Geometric phases and anholonomy for a class of chaotic classical systems

C. Jarzynski

University of California, Department of Physics,
and Lawrence Berkeley Laboratory

Berkeley, CA 94720

beginning July, 1994:

Institute for Nuclear Theory, University of Washington,

Seattle, WA 98195

(November 20, 2018)

Abstract

Berry’s phase may be viewed as arising from the parallel transport of a quantal state around a loop in parameter space. In this Letter, the classical limit of this transport is obtained for a particular class of chaotic systems. It is shown that this “classical parallel transport” is anholonomic — transport around a closed curve in parameter space does not bring a point in phase space back to itself — and is intimately related to the Robbins-Berry classical two-form.

PACS numbers: 03.65.Bz, 05.45.+b
Ordinarily, Berry’s phase is defined as the unexpected phase \( \Delta \gamma_n \) picked up by a quantal eigenstate \(|n\rangle\) evolving under a parameter-dependent Hamiltonian \( \hat{h}(R) \), when \( R \) is made to slowly trace out a loop \( \Gamma \) in parameter space \([1,2]\). This phase is geometric: its value is given in terms of the flux of a 2-form \( V_n(R) = -i\hbar \langle \nabla n \times |\nabla n\rangle \) through a surface bounded by \( \Gamma \). (Here, \(|n\rangle\) is the \( n \)th eigenstate of \( \hat{h} \), and \(|\nabla n\rangle \equiv \partial |n\rangle / \partial R \). \( R \)-space is taken to be ordinary 3-space, hence 2-forms are simply vector fields.) The search for classical counterparts of Berry’s phase has been particularly challenging for chaotic systems. While Robbins and Berry \([3]\) have obtained the classical limit of the 2-form \( V_n(R) \), the analogue of the phase \( \Delta \gamma_n \) itself has proven elusive. It is the purpose here to show that, if one interprets Berry’s phase as an anholonomy effect \([2,4]\), rather than as the dynamical effect mentioned above, then for a certain class of chaotic systems, \( \Delta \gamma_n \) does indeed have a classical analogue.

This Letter is arranged as follows. First, the interpretation of Berry’s phase as an anholonomy effect — arising from the parallel transport of an eigenstate around a loop in parameter space — is reviewed. Next, this transport is expressed in terms of its generator \( \hat{\xi}(R) \). The classical limit \( \xi(z,R) \) of this operator is then obtained, and classical parallel transport is defined as the flow in phase space (\( z \)-space) generated by \( \xi(z,R) \). Finally, this flow is studied, and the classical analogue of \( \Delta \gamma_n \) is derived. Results similar to those presented here have been obtained independently by Dr. Jonathan Robbins (personal communication).

First, let us define \( h(z,R) \) (or simply \( h(R) \)) to be the classical Hamiltonian which is the classical limit of \( \hat{h}(R) \). Motion under \( h(R) \), with \( R \) fixed, is assumed bounded, and ergodic over the energy shell. (This implies that, under the Poisson bracket, \( h(z,R) \) commutes only with functions of the form \( f(h,R) \), a fact which will come in handy.) Phase space is \( 2N \)-dimensional, where \( N > 1 \).

Now, consider the following definition of the “parallel transport” of a quantal state in \( R \)-space: along a curve \( R(\tau) \) starting from \( R_0 \), the \( n \)th eigenstate of \( \hat{h}(R_0) \) gets transported to the \( n \)th eigenstate of \( \hat{h}(R') \), for each point \( R' \) along the curve. To remove ambiguity about how the phase of the state changes along the curve, we impose the condition \( \langle \psi(\tau)|\psi(\tau + \delta \tau)\rangle = 1 + O((\delta \tau)^2) \) on an eigenstate thus transported. (Here, \( \tau \) is a dummy variable,
labelling points along the curve in $\mathbf{R}$-space, and also labelling the state $|\psi\rangle$ found at each such point.) If we extend this definition to include linear combinations of eigenstates (by assuming the principle of superposition) then we have a prescription for how an arbitrary state $|\psi\rangle$ “evolves” along an arbitrary curve in parameter space. It was shown by Simon \[4\] that, under the transport thus defined, an eigenstate $|n\rangle$ taken around a loop $\Gamma$ picks up a net phase equal to Berry’s phase. Berry’s phase thus emerges as an anholonomy effect: when $\mathbf{R}$ completes its circuit, the quantal phase does not return to its initial value. (The term “anholonomy” refers to the situation when a non-zero change in some quantity is induced by taking a parameter $\mathbf{R}$ around a closed circuit \[2\]. For instance, a vector parallel transported around a loop in a curved space typically does not return to its original orientation.)

