Physics 556 Spring 2007 **Note 1** Philip B. Allen

"Berry phase" of π under rotation by 2π in simple quantum systems.

A sign change of the wavefunction under cyclic adiabatic evolution was found by Longuet-Higgins in molecules. The Hamiltonian is purely real and the wavefunctions can also be chosen purely real. Berry's fundamental contribution was to formulate a general way of understanding how the complex phase evolves when a wavefunction undergoes cyclic adiabatic evolution, and the sign change of real wavefunctions is a special case of a complex phase $e^{i\phi}$ with $\phi = \pm\pi$. This phase change of π occurs when the molecule has a two-dimensional configuration space that contains a point where the ground state is doubly degenerate, and when the adiabatic path surrounds this point. The same phase change occurs in two-dimensional solids (graphene, for example) when the wavevector is altered adiabatically around a special $\vec{k}$-point in the 2-dimensional $\vec{k}$-space where the Bloch state is doubly degenerate. The mathematics, although elementary, can get quite confusing. This note is intended to introduce the needed mathematics of 2 x 2 matrices, and subsequent notes will give examples.

The archetype of eigenfunction sign change (phase change by π) upon circulation by 2π is the system of matrix and eigenvectors

$$\hat{M} = \begin{pmatrix} \cos\psi & \sin\psi \\ \sin\psi & -\cos\psi \end{pmatrix},\ \hat{M}|\pm\rangle = \pm|\pm\rangle,\ |+\rangle = \begin{pmatrix} \cos(\psi/2) \\ \sin(\psi/2) \end{pmatrix}, \text{ and } |-\rangle = \begin{pmatrix} \sin(\psi/2) \\ -\cos(\psi/2) \end{pmatrix}. \quad (1)$$

These eigenvectors, which are purely real, change sign on a complete rotation $0 \rightarrow \psi \rightarrow 2\pi$. The key property is not that the matrix elements $M_{\alpha\beta}$ need to be exactly sine and cosine, but that they should evolve in sign in the same way as sine and cosine when the "angle" ψ revolves once. This needs clarification, because, for example, ψ is not always a true physical angle.

Consider a general 2 x 2 real symmetric matrix,

$$\begin{pmatrix} a(\phi)+g(\phi) & f(\phi) \\ f(\phi) & a(\phi)-g(\phi) \end{pmatrix} = a\hat{1} + \sqrt{g^2+f^2}\begin{pmatrix} \cos\psi & \sin\psi \\ \sin\psi & -\cos\psi \end{pmatrix} \text{where } \tan[\psi(\phi)] = \frac{f(\phi)}{g(\phi)}. \quad (2)$$

Assume that the parameter ϕ lives in a physical space and can be evolved $0 \rightarrow \phi \rightarrow 2\pi$. Also assume that the Hamiltonian matrix is invariant under such a full rotation by 2π. Thus $f(\phi)$ and $g(\phi)$ are periodic with period 2π. Let us also assume they are smooth. The eigenstates of (2) are those of Eq.(1), and change sign under $0 \rightarrow \psi \rightarrow 2\pi$. The problem is to figure out how the abstract parameter ψ evolves when the physical parameter ϕ undergoes a full rotation. It may or may not increase by 2π. There are many possibilities. If either $f(\phi)$ or $g(\phi)$ has no sign change during $0 \rightarrow \phi \rightarrow 2\pi$, then the evolution of ψ is $\psi_0 \rightarrow \psi \rightarrow \psi_0$, that is, it returns to its original value with no complete circuit. In this case, the rotation of ϕ by 2π does not yield a change of sign of the eigenvector (no Berry phase.) The next possibility is that both f and g have two sign changes. Since they are periodic and smooth, they cannot have an odd number of sign changes. Both sine and cosine have two sign changes. Then the angle ψ evolves as $\psi_0 \rightarrow \psi \rightarrow \psi_0 + 2\pi$, one circulation, if the zeros of f and g are interleaved on the path $0 \rightarrow \phi \rightarrow 2\pi$, as are the zeros of sine and cosine. This case gives a Berry phase of π.

But if both zeros of *f* lie between the two zeros of *g*, or *vice versa*, then $\psi_0 \to \psi \to \psi_0$ without circulation, and there is no Berry phase. A general rule is not necessarily needed, since each case has to be examined separately anyway.

A real Hamiltonian does not have to look real if the basis functions are complex. For example, the matrix (1) takes the form

$$U^{+}MU = \tilde{M} = \begin{pmatrix} 0 & e^{i\theta} \\ e^{-i\theta} & 0 \end{pmatrix} \text{ with eigenvectors } |+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{i\theta/2} \\ e^{-i\theta/2} \end{pmatrix} \text{ and } |-\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{i\theta/2} \\ -e^{-i\theta/2} \end{pmatrix}$$

after unitary transformation by $U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix}$. Once again, note that a full rotation of the elements of the matrix by 2π generates a rotation by π of the eigenfunctions. The Berry phase is gauge-invariant, as Berry showed in full generality. If the matrix is fully complex Hermitean, the equations become

$$\begin{pmatrix} a & c \\ c^* & b \end{pmatrix} = \frac{1}{2}(a+b)\hat{1} + \sqrt{\left(\frac{1}{2}[a-b]\right)^2 + |c|^2}\begin{pmatrix} \cos\theta & \sin\theta e^{i\phi} \\ \sin\theta e^{-i\phi} & -\cos\theta \end{pmatrix} \text{ where } \theta = \tan^{-1}\left(\frac{2|c|}{a-b}\right) \text{ and}$$

$c = c_1 + ic_2 = |c|\exp(i\phi)$. The corresponding eigenvectors are

$$|+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} \cos(\theta/2)e^{i\phi/2} \\ \sin(\theta/2)e^{-i\phi/2} \end{pmatrix} \text{ and } |-\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} \sin(\theta/2)e^{i\phi/2} \\ -\cos(\theta/2)e^{-i\phi/2} \end{pmatrix}$$

Note that in this case, a phase change of π of the wavefunction follows from a phase change of 2π in either angle θ or ϕ, but, if both angles change by 2π, then there is no phase change in the wavefunction. The more complete analysis of Berry is needed to classify the behavior. The subsequent notes will be concerned only with the case of real Hamiltonian matrices.

One of the important special cases of non-zero Berry phases concerns circulation on a path that surrounds a "point" where the Hamiltonian has a degeneracy. The equation above shows an elementary fact about double degeneracy in a 2 x 2 matrix. It is possible to have a double degeneracy only if three equations are simultaneously satisfied: (1) $a=b$, (2) $c_1=0$, and (3) $c_2=0$. Usually this only happens if forced by some symmetry. When the Hamiltonian is not fundamentally complex but can be transformed to purely real, then c_2 is automatically zero and only the first two equations need to be satisfied. In 3-dimensional solids, the $\vec{k}$ -space is 3-dimensional. This means that if there is a degeneracy at some point $\vec{k}_0$, then there is a two-dimensional space of angles evolving from $\vec{k}_0$, and one can expect to satisfy both Eqs.(1) and (2) for some special angles. Therefore, a line of double degeneracies is expected generically, often containing a point of symmetry-forced degeneracy, which might be considered the source of the line. This is the topic of one of the other sets of notes.