Geometric Phase with Nonunitary Evolution in the Presence of a Quantum Critical Bath

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(Received 8 June 2010; published 10 December 2010)

Geometric phases, arising from cyclic evolutions in a curved parameter space, appear in a wealth of physical settings. Recently, and largely motivated by the need of an experimentally realistic definition for quantum computing applications, the quantum geometric phase was generalized to open systems. The definition takes a kinematical approach, with an initial state that is evolved cyclically but coupled to an environment—leading to a correction of the geometric phase with respect to the uncoupled case. We obtain this correction by measuring the nonunitary evolution of the reduced density matrix of a spin one-half coupled to an environment. In particular we are interested in baths near a quantum phase transition, which are known to induce strong decoherence. The experiments are done with a NMR quantum simulator, where we emulate qualitatively the influence of a critical environment using a simple one-qubit model.

DOI: 10.1103/PhysRevLett.105.240406 PACS numbers: 03.65.Vf, 03.65.Yz, 03.67.Ac, 05.30.Rt

For decades, the geometric phase [1] (GP) has fascinated physicists for its elegant theoretical grounds and its practical applications [2]. The GP is resilient to dynamical perturbations; thus, it might serve as a naturally fault-tolerant quantum information processing device [3]. In order to explore such applications, and unlike traditional studies of the GP in closed systems with pure states, one must take into account realistic experimental conditions—i.e., the explicit presence of noise and environments. Uhlmann was the first in considering a system in a mixed state, embedded, as a subsystem, in a larger system that is in a pure state [4]. Later, Sjöqvist *et al* [5] put forward a definition of the GP for a general mixed state undergoing a cyclic unitary evolution—subsequently measured using NMR interferometry in Ref. [6]. Different approaches to the problem were proposed [7]. In the present Letter, we will follow the line of Tong *et al.* [8], who developed a kinematic generalization of the GP to open systems that takes into account the coupling to an environment (leading to a *nonunitary* evolution of the reduced density matrix of the system [9]). Arguably, this approach is better suited to explore the usefulness of the GP in a real quantum computer undergoing decoherence processes [10]. Here we report a measurement of the GP for a spin $1/2$ undergoing nonunitary evolution induced by the coupling to an environment, using the decoherence factor or fidelity decay [11]. In particular—motivated by the recent observation that baths near quantum criticality induce strong decoherence [11]—we choose environments that can be tuned near a quantum phase transition (QPT). This choice not only adds richness to the behavior of the GP, but also advances the program of understanding it in general open systems [10]. In our experiments, performed in a NMR quantum simulator, we measure the full time dependence of the decoherence factor of the system spin—from which we can determine the GP using the results of Ref. [8]. To emulate the effect of a critical environment, we introduce a simple qualitative model of the ground state degeneracy that occurs at QPTs. Apart from demonstrating an alternative to traditional interferometry-based approaches for measuring the GP in open systems, our results further establish the strong connections between quantum information, quantum criticality, decoherence, and the quantum geometric phase [11–14] that have been the focus of much recent research (especially in the context of quantum simulations [15,16]).

The correction to the GP by a critical environment was first studied by Yi and Wang [17], who gave some general analytical results and found numerical instabilities in the GP of a qubit near criticality of the bath (an XY spin chain). More recently, it was shown that the GP of a spin coupled to an antiferromagnetic environment changes suddenly when the bath undergoes a first order QPT [18]. Notice that our problem is seemingly related to, but different than, the use of the GP as an order parameter in a QPT of a *closed* system, as studied first by Carollo and Pachos and others [12,14].

