ Lanzhou Center for Theoretical Physics and Key Laboratory of Theoretical Physics of Gansu Province, Lanzhou University, Lanzhou 730000, People's Republic of ChinaE-mail: junchang@snnu.edu.cn**Keywords:** phase transition, Pancharatnam-Berry phase, dynamics, qubitsSupplementary material for this article is available [online](#)**Abstract**

Dynamical anomalies are often observed near both the continuous and first-order phase transition points. We propose that the universal anomalies could originate from the geometric phase effects. A Pancharatnam-Berry phase is accumulated continuously in quantum states with the variation of tuning parameters. Phase transitions are supposed to induce an abrupt shift of the geometric phase. In our multi-level quantum model, the quantum interference induced by the geometric phase could prolong or shorten the relaxation times of excited states at phase transition points, which agrees with the experiments, models under sudden quenches and our semi-classical model. Furthermore, we find that by setting a phase shift of π , the excited state could be decoupled from the ground state by quantum cancellation so that the relaxation time even could diverge to infinity. Our work introduces the geometric phase to the study of conventional phase transitions as well as quantum phase transition, and could substantially extend the dephasing time of qubits for quantum computing.

1. Introduction

Phase transitions are of crucial importance in physics since a variety of static and dynamic properties of systems are changed [1–5]. In a long history, the study of phase transition focuses on the static thermodynamic properties in equilibrium states. Recently, it was shown that dynamical measurements could provide a direct insight into the investigation of the complex transitions [6–15]. Remarkably, the slowing-down dynamics near the phase transition point have been observed in solids [9, 15–17], glasses [18] and even microbial systems [19]. In the symmetry-breaking phase transition, the critical slowing down under perturbation could clearly be observed in both experiments and theoretical models at critical points [16, 20–23]. The divergence of the relaxation time is attributed to the divergent correlation length according to the renormalization group theory [24]. However, near the first-order phase transition, the ultrafast relaxation time from the photoexcited state to the equilibrium state also increases by orders of magnitude in charge-ordered LaSrFeO [9]. Similarly, slowing-down dynamics were observed near the first-order Mott transition and structural phase transition [15, 17]. More surprisingly, in the superconducting and antiferromagnetic phase transitions, the lifetimes of the decay are even shortened at the critical point [12, 14]. Furthermore, in some 1D short-range spin models under sudden quenches, the fastest relaxations are unexpectedly found at the critical points, in contrast to the critical slowing down [5, 25–27]. Therefore, the dynamical anomalies near phase transition points are expected to be universal phenomena in a vast number of systems.

In this paper, we propose that the universal anomalies of dynamics near phase transition points could originate from the effect of the geometric phase. Date back to 1956, Pancharatnam proposed that the relative



phase between two polarized light beams determines the intensity of the interferogram [28]. Later in 1984, Berry realized that besides the dynamical phase, the quantum state acquires a geometric phase in the adiabatic and cyclic evolution of the time-dependent Hamiltonian [29]. The geometric phase is then generalized by loosening the constraint of adiabaticity, cyclicity and unity [30, 31], and applied in many fields ranging from high-energy physics [32] to condensed matter [33], statistics [34, 35], molecular [36, 37], ultracold atoms [38], optics [39, 40] and quantum computation [41].