The quantal parallel transport thus defined is unitary, and may be described in terms of its generator, the vector operator $\hat{\xi}(\mathbf{R})$ such that

$$i\hbar \frac{d}{d\tau} |\psi\rangle = \frac{d\mathbf{R}}{d\tau} \cdot \hat{\xi} |\psi\rangle$$

for any $|\psi(\tau)\rangle$ enjoying parallel transport along $\mathbf{R}(\tau)$. (I.e. if parallel transport is a rule for associating an infinitesimal step $|\delta\psi\rangle$ in Hilbert space with a given step $\delta\mathbf{R}$ in parameter space, then $\hat{\xi}(\mathbf{R})$ is the operator such that $i\hbar|\delta\psi\rangle = \delta\mathbf{R} \cdot \hat{\xi}|\psi\rangle$.) It is a straightforward exercise to show that $\hat{\xi}$ is determined by the conditions

$$[\hat{\xi}, \hat{h}] = i\hbar(\hat{\nabla}h - \hat{D})$$

$$\langle n|\hat{\xi}|n\rangle = 0,$$

where $\langle m|\hat{D}|n\rangle \equiv \langle m|\hat{\nabla}h|n\rangle \delta_{mn}$. (Eqs.\[2\] and \[3\], and their classical counterparts \[\xi\] and \[\xi\], appear as well in the context of Born-Oppenheimer forces, where $\mathbf{R}$ is a dynamical quantity rather than an externally driven parameter; see Aharonov et al \[3\].)

Given this quantal picture, what might the corresponding classical picture be? Since Eq.\[1\] is essentially a prescription for lifting a curve $\mathbf{R}(\tau)$ from parameter space to a curve $|\psi(\tau)\rangle$ in Hilbert space (given an initial state $|\psi_0\rangle$), we might expect the classical version to be a prescription for lifting $\mathbf{R}(\tau)$ to a curve $z(\tau)$ in phase space (given an initial $z_i$).
With this in mind, let us obtain the vector function $\xi(z, R)$ which is the classical limit of $\hat{\xi}(R)$, and then define classical parallel transport to be the flow in phase space generated by $\xi(z, R)$, according to

$$\frac{dz}{d\tau} = \frac{dR}{d\tau} \cdot \{z, \xi\}. \quad (4)$$

(As in the quantal case, $dR/d\tau \cdot \hat{\xi}$ acts as a Hamiltonian along $R(\tau)$. This makes classical parallel transport a canonical flow, just as the quantal version is unitary.) Once $\xi$ is obtained, we will be able to study what happens when a point $z_i$ gets transported around a closed curve in parameter space: will $z_i$ return to itself, and if not will the anholonomy bear any resemblance to Berry's phase?

To obtain $\xi(z, R)$ from $\hat{\xi}(R)$, we exploit the fact that $\hat{\xi}(R)$ is specified by Eqs. 2 and 3, whose classical limits, using the simplest of semiclassical approximations, are:

$$\{\xi, h\} = \nabla h - \langle \nabla h \rangle_{h, R} \quad (5)$$

$$\langle \xi \rangle_{E, R} = 0. \quad (6)$$

Here, $\langle \cdots \rangle_{E, R}$ denotes a phase space average over an energy shell of $h(R)$:

$$\langle \cdots \rangle_{E, R} = \left( \frac{\partial \Omega}{\partial E} \right)^{-1} \int dz \delta(E - h) \cdots \quad (7)$$

where $\Omega(E, R) = \int dz \theta(E - h)$ is the volume of phase space enclosed by this shell. Note that the left side of Eq.5 is evaluated at some $(z, R)$; the value of the subscript $h$ on the right side is evaluated at the same $(z, R)$.

