A PROBLEM IN SEMICLASSICAL ADIABATIC THEORY

by

M.V.BERRY

H.H.Wills Physics Laboratory, Tyndall Avenue, Bristol

BS81TL, UK

Consider a family of quantal Hamiltonians (Hermitian operators) parameterized by $R=(X,Y,Z\ldots)$ and denoted by $\hat{H}(R)$. For any R let the spectrum be discrete, with eigenvalues $E_n(R)$ and eigenstates $|n;R\rangle$ $(n=1,2,3\ldots)$. Now imagine $\hat{H}$ taken slowly round a circuit C in parameter space, i.e. $R=R(t)$ with $R(T)=R(0)$ and $T\rightarrow\infty$ (for example $\hat{H}$ could describe a quantum particle influenced by slowly-varied external electromagnetic fields). The system's state $|\Psi(t)\rangle$ evolves according to the Schrödinger equation

$$\hat{H}(R(t))\,|\Psi(t)\rangle = i\hbar\frac{\partial}{\partial t}\,|\Psi(t)\rangle. \tag{1}$$

Then the quantal adiabatic theorem [1] guarantees that if the initial state is an eigenstate, i.e. if

$$|\Psi(0)\rangle = |n;R(0)\rangle \tag{2}$$

then the system will remain in the state $|n;R(t)\rangle$ as R varies, and in particular will return to the original state at t=T when the circuit is completed. But it will acquire a phase factor [2] given by

$$\langle\Psi(0)|\Psi(T)\rangle = \exp\{-i\int_0^T E_n(R(t)dt/\hbar\}\exp\{i\gamma_n(C)\} \tag{3}$$

In this formula, the first factor gives the expected 'dynamical phase' which accompanies the evolution of any state even if the parameters are kept constant. The second factor represents a new phenomenon: a 'geometrical phase' $\gamma_n(C)$ that is independent of the time T taken to traverse the circuit. As shown in [2], $\gamma_n(C)$ is given by the flux through C of a phase 2-form $V_n(R)$, i.e.

$$\gamma_n = -\int_{\partial S = C} V_n \ (R) \tag{4}$$

where

$$V_n(R) = \text{Im} \langle dn;R| \wedge |dn;R\rangle$$
$$= \text{Im} \sum_{m \neq n} \frac{\langle n;R|d\hat{H}(R)|m;R\rangle \wedge \langle m;R|d\hat{H}|n;R\rangle}{[E_m(R) - E_n(R)]^2} \tag{5}$$

and where the differential forms $|dn;R\rangle$ and $d\hat{H}(R)$ give the changes in the state and the Hamiltonian associated with small displacements in parameter space. The geometrical phase has a variety of physical applications [2-6] and can be interpreted in terms of anholonomy for Hermitian line bundles [7].

The problem to which I wish to draw attention is the semiclassical limit ($\hbar \to 0$) of the phase 2-form for systems whose classical motion is chaotic.

Consider first the simpler situation where motion is integrable [8,9], that is where the system (with N freedoms) is such that there exist N constants of motion restricting orbits to N-tori in the 2N-dimensional phase space. Each torus is labelled by its actions $I = (I_1 \ldots I_N)$. If now the classical Hamiltonian H(R) is slowly varied round a circuit C in parameter space, the classical adiabatic theorem [8,10,11] guarantees that the orbit will remain on the torus I as R varies, even though the energy will not be conserved.

But this is not the whole story, because such classical integrable systems also display anholonomy, which manifests itself in the angle variables $\theta = (\theta_1 \ldots \theta_N)$ describing position on the torus I. It was recently discovered [12] that the angles before and after the circuit are related by

$$\theta(T) = \theta(0) + \int_0^T dt \ w(I;R(t)) + \Delta\theta(I;C) \tag{6}$$

This formula is analogous to (3): the integral over the instantaneous frequencies $w = (w_1 \ldots w_N)$(of motion round the irreducible cycles of the torus I) is the expected 'dynamical' evolution of the angles which would occur even if H were kept constant. The shifts $\Delta\theta=(\Delta\theta_1 \ldots \Delta\theta_N)$ are the recently-discovered [12] 'adiabatic angles'. They too can be expressed as the flux of a 2-form through C, i.e.