The quantum criticality have been investigated based on the geometric phase of ground states in the XY Spin model [42, 43], the ground state overlap in Dicke mode [44], the ground-state energy and its derivative in Rabi model [45]. However, in many-body systems, it is difficult or impossible to experimentally measure the ground state energy and the functional dependency of the geometric phase on parameters. Theoretically, the system Hamiltonian often could not be identified for a long time as in cuprates, iron pnictides, manganites and so on. In this paper, we prove the dynamical anomalies at phase transition points are universal as the result of quantum coherence, without the need for the exact system Hamiltonian or the precise dependency of the geometric phases on control parameters. Our model only includes some relevant quantum states of systems and coupling interactions. The information of the energy gaps between the states and the coupling constants could be measured via experiments. Therefore, the multi-level model is not limited to a special system. We suppose that Pancharatnam-Berry phases appear in quantum states and change continuously with tunable parameters such as external fields in the Hamiltonians. In particular, such phases abruptly change at phase transition points. Using the dissipative Schrödinger equation, we study the geometric phase effects on the dynamical evolution of a multi-level system near the phase transition point based on the generalized spin-boson model. Near the phase transition points, the relative phase between the states belonging to neighboring phases induces quantum interference, which results in the universal anomalies of the dynamics. The dynamical anomalies could be applied to probe the phase transition in experiments. We also use a semi-classical model to corroborate the geometric phase effects on the relaxation of the excited states. The relaxation time at phase transition points could become longer or shorter, which is in agreement with the experiments. Furthermore, we show that the relaxation time even could go to infinity by setting some peculiar coupling parameters. Our work could contribute to the study of phase transition and the design of qubits with long dephasing time.

2. Quantum model

We set up a quantum model to study the relaxation process around phase transition points as shown in figure 1. To elucidate the dynamical process, we introduce a system with the Hamiltonian $H_s(\xi)$ under a phase transition from phase I to phase II driven by the control parameter ξ , e.g. temperature, pressure, magnetic field and interaction constants. For simplicity and generality, we consider a multi-level system coupled to a bosonic bath, i.e. a generalized spin-boson model. The model is first mapped to another model with the electronic states coupled to a single harmonic mode damped by an Ohmic bath [46–48]. The Hamiltonian of the system is then written as

$$H_s = \sum_i E_i c_i^\dagger c_i + \sum_{ij} V_{ij} (c_i^\dagger c_j + \text{h.c.}) + \sum_i \lambda_i c_i^\dagger c_i (a^\dagger + a) + \hbar\omega a^\dagger a, \quad (1)$$

where E_i is the energy level and $n_i = c_i^\dagger c_i$ gives the occupation in the state i , V_{ij} is the real coupling (hybridization) constant between states j and i , e.g. Heisenberg exchange interaction, spin-orbit coupling constant, atom-field coupling strength. a^\dagger is the creation operator for the bosonic mode with frequency ω . We further define the electron-boson self-energy $\varepsilon_i = \lambda_i^2 / \hbar\omega$, and the self-energy difference $\varepsilon_{ij} = (\lambda_i - \lambda_j)^2 / \hbar\omega$ as well as the energy gap $\Delta_{ij} = (E_i - \varepsilon_i) - (E_j - \varepsilon_j)$ between two states. E_i , V_{ij} , ω and λ_i are the functions of the tuning parameter ξ .

The Ohmic bath damping is introduced by a dissipative Schrödinger equation, in which a dissipative operator iD is added to the Hamiltonian to describe the bath induced dissipation on the system [46],

$$i\hbar \frac{d|\psi(t)\rangle}{dt} = (H_0 + iD)|\psi(t)\rangle, \quad (2)$$

where $H_0 = e^S H_s e^{-S}$ is the Fröhlich transformation of H_s with $S = 1/\hbar\omega \sum_i n_i \lambda_i (a^\dagger - a)$. The eigenvectors $|\psi_{in}\rangle$ of H_0 are selected as the basis of the state i with n excited boson modes. We still need the detailed time evolution formula for $P_{in}(t)$. On one hand, the coupling to the surroundings relaxes a state with n bosons to a $n - 1$ boson state by the emission of bosons. On the other hand, the probability of the n -boson state increases due to the decay of the state with $n + 1$ bosons. This gives a change in the probability of the n -boson state

