Geometric phases and quantum phase transitions in open systems

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The relationship is established between quantum phase transitions and complex geometric phases for open quantum systems governed by a non-Hermitian effective Hamiltonian with accidental crossing of the eigenvalues. In particular, the geometric phase associated with the ground state of the one-dimensional dissipative Ising model in a transverse magnetic field is evaluated, and it is demonstrated that the related quantum phase transition is of the first order.

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A quantum phase transition (QPT) is characterized by qualitative changes of the ground state of a many-body system and occurs at zero temperature. The QPT, being a purely quantum phenomenon driven by quantum fluctuations, is associated with energy level crossing and implies a loss of analyticity in the energy spectrum at the critical points [1]. A first-order QPT is determined by a discontinuity in the first derivative of the ground state energy. A second-order QPT means that the first derivative is continuous, while the second derivative has either a finite discontinuity or a divergence at the critical point. Since the OPT is accomplished by changing some parameter in the Hamiltonian of the system, but not the temperature, its description in the standard framework of Landau-Ginzburg theory of phase transitions fails, and identification of an order parameter is still an open problem [2]. In this connection, an issue of a great interest is the recently established relationship between geometric phases and quantum phase transitions [3-6]. This relation is expected since the geometric phase associated with the energy level crossings has a peculiar behavior near the degeneracy point. It is supposed that the geometric phase, being a measure of the curvature of the Hilbert space, is able to capture drastic changes in the properties of the ground state in the presence of a QPT [4-7].

In this Rapid Communication, we analyze the relation between the geometric phase and the QPT in an open quantum system governed by a non-Hermitian Hamiltonian. We found that the QPT is closely connected with the geometric phase and the latter may be considered as a universal order parameter for description of the QPT. By studying the dissipative one-dimensional Ising model in a transverse magnetic field, we demonstrated that a QPT that is of second order in the absence of dissipation is of first order for an open system.

We consider an open quantum mechanical system which together with its environment forms a closed system. The description of such systems by an effective non-Hermitian Hamiltonian is well known, beginning with the classical papers by Weisskopf and Wigner on metastable states [8,9].¹

For the Hermitian Hamiltonian coalescence of eigenvalues results in different eigenvectors, and the related degeneracy referred to as a "conical intersection" is known also as a "diabolic point." However, in a quantum mechanical system governed by a non-Hermitian Hamiltonian merging not only of eigenvalues of the Hamiltonian but also the associated eigenvectors can occur. The point of coalescing is called an "exceptional point." At the latter the eigenvectors merge, forming a Jordan block (for a review and references, see, e.g., [13,14]).

In the context of the Berry phase the diabolic point is associated with a "fictitious magnetic monopole" as follows. Assume that for adiabatic driving of a quantum system two energy levels may cross. Then the energy surfaces form sheets of a double cone, and its apex is called a diabolic point [15]. Since for a generic Hermitian Hamiltonian the codimension of the diabolic point is 3, it can be characterized by three parameters $\mathbf{R} = (X, Y, Z)$. The eigenstates $|n, \mathbf{R}\rangle$ give rise to the Berry connection defined by $A_n(\mathbf{R})$ $=i\langle n, \mathbf{R}|\nabla_{\mathbf{R}}|n, \mathbf{R}\rangle$, and the curvature $\mathbf{B}_n = \nabla_{\mathbf{R}} \times \mathbf{A}_n$ associated with A_n is the field strength of the magnetic monopole located at the diabolic point [16,17]. The Berry phase γ_n $= \oint_{\mathcal{C}} \mathbf{A}_n \cdot d\mathbf{R}$ is interpreted as a holonomy associated with the parallel transport along a circuit C [18]. A similar treatment of the non-Hermitian Hamiltonian yields the fictitious complex monopole located at the exceptional point [19].

