Control of the geometric phase with time-dependent fields

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If the time evolution of a quantum state leads back to the initial state, a geometric phase is accumulated that is known as the Berry phase for adiabatic evolution or as the Aharonov-Anandan phase for nonadiabatic evolution. We evaluate these geometric phases using Floquet theory for two example systems, namely an ion in a light field and a spin-1/2 particle in a magnetic field. We demonstrate that, contrary to expectations, the low-frequency limit of the Aharonov-Anandan phase does not always coincide with the Berry phase, even though the time evolution becomes adiabatic. On the other hand, for a well-chosen system, both phase definitions agree, nonadiabatic corrections vanish at suitable frequencies, and the dynamical phase is zero, providing an advantageous setup for control of quantum phases. The value of the geometric phase can be controlled by steering the system through a degeneracy of the adiabatic energies, which can cause a π phase shift.

When a quantum-mechanical system undergoes a closed circuit in parameter space, an adiabatically evolving state may acquire a geometric phase, known as the Berry phase \cite{1}, in addition to its dynamical phase, where the latter is essentially the time-integrated energy. Adiabaticity is usually satisfied under sufficiently slow parameter variation. It means that the quantum state remains close to an instantaneous eigenstate of the Hamiltonian at all times. The geometric phase is an important fundamental concept in many fields including molecular physics \cite{2–4}, solid-state physics \cite{5–8}, ultracold atoms \cite{9, 10}, optics \cite{11–15}, and quantum computation \cite{16–18}. Following Berry, the geometric phase can be evaluated from the instantaneous eigenstates by integration of the Berry connection, without reference to time evolution. However, since the adiabatic approximation is not necessarily valid for a cyclic process \cite{19, 20}, one may resort to the nonadiabatic generalization of the geometric phase by Aharonov and Anandan (AA) \cite{21}. A conceptually different approach applicable to time-independent Hamiltonians is the exact factorization of nonadiabatic molecular wavefunctions into nuclear and electronic functions \cite{3, 22}. Focusing on the case of a Hamiltonian with time-varying parameter, we note that both Berry and AA consider the total phase acquired in a period $T$ and subtract the dynamical phase $\theta$, but they define the latter differently. Berry uses the time average $\bar{E}_{\text{ad}}$ of an instantaneous eigenenergy to define $\theta = -\bar{E}_{\text{ad}}T$ (written in atomic units); AA use the averaged energy expectation value $\bar{E}$ to define $\theta = -\bar{E}T$. Although in many applications, the two definitions agree in the adiabatic limit, one result of this Letter is the demonstration of a counter-example, calling for a discussion of the physical meaning.

A systematic way \cite{23–25} to obtain the AA phase \cite{26} follows from Floquet theory \cite{27–29}, the tool to describe periodically driven quantum matter \cite{30, 31}. As temporal analog of the Bloch theorem, the Floquet theorem states that the time-dependent Schrödinger equation (TDSE) with a time-periodic Hamiltonian has cyclic-state solutions that return exactly to the initial state, up to an overall phase determined by the Floquet quasienergy. To investigate the adiabatic limit, it seems natural to consider Floquet states at low-frequency: the quasienergy can be written as a power series in frequency, where the linear term is zero except when there is a nonzero adiabatic Berry phase \cite{32–38}. However, the low-frequency regime is highly nontrivial owing to multiphoton resonances, as we demonstrate below.

In this Letter, we scrutinize the frequency dependence of the geometric phase by considering four examples, involving a periodic laser field or magnetic field. A broad range of situations is covered: multiphoton resonances may be present, depending on the allowed quantum-mechanical transitions; the parameter circuit may lead through a degeneracy; the low-frequency Floquet states may or may not resemble adiabatically evolving states.

