Observation of the Ground-State Geometric Phase in a Heisenberg *XY* Model

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Geometric phases play a central role in a variety of quantum phenomena, especially in condensed matter physics. Recently, it was shown that this fundamental concept exhibits a connection to quantum phase transitions where the system undergoes a qualitative change in the ground state when a control parameter in its Hamiltonian is varied. Here we report the first experimental study using the geometric phase as a topological test of quantum transitions of the ground state in a Heisenberg *XY* spin model. Using NMR interferometry, we measure the geometric phase for different adiabatic circuits that do not pass through points of degeneracy.

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When a quantum system is subjected to cyclic adiabatic evolution, it returns to its original state but may acquire a geometric phase factor in addition to the dynamical one. Berry made this surprising discovery in 1984 [1], so this is also known as Berry's phase. Later, this phase was generalized in various directions to include a more general case of noncyclic and nonadiabatic evolution [2], and even the case of mixed states. Geometric phases (GPs) have been observed in a wide variety of physical systems, e.g., in spin-polarized neutrons [3], NMR [4], and superconducting systems [5]. Moreover, GPs have found applications in many areas, such as molecular dynamics, many-body systems, and quantum computation [6,7].

Very recently, the GP of many-body systems has been shown to be closely connected to quantum phase transitions (QPTs), an important phenomenon in condensed matter physics [8,9]. QPTs occur at zero temperature and describe abrupt changes in the properties of the ground state resulting from the presence of level crossings or avoided crossings [10]. Recently, different methods related to quantum information have been developed for characterizing QPTs, including the fidelity [11], quantum entanglement [12,13], and some other geometric properties [14]. The GP, which is a measure of the curvature of Hilbert space, can reflect the energy-level structure to fingerprint certain features of QPTs. Carollo and Pachos [8] demonstrated that the GP difference between the ground state and the first excited state encounters a singularity when the system undergoes a QPT in the *XY* spin chain. Zhu [9] revealed that a GP associated with its ground state exhibits universality, or scaling behavior, around the critical point. In addition to the study in the thermodynamical limit, it was also shown that a GP could be used to detect level crossings for a two-qubit system with an *XY* interaction [15]. As a complement to these theoretical investigations, it appears highly desirable to have experimental evidence for these effects.

In this Letter, we report the first experiment that shows this important connection between a GP and the energy-level structure (i.e., level crossing points) in a Heisenberg *XY* spin model. In our experiment, the system Hamiltonian changes adiabatically along a closed trajectory in parameter space, while the system, which is in the ground state of the Hamiltonian, accumulates a GP. Depending on the region in parameter space, the resulting GP is zero or has a finite value. These regions in parameter space are separated by a line where the ground state of the system becomes degenerate [15]. Using adiabatic state preparation and NMR interferometry, we observe the transitions of the GP on both sides of the level crossing point. This experiment might be viewed as the first meaningful step to use a GP as a fingerprint for observing QPTs.

Consider a one-dimensional spin-1/2 *XY* model in a uniform external magnetic field along the z axis:

$$\mathcal{H}(\lambda, \gamma) = -\sum_j \left(\frac{1+\gamma}{2} \sigma_x^j \sigma_x^{j+1} + \frac{1-\gamma}{2} \sigma_y^j \sigma_y^{j+1} \right) - \frac{\lambda}{2} \sum_j \sigma_z^j,$$

where $\sigma_\nu^k (\nu = x, y, z)$ denote the Pauli matrices for qubit k, λ is the strength of the external magnetic field, and γ measures the anisotropy of the coupling strength in the *XY* plane. This model is exactly solvable and can be diagonalized by the Jordan-Wigner transformation, Fourier transformation, and then Bogoliubov transformation [16]. However, it still contains a rich phase structure [10]. Barouch and McCoy [17] investigated the statistical mechanics of this model in the thermodynamical limit and showed that a circle ($\lambda^2 + \gamma^2 = 1$) separates the oscillatory phase (inside) from the paramagnetic or ferromagnetic phase (outside). At the level crossing or avoided crossing between the ground state and the first excited state, the ground state changes discontinuously. As a result, the GP

associated with the ground state also changes discontinuously. Theoretical work has demonstrated the close relation between GPs and the energy-level structures, thereby revealing the ground-state properties [8,9], even in the two-qubit case [15].

