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Parameter space analogue of the Aharonov-Bohm effect

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Abstract. A simple dynamical system having a Berry phase component completely analogous to the Aharonov-Bohm circuit phase is presented. The underlying 'magnetic-vector-potential-like' object is identified. This parameter-space vector plays a vector-potential-like role at both quantal and classical levels.

1. Introduction

A magnetic vector potential can have no effect on the motion of a classical charged particle which passes through regions in which the potential has zero curl. Yet such regions significantly affect the wavefunction in the corresponding quantal case (Ehrenburg and Siday 1949, Aharonov and Bohm 1959). Briefly, an interferometer whose two arms encircle an infinitely long solenoid will record a fringe shift proportional to the circuit phase difference $(q/\hbar) \oint A \cdot dl = (q\phi/\hbar)$ when the solenoid is energised. Such classical-quantal contradictions are of general interest and consequently it is natural to enquire whether the Aharonov-Bohm (AB) effect is the sole instance of its kind. That is, are there other ways whereby nature acts in a manner similar to A(r) on the phase of the wavefunction to produce significant physical effects, but fails to touch the motion of the corresponding classical object? It is the purpose of this paper to provide an affirmative answer to this question using a general theoretical development given by Berry (1984).

Berry was concerned with the adiabatic transport of a system (classical or quantal) in the space of its parameters. If the time variation of the parameters is slow enough for the quantal adiabatic theorem to apply then, over and above the usual 'dynamical phase' (i.e. $-\hbar^{-1} \int_0^T dt \varepsilon_n(t)$), there appears an excess phase γ which we shall call the geometric circuit phase (GCP).

The properties of the GCP are most strikingly revealed when the system, initially in some eigenstate, traverses a closed circuit in parameter space. Then, the GCP depends only on the initial eigenstate and on the geometry of the circuit C.

Now, as Berry noted, the AB effect can be viewed as the excess phase generated when (see figure 1) a charge, confined within a small box, is adiabatically transported around, say, a single flux line which never penetrates the box. Since $\hat{H} = H(\hat{p} - (e/c)A(r), \hat{r} - R)$, where R(t) represents the box position in real space, one can readily show that on completion of a single circuit the wavefunction changes its phase by $(q\phi/\hbar)$, where ϕ is the magnetic flux through the closed circuit C.

Next, consider adiabatic transport of the corresponding classical system. Then, provided the Hamiltonian is integrable for every point on C, the motions of the

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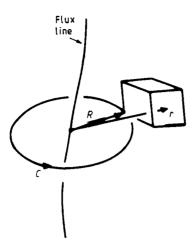


Figure 1. The adiabatic parameter space transport interpretation of the Aharonov-Bohm effect.

phase-space angle variables, θ_i are not just described by the usual formula: $\theta_i = \int_0^T dt \,\omega_i(t)$ given by the classical adiabatic theorem. Excess angles, $\Delta \theta_i$, (see Hannay 1985) whose distinctive features are best seen for cyclic parameter space paths, are generated. The $\Delta \theta_i$ (called Hannay's angles) are found to depend on the conserved tori actions and on the geometry of the closed path C.

 $\Delta \theta_i$ and $\gamma_n(C)$ are conjugate quantities at the semiclassical level. The connection between the two was worked out by Berry (1985) who found that

$$\Delta \theta_i(I_i; C) = -\hbar \frac{\partial}{\partial I_i} \gamma_{n_i}(C) = -\frac{\partial}{\partial n_i} \gamma_{n_i}(C)$$

where the last equality is semiclassically correct, since $I_i = \hbar(n_i + \sigma_i)$ according to the rule of Bohr-Sommerfeld. The σ_i are unimportant constants in the present context.

Returning to the AB effect we can now ask: what is the corresponding Hannay angle? Since **B**, the physically relevant field in an AB experiment, vanishes outside the infinite solenoid, the angle is zero. This verifies the semiclassical connection formula, as the GCP ($= q\phi/\hbar$) is action independent, i.e. it does not depend on the eigenstate of the particle inside the box. Since $\gamma \sim \hbar^{-1}$ we are, in fact, dealing with a purely quantal phenomenon, i.e. $\gamma(\hbar \to 0)$ is undefined.