We consider laser pulses because their time-dependent electric-field vector follows a closed curve in the plane of polarization, i.e., a loop in parameter space. The simplest example is a circularly polarized (CP) single-color field. The shape of the field can be controlled by using more than one color. In particular, bicircular fields, i.e., two-color fields with circularly polarized colors have recently been used for fundamental studies and novel applications \cite{39–48}, including the generation of CP extreme ultraviolet radiation \cite{40} or the study of nonadiabaticity in strong-field ionization \cite{48}. By admixture of a weak counter-rotating second color to the CP field, additional transitions become possible and cause the appearance of multiphoton resonances, which we will interpret within a photon channel perspective \cite{40, 49}. For a bicircular field with equal strengths of both colors, the field crosses zero several times per optical cycle. Therefore, such a 1:1 field can steer a system through a degeneracy if, as in many atomic ions, there are degenerate states at
zero field strength. Although this does not hinder adiabatic evolution, we find a breakdown of the equivalence between AA phase and Berry phase. Another relevant example, proposed already by AA [21] in the context of their nonadiabatic geometric phase, is a spin-1/2 particle in a time-dependent magnetic field that passes through zero once per cycle. Again, we find that the degeneracy does not prevent adiabatic evolution, but one must superpose different low-frequency Floquet states to retrieve the adiabatic state and to find equivalence between AA and Berry phases.

Floquet theory and geometric phase.—According to the Floquet theorem, the TDSE \(i\partial\psi(t)/\partial t = H(t)|\psi(t)\) with periodic Hamiltonian \(H(t) = H(t + T)\) has solutions \(|\psi(t)\rangle = e^{-i\bar{E}T}|P(t)\rangle\) with quasienergy \(\bar{E}_f\) (dressed-state energy) and time-periodic states \(|P(t+T)\rangle = |P(t)\rangle\) satisfying the Floquet equation \((H - i\partial/\partial t)|P(t)\rangle = \bar{E}_f|P(t)\rangle\). The total phase accumulation in one period is \(-\bar{E}T\). Substracting the dynamical phase \(-\bar{E}T\) based on the time-averaged energy expectation value \(\bar{E} = \frac{1}{T}\int_0^T |\langle P(t)|H(t)|\Psi(t)\rangle|dt/T\), we obtain the AA phase \(\gamma_A = (\bar{E} - \bar{E}_f)T\). For practical calculations, the periodic state \(|P(t)\rangle\) is expanded as a Fourier series \(|P(t)\rangle = \sum_ne^{-i\omega nT}|F_n\rangle\), \(\omega = 2\pi/T\), so that the Floquet states are determined by a time-independent matrix eigenvalue equation [27, 28]. The AA phase takes the form \(\gamma_A = 2\pi n\bar{n}\) with \(n = \sum_n\langle F_n|\rho_F\rangle\), see also [24, 34]. We interpret this result from the photon channel perspective: When an eigenstate of the field-free Hamiltonian is exposed to the external field, the initial state is a Floquet state with only \(n = 0\) populated. If the system remains in a single Floquet state while turning on the field, populations are redistributed by photon absorption/emission and \(\langle F_n|\rho_F\rangle\) is the weight of the contribution reached by absorption of the photon energy \(n\omega\). The AA phase equals the mean absorbed photon energy, in units of \(\omega\), multiplied by \(2\pi\). An alternative view on geometric phases is provided by low-frequency Floquet theory, where the quasienergy is expanded as \(\bar{E}_f = \bar{E}_\text{ad} + \omega\bar{E}^{(1)} + \omega^2\bar{E}^{(2)} + \ldots\) [32–38] with \(\bar{E}_\text{ad} = \frac{1}{T}\int_0^T \bar{E}_\text{ad}(t)dt/T\) and \(\bar{E}_\text{ad}(t)\) being an eigenvalue of \(H(t)\). Using the dynamical phase \(-\bar{E}_\text{ad}T\) as in [1], we find a Berry phase \(\gamma_B = (\bar{E}_\text{ad} - \bar{E}_f)T\) including nonadiabaticity via \(\bar{E}_f(\omega)\). The adiabatic Berry phase is given by the low-frequency limit \(\gamma_B^{(0)} = -2\pi\bar{E}_f^{(1)}\). It can be observed by measuring the quasienergy. For example, positions of peaks in electron spectra from light-induced ionization depend on the bound-state quasienergies [50, 51].