The Berry phase was extended to non-Hermitian systems for the first time by Garrison and Wright as follows [20]. Let an adjoint pair $\{|\Psi(t)\rangle, \langle \tilde{\Psi}(t)|\}$ be a solution of the timedependent Schrödinger equation and its adjoint equation $(\hbar = 1)$,

$$i\frac{\partial}{\partial t}|\Psi(t)\rangle = H(\lambda(t))|\Psi(t)\rangle, \qquad (1)$$

$$-i\frac{\partial}{\partial t}\langle \tilde{\Psi}(t) | = \langle \tilde{\Psi}(t) | H(\lambda(t)), \qquad (2)$$

where $\lambda \in \mathfrak{M}$, the parameter space being \mathfrak{M} . Let $|\psi_n(\lambda)\rangle$ and $\langle \tilde{\psi}_n(\lambda)|$ be right and left eigenvectors of the Hamiltonian: $H(\lambda)|\psi_n(\lambda)\rangle = E_n(\lambda)|\psi_n(\lambda)\rangle, \qquad \langle \tilde{\psi}_n(\lambda)|H(\lambda) = E_n(\lambda)\langle \tilde{\psi}_n(\lambda)|.$ Now suppose that there exists a time period *T* for which

¹For discussion and recent development, see, e.g., [10–12]

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 $\lambda(T) = \lambda(0)$; then a complex geometric phase γ_n is given by the integral [13,20]

$$\gamma_n = \oint_{\mathcal{C}} A^{(n)} = i \oint_{\mathcal{C}} \frac{\langle \tilde{\psi}_n(\lambda) | \nabla_a | \psi_n(\lambda) \rangle d\lambda^a}{\langle \tilde{\psi}_n(\lambda) | \psi_n(\lambda) \rangle}, \qquad (3)$$

where the integration is performed over the contour C in the parameter space, and $a=1,\ldots,\dim \mathfrak{M}, A^{(n)}$ being the connection one-form. Further, we assume that the instantaneous eigenvectors form a biorthonormal basis $\langle \tilde{\psi}_m | \psi_n \rangle = \delta_{mn}^2$.

To analyze the relation between the QPT and the geometric phase we begin with consideration of a two-level system described by a generic non-Hermitian Hamiltonian $H=\lambda_0\mathbf{1}+\mathbf{R}(t)\cdot\boldsymbol{\sigma}$, where σ_i are the Pauli matrices, $\mathbf{R}(t) = (X, Y, Z)$ is slowly varying, and $\lambda_0, X, Y, Z \in \mathbb{C}$. Using the spinless fermionic creation and annihilation operators, which obey anticommutation relations $\{C, C\}=0, \{C^{\dagger}, C^{\dagger}\}=0$, and $\{C, C^{\dagger}\}=1$, one can rewrite the Hamiltonian as $H=(\lambda_0-R)\mathbf{1}+2RC^{\dagger}C$, where $R=(X^2+Y^2+Z^2)^{1/2}$. The ground state $|u_-\rangle$ is defined as the vacuum state determined by $C|u_-\rangle=0$.

The instantaneous eigenvectors are found to be

$$|u_{-}\rangle = \begin{pmatrix} -e^{-i\varphi}\sin\frac{\theta}{2}\\ \cos\frac{\theta}{2} \end{pmatrix}, \quad \langle \widetilde{u}_{-}| = \left(-e^{i\varphi}\sin\frac{\theta}{2}, \cos\frac{\theta}{2}\right), \\ |u_{+}\rangle = \begin{pmatrix} e^{-i\varphi}\cos\frac{\theta}{2}\\ \sin\frac{\theta}{2} \end{pmatrix}, \quad \langle \widetilde{u}_{+}| = \left(e^{i\varphi}\cos\frac{\theta}{2}, \sin\frac{\theta}{2}\right), \quad (4)$$

where θ, φ are the complex angles of the complex spherical coordinates, and the complex energy spectrum is given by $E_{\pm} = \lambda_0 \pm R$. Coupling of eigenvalues occurs when R = 0, and there are two cases. The first one is the diabolic point located at the origin of coordinates. The second case yields the exceptional point (X_0, Y_0, Z_0) . At the latter the eigenvectors coincide up to a phase factor, $|u_+\rangle = e^{i\kappa}|u_-\rangle$ and $\langle \tilde{u}_+| = e^{-i\kappa} \langle \tilde{u}_-|$ [14,26].

The geometric phase of the ground state is given by $\gamma = (1/2)\oint_{C}q(1-\cos\theta)d\varphi$, where integration is performed over the contour C on the complex sphere S_c^2 . Let us assume that the contour C of integration is chosen as $\theta = \text{const.}$ Then the geometric phase of the ground state is given by $\gamma = \pi(1 - Z/R)$ and can be written as $\gamma = \pi(1 + \partial E_{-}/\partial Z)$, where E_{-} is the ground state energy. As can be observed, lost of analyticity occurs at the degeneracy point defined by R=0 and on the Dirac string attached to the complex fictitious monopole and crossing the complex sphere S_c^2 at the south pole.