We now consider the GP that results in this system if the Hamiltonian rotates around the z axis, $\tilde{\mathcal{H}}(\lambda, \gamma, \phi) = U_z^\dagger(\phi)\mathcal{H}(\lambda, \gamma)U_z(\phi)$ with $U_z(\phi) = \prod_k e^{-i(\phi/2)\sigma_z^k}$ [8]. $\tilde{\mathcal{H}}$ has the same spectrum as $\mathcal{H}$, independent of ϕ. Here we study a minimal model of two qubits coupled by an XY-type interaction [15]. The eigenvalues of $\tilde{\mathcal{H}}$ are ± 1 and $\pm r$, where $r = \sqrt{\lambda^2 + \gamma^2}$. The ground state is

$$|\Psi_g(\phi)\rangle = \begin{cases} \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle) & r < 1 \\ \cos\frac{\theta}{2}|00\rangle + \sin\frac{\theta}{2}e^{-i2\phi}|11\rangle & r > 1, \end{cases} \quad (1)$$

where $\tan\theta = \gamma/\lambda$. For $r < 1$, the ground state is thus invariant; for $r = 1$, it is doubly degenerate; and for $r > 1$, it is spanned by the two states $|00\rangle$ and $|11\rangle$, with coefficients that depend on the angle θ.

If we let the Hamiltonian travel along a cyclic path in the parameter space (λ, γ, ϕ), we can consider the subspace spanned by $|00\rangle$ and $|11\rangle$, which contains the ground state, as a pseudospin $1/2$, where the spin evolves in an effective magnetic field $\mathbf{B} = r(\sin\theta\cos 2\phi, \sin\theta\sin 2\phi, \cos\theta)$. Using the standard formula $\beta_g = i\oint_0^\pi \langle\Psi_g|\partial_\phi|\Psi_g\rangle$ [1], the ground state accumulates a GP,

$$\beta_g(\phi: 0 \to \pi) = \begin{cases} 0 & r < 1 \\ \pi(1 - \cos\theta) & r > 1. \end{cases} \quad (2)$$

As shown in Fig. 1(a), it is useful to represent the trajectory in a parameter space spanned by $\gamma\cos(2\phi)$, $\gamma\sin(2\phi)$, and λ. Here, the sphere with radius $r = 1$ marks the points where the Hamiltonian is degenerate. Inside this sphere ($r < 1$), the GP vanishes, while it has a finite value that depends on the opening angle θ of the cone subtended by the circuit when $r > 1$. A special case is the XX spin model (i.e., $\gamma = 0$). Here, the GP always vanishes, because the operation U_z does not change the Hamiltonian of the system. While we are considering here only a minimal two-spin model, the ground state and the ground-state energy of the XY model in the thermodynamic limit are similar [17].

When the system undergoes cyclic adiabatic evolution along $\tilde{\mathcal{H}}$, there will also be an additional dynamic phase generated, relative to the instantaneous energy of the system, besides the GP. Hence, in order to acquire the pure geometric part, we have to eliminate the dynamical contribution. To eliminate the dynamical contribution to the phase shift, we combine two experiments with the closed paths C and $\bar{C}$ [2], which generate the same geometrical phases, but opposite dynamical phases. The two trajectories have the same geometrical shape (cones), but their Hamiltonians $\tilde{\mathcal{H}}$ and $-\tilde{\mathcal{H}}$, and thus their dynamical phases, add to zero. During the first period, the Hamiltonian $\tilde{\mathcal{H}}(\lambda, \gamma, \phi)$ follows the closed curve C in the parameter space $\mathbf{r} = (r, \theta, \phi)$, with ϕ changing from 0 to π, as schematically shown by the red circles (labeled by C in the upper part) for $\lambda > 0$ in Fig. 1(a). During the second period, the Hamiltonian $-\tilde{\mathcal{H}} = R_{kz}^\dagger(\pi)\tilde{\mathcal{H}}(-\lambda, \gamma, \phi)R_{kz}(\pi)$ follows the curve $\bar{C}$, shown in the lower part of Fig. 1(a). Here $R_{kz}(\pi) = e^{-i(\pi/2)\sigma_z^k}$ ($k = 1$ or 2) rotates one of the two spins around the z axis. For the circuit C, the resulting phase is $\beta_C = \pi(1 - \cos\theta) - rT$, where T is the cycle time and we have assumed $r > 1$. For $\bar{C}$, $\beta_{\bar{C}} = \pi(1 - \cos\theta) + rT$ because the sign of the eigenvalue of the state $|\Psi_g\rangle$ changes for $-\tilde{\mathcal{H}}$. The sum of the two phases, $\beta_C + \beta_{\bar{C}} = 2\pi(1 - \cos\theta)$, is thus purely geometrical. If $r < 1$, the dynamical component changes to $-T$ for C and T for $\bar{C}$, while the GP vanishes.

