CHAPTER VI

DISCUSSION AND CONCLUSION

A system slowly transported round a circuit will return in its original state, this is the content of the adiabatic theorem. In Berry's paper, he assumes that the energy eigenstate undergoing adiabatic evolution is non-degenerate. If this is so, then a cyclic variation C of the external parameters will return the system to its original state, multiplied by a complex number of unit modulus, the product of a dynamical phase and a geometric phase. He shows that the total phase of the transported state

$$|\psi(T)\rangle = \exp[i\gamma_n(C)] \exp\left[-\frac{i}{\hbar}\int_0^T dt\, E_n(\mathbf{R}(t))\right]|\psi(0)\rangle$$

is dominated by the dynamical part, because the time $T \rightarrow \infty$ in the adiabatic limit, and it might be thought that this must overwhelm the geometrical phase γ_n and make its physical effects difficult to detect.

The phase factor experienced by a Born-Oppenheimer wave function under traversal by the nuclei of a closed path was discussed in a more general way by Mead and Truhlar, who showed that the resulting multiple-valuedness of the electronic wave function can be removed, but only at the cost of introducing a vector potential like effect was analogous to that of Aharonov and Bohm, the name molecular Aharonov-Bohm effect was proposed for this phenomenon. If we will change the Berry phase. This is akin to making a gauge choice in electromagnetism.

$$|n(\mathbf{R})\rangle \rightarrow \exp[i\,\Lambda(\mathbf{R})]\,|n(\mathbf{R})\rangle$$

then the vector potential will change and with it $\gamma_n(C)$,

$$\mathbf{A}_n(\mathbf{R}) \rightarrow \mathbf{A}_n(\mathbf{R}) + \nabla_{\mathbf{R}}\Lambda\ (\mathbf{R})$$

In the context of the Born-Oppenheimer approximation. Kuratsuji and Iida were found the Berry's phase in a path integral framework, as opposed to a Schrödinger description. Such a framework lends itself well to the study of Born-Oppenheimer systems, where one is interested in separating the integrations over fast electronic variables and slow nuclear variables. Typically, one performs the electronic path integration first, in a fixed nuclear background, and making the adiabatic approximation that electronic transitions do not occur. The result is an effective action involving only the nuclear coordinates. They have presented a path integral including the topological structure associated with the quantum adiabatic process. By considering the trace of the evolution operator $\mathrm{Tr}\left(\exp\left[-\frac{i}{\hbar}\hat{H}\,T\right]\right)$, in adiabatic approximate, they show that it is given by

$$K^{\mathrm{eff}}(T) = \sum_n \int \exp\left[\frac{i}{\hbar}\left(S_n^{ad} + \hbar\,\gamma_n(C)\right)\right] \prod_t d\mu\,(\mathbf{R}_t\,,\mathbf{P}_t)$$

where $\mathbf{R}(T) = \mathbf{R}_0$ (since for the trace we want to return to the same state at t = T), and where γ_n is now evaluated over closed loops $\mathbf{R}_0 \rightarrow \mathbf{R}(t) \rightarrow \mathbf{R}(T) = \mathbf{R}_0$ in parameter space (R-space).

$$\gamma_n(C) = i\oint_C \langle n(\mathbf{R})|\nabla_{\mathbf{R}}\, n(\mathbf{R})\rangle \cdot d\mathbf{R} = \oint_C \mathbf{A}_n(\mathbf{R}) \cdot d\mathbf{R}$$

Here Berry's phase has a strikingly direct effect on the energy levels. If C is a closed classical path and (P(t), Q(t)) the corresponding trajectory in phase space, then they find the following quantization rule

$$\oint_C \mathbf{P}\cdot d\mathbf{R} = \left(n + \frac{\alpha}{4} - \frac{\gamma(C)}{2\pi}\right) 2\pi\hbar.$$

The form of this phase is particularly simple near a point in parameter space where two eigenstates become degenerate. In this case, the two states acquire phase equal to plus or minus one half the solid angle $\Omega(C)$ subtended by the Hamiltonian trajectory at the degeneracy. And can shows that geometrical phase is the flux though C of the magnetic field of a monopole strength 1/2 located at the origin of magnetic field space (at the degeneracy).

$$\gamma_{\uparrow}(t) = \oint\!\!\oint_S \mathbf{B}(\mathbf{R}) \cdot d\mathbf{S} = \pm\pi\left(1 - \cos\theta\right)$$

$$= \pm\frac{\Omega(C)}{2}$$

This is further confirmation of the geometrical nature of Berry's phase. By using this result, we were able to rederive Dirac's famous relation between electric and the magnetic charge (Holstein, 1989; Kuratsuji and Iida, 1985). One should extend the present treatment to the spin 1/2 charged particles circling a magnetic field where adiabatic not hold.

Now, the geometrical phase has been generalized in various ways. Wilczek and Zee showed that even for a system with degenerate states, where the adiabatic theorem does not hold, it is possible to define and calculate a geometrical phase (Wilczek and Zee, 1983; 1984). Berry developed a method of calculating the relevant phase when the change in the Hamiltonian is not sufficiently slow for the adiabatic approximation to hold (Berry, 1985). A nonadiabatic process was discussed by Bulgac (1987) in path integral framework. An important generalization was made by Aharonov and Anandan (1987). They showed that the geometrical phase is directly related to the cyclic evolution of the wave function, and not to the change in the Hamiltonian. In particular, adiabaticity is not necessary for this phase to appear.