We consider a spin $1/2$ coupled to an environment with a total Hamiltonian $H = \Omega Z_{\mathcal{S}} \otimes I_{\mathcal{E}} + Z_{\mathcal{S}} \otimes H_{\mathcal{S}\mathcal{E}} + I_{\mathcal{S}} \otimes H_{\mathcal{E}}$, where $H_{\mathcal{E}}$ is the Hamiltonian of the bath, $Z_{\mathcal{S}}$ is the z Pauli matrix of the system (in this notation, X and Y are, respectively, the x and y Pauli matrices), $I_{\mathcal{S}}$ is the identity operator of the system and $I_{\mathcal{E}}$ the one of the bath. For simplicity, we only consider a dephasing spin-bath interaction, $Z_{\mathcal{S}} \otimes H_{\mathcal{S}\mathcal{E}}$, neglecting relaxation effects and limiting the relevance of the initial state (see discussion below). We take a product initial state for the spin-bath system, $\rho(0) = |\psi_0\rangle\langle\psi_0| \otimes |\varepsilon(0)\rangle\langle\varepsilon(0)|$, where $|\psi_0\rangle = \sin(\theta/2)|0\rangle + \cos(\theta/2)|1\rangle$ and $|\varepsilon(0)\rangle$ is a general initial state of the bath. In absence of the bath, the spin follows an evolution around the Bloch sphere, reaching again the initial state for $\tau = 2\pi/\Omega$. To compute the global phase gain during the evolution, one can use Pancharatnam's definition [19], which contains a gauge dependent part [i.e., a *dynamical* phase $\Phi_d = \pi\cos(\theta)$] and a gauge independent part, commonly known as *geometric* phase $\Phi_g = \pi[1 - \cos(\theta)]$. When coupled to the bath, the reduced density matrix of the system at time t is

$$\rho_r(t) = \sin^2(\theta/2)|0\rangle\langle 0| + \cos^2(\theta/2)|1\rangle\langle 1| + \frac{\sin\theta}{2} e^{-i2\Omega t} r(t)|0\rangle\langle 1| + \frac{\sin\theta}{2} e^{i2\Omega t} r^*(t)|1\rangle\langle 0|. \quad (1)$$

Here, $r(t) = \langle\varepsilon_0(t)|\varepsilon_1(t)\rangle$ is the decoherence factor induced by the environment, with $|\varepsilon_k(t)\rangle = e^{-it[H_{\mathcal{E}}+(-1)^k H_{\mathcal{S}\mathcal{E}}]}|\varepsilon(0)\rangle$. The phase Φ acquired by the open system after a period τ is defined as [8],

$$\Phi = \arg\left[\sum_k \sqrt{\epsilon_k(\tau)\epsilon_k(0)}\langle k(0)|k(\tau)\rangle e^{-\int_0^\tau dt \langle k(t)|(\partial/\partial t)|k(t)\rangle}\right], \quad (2)$$

where $|k(t)\rangle$ and $\epsilon_k(\tau)$ are, respectively, the instantaneous eigenvectors and eigenvalues of $\rho_r(t)$. Of the two k modes ($+$ and $-$) of the one-qubit model we are treating, only the $+$ mode contributes to the GP. Because our environments can induce a complex decoherence factor, i.e., $r(t) = |r(t)|e^{-i\varphi}$, we obtain a slightly different expression than that shown in Ref. [9], namely

$$\Phi = \int_0^\tau dt\left(\Omega - \frac{\partial\varphi}{\partial t}\right)\sin^2\left(\frac{\theta_t^+}{2}\right) + \tan^{-1}\frac{\sin\varphi(\tau)\sin(\frac{\theta_\tau^+}{2})\sin(\frac{\theta}{2})}{\cos\varphi(\tau)\sin(\frac{\theta_\tau^+}{2})\sin(\frac{\theta}{2}) + \cos(\frac{\theta_\tau^+}{2})\cos(\frac{\theta}{2})}, \quad (3)$$

where we have defined

$$\cos(\theta_t^+/2) = \frac{2(\epsilon_+ - \sin^2\theta/2)}{\xi(t)}, \quad \sin(\theta_t^+/2) = \frac{|r(t)|\sin\theta}{\xi(t)},$$
$$\xi(t) = \sqrt{|r(t)|^2\sin^2(\theta) + 4[\epsilon_+ - \sin^2(\theta/2)]^2}. \quad (4)$$

During normal quantum evolution, the system gains a global phase. The central result of Eq. (3) is to extract (by a proper choice of the "parallel transport condition") the purification independent part of the phase—which can be called a geometric phase because it is gauge invariant and reduces to the known unitary evolution limit.

In order to study the behavior of the GP when the bath is near a quantum phase transition, we have solved Eq. (3) both numerically and analytically with an Ising spin chain environment (see supplementary material [20]). In particular, the nonanalyticity of the GP at the critical point in the thermodynamical limit becomes evident in the limit of weak system-bath coupling [20]. Nevertheless, a full quantum simulation of a large enough critical system is on the edge of current technology, and beyond the scope of this Letter. Therefore, we opt for emulating the most relevant aspects of a critical bath qualitatively with a simplified model that is within experimental reach.

