BERRY'S PHASE —
TOPOLOGICAL IDEAS FROM ATOMIC, MOLECULAR AND OPTICAL PHYSICS*

R. Jackiw

Center for Theoretical Physics
Laboratory for Nuclear Science
and Department of Physics
Massachusetts Institute of Technology
Cambridge, Massachusetts 02139 U.S.A.

Annual Meeting of the Division of Atomic, Molecular and Optical Physics
American Physical Society, Cambridge, MA, U.S.A.
May 1987

To be published in: Comments on Atomic and Molecular Physics

Typeset in TeX by Roger L. Gilson

CTP#1475
May 1987

* This work is supported in part by funds provided by the U. S. Department of Energy (D.O.E.) under contract #DE-AC02-76ER03069.
BERRY'S PHASE —
TOPOLOGICAL IDEAS FROM ATOMIC,
MOLECULAR AND OPTICAL PHYSICS

R. Jackiw

ABSTRACT

Berry's modification of the quantum adiabatic theorem is described and its
experimental status is mentioned. The relation of these ideas to phenomena
seen in second-quantized field theory is explained.

When analyzing a physical system, it is sometimes useful to divide its dynamical
variables into two sets, first deal with the motion of one set of variables, keeping
the others fixed but arbitrary, and then complete the analysis of the entire system by
allowing variation of the previously fixed coordinates. The quantum adiabatic theorem
and the molecular Born-Oppenheimer approximation are closely related and well-
known examples of this program, which has been used for over half a century. It was
a surprise, therefore, when a few years ago M. V. Berry made some new observations
in this area, which advanced our understanding of this procedure and clarified some
puzzles that were encountered by practitioners of the technique.\textsuperscript{1,2} This is what I shall
describe to you, and also I shall speak about further applications of Berry's results to
elementary particle physics.

Consider a system described by a Hamiltonian with two sets of variables.

\[ H = \frac{\mathbf{p}^2}{2M} + \frac{\mathbf{p}^2}{2m} + V(R, r) \]  

(1)

The capitalized coordinates and momenta, $\mathbf{P}$ and $\mathbf{R}$, will be called slow variables, the
others, $\mathbf{p}$ and $r$, are fast variables — for molecules the former are the nuclear variables,
the latter, electron variables. In the most drastic approximation, one ignores the kinetic
energy and the motion of the slow coordinates, and solves for the energy eigenvalues
and eigenvectors of the fast Hamiltonian, with parametric dependence on the slow
coordinate $R$.

\[ h(p, r; R) = \frac{p^2}{2m} + V(R, r) \]  

(2a)

\[ h(p, r; R)|n; R\rangle = \epsilon_n(R)|n; R\rangle \]  

(2b)

In the adiabatic approximation, one allows the parameter $R$ to vary with time, suf-
ficiently slowly so that its kinetic energy may be still ignored and so that its time
evolution may be viewed as a prescribed, classical motion: $\mathbb{R} \rightarrow \mathbb{R}(t)$. The adiabatic theorem then states that the time evolution of a non-degenerate eigenstate of $\hbar$ is given by
\[ |t\rangle = e^{-\frac{i}{\hbar} \int_0^t dt' \epsilon_n(R(t'))} e^{i \gamma_n(t)} |n; R(t)\rangle \] (3)
where
\[ \dot{\gamma}(t) = i \left\langle n; R(t) \right| \frac{d}{dt} n; R(t) \right\rangle \]
\[ = \dot{R}(t) \cdot i \left\langle n; R(t) \right| \nabla n; R(t) \right\rangle \] (4)
[The time derivative and the gradient with respect to $R$ act on the fast wavefunction.]
Because $|n; R\rangle$ is normalized, $\gamma$ is real. Equations (3) and (4), which are derived by projecting the time-dependent Schrödinger equation
\[ i\hbar \partial_t |t\rangle = \mathcal{H} |t\rangle \] (5)
on $|n; R(t)\rangle$ and ignoring off-diagonal matrix-elements, are discussed in most quantum mechanics textbooks, except that the phase $\gamma_n(t)$ is omitted. The textbook argument for ignoring this phase is that the eigenvalue equation (2) does not determine phases of the fast eigenfunctions; it is said that $e^{i \gamma_n(t)}$ can be absorbed into $|n; R(t)\rangle$ by a redefinition of phases and therefore no meaning can be attached to them.