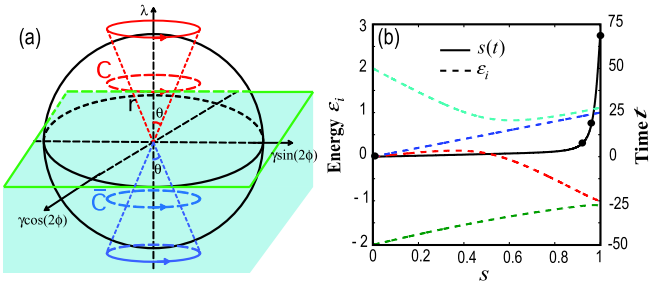

FIG. 1 (color online). (a) Parameter-space representation of the cyclic adiabatic evolutions that generate the GP. Two closed paths C and $\bar{C}$, related by inversion symmetry, were combined for observing a purely GP. The cycles are horizontal; i.e., λ is constant and γ is constant. The observed GP depends on the angle θ if the circles are outside the sphere $r = 1$ (shown in black) and vanish if the curves are inside the sphere. (b) Energy-level diagram of the time-dependent $\mathcal{H}_{ad}(s)$ for ASP (denoted by the dashed lines), and the optimal function of the adiabatic parameter $s(t)$ (denoted by the solid line) calculated for a constant adiabaticity factor, when $\gamma = 0.5$, $\lambda = 0.9920$. The black dots represent the experimental values for the discretized scan.

To measure the GP, we use NMR interferometry [4,18]. This requires an ancilla qubit that is coupled to the system undergoing the circuit. Figure 2 shows the experiment schematically, including the adiabatic state preparation (ASP) of the two-qubit system into the ground state of the Heisenberg XY model, and the generation of a superposition of the ancilla qubit by a Hadamard gate. The subsequent adiabatic circuit U_i, which is conditional on the state of the ancilla qubit, implements the interferometer $\mathcal{U}_i = |0\rangle\langle 0|_a \otimes \mathbf{1} + |1\rangle\langle 1|_a \otimes U_i$, where $\mathbf{1}$ represents a 4×4 unit operator and the unitary operator U_i is the cyclic adiabatic evolution on the system qubits along the chosen path C or $\bar{C}$. The phase acquired during this path then appears directly as a relative phase in the superposition of the two ancilla states and can be measured in the NMR spectrum of the ancilla spin [24].

The experiment was carried out on a Bruker Avance III 400 MHz (9.4 T) spectrometer at room temperature. The three qubits 0, 1, and 2 in the quantum circuit (Fig. 2) were represented by the ^{1}H, ^{13}C, and ^{19}F nuclear spins in

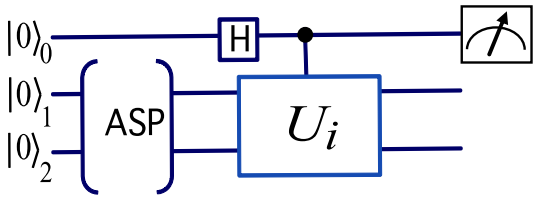

FIG. 2 (color online). Quantum circuit for measuring the ground-state GP. H is the Hadamard gate, and following the ASP, the operation U_i performs a cyclic adiabatic evolution of the system qubits (1 and 2), conditionally, when the ancilla path qubit 0 is in the state $|1\rangle$.

diethyl-fluoromalonate. The relaxation time for all three spins is $T_2 \approx 1$ s. The natural Hamiltonian of this system is $\mathcal{H}_{\mathrm{NMR}} = -\sum_{i=0}^{2} \frac{\omega_i}{2}\sigma_z^i + \sum_{i<j}\frac{\pi J_{ij}}{2}\sigma_z^i\sigma_z^j$, where ω_i is the Larmor frequency for spin i and J_{ij} are the coupling constants $J_{01} = 160.7$ Hz, $J_{12} = -194.4$ Hz, and $J_{02} = 47.6$ Hz. As the sample is not labeled, the relative phase information on ^{1}H at the end of the quantum circuit was obtained through the ^{13}C spectrum by a SWAP operation between ^{13}C and ^{1}H [13].