We can now ask whether there are other systems which have such purely quantal geometric phases. That is, are there Hamiltonians whose cyclic, adiabatic excursions in parameter space generate a quantal GCP, while the very same excursions are classically 'hidden'. To date no such system has been identified. However, no simple *a priori* reason suggests that they do not exist. On the contrary, no physical principle suggests a unique role for the magnetic vector potential in nature.

We have found one such system, which is a generalisation of the generalised simple harmonic oscillator (GSHO) of Berry (1985) and Hannay (1985) as introduced in § 2. Our generalisation (GGSHO) is to augment the GSHO Hamiltonian by a constant external force field. The GCP is calculated using the Berry (1984) prescription. An alternate derivation is provided in § 3. The 'first principles' derivation is included since it makes clear the simple, physical reasons that lie behind Berry's GCP. The two derivations are shown to give identical answers. Additionally, the second derivation is much more general and covers any time variation of the parameters of the system Hamiltonian. Section 4 is devoted to the classical analysis, i.e. calculation of Hannay's angle. In § 5, the results obtained are compared using the semiclassical connection formula of Berry (1985). It is shown that we have indeed produced a system which behaves, in the sense discussed, as a parameter-space analogue of the AB system. The GCP has a component that is entirely quantal. Its classical manifestation, like that of the magnetic vector potential in the AB effect, is entirely 'hidden'.

Berry has pointed out that this paper draws attention to action-independent parts of classical 2-forms or, equivalently, *n*-independent quantal phases $\gamma_n(C)$.

2. Model system and its geometric phase

The model Hamiltonian is

$$\hat{H} = \frac{1}{2} [Z\hat{p}^2 + Y(\hat{p}\hat{q} + \hat{q}\hat{p}) + X\hat{q}^2] + F\hat{q}$$
(1)

with $\mathbf{R}(t) \equiv (X(t), Y(t), Z(t))$ being a time-dependent 3-vector and F being kept constant. The latter restriction is not at all essential and is used so that we may employ the familiar vector calculus instead of the much more general, but less familiar, language of 2-forms (Arnold 1978). The formula derived by Berry (1984) for the adiabatic GCP is

$$\gamma_n(C) = - \oiint d\mathbf{A} \cdot \mathbf{V}(n; \mathbf{R})$$

$$\mathbf{V}(n; \mathbf{R}) = \operatorname{Im} \nabla_{\mathbf{R}} \times \langle n(\mathbf{R}) | \nabla_{\mathbf{R}} n(\mathbf{R}) \rangle.$$
(2)

It may readily be verified that the instantaneous eigenfunctions are:

$$|n(x; \mathbf{R}) = \frac{1}{\pi^{1/4}} \frac{1}{l^{1/2}} \exp\left(-\frac{(x-a)^2}{2l^2}\right) h_n\left(\frac{x-a}{2l^2}\right) \exp\left(-\frac{i\,Yx^2}{2Z\hbar}\right)$$
(3)

where $\{h_n\}$ are the series parts of the usual Hermite polynomials and

$$a = -\left(\frac{FZ}{\omega^2}\right) \qquad l = \left(\frac{\hbar Z}{\omega}\right)^2 \omega = (XZ - Y^2)^{1/2}.$$
(4a)

The energy of the *n*th eigenstate is

$$\varepsilon_n(\boldsymbol{R}; F) = \hbar\omega(n+\frac{1}{2}) - \frac{1}{2} \frac{\omega^2 a^2}{Z}.$$
(4b)