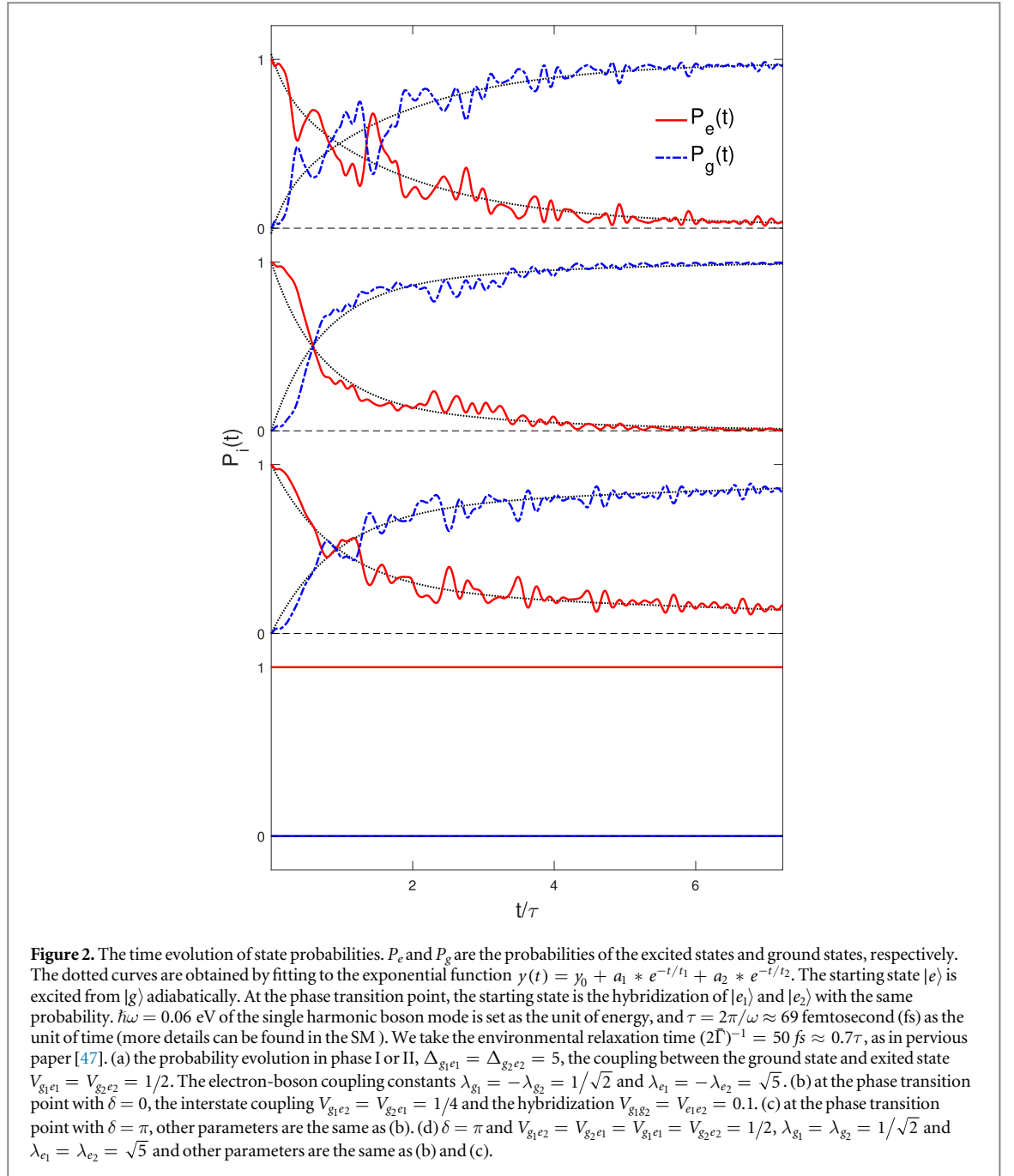
$$\frac{dP_{in}(t)}{dt} = -2n\bar{\Gamma}P_{in}(t) + 2(n+1)\bar{\Gamma}P_{i,n+1}, \quad (3)$$

where $P_{in}(t) = |\langle \psi_{in} | \psi(t) \rangle|^2$, $\bar{\Gamma} = \pi\bar{\rho}\bar{V}^2/\hbar$ is the environmental relaxation constant, where $\bar{\rho}$ is the effective environmental boson density of states and \bar{V} is the interaction between the local system and the environment. The dissipative Schrödinger equation effectively incorporates both the strong electron-boson coupling and environment memory effects by introducing the bosonic mode in the system, which were described previously [49]. Details of the dissipative Schrödinger equation are provided in the Supplemental Materials (SM) [50].