In the experiment, we first initialized the system into the pseudopure state $\rho_{000} = \frac{1-\epsilon}{8}\mathbf{1} + \epsilon|000\rangle\langle 000|$ by spatial averaging [13], with the polarization $\epsilon \approx 10^{-5}$. Then we prepared the ground state of the Heisenberg XY Hamiltonian by an adiabatic passage: A rf pulse rotated the spins from the z to the $-x$ axis, i.e., to the ground state of $\mathcal{H}_0 = \sum_i \sigma_x^i$, and then this Hamiltonian was slowly changed into the target XY Hamiltonian $\mathcal{H}(\lambda, \gamma)$, always fulfilling the adiabatic condition $\kappa \ll 1$ [19]. This assures that the resulting final state is close to the desired ground state of the XY model. We optimized the time dependence of the transfer by choosing $\mathcal{H}_{ad}(t) = [1 - s(t)]\mathcal{H}_0 + s(t)\mathcal{H}$ with $0 \le s(t) \le 1$. The solid line in Fig. 1(b) shows the corresponding time dependence for a constant κ. The time dependence of $s(t)$ was chosen such that the adiabaticity parameter $\kappa < 0.25$ at all times.

In the experiment, the adiabatic transfer was performed in discrete steps. The parameter $s(t)$ therefore assumes discrete values s_m with $m = 0, \ldots, M_P$, and for each period of duration δ, the corresponding Hamiltonian $\mathcal{H}_{ad}[s_m]$ was generated by a multiple pulse sequence: $U_P(\delta) = e^{-i\mathcal{H}_{ad}[s_m]\delta} = e^{-i[1-s_m]\mathcal{H}_0(\delta/2)}e^{-is_m\mathcal{H}(\lambda,\gamma)\delta}e^{-i[1-s_m]\mathcal{H}_0(\delta/2)} + O(\delta^3)$, via the use of Trotter's formula. δ and M_P were chosen by simultaneously considering this stepwise approximation and the adiabaticity criterion. The experimental values s_m for the discretized scan are represented by black dots in Fig. 1(b). The theoretical fidelity of this stepwise transfer process was >0.99, and the experimental fidelity was >0.98.

After the preparation of the ground state, we applied the cyclic adiabatic variation C or $\bar{C}$. The corresponding control operation $\mathcal{U}_C$ or $\mathcal{U}_{\bar{C}}$ was generated in the form of a discretized adiabatic scan, as described for the ASP part. Again, the parameters of the scan were optimized to keep the fidelity >0.99. At the end of the scan, the accumulated phase was measured.

Figure 3(a) shows two representative examples of the resulting data: The spectra on the left-hand side correspond to the states before the adiabatic circuit, after traversing the circuit C, and after traversing $\bar{C}$ for the Hamiltonian parameters $(\lambda, \gamma) = (0, 0.5)$. Clearly, in this situation, we are within the sphere $r = 1$, so the ground state of the system is $\frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$. This is verified by the experimental data, where only the two resonance lines that correspond to the states $|01\rangle$ and $|10\rangle$ of the system are visible. In the initial state, the two lines appear in absorption; this corresponds to the reference phase $\varphi = 0$. During the circuit C or $\bar{C}$, which is traversed over a time $T = 3$, the system should acquire a phase T. In the experimental data, we find that the lines are inverted; a numerical analysis of the lines yields phases of $\beta_t(\bar{C}) \approx 170.6°$ and $\beta_t(\bar{C}) \approx -173.0°$. Thus the resulting GP $\beta_g = [\beta_t(C) + \beta_t(\bar{C})]/2 \approx -1.2°$, which is close to the theoretically expected value of zero. The right-hand part of Fig. 3(a) shows the corresponding results for an adiabatic circuit outside of the sphere $r = 1$, where we expect to observe a nonvanishing GP. In this case, we observe clearly different phases for the two circuits, whose duration is now $T = 10.7$. The measured phases are $\beta_t(C) \approx -62.6°$ and $\beta_t(\bar{C}) \approx 114.2°$, corresponding to a GP of 25.8°.