Clearly, the only contribution to $\text{Im} \langle n(\mathbf{R}; x) | \nabla_{\mathbf{R}} n(\mathbf{R}; x) \rangle$ comes from the phase of $|n(\mathbf{R}, x)\rangle$. The **R** dependences of a and l must, insofar as they enter into the real part of $|n(x; \mathbf{R})\rangle$, necessarily give a net zero contribution to V. We obtain

$$V(n; \mathbf{R}) = -\frac{1}{2}(n+\frac{1}{2})\nabla_{\mathbf{R}}\left(\frac{Z}{\omega}\right) \times \nabla_{\mathbf{R}}\left(\frac{Y}{Z}\right) - \frac{1}{2\hbar}\nabla_{\mathbf{R}}\left(\frac{F^2Z^2}{\omega^4}\right) \times \nabla_{\mathbf{R}}\left(\frac{Y}{Z}\right).$$
 (5)

The first term in (5) is identical to that for the GSHO (Berry 1985). The new second term arises from a time dependent displacement of the centre of the wavefunction. The R dependence of a lies behind this finite second term. Notice the inverse

dependence on the quantum of action, \hbar . Notice too, that this part of the phase makes a distinct contribution to the total GCP, i.e. its magnitude reflects a different geometrical aspect of the circuit C.

In the next section we obtain the GCP in a different and much more intuitive manner which, as will be seen, elucidates the rather abstruse-looking basic formula (2) by linking it to more familiar physical concepts.

3. A physically motivated deduction of the phase anholonomy

For the GGSHO we work with the polar form

$$\psi(x, t) = N(x, t) \exp -(\mathrm{i}S(x, t)/\hbar)$$

to obtain

$$\frac{\partial S}{\partial t} + \frac{Z}{2} \left(\frac{\partial S}{\partial x} \right)^2 + \frac{Xx^2}{2} + Fx + Yx \frac{\partial S}{\partial x} - \frac{Z\hbar^2}{2N} \frac{\partial^2 N}{\partial x^2} = 0$$
(6a)

$$\frac{1}{N}\frac{\partial N}{\partial t} = -Z\left(\frac{1}{N}\frac{\partial N}{\partial x}\frac{\partial S}{\partial x} + \frac{1}{2}\frac{\partial^2 S}{\partial x^2}\right) - \frac{Y}{2}\left(1 + \frac{2x}{N}\frac{\partial N}{\partial x}\right).$$
(6b)

Considerable progress can be made by using the fact that the quantal motion will be a compound of a time-dependent motion of the centre of the eigenpacket together with time-dependent changes in packet shape. The real part of the eigenpacket must clearly be a displaced Gaussian, for the ground state case. We can therefore make the tentative ansätze:

$$N_0 = \frac{1}{\pi^{1/4} l_0^{1/2}} \exp\left(-\frac{(x-a)^2}{2l_0^2}\right) \qquad S = \Gamma(t) + \alpha(t)x + \frac{1}{2}\beta(t)x^2 \tag{7}$$

for the amplitude and phase parts of the evolving ground state. The meanings of a_0 and l_0 , the two physical parameters whose time-dependences we seek, are clear. The meanings of α , β and Γ will follow in a moment. We find, using the above ansätze, from (6b), that:

$$\alpha = \frac{1}{Z} \left[\frac{\mathrm{d}a_0}{\mathrm{d}t} - \left(\frac{a_0}{l_0} \right) \frac{\mathrm{d}l_0}{\mathrm{d}t} \right]$$

$$\beta = \frac{1}{Z} \left(\frac{1}{l_0} \frac{\mathrm{d}l_0}{\mathrm{d}t} - Y \right).$$
 (8)

From the quantal Hamilton-Jacobi equation, on the other hand,

$$\frac{\mathrm{d}\alpha}{\mathrm{d}t} + \sigma\beta Z + F + \alpha Y + Z\hbar^2 a_0 / l_0^4 = 0$$
(9a)

$$d\beta/dt + Z\beta^2 + X + 2\beta Y - Z\hbar^2/l_0^4 = 0$$
(9b)

$$\frac{\mathrm{d}\Gamma}{\mathrm{d}t} + \frac{1}{2}(Z\alpha^2) - \frac{1}{2}Z\hbar^2(a_0^2/l_0^4 - 1/l_0^2) = 0$$
(9c)

are readily obtained.