Ne\textsuperscript{+} ion in a light field.—This set of examples is motivated by the experimental feasibility of preparing ringing current states in rare-gas ions [52, 53]. We treat a single active electron in an effective potential [54] and we restrict the analysis to the 2p\(\pm\) states with magnetic quantum numbers \(m = \pm 1\) and the 2s state [55–57]. The bicircular electric field composed of frequencies \(\omega\) and \(2\omega\) as a function of the field. One of the orbitals tends to spatially align along the field (labeled \(p_{\perp}\)) exhibiting a parabolic energy surface, whereas the other one tends to align perpendicularly (labeled \(p_{\parallel}\)) with flat energy surface [55]. The degeneracy at \(E = 0\) is reminiscent of a Renner-Teller level touching, which shows no Berry phase when encircled by an adiabatic path [58]. In the Floquet calculation, we expand \(\langle F_n|\rho_F\rangle = \sum_j c_{nj}\langle \phi_j|\rangle\) where \(\langle \phi_j|\rangle\) are the field-free states \((j = p_{\parallel}, s, p_{\perp})\). All solutions within an infinite set of quasienergies \(\bar{E}_f = \bar{E}_f + k\omega\) with integer \(k\) correspond to the same time-dependent state \(|\Psi(t)\rangle\). Therefore, one obtains only three different states \(|\Psi(t)\rangle\), describing the laser-dressed 2p and 2s states. Field-induced transitions are possible only within angular-momentum conservation rules. The possible photon channels from 2p\(\_\) and 2s as initial states are illustrated in Fig. 1(b). For a CP field, there are only few channels, indicated by the thick arrows.

The numerically calculated AA phases for a CP field with intensity \(I = 5 \times 10^{14}\) W/cm\(^2\) and variable \(\omega\) are presented in Fig. 2(a) as a function of the dimensionless parameter \(N = 2D^2E_0^2/(\omega\Delta\bar{E})\), where \(E_0^2 = E_1^2 + E_2^2\), \(\Delta\bar{E} = 0.8509\) a.u. is the gap between the field-free 2p and 2s energies, and \(D = \langle \phi_{p_{\perp}}|x|\phi_{p_{\perp}}\rangle = -0.3513\) a.u. We find nonzero \(\gamma_A\) with opposite signs for the 2p states, varying continuously from 0 at small \(N\) to \(\pm 2\pi\) at \(N\rightarrow\infty\), when we select the Floquet solutions with quasienergies close to \(\bar{E}\) at the smallest considered \(N\) [59]. It is intuitive that \(\gamma_A\) vanishes at large frequencies as there is no time \((T \rightarrow 0)\) to accumulate phase. To understand the low-frequency limit, we compare the Floquet state \(|\Psi(t)\rangle\) with
the instantaneous eigenstates,
\[ \Psi_{p_j}^{ad}(t) \propto \left( e^{i\omega t}, \frac{e^{i\omega t} \sqrt{\Delta \omega^2 + 8 \Delta D E_0^2 - \Delta \omega^2}}{2DE_0}, 1 \right)^T \]  
and \[ \Psi_{p_j}^{ad}(t) \propto (-e^{i\omega t}, 0, 1)^T, \]  
where the three components are the expansion coefficients in the field-free states \( p_-, s, p_+ \), respectively. To this end, we evaluate the time-dependent fidelity \( F_j(t) = |(\Psi_{p_j}^{ad}|\Phi(t))|^2 \) and we define the adiabaticity indicator \( F = \max_j F_j(t) \), plotted in Fig. 2(c). \( F \) converges to 1 for \( N \to \infty \) indicating low-frequency adiabatic behavior. Furthermore, since \( |(\phi_{p_-}^{ad}|\Psi_{p_j}^{ad})|^2 = |(\phi_{p_+}^{ad}|\Psi_{p_j}^{ad})|^2 = (1 - |(\phi_s|\Psi_{p_j}^{ad})|^2)/2 \), the mean number of absorbed quanta \( \omega \) when transiting from \( p_- \) (in Floquet channel \( n = 0 \)) to \( s \) and \( p_+ \) (cf. Fig. 1(b)) is \( \bar{n} = 1 \), and \( \gamma_A = 2\pi \) at \( \omega \to 0 \). In analogy, one finds \( -2\pi \) for the other \( p\)-type state. At intermediate \( N \), the system deviates from adiabaticity, resulting in nontrivial values of \( \gamma_A \). For the \( 2s \) state, the transitions from \( s \) to \( p_+ \) via absorbing/emitting photons are symmetric, so that \( \bar{n} = 0 \) and \( \gamma_A = 0 \). Apparently, symmetry breaking of the photon channels for initial states carrying ring current causes nonzero geometric phases in this system. A similar conclusion drawn for pseudorotating molecules was that the nuclear ring currents allowed by a degeneracy play a crucial role in the nonzero geometric phase [22]. The adiabatic limit of the AA phase is (up to multiples of \( 2\pi \)) the same as the adiabatic Berry phase obtained from the instantaneous eigenstates by integration of the Berry connection.