Berry’s contribution consists in realizing that a meaningful question can be asked about the phase: to wit, if the time evolution is periodic so that the parameter $R(t)$ returns to its original value at some later time $t = T$, $R(T) = R(0)$, one may ask whether the fast eigenfunction returns to its original form at $t = 0$, times the familiar dynamical phase $\frac{1}{\hbar} \int_0^T dt \epsilon_n(R(t))$, already present even if the parameters remain constant, or whether the wavefunction picks up an additional phase. Berry further showed that there are physical systems where the latter happens. Evidently, the accumulated additional phase in a cycle, now called Berry’s phase, is
\[ \gamma_n = \int_0^T dt \dot{\gamma}_n(t) = \int_0^T dt \dot{R}(t) \cdot A(R(t)) \]
\[ = \oint dR \cdot A(R) \] (6)
where a suggestive notation in terms of a vector potential has been introduced.

\[ A(R) = i \left\langle n; R \right| \nabla n; R \right\rangle \] (7)

The use of a vector potential brings out the fact that our description possess the freedom of performing gauge transformations in analogy with electromagnetism: if the phase of $|n; R\rangle$ is changed, $A$ changes by a gradient.
\[ |n; R\rangle \rightarrow e^{i \Theta(R)} |n; R\rangle \]
\[ A(R) \rightarrow A(R) - \nabla \Theta \] (8)
Nevertheless, Berry’s phase is gauge invariant because by Stoke’s law the line integral in (6) may be converted to an integral of the curl of $\mathbf{A}$ over any surface enclosed by the contour. It is seen that $\gamma_n$ is given by the flux of a gauge invariant magnetic field through the area enclosed by the adiabatic path.

$$\gamma_n = \oint d\mathbf{R} \cdot \mathbf{A}(\mathbf{R}) = \int d\mathbf{S} \cdot (\nabla \times \mathbf{A}) = \int d\mathbf{S} \cdot \mathbf{B}$$  \hspace{1cm} (9)$$

$$\mathbf{B} \equiv \nabla \times \mathbf{A}$$  \hspace{1cm} (10)

This is an invariant and unambiguous measure, unaffected by choices of phases on wavefunctions. Indeed, if the phases can be removed, but for some reason are not, $\mathbf{A}$ will be a pure gauge $\mathbf{A} = \nabla \Theta$, and Berry’s phase will vanish, because $\mathbf{B} = \nabla \times \nabla \Theta = 0$, provided $\Theta$ is non-singular.

The analogy with electromagnetic potentials and fields does not mean that the effects are necessarily of electromagnetic origin. Therefore, I shall use a mathematical terminology, which makes no reference to electrodynamics, and call the vector potential $\mathbf{A}$ a connection and the field $\mathbf{B} = \nabla \times \mathbf{A}$ a curvature. This terminology also highlights the fact that the phase arises from the non-trivial topological properties of the space spanned by the parameters.

Rather than treating the slow variables as adiabatically evolving in a prescribed way, one can quantize them. This is the content of the Born-Oppenheimer approximation$^4$ which seeks eigenfunctions of the complete Hamiltonian $H$ (1) in factorized form.

$$\Psi(\mathbf{R}, r) = \psi(\mathbf{R})|n; \mathbf{R}\rangle$$  \hspace{1cm} (11)

By projecting the complete eigenvalue equation

$$H\Psi = E\Psi$$  \hspace{1cm} (12)

on $|n; \mathbf{R}\rangle$ and ignoring off-diagonal matrix elements, one obtains an equation for $\psi(\mathbf{R})$, when $|n; \mathbf{R}\rangle$ is non-degenerate.

$$\left[ \frac{1}{2M} (\mathbf{P} - \mathbf{A}(\mathbf{R}))^2 + V(\mathbf{R}) \right] \psi(\mathbf{R}) = E\psi(\mathbf{R})$$  \hspace{1cm} (13a)

$$V(\mathbf{R}) = \epsilon_n(\mathbf{R}) + \frac{1}{2M} \sum_{n' \neq n} \langle \nabla n; \mathbf{R} | n' ; \mathbf{R}\rangle \langle n' ; \mathbf{R} | \nabla n; \mathbf{R}\rangle$$  \hspace{1cm} (13b)

$$= \epsilon_n(\mathbf{R}) + \frac{1}{2M} \left( \langle \nabla n; \mathbf{R} | \nabla n; \mathbf{R}\rangle - A^2(\mathbf{R}) \right)$$

The effective Born-Oppenheimer potential $V(\mathbf{R})$ consists of the fast eigenvalue at coordinate $\mathbf{R}$ and a small correction coming from the slow motion; the kinetic energy is that of a particle moving on a space endowed with a connection $\mathbf{A}$. Equation (13) is derived in many textbooks, but with the assumption that phases of the fast wavefunctions may be always chosen, so that the wavefunctions are real, in which case $\mathbf{A}$ vanishes. On the contrary, in view of Berry’s work, we know that it may be
impossible to remove all phases, and in general one should work with (13a), which is
gauge covariant, in the sense that any change in the phase of \( |n; \mathbb{R} \rangle \), which induces
a gauge transformation on \( A \), can be compensated in (13a) by a change of phase in \( \psi \), just as for couplings with external electromagnetic fields. Only connections with
non-vanishing curvature, \( \nabla \times A = B \neq 0 \), lead to physical, observable effects.