Using (8) we can rewrite (9a) and (9b) as ODE in the width $l_0(t)$ and centre $a_0(t)$ of the wavefunction. The results obtained are

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{1}{Z}\frac{\mathrm{d}l_{0}}{\mathrm{d}t}\right) + l_{0}\left[X - \frac{Y^{2}}{Z} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{Y}{Z}\right)\right] - \frac{Z\hbar^{2}}{l_{0}^{3}} = 0$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{1}{Z}\frac{\mathrm{d}a_{0}}{\mathrm{d}t}\right) + a_{0}\left[X - \frac{Y^{2}}{Z} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{Y}{Z}\right)\right] = -F.$$
(10)

These two equations determine, exactly, the evolution of the ground-state wavefunction in all cases, i.e. they are true not only in the adiabatic limit but for all parameter excursions. Their correctness can be seen by taking the time-independent limit and assuming Y = 0. Then we obtain the standard result for the quantal displaced sho. Further confirmation is provided by the fact that the centre of the state, $a_0(t)$, follows the correct equation of motion for the corresponding classical oscillator (compare Berry (1985) equation (A1.1) for the F = 0 case). The equation for the state width $l_0(t)$ is non-classical compared with the typical quantum potential term $(= Z\hbar^2/l_0^3)$. In the adiabatic limit the solutions

$$l_{0} = \hbar^{1/2} \left[X - \frac{Y^{2}}{Z} - \frac{d}{dt} \left(\frac{Y}{Z} \right) \right]^{-1/2}$$

$$a_{0} = -F \left[X - \frac{Y^{2}}{Z} - \frac{d}{dt} \left(\frac{Y}{Z} \right) \right]^{-1}$$
(11)

are obtained. We see that, even in the adiabatic limit, the time-dependent wavefunction does not adjust to the instantaneous values of X, Y and Z. There occurs the characteristic rate-dependent quantity (d/dt)(Y/Z) which spoils an exact following of the varying system parameters. We shall soon see that it is this property—which the conventional adiabatic theorem neglects—that leads to the Berry geometric phase. To calculate the overall phase we must integrate the equation for $\Gamma(t)$. In the adiabatic limit the second term (9c) contributes nothing and so

$$\Gamma(t) = \frac{1}{2} \left\{ \int_0^T dt \, F^2 \left[X - \frac{Y^2}{Z} - \frac{d}{dt} \left(\frac{Y}{Z} \right) \right]^{-1} - \hbar \int_0^T dt \left[XZ - Y^2 - Z \frac{d}{dt} \left(\frac{Y}{Z} \right) \right]^{1/2} \right\}.$$
 (12)

The geometric phase is, in general, that part of Γ/\hbar which is in excess of the dynamical phase. We find

$$\gamma_{0}(C) = \frac{1}{2\hbar} \int_{0}^{T} dt \left(a^{2} + \frac{1}{2}l^{2}\right) \frac{d}{dt} \left(\frac{Y}{Z}\right)$$
$$= \frac{1}{2\hbar} \oint d\mathbf{R} \cdot \left(a^{2} + \frac{1}{2}l^{2}\right) \nabla \mathbf{R} \left(\frac{Y}{Z}\right)$$
$$= \frac{1}{2\hbar} \oint d\mathbf{A} \cdot \nabla_{\mathbf{R}} \left(a^{2} + \frac{1}{2}l^{2}\right) \times \nabla_{\mathbf{R}} \left(\frac{Y}{Z}\right)$$
(13*a*)

where we have expanded around the instantaneous frequency $\omega = (XZ - Y^2)^{1/2}$ and kept only the leading terms $\sim d/dt(Y/Z)$. The second term is the Berry phase for the GSHO—a result already obtained in Berry (1985). The first term is the extra phase due to the presence of the external field. Note that, as in the case of the Aharonov-Bohm phase, this term is inversely proportional to \hbar . In contrast the other term is independent of \hbar . It is curious that the more classical object $a_0(t)$ produces a Bohm-Aharonov-like phase, rather than $l_0(t)$ which is the more quantal of the two. Excited state GCP can be similarly worked out. We do not do so here; instead an alternative method applicable to a larger class of systems is derived in the appendix. From that general method (A5) we find the excited state GCP to be