The geometric phase is reflected in the low-frequency behavior of the quasienergies. As shown in Fig. 2(e), the quasienergies of dressed \( p \) states converge to the adiabatic energies. In the special case of CP, we have \( \tilde{\omega}_ad = \tilde{\omega}_ad \). We find that the difference \( \tilde{\omega}_ad - \tilde{\omega}_f \) (mod \( \omega \)) converges to 0 quadratically in \( \omega \). In this case, the Berry phase \( (\tilde{\omega}_ad - \tilde{\omega}_f)T \) vanishes at \( \omega \to 0 \). Similarly, \( \tilde{\omega} - \tilde{\omega}_f \) (mod \( \omega \)) vanishes as \( \omega^2 \), implying that \( \gamma_A \) approaches zero.

For a bicircular field with field-strength ratio \( 5:1 \) of the \( \omega \) and \( 2\omega \) components and total intensity \( I = 5 \times 10^{14} \) W/cm\(^2\), nontrivial AA phases are again obtained for the ring-current \( 2p_{\pm} \) while \( \gamma_A = 0 \) for the \( 2s \) state, see Fig. 2(b). The most important new phenomenon is the appearance of multiphoton resonances. They cause avoided crossings of the quasienergy curves in Fig. 2(f). At a resonance, \( \gamma_A \) jumps by a large amount. The photon channel perspective explains this behavior. For example, at the avoided crossing between \( |p_-, 0 \rangle \) and \( |p_+, -1 \rangle \), indicated by the first double-headed arrow in Fig. 2(f), the Floquet state emits the photon energy \( \omega \) as \( n \) changes from 0 to -1. Additionally, as in the CP case, the difference between dressed state and field-free \( p_+ \) state implies slightly increased photon-energy emission so that \( \gamma_A \) drops below \(-2\pi \). Similarly, the state changes to \( |p_-, +3 \rangle \) at the second avoided crossing and \( \gamma_A \) jumps to above \( 3 \times 2\pi \).

![Figure 2](image-url)

**FIG. 2.** (a),(b) AA phases for the CP and 5:1 bicircular fields. (Points have been shifted by integer multiples of \( 2\pi \)). (c),(d) Adiabaticity indicator for \( p \)-type states. (e) Energy curves for the CP field. The label \( |p_-, 0 \rangle \) denotes a solution for \( |P(t)\rangle \) that resembles the \( p_- \) state at the smallest considered \( N \), while \( |p_-, n \rangle \) denotes a solution with quasienergy differing by \( -n\omega \). (f) Energy curves for the 5:1 bicircular field. The labels \( |p_-, n \rangle \) refer to “diabatic” curves that would show as continuous lines in the absence of avoided crossings. In (e),(f), the dot-dashed curves correspond to the same Floquet states as the red curves.