Near its critical point, the spectrum of a quantum critical system is characterized by the closing of the energy gap between the ground and the first excited state. In the thermodynamical limit, the gap closes with a power law $\sim|\lambda - \lambda_c|^{z\nu}$ (where z and ν are critical exponents), but for all finite size systems there is a minimum gap Δ near λ_c. It is remarkable that, for many purposes, this feature of the spectrum is enough to describe qualitatively the effects of a critical environment: as long as the excitations involved are small, and one is only interested in qualitative behavior, a small energy expansion of the decoherence factor can justify considering just two levels with appropriate dynamics [16]. Thus, we propose to emulate a complex critical bath using a simple two-level system model with Hamiltonian $H_{\mathcal{E}} = \lambda|\lambda|^{z\nu-1}\Delta Z_{\mathcal{E}} + \Delta X_{\mathcal{E}}$, where $\lambda_c = 0$ represents the "critical point" or QPT. The simplification might seem excessive, but it has been successful in previous studies: For $z\nu = 1$ (the mean field case), it gives a correct qualitative description of the creation of topological excitations during a finite speed quench [21]. In essence, the model is quantitatively not far away from the small systems used in demonstrations of quantum phase transitions [15,22]. A complete characterization of when this model does not describe the correct physics of a critical model is missing (one such case is the calculation of the path length of an adiabatic evolution [23]). For example, our simplified model cannot capture one feature observed in the Ising chain case: the total number of environment modes that contribute significantly to the geometric phase appears to be larger in the paramagnetic phase than in the ferromagnetic phase. This behavior could be related to the different nature of the excitations in both phases. Nevertheless, our results show that for the GP problem the model gives a fair qualitative description when the gap Δ is much smaller than the natural frequency Ω of the system spin.

Using a tomographic approach, we measure the GP of a qubit coupled to a critical environment using a nuclear magnetic resonance (NMR) quantum simulator, with the environment represented by the two-level model described above (with critical exponents $z\nu = 1$ and a transverse field strength $B = \lambda\Delta$). The target Hamiltonian to simulate experimentally is: $H = \Omega Z_{\mathcal{S}} + \delta Z_{\mathcal{S}} Z_{\mathcal{E}} + B Z_{\mathcal{E}} + \Delta X_{\mathcal{E}}$, where $Z_{\mathcal{S}}$ and $Z_{\mathcal{E}}$ are the z Pauli matrices of the system and environment, respectively. We obtain the GP by measuring the magnetization of the system spin in the $X - Y$ plane, which gives us the decoherence factor $r(t)$.

Denoting by $\epsilon_\pm = \pm\Delta\sqrt{1 + \lambda^{2z\nu}}$ the eigenenergies of $H_{\mathcal{E}}$, the decoherence factor of this model is

$$r(t) = e^{i\epsilon_-(\lambda)t}\Big[\cos\epsilon_-(\lambda+\delta)t - i\frac{\epsilon_-^2(\lambda+\delta) - \Delta^2\delta^2}{\epsilon_-(\lambda)\epsilon_-(\lambda+\delta)} \times \sin\epsilon_-(\lambda+\delta)t\Big], \tag{5}$$

where, to simplify notation, we have chosen the system-environment interaction to be $H_{\mathcal{SE}} = \delta(I_{\mathcal{S}} - Z_{\mathcal{S}})Z_{\mathcal{E}}$. The correction to the GP due to this decoherence factor [shown in Fig. 1 with the experimental results to be discussed below] contains the main elements observed in more complex models, as Ising spin chains [20]: a maximum correction of the GP at criticality, and a small asymmetric correction far away from the critical point.

The experimental sequence is as follows: We first fix Ω, δ, and Δ. Then, for each value of B, we initialize the system, and measure the decoherence factor $r(t)$ of the system after evolution with an operator $U = e^{-iHt}$ for various times $t \in [0, 2\pi/\Omega]$. The measured decoherence factor is shown in Figs. 1(a) and 1(b). The GP is calculated using a numerical interpolation of $r(t)$ in Eq. (3).

We choose the C^{13} and H^1 spins in the molecule of carbon-13 labeled chloroform ($CHCl_3$) dissolved in d6-acetone as the quantum registers (qubits) for the demonstration. The C^{13} atom simulates the system, and the H^1 the environment, where the scalar coupling between them is measured to be $J = 215$ Hz. Data were taken with a Bruker DRX 700 MHz spectrometer.