$$\gamma_n(C) = \bigoplus d\mathbf{A} \cdot \left[\frac{(n+\frac{1}{2})}{2} \nabla_{\mathbf{R}} \left(\frac{Z}{\omega} \right) \times \nabla_{\mathbf{R}} \left(\frac{Y}{Z} \right) + \frac{1}{2\hbar} \nabla_{\mathbf{R}} (a^2) \times \nabla_{\mathbf{R}} \left(\frac{Y}{Z} \right) \right].$$
(13b)

4. The classical case

The formula for the Hannay angle is (Berry 1985)

$$\Delta \theta(I; C) = -\frac{\partial}{\partial I} \oint d\mathbf{A} \cdot \mathbf{W}(I; \mathbf{R})$$

$$\mathbf{W} = \frac{1}{2\pi} \oint d\theta(\nabla_{\mathbf{R}} p) \times (\nabla_{\mathbf{R}} q)$$
(14)

where $(p, q; I, \theta)$ refers to the 'instantaneous Hamiltonian'. Now the classical equation of motion, for the coordinate q, corresponds to an oscillator with parametrically forced frequency in an external field of strength F. Therefore, the action-angle variables for the fixed (X, Y, Z) problem are easily calculated. Taking

$$q = \left(\frac{2IZ}{\bar{\omega}}\right)^{1/2} \cos \theta + Q$$

$$p = -\left(\frac{2IZ}{\bar{\omega}}\right)^{1/2} \left(\frac{\bar{\omega}}{Z} \sin \theta + \frac{Y}{Z} \cos \theta\right) + p$$
(15)

it is readily verified that

$$\bar{\omega} = (XZ - Y^2)^{1/2} = \omega$$

$$Q = -(FZ/\omega^2)$$

$$P = (FY/\omega^2).$$
(16)

The action Hamiltonian, again at fixed X, Y, Z, is

$$H = I\omega - \frac{1}{2}(F^2 Z/\omega^2) \tag{17}$$

and

$$\boldsymbol{W}(I;\boldsymbol{R}) = -I\nabla_{\boldsymbol{R}}\left(\frac{Y}{2Z}\right) \times \nabla_{\boldsymbol{R}}\left(\frac{Z}{\omega}\right) + (\nabla_{\boldsymbol{R}}P) \times (\nabla_{\boldsymbol{R}}Q).$$
(18)

Therefore, using (14), we obtain

$$\Delta\theta(I; C) = \oiint \frac{1}{2} \left[\nabla_R \left(\frac{Y}{Z} \right) \times \nabla_R \left(\frac{Z}{\omega} \right) \right] \cdot dA$$
(19)

a result identical to that found for the GSHO.

5. A comparison of the classical and quantal results

From

$$\boldsymbol{V}(\boldsymbol{n};\boldsymbol{R}) = -\frac{(\boldsymbol{n}+\frac{1}{2})}{2} \nabla_{\boldsymbol{R}} \left(\frac{Z}{\omega}\right) \times \nabla_{\boldsymbol{R}} \left(\frac{Y}{Z}\right) - \frac{1}{2\hbar} (\nabla_{\boldsymbol{R}} a^2) \times \nabla_{\boldsymbol{R}} \left(\frac{Y}{Z}\right)$$

and in view of the semiclassical rule (exact here), $I = \hbar (n + \frac{1}{2})$ we find, using Berry's connection formula, that

$$W(I; \mathbf{R}) = -\hbar V(n; \mathbf{R})$$

where use has been made of the identity

$$(\nabla_{\mathbf{R}}P)\times(\nabla_{\mathbf{R}}Q)=-\frac{1}{2}(\nabla_{\mathbf{R}}a^2)\times\nabla_{\mathbf{R}}\left(\frac{Y}{Z}\right).$$

At this level the classical and quantal behaviours are very similar. Any parameter-space motion which contributes to V has to contribute to W. However, V and W are not observables, and it is at the observable level that we do find striking differences between the two kinds of mechanics. Any action-independent contribution to V gives (compared with Berry's connection formula) a zero Hannay angle, yet it contributes freely to the quantal phase. In other words the motion of the phase space point (Q, P), which represents the centre of the moving, constant area, phase-plane ellipse, is ignored classically. The quantal system's phase, however, registers the motion of (Q, P).