The adiabaticity indicator for the 5:1 bicircular field in Fig. 2(d) shows that the system is far from adiabaticity at resonances. At frequencies off resonances, we observe \( F \approx 1 \) at large \( N \), as the \( p \)-type Floquet states approach either \( \Psi_{p_\pm}^{ad} \) or \( \Psi_{p_\mp}^{ad} \) (calculated for the 5:1 field). In this sense, the system behaves adiabatically at low frequencies. We choose representative points in the middle between each pair of adjacent avoided crossings and plot the corresponding \( \gamma_A \) shifted by an integer multiple of \( 2\pi \) into the interval \([-2\pi, 0]\) or \([0, 2\pi]\), see Fig. 2(a), revealing a gradual change from 0 to \( \pm 2\pi \), as in the CP field. At these points, also \( |\tilde{\omega} - \tilde{\omega}_f| \) (mod \( \omega \)) decrease as \( \omega^2 \) when \( \omega \to 0 \). Again, the phase obtained by integration of the Berry connection is an integer multiple of \( 2\pi \). In short, \( \gamma_A = \gamma_B \) in the adiabatic limit.

For the 1:1 bicircular field, the electric field (yellow curve in Fig. 1(a)) passes through zero three times per cycle. We find avoided crossings, see Fig. 3(a), and nontrivial AA phases of the \( p \)-type Floquet states, exhibiting phase jumps at the resonances, similar to Fig. 2(b). Figure 3(b) shows that the low-frequency evolution becomes adiabatic except at the avoided crossings. However, we
find an anomalous behavior of $\gamma_A$, see Fig. 3(c), where a series of points between each pair of adjacent avoided crossings is selected and $\gamma_A$ is shifted into $[-\pi, \pi]$. The AA phase does not seem to converge to a well-defined adiabatic limit even when extending this calculation to $N = 900$, although $E - E_f \rightarrow 0$ at $\omega \rightarrow 0$. For deeper understanding, we consider the instantaneous eigenstate $\Psi_{p\perp}^{ad}(t) \propto (-e^{-i\omega T}, 0, 1)^T$. Unlike the examples without degeneracy, integration of the Berry connection yields $\pi$ (mod 2$\pi$). Indeed, $\gamma_B = (\tilde{E}_{ad} - E_f)T$ calculated at points in the middle between avoided crossings also converges to $\pm\pi$, see Fig. 3(c). The striking conclusion is that AA phase and Berry phase differ in the adiabatic limit. At first sight, this may contradict the agreement of the two energies $\tilde{E}$ and $\tilde{E}_{ad}$ at $\omega \rightarrow 0$. But in the dynamical phase expressions $-\tilde{E}T$ and $-\tilde{E}_{ad}T$, energies are multiplied with a diverging factor $T \rightarrow \infty$ and $|E - E_f|$ does not decrease fast enough to let $\gamma_A$ converge. The adiabatic Berry phase $\pi$ can be understood as follows. When the field goes through zero, its direction is suddenly reversed, whereas the aligned time-dependent wavefunction evolves continuously. After one cycle with $N$ zero crossings, the field returns to its initial direction, whereas, relative to the field, the $p$ orbital has reversed $N$ times and gained the phase $N\pi$. Hence, one can effectively control the geometric phase by steering the system through the degeneracy. The exemplary time evolution in Fig. 3(d) (see also the supplementary movie) shows that within one period of the field, the $p$ orbital rotates by 180 degrees and gains a Berry phase of about $0.8\pi$. Because of nonadiabaticity, this value is not exactly $\pi$. More generally, a 1:1 bicircular field with frequencies $\omega$ and $(N-1)\omega$ has $N$ zero crossings [44] and therefore $\gamma_B^{(0)} = N\pi$ (mod 2$\pi$).