$$\Delta\theta(I;C) = -\frac{\partial}{\partial I}\int_{\partial S=C} W(I;R) \tag{7}$$

where the angle 2-form can be written in terms of W, which is given [13] as an integral over the angles θ of the torus I at R by

$$W(I;R)=\frac{1}{(2\pi)^N}\oint d\theta \sum_{i=1}^{N} dp_i \wedge dq_i \tag{8}$$

(Note that dp_i and dq_i are parameter-space forms and not phase-space ones.) The semiclassical connection between the quantal 2-form V (equations 4 and 5) and the classical 2-form W can be shown [13] to be

$$V_n(R) \xrightarrow[\hbar\to 0]{} -\frac{1}{\hbar}\, W(I;R) \tag{9}$$

where the quantum state is now labelled by $n=(n_1 \ldots n_N)$, related to I by the Bohr-Sommerfeld ('torus quantization' [14]) association

$$I = (n+\sigma)\hbar \tag{10}$$

in which $\sigma = (\sigma_1 \ldots \sigma_N)$ are the Maslov indices.

For classically chaotic systems, equations (6-10) have no meaning, because there are no tori and hence no actions or angles. But the quantal phase 2-form V_n still exists, and must have a semiclassical interpretation. A clue to the direction in which to search for this interpretation comes from the observation [2,3,15] that $V_n(R)$ has singularities at points $R=R^*$ where the state $|n\rangle$ is degenerate with the state $|n\pm 1\rangle$. The singularity at R^* is that of a monopole, with strength $\pm 1/2$ if $|n\rangle$ degenerates with $|n\mp 1\rangle$. It has long been known [16] that degeneracies have codimension 3 in families of generic Hermitian matrices. Thus in a space of three parameters R=(X,Y,Z) the singularities can be written in terms of the divergence of V_n as

$$dV_n(R) = dX_\wedge dY_\wedge dZ \sum_\ell \varepsilon_\ell \delta(R-R_\ell^*), \qquad (11)$$

where ℓ labels the points of degeneracy and $\varepsilon_\ell = \pm 2\pi$ if the strength is ± 1.

Semiclassically, the average of the divergence of V_n (over a small domain in R space) must give the signed density of degeneracies involving the state $|n\rangle$. But how is this related to the system's chaotic dynamics? For a special class of real symmetric Hamiltonians, the density of (codimension 2) degeneracies ('diabolical points') can be estimated [17], but it is proving difficult to find a general formulation.

REFERENCES

[1] Berry, M.V. 1984, Proc.Roy.Soc.Lond.A.392 45-57.

[2] Messiah,A 1962 Quantum Mechanics (North-Holland: Amsterdam)

[3] M.V.Berry 1985, Quantum, Classical and Semiclassical Adiabaticity in proceedings of XVIth ICTAM congress (North-Holland: eds.F.Niordson and N.Olhoff). In press.

[4] Wilkinson,M 1984 J.Phys.A. In press.

[5] Avron, J.E. and Seiler, R,1984. To be published.

[6] Mead, C.A. and Truhlar, D.G. 1979 J.Chem.Phys. 70 2284-2296.

[7] Simon, B 1983 Phys.Rev.Lett. 51 2167-2170.

[8] Arnold, V.I. 1978 Mathematical Methods of Classical Mechanics (Springer: New York).

[9] Lichtenberg,A.J. and Lieberman, M.A. 1983 Regular and Stochastic Motion (Springer: New York).

[10] Arnold,V.I. 1983 Geometrical Methods in the Theory of Ordinary Differential Equations (Springer: New York).

[11] Dirac,P.A.M. 1925 Proc.Roy.Soc.Lond. 107 725-734.

[12] Hannay, J.H. 1984 J.Phys.A. In press.

[13] Berry, M.V. 1984 J.Phys.A. In press.

[14] Berry, M.V. 1983, Semiclassical Mechanics of Regular and Irregular Motion in Chaotic Behavior of Deterministic Systems (Les Houches Lectures XXXVI,

eds. G. Iooss, R.H.G. Helleman and R. Stora (North--Holland: Amsterdam) pp171-271.

[15] Berry, M.V. 1984 'Aspects of Degeneracy' in Proc. Como Conference on Quantum Chaos (G. Casati, ed) (Plenum:-London). In press.

[16] Von Neumann, J. and Wigner, E. 1929 Phys.Z. **30** 467-470.

[17] Berry, M.V. and Wilkinson, M. 1984 Proc.Roy.Soc.Lond. **A392**, 15-43.