The Lagrangian corresponding to the effective Born-Oppenheimer Hamiltonian in
(13) is
\[
L = \frac{1}{2} M \dot{R}^2 + \dot{R} \cdot A - V(R)
\]
(14)
The velocity dependent force, induced by the fast variables, changes the velocity com-
mutator.
\[
[\dot{R}^i, \dot{R}^j] = \frac{i \hbar}{M^2} \epsilon^{ijk} B^k
\]
(15)
This is an example of dynamical modification of canonical commutation relations, a
phenomenon observed in quantum field theory for many years,\(^6\) which I shall speak
about later.

The concepts of gauge connection and curvature permeate modern particle physics,
and it is most remarkable that they now emerge in the description of atoms and
molecules. Particle physicists also consider gauge connections and curvatures that are
matrix valued quantities — these comprise the non-abelian Yang-Mills theory, which
is at the core of modern fundamental physics. Such matrices also arise in the atomic
and molecular context:\(^6\) recall that throughout I have ignored off-diagonal terms like
\( \langle n; R | \nabla \left| n'; R \right\rangle \) but these are equal to \( \frac{\epsilon_{nm}}{\epsilon_{nn'} - \epsilon_{nn}} \), unless the states are degenerate, in
which case the entire discussion must be modified along lines familiar from degenerate
perturbation theory. Final results, in the presence of degeneracy, are similar to what I
have presented above, except that the connection becomes a matrix in the degenerate
subspace.

\[
A_{ab} = i \langle n, a; R | \nabla n, b; R \rangle
\]
(16a)
and the formula for the curvature, which now also is a matrix, acquires an additional
term, beyond the curl of \( A \).

\[
B_{ab} = \nabla \times A_{ab} + i(A \times A)_{ab}
\]
(16b)
Eq. (16b) is exactly what are constructs in Yang-Mills theory.

Can one decide \textit{a priori} whether phases are trivial or whether a non-vanishing
curvature is induced by the fast variables? a general discussion is too lengthy to
present here. Suffice it to state that it is necessary that the fast energy eigenvalues
should cross somewhere in the parameter space, but not, of course, along the adiabatic
path.\(^7\)

Finally, let me remark that a correction to the \textit{classical} adiabatic theorem about
action-angle variables \( (I, \theta) \) has also been identified and the effect on angle variables
called Hannay’s angle\(^8\) is related to the semi-classical limit of Berry’s phase.

\[
\delta \theta = \lim_{\hbar \to \infty} - \frac{\partial \gamma}{\partial n}
\]
(17)
Moreover, for quadratic systems, the semi-classical result is quantum mechanically exact.9

Verification of Berry's phase, and of its consequences, falls into two categories. When the variation of parameters is under experimental control, one uses the adiabatic theorem and seeks to measure the phase change of the wavefunction, for example by interference experiments. Of course, one must be in a situation where the dynamical phase \( \int_0^T dt \epsilon_n (R(t)) \) does not dominate Berry's phase. When the parameters are themselves dynamical variables in a larger system only more indirect effects can be tested. Here one is dealing with the Born-Oppenheimer approximation, and the complete wavefunction for slow and fast variables \( \psi(R)|n; R \rangle \) does not possess any peculiar phase: Berry's phase is absorbed in \( \psi(R) \). In these cases, the presence of the connection in the kinetic energy for the slow variables is established, by studying the energy spectrum of the complete system.

In fact, the need of a connection in the Born-Oppenheimer theory for some molecules was appreciated even before Berry explicated the phenomenon in its full generality. This happened because some chemists did not begin with the textbook version of the Born-Oppenheimer Hamiltonian, but attempted to derive it from first principles. They noticed that it was not always possible to choose phases of the fast wavefunctions so that they be real and single-valued. Consequently a "vector-potential-type term" was added to the slow Hamiltonian to deal with the problem.10 With the advent of Berry's analysis, several such systems have been studied and it is claimed that the observed vibrational levels do indeed verify the need for a connection.11 The indirect effect of Berry's phase in other physical situations has also been analyzed. These include the Hall effect,12 spin and statistics of quasiparticles such as vortices in two-dimensional systems,13 and conductance in low dimensional metals.14

Direct measurement of the phase change when parameters are experimentally controlled has been accomplished in optical experiments concerned with the rotation of the polarization vector of light in helically wound optical fibers and in circularly polarized NMR experiments.15