3. Dynamics at phase transition point

The cascade decay in a multi-level system could be effectively described by a two-level system. One of them is the excited state and the other is the ground state [46]. Therefore, in this paper, we only consider the relaxation process in such a two-level system. We assume that the Ohmic bath is the same in two different phases. The ground states are represented by $|g_1\rangle$ and $|g_2\rangle$, and the excited states $|e_1\rangle$ and $|e_2\rangle$ in phase I and II, respectively. At the phase transition point, we assume the four states in phase I and II coexist due to phase fluctuation. There are inter couplings between the states in phase I and II, such as $V_{g_i e_j}$, $V_{g_i g_j}$ and $V_{e_i e_j}$ with $i \neq j$. Importantly, we assume that the quantum state acquires a Pancharatnam-Berry phase $\theta_i(\xi)$ with the change of the control parameters ξ in the i th phase. The phase transition induces a geometric phase difference between the two ground states with $e^{i\delta} = e^{i(\theta_2 - \theta_1)} = \langle g_1 | g_2 \rangle / | \langle g_1 | g_2 \rangle |$ at ξ_c . The total probability $P = P_e + P_g$ is normalized to 1 with $P_e = P_{e_1} + P_{e_2}$ for the excited states and $P_g = P_{g_1} + P_{g_2}$ for the ground states. To study the relaxation of excited states, we assume the initial state is $|e_1\rangle$ or $|e_2\rangle$ adiabatically excited from $|g_1\rangle$ or $|g_2\rangle$ in phase I or phase II, or the superposition of $|e_1\rangle$ and $|e_2\rangle$ at the phase transition point. Solving the dissipative Schrödinger equation numerically, the evolution of all the states as a function of time clearly reflects the dynamic processes in phase I, II and at the phase transition point. In this paper, we set $\hbar\omega$ of the single harmonic boson mode as the energy unit, and $\tau = 2\pi/\omega$ as the unit of time.

To underscore the dynamical anomaly at the phase transition points, firstly, we set the parameters E_i , λ_i and V_{ij} to ensure that the decay processes are the same in both phases. We assume E_i , V_{ij} and ω are independent of the control parameter ξ , and only λ_i may change with ξ . For example, the abrupt change of the λ_i with respect to ξ could be selected as the order parameter of phase transition. The energies of the ground states E_{g_1} and E_{g_2} are set to be zero in both phases, and the energies of the excited states $E_{e_1} = E_{e_2}$. The coupling constants between the ground state and excited state are the same $V_{g_1 e_1} = V_{g_2 e_2}$. For the electron-boson coupling, we take $\lambda_{g_1} = -\lambda_{g_2}$ and $\lambda_{e_1} = -\lambda_{e_2}$, and hence $\varepsilon_{g_1} = \varepsilon_{g_2}$, $\varepsilon_{e_1} = \varepsilon_{e_2}$ and $\Delta_{g_1 e_1} = \Delta_{g_2 e_2}$. Therefore, the excited states in the both phases decay in the same way, as shown in figure 2(a). On the other hand, at the phase transition point, we assume that the four states coexist due to the fluctuation. The intercoupling constants between the ground states and excited states are supposed to be the same $V_{g_1 e_2} = V_{g_2 e_1}$. Furthermore, there are fluctuations within the ground and excited states with $V_{g_1 g_2} = V_{e_1 e_2}$. The starting states are excited adiabatically from the ground states $|g_1\rangle$, $|g_2\rangle$ or the mixture. We assume that there is a Pancharatnam-Berry phase difference δ between the ground state $|g_1\rangle$ and $|g_2\rangle$ of phase I and II. It is expected that the relaxation time at the phase transition point should be quite close to that in phase I and II. However, we find that the relaxation strongly depends on the relative phase δ due to quantum interference effects. When there is no phase difference or $\delta = 0$, the relaxation time at the phase transition point



is even slightly shorter than that in phase I or II as shown in figure 2(b), which is in agreement with the reduction of relaxation time observed in the experiment at the critical point [12, 14]. On the other hand, in figure 2(c) for $\delta = \pi$, the decay time at the phase transition point could be much longer than that in phase I or II, as the slowing down observed in many experiments [9, 16, 21, 51, 52].