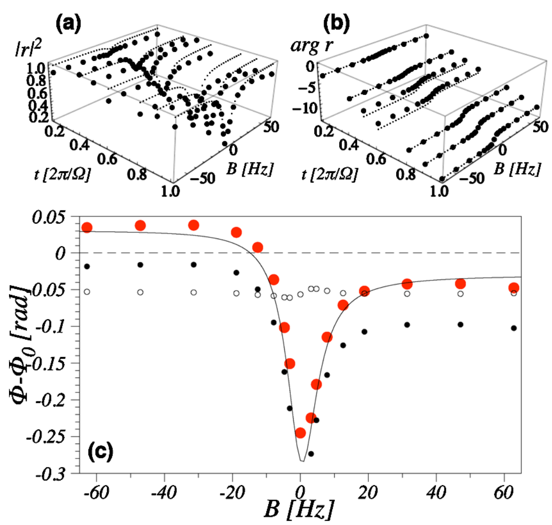

FIG. 1 (color online). (a) Observed absolute value squared of the decoherence factor and (b) its argument, both as a function of time and external magnetic field strength. (c) Computed correction to the geometric phase for a choice of $\theta = \pi/4$. Large filled circles are the experimental data, and the solid line is the theoretically expected value (without free parameters). Also shown is the difference between the GP measured *in presence* of the environment (small filled circles), and the GP measured when the system and environment are *decoupled* (small empty circles). Here, $\Omega = 100\ \pi$Hz, $\Delta = 0.02\Omega$, and $\delta = 0.1\Omega$.

Our choice of system-environment coupling makes the decoherence factor $r(t)$ independent of the initial state of the system (given by the angle θ) [see Eq. (1)]. This, in turn, makes the GP depend trivially on θ, which can be fully appreciated when approximating Eq. (3) in the weak coupling regime (see supplementary material [20]). Because we concentrate on how the criticality properties of the bath affect the GP, it is experimentally convenient to fix an initial state of the system that maximizes the signal-to-noise ratio, and change only the parameters of the environment spin. In particular, we choose the input state of the system to be $(|0\rangle_{\mathcal{S}} + |1\rangle_{\mathcal{S}})/\sqrt{2}$. The corresponding decoherence factor can then be used to compute Eq. (3) for any other initial state of the system. From Eq. (1) we can see that $r(t)$ is encoded in the coherent terms proportional to $\langle 2\sigma_+\rangle$ [see Fig. 2(b)], which can be observed directly in NMR by adding the two complex amplitudes of the peaks in the C^{13} spectra.

We use the gate sequence of Fig. 2(a) [24–26] to prepare the pseudopure state $|00\rangle_{\mathcal{SE}}$, to which we apply the unitary $e^{-i\pi Y_{\mathcal{S}}/4}e^{i\alpha Y_{\mathcal{E}}/2}$ to reach the input state $|\psi_{\rm in}\rangle = (|0\rangle + |1\rangle)_{\mathcal{S}}|g\rangle_{\mathcal{E}}/\sqrt{2}$. Here $|g\rangle_{\mathcal{E}} = |0\rangle\cos(\alpha/2) - |1\rangle \times \sin(\alpha/2)$ is the ground state of the environment for a given B value, where $\tan\alpha = -\Delta/B$ with $\alpha \in (0, \pi)$. Because the decoherence factor is independent of the initial state of the system, we chose it such that it maximizes the signal-to-noise ratio of the experiment.

The quantum simulated evolution U for a time t can be implemented with a Trotter approximation [27,28],