Eqs. 5 and 6 are solved by:

$$\xi(z, R) = \lim_{\alpha \to 0} \int_{-\infty}^{0} ds e^{-\alpha s} \nabla \tilde{h}(z_s, R), \quad (8)$$

where, as in Ref. [6], $\nabla \tilde{h} \equiv \nabla h - \langle \nabla h \rangle_{h, R}$, and $z_s(z, R)$ is the point in phase space reached by evolution from $z$, for time $s$, under $h(R)$. If Eq. 8 converges, it solves Eqs. 5 and 6 uniquely. Generically, however, Eq. 8 approaches an infinitely convoluted distribution [6], rather than a smooth vector function on phase space. Since it is not clear how such an
object could serve as the generator of flow, we assume that Eq. 8 converges. This places a
restriction (discussed below) on the class of systems for which the results to be derived are
valid.

Eqs. 4 and 8 together specify how a point in phase space gets transported along a curve
in parameter space. This flow has a number of properties that simplify the investigation of
transport around a \textit{closed} curve:

\begin{itemize}
  \item First, consider a new Hamiltonian \( h' \) of the form \( h'(z, R) = f(h(z, R), R) \). Then any
    \( \xi \) satisfying Eq. 3 also satisfies \( \{ \xi, h' \} = \nabla h' - \langle \nabla h' \rangle \), i.e. \( h(R) \) and \( h'(R) \) give rise to the
    same generator \( \xi(R) \). Since \( h'(R) \) simply relabels the energy shells of \( h(R) \), this means that \textit{parallel transport is determined by the manner in which \( h(R) \) divides phase space into energy shells} (at each \( R \)), but is independent of the energy values that happen to be assigned to those shells. (In Ref. [3], where the classical limit of the quantal 2-form \( V_n \) is obtained, it is shown that the resulting \textit{classical 2-form} \( V^c \) shares this property.)

  Thus, for studying the flow generated by \( \xi(R) \), we may replace \( h(R) \) with any \( h'(R) \) of
the form given above. A convenient replacement is the “volume Hamiltonian” \( \Omega \)\n\begin{equation}
\Omega_P(z, R) = \Omega(h(z, R), R),
\end{equation}
with \( \Omega \) as defined earlier. \( \Omega_P(R) \) relabels the energy shells of \( h(R) \), assigning to each a value
equal to the volume of phase space it encloses. Note that the dynamics under \( \Omega_P(z, R) \),
with \( R \) fixed, is the same as under \( h(z, R) \), only with time re-scaled.

  \item For an arbitrary curve \( R(\tau) \) from \( R_0 \) to \( R_1 \), parallel transport defines a mapping
  \( z \rightarrow z' \) of phase onto itself: \( z' \) is the point reached by transport from \( z \) along \( R(\tau) \).
  Let \( z(\tau) \) then denote the curve connecting \( z \) to \( z' \), satisfying Eq. 4. From Eq. 4 and the
  identity \( \langle \nabla \Omega_P \rangle_E.R = 0 \), we get
  \begin{equation}
  \frac{d}{d\tau} \Omega_P(z(\tau), R(\tau)) = 0.
  \end{equation}
In words, \textit{parallel transport conserves the value of} \( \Omega_P(z, R) \) (just as the quantal version
conserves quantum number \( n \).) This tells us that the canonical transformation \( z \rightarrow z' \) maps
each energy shell $A_0$ of $\Omega_P(R_0)$ to the same-valued shell $A_1$ of $\Omega_P(R_1)$. (Thus, under parallel transport around a closed curve, $A_0$ gets mapped to itself.)