More surprisingly, when we set $\delta = \pi$, $V_{g_1e_2} = V_{g_2e_1} = V_{g_1e_1} = V_{g_2e_2}$, $\lambda_{g_1} = \lambda_{g_2}$, $\lambda_{e_1} = \lambda_{e_2}$ and keep the rest of the parameters the same as in figure 2(c), the relaxation time of the excited states at the transition point even could stretch into infinity as shown in figure 2(d), which is similar to the critical slowing down in the continuous phase transitions but it is independent of the divergent correlation length. As a contrast, for $\delta = 0$, the relaxation time of the excited states is close to that in phase I or II (not shown). Actually, it has been realized in experiments since several decades ago that the superconducting qubits composed by Josephson junctions with π phase shifters could be efficiently decoupled from environments and extend the phase coherence time [53–55]. To apprehend this puzzling result, we consider a four-level system without a bath. We assume that $|g_1, g_2\rangle$ are the wave vectors for the ground states and $|e_1, e_2\rangle$ the wave vectors for the excited states. The time-dependent Schrödinger equation of the four states is written as

$$i\hbar \frac{d}{dt} \begin{bmatrix} |e_1\rangle \\ |e_2\rangle \\ |g_1\rangle \\ |g_2\rangle \end{bmatrix} = \begin{bmatrix} E_e & \nu & V & V \\ \nu & E_e & V & V \\ V & V & E_g & \nu \\ V & V & \nu & E_g \end{bmatrix} \begin{bmatrix} |e_1\rangle \\ |e_2\rangle \\ |g_1\rangle \\ |g_2\rangle \end{bmatrix}, \quad (4)$$

where $E_{e,g}$ are the energies of the four states, ν and V are the state coupling constants. One has

$$i\hbar \frac{d|g_1\rangle}{dt} = E_g|g_1\rangle + \nu|g_2\rangle + V|e_1\rangle + V|e_2\rangle. \quad (5)$$

When $|e_1\rangle$ has a π phase difference with respect to $|e_2\rangle$, i.e. $|e_1\rangle = e^{i\pi}|e_2\rangle$, then the two last terms in equation (5) cancel each other and the ground states are decoupled from the two excited states. Interestingly, figure 2(d) indicates that even the environmental dissipation is involved, the excited states and ground states still could be decoupled from each other by canceling. Consequently, the quantum cancellation induced by the π phase shift is the key to extending the phase coherence time in the experiments [53–55].

4. Semiclassical relaxation model

To qualitatively understand the time relaxation in the quantum model, we appeal to a semiclassical model. A general phenomenological model is proposed to study the time evolution of the excited states near the phase transition points. We assume that $|e_1, e_2\rangle$ are the wave vectors of the excited states in the neighboring phase I and phase II. At the phase transition point, two excited states coexist and are weakly coupled to each other due to phase fluctuation. The quantum coherence is set up between the two excited states. We study the time evolution of the two excited states by mimicking the method in the Feynman's phenomenological model of the Josephson junction [50].

$$i\hbar \frac{\partial |e_1\rangle}{\partial t} = (E_{e_1} - i\Gamma_1)|e_1\rangle + (K - iK')|e_2\rangle, \quad (6)$$

$$i\hbar \frac{\partial |e_2\rangle}{\partial t} = (E_{e_2} - i\Gamma_2)|e_2\rangle + (K - iK')|e_1\rangle, \quad (7)$$

where E_{e_1}, E_{e_2} are the energies, Γ_1, Γ_2 are the relaxation rates of the two excited states, respectively. While K is the state coupling constant and K' is relaxation rate constant. If K and K' are zero, then the two Schrödinger equations describe the two excited states in the phase I and II, respectively. Near the critical point, the coupling or fluctuation between the two states may induce tunneling from one state to the other. Defining the total excited quasiparticle density $P_e = P_{e_1} + P_{e_2}$ with $P_{e_1} = \langle e_1|e_1\rangle$ and $P_{e_2} = \langle e_2|e_2\rangle$, and the phase difference $e^{i\delta} = \langle e_1|e_2\rangle / |\langle e_1|e_2\rangle|$, then one has