Further simplification can be made by writing $\mathbf{R} = \boldsymbol{\rho} - i\boldsymbol{\varepsilon}$, where we set $\boldsymbol{\rho} = (x, y, z)$. Without loss of generality we may choose the coordinate system such that $\boldsymbol{\varepsilon} = (0, 0, \boldsymbol{\varepsilon})$. Then computation of the geometric phase yields

$$\gamma = \pi \left(1 - \frac{z - i\varepsilon}{\sqrt{r^2 + (z - i\varepsilon)^2}} \right)$$
(5)

where $r = \sqrt{x^2 + y^2}$.





FIG. 1. (Color online) Left panel (ε =0): Clear step function behavior of the geometric phase at the diabolic point *r*=*z*=0. Right panel: Re γ near the exceptional point (ε =0.5).

In what follows we consider the behavior of the geometric phase near the critical points, starting with the Hermitian Hamiltonian. Inserting $\varepsilon = 0$ in Eq. (5), we obtain $\gamma = \pi [1 - z/(r^2 + z^2)^{1/2}]$. This implies that the geometric phase behaves as a step function near the diabolic point. Considering the general case, we obtain

Re
$$\gamma = \begin{cases} \pi & \text{if } r > \varepsilon \quad (z=0), \\ \pi \left(1 \mp \frac{\varepsilon}{\sqrt{\varepsilon^2 - r^2}} \right) & \text{if } r < \varepsilon, \quad z \to \pm 0, \end{cases}$$
 (6)

where the upper (lower) sign corresponds to $z \rightarrow \pm 0$, As can be observed in Fig. 1, if $\varepsilon = 0$ the geometric phase behaves as a steplike function near the diabolic point. In addition, Re $\gamma \rightarrow \pm \infty$ at the exceptional point $r = \varepsilon$, and it behaves as a steplike function as $r \rightarrow 0$. Similar consideration of the imaginary part yields

Im
$$\gamma = \begin{cases} 0 & \text{if } r < \varepsilon \quad (z=0), \\ \frac{\pi \varepsilon}{\sqrt{r^2 - \varepsilon^2}}, & \text{if } r > \varepsilon \quad (z=0); \end{cases}$$
 (7)

clearly it diverges at the exceptional point, Im $\gamma \rightarrow \infty$.

We return to the general non-Hermitian *N*-dimensional problem and consider the non-Hermitian diagonalizable Hamiltonian $H(\lambda) = \sum_{i=1} E_i |\psi_i\rangle \langle \tilde{\psi}_i|$. The ground state is given by $|\psi_g(\lambda)\rangle = \bigotimes_{i=1}^N |\psi_i(\lambda)\rangle$, and computation of the geometric phase yields

$$\gamma = i \oint_{\mathcal{C}} \langle \tilde{\psi}_g(\lambda) | \frac{\partial}{\partial \lambda^a} | \psi_g(\lambda) \rangle d\lambda^a = \sum_{i=1}^N \gamma_i, \tag{8}$$

where γ_i is the geometric phase associated with the eigenvector $|\psi_i(\lambda)\rangle$. Then, applying the Stokes theorem and the Schrödinger equation $H|\chi_m\rangle = E_m|\chi_m\rangle$ together with its adjoint equation $\langle \tilde{\chi}_m | H = E_m \langle \tilde{\chi}_m |$, we obtain

$$\gamma = -i\sum_{i=1}^{N}\sum_{m\neq i}^{N}\int \int_{\Sigma} \frac{\langle \tilde{\chi}_{i} | \nabla_{a} H | \chi_{m} \rangle \langle \tilde{\chi}_{m} | \nabla_{b} H | \chi_{i} \rangle d\lambda^{a} \wedge d\lambda^{b}}{(E_{m} - E_{i})^{2}}.$$

It follows from this that the curvature $F^{(i)} = dA^{(i)}$ diverges at the degeneracy points, where the energy levels, say E_n and E_{n+1} , are crossing, and reaches its maximum values at the avoided level crossing points. Thus, the critical behavior of the system is reflected in the geometry of the Hilbert space through the geometric phase of the ground state.