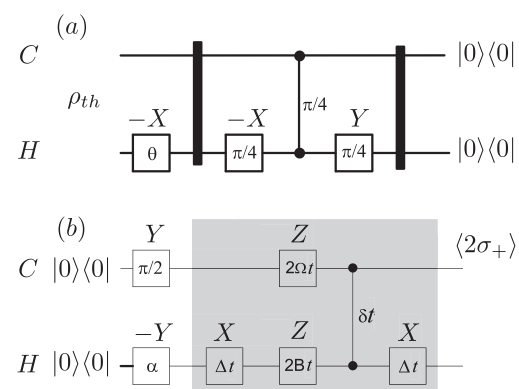

FIG. 2. (a) Gate sequence for preparing the pseudopure state $|00\rangle_{\mathcal{SE}}$ from the thermal state $\rho_{\rm th} = \gamma_C Z_{\mathcal{S}} + \gamma_H Z_{\mathcal{E}}$, where γ_C and γ_H are the gyromagnetic ratio of C^{13} and H^1. (b) Gate sequence for the quantum simulation of the system and measurement of the decoherence factor $r(t)$, proportional to $\langle 2\sigma_+\rangle = \langle X + iY\rangle$. The rectangles denote single-qubit gates, implemented through radio-frequency pulses. The rotation angle is shown inside the rectangle, and the direction above. We used $\cos\theta = 2\gamma_C/\gamma_H \approx 1/2$ and $\tan\alpha = -\Delta/B$ with $\alpha \in (0, \pi)$. The narrow black rectangles represent the gradient pulses along Z axis. The two connected circles denote the J-coupling evolution $e^{-i\phi Z_{\mathcal{S}}Z_{\mathcal{E}}}$, where ϕ is indicated next to the line. The grayed area marks the quantum simulation of the desired Hamiltonian, to the left is the initial state preparation, and to the right the measurement.

$$U \approx e^{-i\Delta t X_\mathcal{E}/2} e^{-i\delta t Z_\mathcal{S} Z_\mathcal{E}} e^{-i\Omega t Z_\mathcal{S}} e^{-iBtZ_\mathcal{E}} e^{-i\Delta t X_\mathcal{E}/2} \quad (6)$$

where we choose $\Omega = 100\pi$ Hz, $\Delta = 0.02\Omega$, $\delta = 0.1\Omega$, and the time t goes from zero to the maximum time of the evolution, τ. We checked numerically that the Trotter approximation reduces the fidelity less than 0.3% for $B \in [-0.2\Omega, 0.2\Omega]$. Furthermore, we decompose the unitary operations $e^{-iBtZ_\mathcal{E}}$ as $e^{-i\pi X_\mathcal{E}/4} e^{-iBtY_\mathcal{E}} e^{i\pi X_\mathcal{E}/4}$, and $e^{-i\Omega t Z_\mathcal{S}}$ as $e^{-i\pi X_\mathcal{S}/4} e^{-i\Omega t Y_\mathcal{S}} e^{i\pi X_\mathcal{S}/4}$ so that we can implement them with standard rf pulses. The coupling operation $e^{-i\delta t Z_\mathcal{S} Z_\mathcal{E}}$ is realized using the natural spin coupling with an evolution time $2\delta t/(\pi J)$. After the evolution U, we measure the magnetization in the XY plane, which is proportional to the decoherence factor $r(t)$. The whole gate sequence for each measurement is shown in Fig. 2(b). Notice that we measure the absolute value as well as the complex phase of $r(t)$, necessary for the GP. The total evolution time was always well below the natural decoherence time of the quantum simulator.

To eliminate systematic errors, we repeat the experiment but uncoupling the system and the environment ($\delta = 0$). From this we compute a baseline GP, which we subtract from the full (coupled) experiment. Thus, we obtain the *correction* to the GP due to the presence of the critical environment, which agrees well with theoretical expectations [see Fig. 1(c)].

Conclusions.—Using a NMR quantum simulator, we obtained the quantum geometric phase of an open system undergoing nonunitary evolution. The GP is computed in a tomographic manner; i.e., we measure the off-diagonal elements of the reduced density matrix of the system, from which we extract the decoherence factor that we use in the definition of the open system GP. Our experiments support the observation that when the environment is near a second order quantum phase transition, the correction to the GP becomes singular. For our experiments we introduced a simplified two-level model that captures the closing of the gap typical of quantum phase transitions. This, in turn, gave us a way to represent the well-known suppression of the decoherence factor observed from critical environments, and confirm qualitatively our numerical and analytical results. In future work, we will introduce a third (probe) spin to perform an independent and direct measurement of the GP using traditional interferometry-based techniques [6]. Furthermore, by adding stochastic fields and further spins, we can quantum simulate more realistic environments and couplings to the system. Despite the apparent simplicity of our experiment, we believe that the techniques we developed are quite general and applicable to more complex quantum simulations, and to related approaches such as bath engineering [29]—designing an environment so that it induces a system to relax and decohere to interesting quantum many-body pure states.

We acknowledge helpful discussions with A. Acín, J. I. Cirac, P. Hauke, M. Lewenstein, G. Morigi, A. Roncaglia, and A. M. Souza. F. M. C. acknowledges financial support from Spanish MEC project TOQATA, ERC Advanced Grant QUAGATUA, and Caixa Manresa. F. C. L is supported by UBA, CONICET and ANPCyT–Argentina. P. I. V acknowledges financial support from the UNESCO LOREAL Women in Science Programme.

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