$$\hbar \frac{\partial P_e}{\partial t} = -2\Gamma' P_e, \quad (8)$$

with the effective relaxation rate

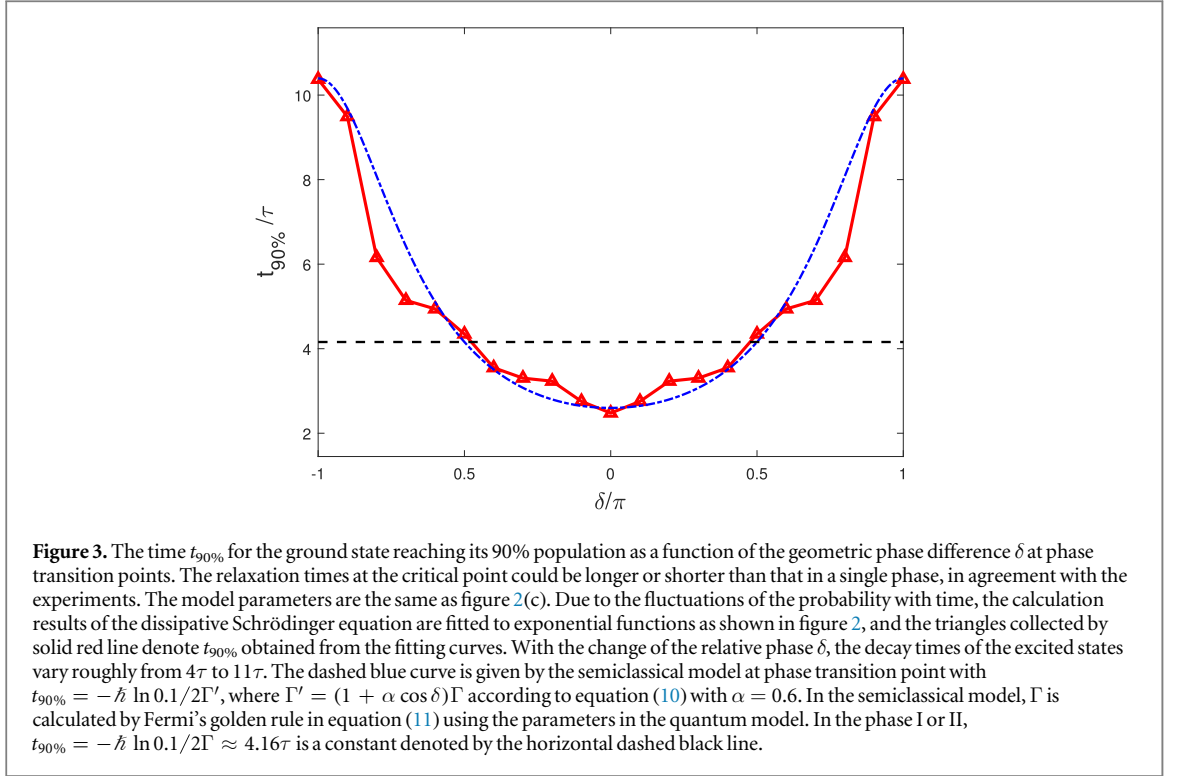
$$\Gamma' = \frac{\Gamma_1 P_{e_1} + \Gamma_2 P_{e_2}}{P_e} + \alpha K' \cos \delta, \quad (9)$$

where $\alpha = 2|\langle e_1|e_2\rangle|/P_e$ and $0 \leq \alpha \leq 1$. Since $\max(\Gamma_1, \Gamma_2) > (\Gamma_1 P_{e_1} + \Gamma_2 P_{e_2})/P_e > \min(\Gamma_1, \Gamma_2)$, the relaxation rate should change smoothly from one phase to the other if the quantum coherence in the last term of equation (9) is ignored. However, the quantum coherence could strongly affect the relaxation rate. For example, if we further assume $K' = \Gamma_1 = \Gamma_2 = \Gamma$, then, the effective relaxation rate reads,

$$\Gamma' = (1 + \alpha \cos \delta)\Gamma. \quad (10)$$

Since $\cos \delta$ could be zero, positive or negative, one has $0 \leq \Gamma' \leq 2\Gamma$. When $\delta = 0$, Γ' is larger than Γ . While $\Gamma' = 0$ signifies the relaxation time $\tau' = 1/\Gamma'$ approaching infinity, similar to the critical slowing down.