Therefore, the vector $\mathscr{A}(\mathbf{R}) = \frac{1}{2}a^2\nabla_{\mathbf{R}}(Y/Z)$ is analogous to the magnetic vector potential in the AB problem. $\mathscr{A}(\mathbf{R})$ like $A(\mathbf{r})$ does not touch the classical motion. Yet, the flux of its curl through the circuit C gives us the quantal GCP. So $\mathscr{B} = \nabla_{\mathbf{R}} \times \mathscr{A}$ is a magnetic-field-like object. Even if, all along C, \mathscr{B} vanishes, we shall still see a quantal phase, provided only that the flux of \mathscr{B} through C is finite. Although the vector $l^2 \nabla_{\mathbf{R}} (Y/Z)$ has similar properties yet it differs crucially from \mathscr{A} in that it effects both classical and quantal motions.

6. Discussion

We have described a system where adiabatic parameter-space transport generates a vector-potential-like object $\mathscr{A}(\mathbf{R})$. The fact that \mathscr{A} exists in parameter-space while the magnetic vector potential is a real-space field is irrelevant, as the AB phase can be viewed as stemming from adiabatic transport. Both vectors have identical effects on the dynamics of the cylically transported system; the effects depend, however, on whether the system obeys quantal or classical laws. A mysterious quantal phase, having no classical counterpart is generated by $\mathscr{A}(\mathbf{R})$. This phase, for $\hbar \rightarrow 0$, is undefined, just as the AB phase is undefined in the same limit. This represents the central result of the present work and it shows that there exist systems in which slow cyclic parameter variations do or do not affect the system evolution depending on whether we are using quantal or classical laws to describe the dynamics.

A subsidiary calculation (see § 3) yields a different and more physical way of understanding Berry's phase for a large class (GGSHO) of systems. Berry's formula, though correct, is not readily understandable. As we have shown, however, it arises simply because at every instant the system lags behind the instantaneous Hamiltonian. It is this lag that accumulates to give the non-zero Berry phase, $\gamma_n(C)$. Thus, this way of looking at γ parallels the analysis of Berry (1985) for the classical motion of the angle variable. That analysis, too, was physically motivated. The analysis of § 3 can also be used to calculate the Berry phase for systems which are not, at t=0, in an eigenstate of the corresponding initial Hamiltonian. It has been shown (Ghosh and Dutta-Ray 1987) that much interesting information is obtained when we look at the Berry phase for non-stationary initial states.

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Appendix. Calculation of Berry's phase for the generalised particle in a potential problem

The Hamiltonian is

$$\hat{H} = \frac{1}{2} [Z\hat{p}^2 + Y(\hat{p}\hat{q} + \hat{q}\hat{p}) + X\hat{q}^2] + V_{\text{ex}}(\hat{q})$$
(A1)

where the total potential has been split up, for reasons of mathematical convenience, into two parts. V_{ex} is all of the potential that is other than harmonic in the coordinate. Using the polar form for $\psi(x, t)$ we obtain

$$\frac{\partial S}{\partial t} + \frac{Z}{2} \left(\frac{\partial S}{\partial x} \right)^2 + \frac{Xx^2}{2} + V_{ex}(x) + Yx \frac{\partial S}{\partial x} - \frac{Z\hbar^2}{2N} \frac{\partial^2 N}{\partial x^2} = 0$$

$$\frac{1}{N} \frac{\partial N}{\partial t} = -Z \left(\frac{1}{N} \frac{\partial N}{\partial x} \frac{\partial S}{\partial x} + \frac{1}{2} \frac{\partial^2 S}{\partial x^2} \right) - \frac{Y}{2} \left(1 + \frac{2x}{N} \frac{\partial N}{\partial x} \right).$$
(A2)