• While the statement that parallel transport takes $A_0$ to $A_1$ is true for any $R(\tau)$ from $R_0$ to $R_1$, the specific point $z'$ on $A_1$ to which a given $z$ on $A_0$ gets mapped depends on $R(\tau)$. Thus, a slight change $\delta R(\tau)$ in the path from $R_0$ to $R_1$ induces a slight shift $\delta z'$ in the final point $z'$. The mapping $z' \rightarrow z' + \delta z'$ induced by this change of path is itself a canonical transformation which maps $A_1$ onto itself. Since any continuous deformation of $R(\tau)$ (with endpoints fixed) may be constructed from a sequence of such infinitesimal changes in path, we are led to conclude that, by continuously deforming the path from $R_0$ to $R_1$, we generate a canonical flow of the point $z'$ to which a fixed $z$ gets mapped. Now, the assumption of ergodicity guarantees that the only canonical flow on the energy shell $A_1$ is that generated by $\Omega_P(z, R_1)$ — or $h(z, R_1)$ — itself. Thus, a continuous deformation of the path from $R_0$ to $R_1$ displaces $z'$ along a trajectory of the Hamiltonian $\Omega_P(R_1)$. Assuming further that any closed curve in $R$-space can be shrunk to a single point, we conclude that, if a point $z_i$ is transported around a curve starting and ending at $R_0$, to a point $z_f$, then $z_i$ and $z_f$ lie on a single trajectory of $h(R_0)$.

Since the energy shells of $h(R)$ are identical to those of $\Omega_P(R)$, parallel transport from $R_0$ to $R_1$ maps the shells of $h(R_0)$ to those of $h(R_1)$. This mapping conserves the value of $\Omega_P$, but not necessarily of $h$. Thus, the assumption that Eq. 5 converges has restricted us to systems with the non-generic property that (for any $R_0$ and $R_1$), $h(z, R_0)$ is related to $h(z, R_1)$ by a canonical transformation, along with a possible relabelling of the values of the energy shells. Let us call such a system a generalized canonical family. This follows Ref. [7], where a canonical family is defined by the property that the Hamiltonians at different points in $R$-space are related by canonical transformation, without any relabelling of energy shells. $\Omega_P(z, R)$ constitutes a canonical family.

As discussed in Ref. [7], for a canonical family, e.g. $\Omega_P(z, R)$, we may construct a vector function $g(z, R)$ so that the flow generated by $g$ (as per Eq.4, only with $g$ in place of $\xi$) has the following two properties. First, as with $\xi$, this flow, along any path from $R_0$ to $R_1$,
maps an energy shell of $\Omega_P(R_0)$ to the same-valued shell of $\Omega_P(R_1)$. However, unlike with $\xi$, this mapping is independent of the path connecting $R_0$ to $R_1$. The generator $g$ provides the final tool needed to establish exactly where a point $z_i$ gets taken when parallel transported around a closed loop in parameter space.

Since flow under $g$ preserves $\Omega_P$, we have $\{g, \Omega_P\} = \nabla \Omega_P$, as was the case with $\xi$. Thus, $\{\xi - g, \Omega_P\} = 0$, so $g$ and $\xi$ differ at most by some function $A(\Omega_P, R)$: $\xi(z, R) = g(z, R) + A(\Omega_P(z, R), R)$. Since the phase space average of $\xi$ over any energy shell of $\Omega_P(R)$ is zero, we have

$$A(\omega, R) = -\langle g(z, R) \rangle_{\omega, R},$$

where $\omega$ denotes the volume enclosed by the energy shell of $\Omega_P(R)$ over which the average is taken. As shown in Ref. \[7\], we may choose $g$ so that

$$\nabla \times A(\omega, R) = V^c(\omega, R),$$

where $V^c$ is the Robbins-Berry classical 2-form (the classical limit of the quantal 2-form $V_n$) associated with $\Omega_P(z, R)$. In what follows we assume Eq. \[12\] holds.

We are finally prepared to investigate parallel transport around a loop $\Gamma$, starting and ending at $R_0$. Let $R(\tau)$ explicitly represent this loop, with $\tau$ running from $\tau_i$ to $\tau_f$. Let $z_i$ be an initial point in phase space, and $z_f$ the point reached from $z_i$ by transport around $\Gamma$. We already know that $z_f$ and $z_i$ lie on a single trajectory of $\Omega_P(R_0)$; let us use $\Delta \sigma$, the time of evolution under $\Omega_P(R_0)$ separating $z_f$ from $z_i$, as the measure of “distance” between these two points along the trajectory. $\Delta \sigma$ thus measures the anholonomy associated with transport around $\Gamma$. (This definition of distance along a trajectory is meant to be unaffected by a relabelling of the energy shells: for any Hamiltonian $h$, we take distance along a trajectory to mean time of evolution under the associated “volume Hamiltonian” $\Omega_P$. In one degree of freedom, this reduces to the ordinary angle variable of action-angle variables, divided by $2\pi$.)