In order to compare the quantum and semiclassical models, we study the influence of the relative phase δ on the relaxation time quantitatively in both models. We define $t_{90\%}$ as the time for the ground state reaching 90 percent of the total population. As shown in figure 3, the dependence of $t_{90\%}$ on δ in the quantum model agrees well with that in the semiclassical model. With δ varying from 0 to π , the decay rate decreases gradually and the value of $t_{90\%}$ is strongly enhanced. For instance, when there is no phase difference or $\delta = 0$, $t_{90\%}$ at the phase transition point is even slightly shorter than that in phase I or II. On the other hand, for $\delta = \pi$, $t_{90\%}$ at the phase transition point is much longer than that in phase I or II. In the semiclassical model, using the parameters in the quantum model, Γ of the excited states is calculated by Fermi's golden rule [46]



$$\Gamma = \frac{\pi F_n V_{ge}^2}{\hbar\omega} \quad (11)$$

where V_{ge} is the coupling strength between the ground state and excited state and $F_n = e^{-g} g^n / n!$ is the Franck-Condon factor with $n \approx \Delta_{ge}/\hbar\omega$ with energy gap $\Delta_{ge} = (E_e - \lambda_e^2/\hbar\omega) - (E_g - \lambda_g^2/\hbar\omega)$, and $g = \varepsilon_{ge}/\hbar\omega$ is the Huang-Rhys factor with the electron-phonon selfenergy difference $\varepsilon_{ge} = (\lambda_e - \lambda_g)^2/\hbar\omega$. At phase transition point, the decay time $t_{90\%} = -\hbar \ln 0.1/2\Gamma'$ with $\Gamma' = (1 + \alpha \cos \delta)\Gamma$. In the phase I or II, $t_{90\%} = -\hbar \ln 0.1/2\Gamma$ is a constant around 4.16τ .

5. Discussion and conclusions

The phase difference between the ground state and the excited state is not always exactly the same. For example, in the XX spin model, the phase difference between the ground state and the excited state changes from 0 to π near the critical point [43]. Interestingly, the anomaly of the relaxation time dominantly originates from the relative phase difference between the two excited states belonging to the phase I and II, respectively, which could be roughly understood from our semiclassical model and the equation (5) of the 4-level model without dissipation. Furthermore, within the single phase I or II, the phase difference between the ground state and the excited state has limit effects on the relaxation time. The relative phase between different states could be tuned by external fields.

To conclude, we have proposed that the conventional phase transition and quantum phase transition could be featured by the Pancharatnam-Berry phase factor. We assumed that with the change of the control parameter in the Hamiltonian, the quantum state accumulates a geometric phase and there is abrupt shift of the phase at phase transition points. Applying the dissipative Schrödinger equation, we studied the dynamical evolution of the generalized spin-boson model. At the phase transition point, the geometric phase difference between the states belonging to neighboring phases results in the universal anomalies of dynamics via quantum interference. Since the geometric phase strongly affect the dynamical relaxation near phase transition points, experimental measurements of the dynamical anomalies could be applied to probe the phase transition. The effects of the geometric phase on the relaxation times in the quantum model qualitatively agrees with our semiclassical model. The geometric phase can increase or decrease the relaxation time at phase transition points, which coincides with the experiments and existing models. Furthermore, by adjusting some parameters and setting a π phase shift, we found that the relaxation time of the excited states even could be divergent, which agrees well with experiments of the superconducting π -junction. Our work presented theoretical evidences for studying the phase transition by introducing the geometric phase, which is benefited for the design of qubits with a long dephasing time for quantum computation and communications.

Acknowledgments

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Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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