Figure 3(b) shows the GP measured for different parameters (λ, γ). The symbols show experimental data points, while the curves that connect the points show the theoretically expected GP as a function of the magnetic

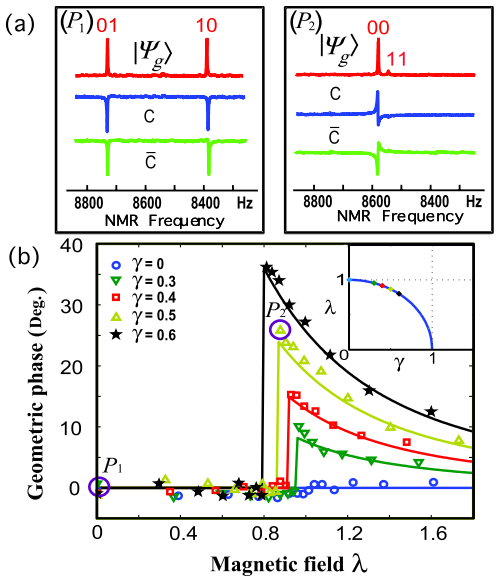

FIG. 3 (color online). (a) Experimental NMR spectra for two specific parameter sets, P_1 for $\mathcal{H}(0, 0.5)$ and P_2 for $\mathcal{H}(0.878, 0.5)$. From top to bottom, the spectrum corresponds to the initial ground state $|\Psi_g(\lambda, \gamma)\rangle$, $U_C|\Psi_g(\lambda, \gamma)\rangle$ for the adiabatic path C and $U_{\bar{C}}|\Psi_g(\lambda, \gamma)\rangle$ for the adiabatic path $\bar{C}$. (b) Measured ground-state GPs of the Heisenberg XY model (points) for different parameter sets (λ, γ) compared to the theoretical expectations (solid curves).

field strength λ, for a constant anisotropy parameter γ. In all cases, the observed GPs are compatible with the theoretically expected values: zero if the parameters $(\lambda, \gamma, \varphi)$ fall inside the sphere with radius $r = 1$, a sudden increase to the maximum value if the parameters are just outside the sphere, where the opening angle θ of the cone subtended by the circuit reaches a maximum, and then decreases as the circuit C is moved away from the origin. Increasing values of γ correspond to larger circles C and thus bigger values of θ. The points marked P_1 and P_2 correspond to the spectra shown in the upper part of the figure.

The relevant sources of experimental errors mainly came from undesired transitions induced by the time-dependent Hamiltonian, inhomogeneities of rf fields and static magnetic fields, imperfect calibration of rotations, and relaxation. We used a numerical optimization procedure to minimize undesired transitions during the adiabatic passage. The duration of individual experiments ranged from 30 ms to 90 ms, short compared to the relaxation time $T_2 \sim 1s$. The experimental error of the geometric phase was less than 3°. The imperfection of the initial state would also contribute to this. Using the experimentally reconstructed density matrices for the initial states, we found that this effect contributed $\approx 1°$ to the errors.

In summary, we have detected the ground-state GP in the Heisenberg XY model, after preparing the initial state by an adiabatic passage. The Heisenberg XY model was simulated by a multiple-pulse sequence, and the phase was measured by NMR interferometry. Our proof-of-principle experiment illustrates that the ground-state GP can serve as a fingerprint of the energy-level crossing points that result in a QPT in the thermodynamic limit. The ground-state GP is a robust indicator that is immune to some experimental imperfections [20] and provides an experimental method that does not need to cross the critical point.