**Spin-1/2 particle in a magnetic field.**—We consider the time-varying field

$$B(t) = B_0\hat{e}_z + B_0[\cos(\omega_B t)\hat{e}_z + \sin(\omega_B t)\hat{e}_x],$$

(3)
describing a circle through zero. The Hamiltonian is $H(t) = \mathbf{B} \cdot \mathbf{\sigma}/2$ with the Pauli vector $\mathbf{\sigma}$. An aligned spin following the field direction cannot reverse suddenly when the field crosses zero (degeneracy of the adiabatic states), see Fig. 4(a) and the supplementary movie. Thus, the system is expected to return to the initial state only after two rotations of the magnetic field [21]. We therefore choose the Floquet frequency $\omega = \omega_B/2$. For both instantaneous eigenstates $\Psi_{1\perp}^{ad}(t) = (\cos \frac{\omega_B t}{2}, \sin \frac{\omega_B t}{2})^T$ and $\Psi_{2\perp}^{ad}(t) = (-\sin \frac{\omega_B t}{2}, \cos \frac{\omega_B t}{2})^T$, the Berry connection gives an adiabatic Berry phase of $\pi$—the known result for a full rotation of a spin-1/2 particle. Motivated by the anomalous result obtained for the 1:1 bicircular field above, a careful analysis of the nonadiabatic phases is needed.

The Floquet results are presented as a function of $N_B = B_0/\omega_B$ in Fig. 4. We find Floquet states with avoided crossings and $F$ is below 0.5, i.e., Floquet and adiabatic states differ strongly. Nevertheless, we can superpose two different Floquet states with equal weight at those frequencies where two quasienergies are equal, see the intersecting black and red curves in Fig. 4(b). The superpositions have $F \approx 1$ at low frequency, i.e., their time evolution is adiabatic, see Fig. 4(c). While the

*FIG. 3. (a),(b) Same as Fig. 2(f),(d) for the 1:1 bicircular field. (c) AA phase $\gamma_A$ and Berry phase $\gamma_B$ of $p$ orbitals, shifted by multiples of 2$\pi$. (d) Evolution of the $p_{\perp}$-like Floquet orbital at $N = 1.7$. The colors represent the position-dependent phase after subtracting the dynamical phase.*

*FIG. 4. (a) Illustration of the spin-1/2 particle state during one rotation of the magnetic field in the limit $\omega \rightarrow 0$. Thick arrows indicate the spin direction. The colors represent the dynamical phase. (b) Energy curves. (c) Adiabaticity indicator for the Floquet states and superpositions. (d) AA phase $\gamma_A$ and Berry phase $\gamma_B$ shifted by multiples of 2$\pi$ for a Floquet state and superpositions.*
Floquet states have strongly varying $\gamma_A$, see Fig. 4(d), we find $\gamma_A = \gamma_B = \pi$ for the superpositions, surprisingly without frequency dependence. Here, $\gamma_A = \gamma_B$ because $\xi = \xi_{\text{ad}} = 0$. This is due to the antisymmetry about the zero crossing. The accumulated dynamical phase after one rotation of $B(t)$ is always zero, see Fig. 4(a) and the supplementary movie.

**Conclusion.**—Our evaluation of the geometric phase for cyclic states reveals both surprises and useful features. Although the phase defined by Aharonov and Anandan usually agrees with the adiabatic Berry phase in the low-frequency limit, we have presented a counter-example where they differ, although the time evolution is evidently adiabatic. In view of applications of geometric phases in quantum information [17, 18], it is of interest that our study suggests convenient control of geometric phases by tuning the driving frequency and by steering the system through degeneracies. As the Berry phase determines the low-frequency expansion of the quasienergies, it has a direct relation to observable quantities.

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[26] Moore and Stedman [23, 24] use the term “non-adiabatic Berry phase” for the AA phase. We reserve the term “Berry phase” for values obtained with Berry’s definition of the dynamical phase.


Very small $\mathcal{N}$ are excluded from Figs. 2, 3 because of avoided crossings between $s$ and $p$ states that we do not discuss in the present work.