

Quantum Adiabatic Theorem and Berry's Phase Factor

Page Tyler

Department of Physics, Drexel University

Abstract

A study is presented of Michael Berry's observation of quantum mechanical systems transported along a closed, adiabatic path. In this case, a *topological* phase factor arises along with the dynamical phase factor predicted by the adiabatic theorem.

1 Introduction

In 1984, Michael Berry pointed out a feature of quantum mechanics (known as Berry's Phase) that had been overlooked for 60 years at that time. In retrospect, it seems astonishing that this result escaped notice for so long. It is most likely because our classical preconceptions can often be misleading in quantum mechanics. After all, we are accustomed to thinking that the phases of a wave functions are somewhat arbitrary. Physical quantities will involve $|\Psi|^2$ so the phase factors cancel out. It was Berry's insight that if you move the Hamiltonian around a closed, adiabatic loop, the relative phase at the beginning and at the end of the process is not arbitrary, and can be determined.

There is a good, classical analogy used to develop the notion of an adiabatic transport that uses something like a Foucault pendulum. Or rather a pendulum whose support is moved about a loop on the surface of the Earth to return it to its exact initial state or one parallel to it. For the process to be adiabatic, the support must move slow and steady along its path and the

period of oscillation for the pendulum must be much smaller than that of the Earth's.

Adiabatic Theorem says that if a system begins a time t , in an instantaneous eigenstate $\psi_n(x, t)$, then all later times will remain in that same eigenstate, but develop phase factors. It's easy enough to state this theorem. It even seems plausible. But for good practice, we'll prove it, observe how the two types of phase factors emerge and study Berry's phase.

2 Quantum Adiabatic Theorem

If the Hamiltonian is time-dependent, then so are the eigenfunctions and eigenvalues:

$$H(t)\psi_n(t) = E_n(t)\psi_n(t) \quad (1)$$

However, at any particular instant, they still constitute a complete, orthonormal set so $\langle \psi_n(t) | \psi_m(t) \rangle = \delta_{nm}$, and the general solution to the time-dependent Schrodinger equation can be expressed as a linear combination of them:

$$\psi(t) = \sum_n c_n(t) \psi_n(t) e^{i\theta_n(t)} \quad (2)$$

Where the phase factor $\theta_n(t) \equiv -\frac{1}{\hbar} \int_0^t E_n(t') dt'$.

Substituting equation (2) into the time-dependent Schrodinger equation we have:

$$i\hbar \sum_n (\dot{c}_n \psi_n + c_n \dot{\psi}_n + i c_n \psi_n \dot{\theta}_n) e^{i\theta_n} = \sum_n c_n (H\psi_n) e^{i\theta_n} \quad (3)$$

From equation (1), the last two terms cancel leaving $\sum \dot{c}_n \psi_n e^{i\theta_n} = -\sum c_n \dot{\psi}_n e^{i\theta_n}$. Invoking orthonormality and taking the inner product with ψ_m we

obtain $\sum \dot{c}_n \delta_{mn} e^{i\theta_n} = -\sum c_n \langle \psi_m | \dot{\psi}_n \rangle e^{i\theta_n}$ or:

$$\dot{c}_m(t) = -\sum_n c_n \langle \psi_m | \dot{\psi}_n \rangle e^{i(\theta_n - \theta_m)} \quad (4)$$

Taking the time derivative of equation (1) and again the inner product with ψ_m yields

$\langle \psi_m | \dot{H} | \psi_n \rangle + \langle \psi_m | H | \dot{\psi}_n \rangle = \dot{E}_n \delta_{mn} + E_n \langle \psi_m | \dot{\psi}_n \rangle$. So Now, if we exploit the hermiticity of H so that $\langle \psi_m | H | \dot{\psi}_n \rangle = E_m \langle \psi_m | \dot{\psi}_n \rangle$, then:

$$\langle \psi_m | \dot{H} | \psi_n \rangle = (E_n - E_m) \langle \psi_m | \dot{\psi}_n \rangle \quad (5)$$

for $n \neq m$.