²This can alter the definition (3) up to the topological contribution πn , $n \in \mathbb{Z}$ [21]. The geometric phases for systems governed by the non-Hermitian Hamiltonian have been studied by various authors; for details and references see, e.g., [13,17,20,22–25].

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Since in the neighborhood of either a diabolic or an exceptional point only terms related to the invariant subspace formed by the two-dimensional Jordan block make substantial contributions, the *N*-dimensional problem becomes effectively two dimensional (for details see [27,28]). This implies that there exists a map $\varphi: \mathfrak{M} \mapsto S_c^2$ such that, in the vicinity of the degeneracy points, the quantum system can be described by the effective two-dimensional Hamiltonian $H_{\text{eff}} = \lambda_0 \mathbf{I} + \mathbf{R} \cdot \boldsymbol{\sigma}$, where $R = (E_{n+1} - E_n)/2$. Then we have

$$\gamma \approx \frac{1}{2} \int_{\Sigma'} \frac{\mathbf{R} \cdot d\mathbf{S}}{R^3} + \sum_{i \neq n, n+1} \gamma_i(\mathbf{R})$$
(9)

where $\Sigma' = \varphi(\Sigma) \subset S_c^2$. The behavior of the geometric phase described by the first term is independent of the peculiarities of a quantum mechanical system. Therefore, one can consider the complex Bloch sphere as a universal parameter space for description of the QPT in the vicinity of the critical point.

Following [4], we define the overall geometric phase of the ground state as $\gamma_g = (1/N) \sum_{i=1}^{N} \gamma_i$. In the thermodynamic limit $\gamma_g = \int \gamma(x) d\mu(x)$, where $d\mu(x)$ is a suitable measure. As has been shown by Zhu [5] on the example of an XY spin chain, the overall geometric phase associated with the ground state exhibits universality, or scaling behavior in the vicinity of the critical point. In addition, the geometric phase allows one to detect the critical point in the parameter space of the Hamiltonian [3–7]. These works indicate that the overall geometric phase γ_g can be considered as a universal order parameter for description of the QPT.

As an illustrative example we consider the onedimensional Ising model in a transverse magnetic field with dissipation governed by the non-Hermitian Hamiltonian

$$H = -J\sum_{n=1}^{N} \left(h\sigma_n^x + \sigma_n^z \sigma_{n+1}^z - i\frac{\delta}{2}\sigma_n^+ \sigma_n^- \right)$$
(10)

with the periodic boundary condition $\sigma_{N+1} = \sigma_1$. The external magnetic field is described by the parameter *h* and spontaneous decay is described by $\Gamma = \sqrt{\delta}\sigma_n^-$ with the source of decoherence being $\sigma_n^- = (\sigma_n^z - i\sigma_n^y)/2$.

To study the geometric phase in this system we consider the more general Hamiltonian $H(h, \delta, \varphi) = g_{\varphi} H g_{\varphi}^{\dagger}$, where g_{φ} $= \prod_{n=1}^{N} e^{i(\varphi/4)\sigma_n^x}$ and $0 \le \varphi < 2\pi$. After applying the standard Jordan-Wigner transformation and following the procedure outlined in [4,29], we find that the system can be described in terms of noninteracting quasiparticles with the reduced Hamiltonian

N

$$H^{+} = -J\sum_{n=1}^{\infty} (c_{n}^{\dagger}c_{n+1} + e^{i\varphi}c_{n+1}c_{n} + g + i\delta - 2gc_{n}^{\dagger}c_{n} + c_{n+1}^{\dagger}c_{n} + e^{-i\varphi}c_{n}^{\dagger}c_{n+1}^{\dagger}),$$
(11)

where $g=h-i\delta$, and c_n are fermionic operators satisfying the anticommutation relations $\{c_m, c_n^{\dagger}\} = \delta_{mn}$ and $\{c_m, c_n\} = \{c_m^{\dagger}, c_n^{\dagger}\} = 0$. Applying the Fourier transformations $c_n = e^{-i\pi/4} \sum_k c_k e^{ikna} / N^{1/2}$ with the antiperiodic boundary condition $c_{N+1} = -c_1$, we obtain $H^+ = J \sum_k \{2[g - \cos(ka)]c_k^{\dagger}c_k + \sin(ka)(e^{-i\varphi}c_k^{\dagger}c_{-k}^{-+} + e^{i\varphi}c_{-k}c_k) - g - i(\delta/2)\}$, where $k = \pm \pi/Na, \ldots, \pm (N-1)\pi/Na$ is a half-integer quasimomentum, the lattice spacing being a.