Define a new quantity \tilde{S} by

$$\tilde{S}(x, t) = S(x, t) + \frac{1}{2}(Yx^2/Z).$$

Then equations (A2) can be rewritten as

$$\frac{\partial \tilde{S}}{\partial t} + \frac{Z}{2} \left(\frac{\partial \tilde{S}}{\partial x} \right)^2 + \frac{\tilde{X}x^2}{2} + V_{ex}(x) - \frac{Z\hbar^2}{2N} \frac{\partial^2 N}{\partial x^2} = 0$$

$$\frac{1}{N} \frac{\partial N}{\partial t} = -Z \left(\frac{1}{N} \frac{\partial N}{\partial x} \frac{\partial \tilde{S}}{\partial x} + \frac{1}{2} \frac{\partial \tilde{S}}{\partial x^2} \right)$$

$$\tilde{X} = X - \frac{Y^2}{Z} - Z \frac{d}{dt} \left(\frac{Y}{Z} \right) \qquad \tilde{X}_0 = X - \frac{Y^2}{Z}.$$
(A3)

Now (A3) can be interpreted as having been derived from the pseudoHamiltonian

$$\tilde{H} = \frac{1}{2} [Z\hat{p}^2 + \tilde{X}q^2] + V_{ex}(\hat{q})$$
(A4)

whose eigenfunctions are real. Hence, when we change the parameters of \tilde{H} adiabatically, then

$$\operatorname{Im}\langle \tilde{n}(x;\,\tilde{R}) | \nabla_{\tilde{R}} \tilde{n}(x;\,\tilde{R}) \rangle \equiv 0$$

and the standard adiabatic theorem applies, i.e. the phase of the initial wavefunction $|\tilde{n}\rangle$ changes by

$$-\frac{1}{\hbar}\int_0^T \mathrm{d}t\,\tilde{\varepsilon}_n(\tilde{R}(t))$$

in a time interval T. The parameters of \tilde{H} are given by Z, \tilde{X} and the parameters of $V_{\text{ex}}(\hat{q})$. The only contribution to Berry's phase then comes from \tilde{X} and a standard Taylor expansion about $\tilde{X}_0(t)$ gives the result

$$\gamma_{n}(C) = \frac{1}{\hbar} \int_{0}^{T} dt \frac{\partial \tilde{\varepsilon}_{n}}{\partial \tilde{X}_{0}} \nabla_{R} \left(\frac{Y}{Z}\right) \cdot \frac{dR}{dt}$$
$$= \frac{1}{\hbar} \oint dR \cdot \frac{\partial \tilde{\varepsilon}_{n}}{\partial \tilde{X}_{0}} \nabla_{R} \left(\frac{Y}{Z}\right)$$
$$= \frac{1}{\hbar} \oiint dA \cdot \left(\nabla_{R} \frac{\partial \tilde{\varepsilon}_{n}}{\partial \tilde{X}_{0}}\right) \times \left(\nabla_{R} \frac{Y}{Z}\right).$$
(A5)

For the GGSHO, using

$$\tilde{\varepsilon}_n = -\frac{1}{2} \,\tilde{\omega}^2 \tilde{a}^2 / Z + (n + \frac{1}{2}) \,\hbar \tilde{\omega}$$
$$\tilde{\omega}^2 = Z \hbar \left[XZ - Y^2 - Z \frac{d}{dt} \left(\frac{Y}{Z} \right) \right]^{-1}$$
$$\tilde{a} = -FZ \left[XZ - Y^2 - Z \frac{d}{dt} \left(\frac{Y}{Z} \right) \right]^{-1}$$

we find the results quoted in (20).

It is evident that in this reformulation Berry's phase has a purely 'dynamical' origin.

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