My last chapter in this story of Berry's phase concerns its role in modern quantum field theory, where it gives another point of view on the anomaly phenomenon. This peculiar feature of second quantized field theories is probably unfamiliar to you, so let me first explain it.5

I begin by reminding you that the quantum mechanical revolution has not erased our reliance on the earlier classical physics. Indeed when proposing a theory, we begin with classical concepts and construct models according to the rules of classical, pre-quantum physics. We know, however, such classical reasoning is not in complete accord with quantum reality. Therefore, the classical model is reanalyzed by the rules of quantum physics, which comprise the true laws of nature, i.e. the model is quantized. For a long time it was believed that symmetries of a theory are not affected by the transition from classical to quantum rules. However, more recently we have learned that this is not so. In a quantized theory, some symmetries of classical physics may disappear because symmetry violating processes, which are not seen classically, can occur when the analysis is conducted with quantum effects taken into consideration.
Such tenuous symmetries are said to be *anomalously* broken. Although present classically, they are absent from the quantum version of the theory, unless the model is carefully arranged to avoid this effect.

Anomalously or quantum mechanically broken symmetries play a crucial role in our present-day theories of elementary particles. In some instances they save the models from possessing too much symmetry, which would not be in accord with experiment. In other instances, the desire to preserve a symmetry in the quantum theory places strong constraints on model building and gives experimentally verified predictions. For example, the equality in the number of quarks and leptons is understood in these terms. Also, the present-day excitement about strings derives from the fact that only very few string models can be adjusted to avoid quantum mechanical, anomalous breaking of those symmetries that make string theory free of the infinities plaguing conventional field theories. Thus the number of consistent string models appears very limited, and a limitation of theoretical possibilities is what every model builder looks for. Anomalous symmetries are also beginning to play a role in other branches of physics, like condensed matter.

For a specific example of this phenomenon, consider massless fermions moving in an electromagnetic field described by electromagnetic potentials. Since massless fermions possess a well-defined helicity, we shall consider fermions with only one helicity. Such systems are an ingredient in theories of quarks and leptons. Moreover, they also arise in condensed matter physics, not because one is dealing with massless, single-helicity particles, but because a well-formulated approximation to some many-body Hamiltonians can result in a first order matrix equation which is identical to the equation for single-helicity massless fermions, i.e., a massless Dirac equation for a spinor $\psi$. As a first quantized theory, the system is gauge covariant, in that a gauge transformation on the electromagnetic potential can be compensated by a change of the wavefunction, $\psi$. Moreover, the norm of the wavefunction is time-independent: $N = \int \psi^\dagger \psi$, $\frac{d}{dt} N = 0$. So far there are no surprises.

To construct a quantum field theory from the above, the model is second quantized: the wavefunction $\psi$ is promoted to an operator $\Psi$ and the state space for the theory is a many-particle fock space. Moreover, the ground state of the second quantized field theory has to be the filled Dirac sea, so that the negative energy solutions of the first quantized dirac equation are eliminated. Of course all states are functionals of the background electromagnetic potential in which the fermions move.

One expects that the second quantized theory also possesses gauge invariance, and that as a consequence of gauge invariance the total charge, to which the first quantized norm is promoted, $Q = \int \Psi^\dagger \Psi$, is conserved. In fact, this is not true: the charge is not conserved; rather one finds

$$\frac{d}{dt} Q \propto \int E \cdot H$$

where $E$ and $H$ are the background electric and magnetic fields, and correspondingly gauge invariance is lost.$^5$

There are many ways of arriving at the result that the gauge symmetry in this model is anomalously broken. In one physically transparent argument, it is established


that the process of filling the negative energy sea to define the field theoretic ground state necessarily violates gauge invariance.\textsuperscript{5}

Berry’s ideas provide another viewpoint.\textsuperscript{16} The fermion field operators $\psi$ are thought of as fast variables, the analogs of $p$ and $r$. The background electromagnetic potential is viewed as an external parameter; it is the analog of $R$. The Fock-space state vectors are functionals of the background potential; they are analogs of $|n;R\rangle$.

An analysis shows that when the background electromagnetic potentials are gauge transformed — this can be an adiabatic change — the states acquire a phase variation and in this way lose electromagnetic gauge invariance. Thus the anomaly phenomenon is a manifestation of Berry’s phase in quantum field theory.\textsuperscript{16} Moreover, symmetry in quantum theory can also be seen through the realization of the symmetry algebra in the canonical commutation relations. Correspondingly, when the symmetry is anomalously or quantum mechanically broken, the algebra acquires a dynamical modification.\textsuperscript{5} This too is understood from Berry’s analysis, as I have indicated in Eq. (15).

We appreciate Berry’s contribution, not necessarily for the new physics that it exposes, but rather for its universality with which it spans phenomena as diverse as atomic physics and modern particle physics.

REFERENCES