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The Hamiltonian H^+ can be diagonalized by using the Bogoliubov transformation $c_k = \tilde{u}_k b_k + v_{-k} b_{-k}^{\dagger}$, $c_k^{\dagger} = u_k b_k^{\dagger}$ $+ \tilde{v}_{-k} b_{-k}$. The Bogoliubov modes (u_k, v_k) and $(\tilde{u}_k, \tilde{v}_k)$ satisfy the Schrödinger equation and its adjoint equation, respectively, with the Hamiltonian $H(k) = -iJ\delta \mathbf{l} + \mathbf{R}(k) \cdot \boldsymbol{\sigma}$, and $\mathbf{R}(k) = 2J(\sin(ka)\cos\varphi, \sin(ka)\sin\varphi, g - \cos(ka))$. There are two eigenstates for each k with the complex energies $\varepsilon_{\pm}(k)$ $= \varepsilon_0 \pm \varepsilon(k)$, where we set $\varepsilon_0 = -iJ\delta$ and $\varepsilon(k) = 2J[g^2 - 2g\cos(ka) + 1]^{1/2}$. The positive energy eigenstate $|u_+(k)\rangle = (\frac{u_k}{v_k}), \langle \tilde{u}_+(k)| = (\tilde{u}_k, \tilde{v}_k)$, normalized so that $\tilde{u}_k u_k + \tilde{v}_k v_k = 1$, defines the quasiparticle operators $b_k = \tilde{u}_k c_k + \tilde{v}_k c_{-k}^{\dagger}$ and $b_k^{\dagger} = u_k c_k^{\dagger} + v_k c_{-k}$ as follows: $b_k = e^{i\varphi} \cos(\theta_k/2)c_k + \sin(\theta_k/2)c_{-k}^{\dagger}$, $b_k^{\dagger} = e^{-i\varphi} \cos(\theta_k/2)c_k^{\dagger} + \sin(\theta_k/2)c_{-k}$, where

$$\cos \theta_k = \frac{g - \cos(ka)}{\sqrt{g^2 - 2g\cos(ka) + 1}}.$$
 (12)

Using these results, we obtain the diagonalized Hamiltonian as a sum of quasiparticles with half-integer quasimomenta, $H^+ = \sum_k [\varepsilon_0 + \varepsilon(k)(b_k^{\dagger}b_k - \frac{1}{2})]$. Its ground state is given as a product of qubitlike states

$$\begin{split} |\psi_g\rangle &= \bigotimes_k \left(\cos\frac{\vartheta_k}{2}|0\rangle_k|0\rangle_{-k} - e^{-i\varphi}\sin\frac{\vartheta_k}{2}|1\rangle_k|1\rangle_{-k}\right),\\ \langle \widetilde{\psi}_g| &= \bigotimes_k \left(\cos\frac{\vartheta_k}{2}\langle 0|_k\langle 0|_{-k} - e^{i\varphi}\sin\frac{\vartheta_k}{2}\langle 1|_k\langle 1|_{-k}\right), \end{split}$$

where $|0\rangle_k$ is the vacuum state of the mode b_k , and $|1\rangle_k$ is the first excited state, $|1\rangle_k = b_k^{\dagger}|0\rangle_k$. Each single state lies in the two-dimensional Hilbert space spanned by $|0\rangle_k|0\rangle_{-k}$ and $|1\rangle_k|1\rangle_{-k}$. For a given value of k, the state in each of these two-dimensional Hilbert spaces can be presented as a point on the complex two-dimensional sphere S_c^2 with coordinates (θ_k, φ) .