Plugging this all into equation (4), we find that:

$$\dot{c}_m(t) = -c_m \langle \psi_m | \dot{\psi}_m \rangle - \sum_n c_n \frac{\langle \psi_m | \dot{H} | \psi_n \rangle}{E_n - E_m} e^{i(\theta_n - \theta_m)} \quad (6)$$

Next, we can apply the *adiabatic approximation* which is simply to assume that \dot{H} is very, very small and so we can drop off the last term completely. And we are left with just $\dot{c}_m(t) =$

$-c_m \langle \psi_m | \dot{\psi}_m \rangle$ which has the solution:

$$c_m(t) = c_m(0) e^{i\gamma_m(t)} \quad (7)$$

Where $\gamma_m(t) \equiv i \int_0^t \langle \psi_m(t') | \dot{\psi}_m(t') \rangle dt'$.

Therefore, if $c_n(0) = 1$, and $c_m(0) = 0$ ($m \neq n$), then the particle remains in the n th eigenstate of the time-evolving Hamiltonian, only picking up phase factors along the way. And equation (2) is:

$$\Psi_n(t) = e^{i\theta_n(t)} e^{i\gamma_n(t)} \psi_n(t) \quad (8)$$

The phase factor, $\theta_n(t)$ is commonly referred to as the "dynamic phase". And $\gamma_n(t)$ is the so-called "geometric phase".

3 Geometric Phase

Consider that $\psi_n(t)$ is time-dependent due to some parameter of the Hamiltonian that is changing with time. Say, for example, the width of an expanding, square well $R(t)$. Thus

$\frac{\partial \psi_n}{\partial t} = \frac{\partial \psi_n}{\partial R_n} \frac{dR}{dt}$. Here, the geometric phase would look something like:

$$\gamma_n(t) = i \int_{R_i}^{R_f} \left\langle \psi_n \left| \frac{\partial \psi_n}{\partial R} \right\rangle dR \quad (9)$$

Where R_i and R_f are the initial and final values for $R(t)$. And if the Hamiltonian returns to its original form so that $R_i = R_f$, then the geometric phase would equal zero and there really isn't much to see. But now, let's consider there being multiple, changing parameters (R s) so that there are at least two dimensions changing in our expanding, square well. In this case, we have:

$$\frac{\partial \psi_n}{\partial t} = (\nabla_R \psi_n) \cdot \frac{dR}{dt} \quad (10)$$

Where $\mathbf{R} \equiv (R_1, R_2, \dots, R_N)$ and $\nabla_{\mathbf{R}}$ is the gradient with respect to each time-dependent parameter. Now, for the geometric phase, equation (9) becomes $\gamma_n(t) = i \int_{R_i}^{R_f} \langle \psi_n | \nabla_{\mathbf{R}} \psi_n \rangle \cdot d\mathbf{R}$ and if the Hamiltonian now returns to its original form, the total geometric phase change is represented by a line integral around a closed loop.

$$\gamma_n(T) = i \oint \langle \psi_n | \nabla_{\mathbf{R}} \psi_n \rangle \cdot d\mathbf{R} \quad (11)$$

And is not always zero. This equation was first obtained in 1984 by Michael Berry and it is what is known as "Berry's phase". You can see that Berry's phase only depends on the path taken and not the velocity around the path. On the other hand, dynamic phase depends very much on elapsed time.

4 Conclusion

Aharonov-Bohm is another well-known instance of where our classical preconceptions are misleading. Interestingly, Berry's formula can confirm the Aharonov-Bohm result and reveals that the effect is in fact a particular instance of geometric phase. Another physically relevant and rather simple case is any of which the eigensystem of a real Hamiltonian operator H depending on a set of external parameters q . The eigenstates of a real operator may always be chosen to be real, at any q -point. It is straightforward to check that continuous real eigenstates realize parallel transport. In the real case, it is therefore easy to get rid of complex phases coming from the time evolution.