It would be very interesting to extend this experiment to larger spin systems. For this, two issues are relevant: (i) the effectiveness of the ASP and (ii) the realization of a quantum circuit consisting of a quantum interferometer and quantum simulation. For the first issue, although a decisive mathematical analysis of the efficiency of ASP is difficult, numerical simulations (up to 128 qubits) [21] indicate a polynomial growth of the median runtime of an adiabatic evolution with the system size. On the second issue, quantum interferometry has become a mature technique, and the Heisenberg XY model has been efficiently simulated by a universal quantum circuit only involving the realizable single- and two-qubit logic gates [22]. Moreover, the diagonalization theory of the XY model shows a valid energy gap between the two lowest energies, which guarantees the viability of cyclic adiabatic evolution to generate the ground-state GP, even in the thermodynamic limit [8]. Recent research also shows that a 10-qubit system already represents a good approximation to the thermodynamical limit [23]. Therefore, the present scheme is, in principle, applicable to larger spin systems, when the technical difficulties in building a medium-scale quantum computer are overcome. This significant connection between GPs and QPTs is not a specific feature of the XY model, but remains valid in a general case [8,9]. We hope that this experimental work will contribute to an improved understanding of the ground-state properties and QPTs in many-body quantum systems.

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[1] M. V. Berry, Proc. R. Soc. A **392**, 45 (1984).
[2] Y. Aharonov and J. Anandan, Phys. Rev. Lett. **58**, 1593 (1987).
[3] T. Bitter and D. Dubbers, Phys. Rev. Lett. **59**, 251 (1987).
[4] D. Suter, K. T. Mueller, and A. Pines, Phys. Rev. Lett. **60**, 1218 (1988); J. Du *et al.*, *ibid.* **91**, 100403 (2003).
[5] P. J. Leek *et al.*, Science **318**, 1889 (2007).
[6] J. A. Jones *et al.*, Nature (London) **403**, 869 (2000).
[7] *Geometric Phases in Physics*, edited by A. Shapere and F. Wilczek (World Scientific, Singapore, 1989); Q. Niu *et al.*, Phys. Rev. Lett. **83**, 207 (1999); P. Bruno, *ibid.* **93**, 247202 (2004); **94**, 239903(E) (2005); G. Schutz, Phys. Rev. E **49**, 2461 (1994).
[8] A. C. M. Carollo and J. K. Pachos, Phys. Rev. Lett. **95**, 157203 (2005).
[9] S.-L. Zhu, Phys. Rev. Lett. **96**, 077206 (2006).
[10] S. Sachdev, *Quantum Phase Transitions* (Cambridge University Press, Cambridge, England, 1999).
[11] P. Zanardi and N. Paunkovic, Phys. Rev. E **74**, 031123 (2006); J. Zhang *et al.*, Phys. Rev. Lett. **100**, 100501 (2008).
[12] A. Osterloh *et al.*, Nature (London) **416**, 608 (2002).
[13] X. Peng, J. Zhang, J. Du, and D. Suter, Phys. Rev. Lett. **103**, 140501 (2009); X. Peng, J. Du, and D. Suter, Phys. Rev. A **71**, 012307 (2005).
[14] H. T. Quan *et al.*, Phys. Rev. Lett. **96**, 140604 (2006); L. C. Venuti and P. Zanardi, *ibid.* **99**, 095701 (2007); F. M. Cucchietti *et al.*, arXiv:1006.1468.
[15] S. Oh, Phys. Lett. A **373**, 644 (2009).
[16] E. Lieb, T. Schultz, and D. Mattis, Ann. Phys. (N.Y.) **16**, 407 (1961); P. Pfeuty, Ann. Phys. (N.Y.)**57**, 79 (1970).
[17] E. Barouch and B. McCoy, Phys. Rev. A **3**, 786 (1971).
[18] X. Peng *et al.*, Phys. Rev. A **72**, 052109 (2005).
[19] A. Messiah, *Quantum Mechanics* (Wiley, New York, 1976).
[20] A. M. Childs, E. Farhi, and J. Preskill, Phys. Rev. A **65**, 012322 (2001); J. Roland and N. J. Cerf, *ibid.* **71**, 032330 (2005).
[21] A. P. Young, S. Knysh, and V. N. Smelyanskiy, Phys. Rev. Lett. **101**, 170503 (2008).
[22] F. Verstraete, J. I. Cirac, and J. I. Latorre, Phys. Rev. A **79**, 032316 (2009).
[23] A. De Pasquale *et al.*, Eur. Phys. J. Special Topics **160**, 127 (2008).
[24] See supplementary material at http://link.aps.org/supplemental/10.1103/PhysRevLett.105.240405 for a detailed description of the experimental procedure and results.