To solve for $\Delta \sigma$, consider the mapping $z \rightarrow y(z, R)$, where $y$ is reached from $z$ by flow under $g$ along any path from $R$ to $R_0$. This constitutes a kind of projection: for any $R$,
each \( z \) on a given energy shell of \( \Omega_P(R) \) is mapped to a point \( y \) on the corresponding shell of \( \Omega_P(R_0) \). \( y(z, R) \) satisfies

\[
\nabla y(z, R) = -\{y(z, R), g(z, R)\}. \tag{13}
\]

Now, let \( z(\tau) \) be the phase space curve obtained by parallel transport from \( z_i \) along \( R(\tau) \), and let \( y(\tau) \equiv y(z(\tau), R(\tau)) \). Thus, as \( z(\tau) \) traces out some path in phase space, starting and ending at an energy shell \( A_0 \) of \( \Omega_P(R_0) \), its projection \( y(\tau) \) traces out a path wholly confined to \( A_0 \). Since \( R(\tau_i) = R(\tau_f) = R_0 \), we have \( y(\tau_i) = z_i \), and \( y(\tau_f) = z_f \), so we solve for the distance between \( z_i \) and \( z_f \) by solving for \( y(\tau) \):

\[
\frac{dy}{d\tau} = \frac{\partial y}{\partial z} \frac{dz}{d\tau} + \nabla y \cdot \frac{dR}{d\tau} = \frac{\partial y}{\partial z} \frac{dR}{d\tau} \cdot \{z, \xi\} - \frac{dR}{d\tau} \{y, g\} = \frac{dR}{d\tau} \cdot \{y, A\}, \tag{14}
\]

using Eqs. [4] and [13], along with properties of the Poisson bracket. In the last line, \( A = A(\Omega_P(z, R), R) = A(\Omega_P(y, R_0), R) \), hence

\[
\frac{dy}{d\tau} = \frac{dR}{d\tau} \cdot \frac{\partial A}{\partial \omega}(\omega, R) \cdot \{y, \Omega_P(y, R_0)\}, \tag{15}
\]

with \( \partial A/\partial \omega \) evaluated at the constant value \( \omega = \Omega_P(y, R_0) \). Finally, defining

\[
\sigma(\tau) = \int_{R_0}^{R(\tau)} dR' \cdot \frac{\partial A}{\partial \omega}(\omega, R'), \tag{16}
\]

with integration occurring along \( \Gamma \), we get

\[
\frac{dy}{d\sigma} = \{y, \Omega_P(y, R_0)\}. \tag{17}
\]

This means that \( y \) evolves along a trajectory of \( \Omega_P(R_0) \), with \( \sigma \) playing the role of time of evolution. Thus, the distance \( \Delta \sigma \) separating \( z_f = y(\tau_f) \) from \( z_i = y(\tau_i) \) is given by \( \sigma(\tau_f) - \sigma(\tau_i) = \int_{\Gamma} dR \cdot \partial A/\partial \omega \). Using Stokes’s theorem and Eq.[12], we finally have

\[
\Delta \sigma = \frac{\partial}{\partial \omega} \int \int dS \cdot V^c(\omega, R), \tag{18}
\]
where the integral denotes the flux of $V^c(\omega, R)$ through a surface bounded by $\Gamma$.

We have taken $V^c(\omega, R)$ to be the 2-form associated with $\Omega_P(z, R)$. However, since this 2-form is unchanged by a relabelling of the energy shells \[3\], $V^c(\omega, R)$ is equally well the 2-form associated with our original $h(z, R)$. (In either case, however, the integral $\int \int dS \cdot V^c$ is evaluated at fixed $\omega = \Omega(E, R)$, not at fixed $E$.)