For $|g| \ge 1$ the ground state is a paramagnet with all spins oriented along the *x* axis, and from Eq. (12) we obtain $\cos \theta_k \rightarrow 1$ while $|g| \rightarrow \infty$. Thus, the north pole of the complex Bloch sphere corresponds to a paramagnetic ground state. On the other hand, when $|g| \ll 1$, there are two degenerate ferromagnetic ground states with all spins polarized up or down along the *z* axis. The real part of the complex energy reaches its minimum at the point defined by $\cos \theta_k = -1$, and, hence, the south pole of the complex sphere is related to a pure ferromagnetic ground state with broken symmetry when all spins have orientation up or down. However, in the thermodynamic limit, the system passing through the critical point ends in a superposition of the up and down states with finite domains of spins separated by kinks [21].

The geometric phase of the ground state is found to be

$$\gamma = i \int_{0}^{2\pi} \langle \tilde{\psi}_{g} | \frac{\partial}{\partial \varphi} | \psi_{g} \rangle d\varphi = \sum_{k>0} \pi (1 - \cos \theta_{k}).$$
(13)

As can be shown, in the thermodynamic limit the energy gap $\Delta \varepsilon(h,k)$ vanishes and the geometric phase diverges at the exceptional point $h_c = (1 - \delta^2)^{1/2}$, $k_c = \arcsin \delta/a$. However, the overall geometric phase $\gamma_g = (\pi/N) \Sigma_{k>0} (1 - \cos \theta_k)$, written in the thermodynamic limit as

$$\gamma_g = \int_0^{\pi} \left(1 - \frac{g - \cos x}{\sqrt{g^2 - 2g \cos x + 1}} \right) dx,$$
 (14)

has finite jump discontinuity at the exceptional point (Fig. 2). The result of integration can be written in terms of the com-



FIG. 2. (Color online) Real part of the overall geometric phase γ_g (left) and imaginary part of the overall geometric phase γ_g (right) versus δ and h.

plete elliptic integrals of the first and second kinds

$$\gamma_g = \pi + \frac{1-g}{g} K \left(\frac{2\sqrt{g}}{1+g} \right) - \frac{1+g}{g} E \left(\frac{2\sqrt{g}}{1+g} \right).$$
(15)

We note that γ_g can be written as $\gamma_g = \pi(1 + \partial E_g/\partial h)$, where $E_g = \varepsilon_0 - \int_0^{\pi} \varepsilon(x) dx = -iJ\delta - 2(g+1)E[2\sqrt{g}/(g+1)]$ is the ground state energy per spin. Besides, one can show that $\gamma_g = \pi(1 + \langle \sigma_n^z \rangle)$. As known, the total magnetization per spin $\langle \sigma_n^z \rangle$ can be served as the order parameter for Ising model in a transverse magnetic field [1,3]. This supports the statement [3–6] that the geometric phase can be treated as the order parameter for the QPT.

In Figs. 2 and 3 the real and imaginary parts of the overall geometric phase and its derivative as functions of external magnetic field *h* and decay parameter δ are depicted. As can be observed γ_g is a continuous function of *h*, if δ =0, and it behaves as a steplike function, if δ >0. In the limit cases $|g| \leq 1$ and $|g| \geq 1$ we have Re $\gamma_g \rightarrow \pi$ and Re $\gamma_g \rightarrow 0$, respectively.

According to the Ehrenfest classification, the QPT occurring at the exceptional point, which actually is the circle $h_c^2 + \delta_c^2 = 1$, is of the first order. In the absence of dissipation (δ =0), we have the second-order QPT. Indeed, as can be observed in Figs. 2 and 3, the first derivative of the ground

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FIG. 3. (Color online) Real part of derivative of the overall geometric phase $\partial \gamma_g / \partial h$ (left) and its imaginary part (right) versus δ and h.

energy (or, equivalently, the geometric phase) is a continuous function of *h* and its second derivative diverges at the critical point $h_c = 1(\delta = 0)$.

In summary, we established a connection between the geometric phase and the QPT in a generic dissipative system and found the relation between the geometric phase and ground state energy. We showed that the critical point where the QPT occurs can be identified as the degeneracy point in the parameter space. Studying the critical behavior of a dissipative one-dimensional Ising chain in a transverse magnetic field, we found that the related QPT is of the first order. In the absence of dissipation it becomes a second-order QPT. Our results support the claim that the relation between QPTs and geometric phases is a very general result, and the geometric phase may be considered as a good candidate for a universal order parameter for quantum phase transitions [4,5].

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