Eq. [18] is the central result of this Letter; it gives the classical anholonomy resulting from parallel transport around a loop in parameter space. But, does it make sense to call this anholonomy the chaotic classical analogue of Berry’s phase? Let us focus on the fact that both $\Delta\sigma$ and Berry’s phase $\Delta\gamma_n$ are expressed geometrically, in terms of the flux of a 2-form ($V^c$ or $V_n$) through the loop in parameter space. Specifically, since $\Delta\gamma_n = -(1/\hbar) \int \int dS \cdot V_n$ \[3\], and since $V_n \to V^c$ semiclassically, Eq. [18] suggests the correspondence

$$\Delta\sigma = -\hbar \frac{\partial}{\partial \omega} \Delta\gamma_n \quad (19)$$

between the classical and quantal measures of anholonomy. This relationship is the same as that found in Ref. \[8\] between Berry’s phase and Hannay’s angle \[9\] (the classical geometric phase for integrable systems), which suggests that we are on the right track in associating $\Delta\sigma$ with $\Delta\gamma_n$.

On the other hand, the original formulation of Berry’s phase makes a dynamical statement concerning evolution under a slowly time-dependent Hamiltonian. Does $\Delta\sigma$ have a similar significance for chaotic classical systems? That is, does it make a prediction concerning the evolution of trajectories under $h(z, R)$, when $R$ slowly traces out a closed curve? The exponential divergence of chaotic trajectories makes this a difficult question, to which I have no answer. For the time being, then, Eq. [18] is a purely formal result, one more piece of the puzzle, but not the last piece. Its value lies in emphasizing and illuminating the classical chaotic limit of the quantal transport underlying Berry’s phase, and in demonstrating that the anholonomy associated with this classical transport closely resembles its quantal counterpart.

As mentioned, the 2-form $V^c$ was originally derived as the classical limit of $V_n$. Later,
Berry and Robbins [6] demonstrated the significance of $V^c$ within a purely classical context. Namely, when $R(t)$ is itself a dynamical quantity, $V^c$ acts as a magnetic field influencing the evolution of $R(t)$. Perhaps the anholonomy given by Eq.18 will contribute to an intuitive understanding of this geometric magnetism. Incidentally, the restriction in this Letter to generalized canonical families has a simple interpretation in the context of Ref. [6]: for these families, the friction-like reaction force (deterministic friction) is identically zero [7].

The problem of generalizing the analysis of this Letter to systems for which Eq.8 does not converge remains open, and is related to the question of whether or not $V^c$ is closed ($\nabla \cdot V^c = 0$) in the general case [3,7].

In the time since the original submission of this Letter, it has come to my attention that the classical parallel transport studied herein has been discussed by Montgomery [10] and Golin et. al. [11] (These authors obtain this transport classically, rather than as the limit of the quantal version.) Eq.18, however, is a new result.

ACKNOWLEDGMENTS

I would like to thank Wladek Świątecki and Jim Morehead for stimulating discussions. This work was supported by the Director, Office of Energy Research, Division of Nuclear Physics of the Office of High Energy and Nuclear Physics of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098; and by the Department of Energy under Grant No. DE-FG06-90ER40561.
REFERENCES

[1] M.V. Berry, Proc. Roy. Soc. Lond. A 392, 45 (1984).

[2] M.V. Berry, in *Geometric Phases in Physics*, A. Shapere and F. Wilczek, eds. World Scientific: Singapore, 1989. Pages 7-28.

[3] J.M. Robbins and M.V. Berry, Proc. Roy. Soc. Lond. A, 436, 631 (1992).

[4] B. Simon, Phys. Rev. Lett. 51, 2167 (1983).

[5] Y. Aharonov, E. Ben-Reuven, S. Popescu, and D. Rohrlich, Phys. Rev. Lett. 65, 3065 (1990), Nucl. Phys. B350, 818 (1991).

[6] M.V. Berry and J.M. Robbins, Proc. Roy. Soc. Lond. A, 442, 659 (1993).

[7] J.M. Robbins, J. Phys. A 27, 1179 (1994).

[8] M.V. Berry, J. Phys. A 18, 15 (1985).

[9] J.H. Hannay, J. Phys. A 18, 221 (1985).

[10] R. Montgomery, Commun. Math. Phys. 120, 269 (1988).

[11] S. Golin, A. Knauf, and S. Marmi, Commun. Math. Phys. 123, 95 (1989).