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Adiabatic anholonomy and canonical transformations

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Abstract. Biswas and Soni [4] have surmised a semiclassical formula for Berry's phase in terms of a generating function. We derive this formula apart from showing that it is not true in general and investigate its domain of validity. We also derive transformation formulae for Berry's phase (Hannay's angle) under general canonical transformations. A simpler proof for total angle invariance than hitherto available, is given.

Keywords. Berry's phase; Hannay's angle; canonical transformations.

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1. Introduction

Berry's phase [1] (Hannay's angle [2]) has been a subject of considerable interest recently. Berry's (Hannay's) observation is the existence of a contribution of purely geometric origin in the phase (angle) of a system upon adiabatic cycling of parameters on which the system Hamiltonian depends. There has also been a study of the anholonomies under canonical transformations e.g. Giavarini *et al* [3] and Biswas and Soni [4] have talked about the removability of Berry's phase and Hannay's angle. Biswas and Soni (hereafter referred to as BS) have also used a formula, earlier surmised by Biswas [5], to calculate Berry's phase semiclassically in terms of a classical generating function used to transform the system hamiltonian to a hamiltonian that does not exhibit Berry's phase. The aim of our work is many-fold. We investigate the domain of validity of BS's semiclassical formula and show that it is not in general true and is valid for a 'shear transformation' [6] (with shear applied in the momentum coordinate, the position coordinate being unchanged) and a simple translation of the position and momentum coordinates. It is easy to see that the total phase (geometric+dynamical) arg $\langle\psi(0)|\psi(T)\rangle$ is trivially invariant under a unitary transformation $U(T)$ such that $U(0) = U(T)$. In the same spirit we look for a simpler proof of total angle invariance (as against the one given by Giavarini *et al*, see their appendix). We show that using an F_4 type of generating function, total angle invariance indeed turns out to be trivial.

We also derive transformation formulae for Berry's phase (Hannay's angle) under unitary (canonical) transformations and using a gauge in which the dynamical phase (angle) vanishes, we derive useful formulae for the Berry's phase (Hannay's angle) in case of a shear transformation, a general unitary transformation and in the semi-classical case. The shear transformation is considered separately (although it is a special case of the general transformation) because of the following reasons: (i) the shear transformation is directly relevant to a number of systems and as an example we calculate, using the formula derived, Berry's phase for a q-harmonic oscillator [7], a result derived earlier by Soni [8] in a somewhat different manner, (ii) to highlight the fact that the quantum result in this case matches the semi-classical result provided that the quantum expectation value of a quantity in an eigenstate be replaced by the average over the 'fast' angles of the same quantity on the action-angle torus corresponding to the eigenstate. We argue that the 'semi-classical' formula of Biswas and BS works for cases involving the shear transformation and a simple translation of the position and momentum coordinates and not for any general transformation. We have also included a derivation of Berry's phase (arising from a 'time-dependent' Hamiltonian) using 'time-independent' perturbation theory which is an interesting variant of the original one by Berry.

The paper is organized as follows. We begin with the derivation of Berry's phase mentioned above. We then study the transformations of Hannay's angle and Berry's phase under a shear transformation and use the results derived to calculate Berry's phase for a q-harmonic oscillator. The above analysis is then carried out for a general unitary transformation. This is followed by a proof of total angle invariance and finally the semi-classical treatment.

A Hamiltonian $H(t)$ describing a system at time t may be related to the Hamiltonian at time $t+\delta t$ (where δt is small) as follows

$$H(t+\delta t) = H(t) + \delta t \frac{\partial H}{\partial t}. \tag{1}$$

Treating the second term on RHS of (1) as a perturbation and using 'time independent' perturbation theory [9], we can relate the eigenstates $u_n(t)$ and $u_n(t+\delta t)$ corresponding to the Hamiltonians $H(t)$ and $H(t+\delta t)$ respectively as follows

$$u_n(t+\delta t) = u_n(t)(1 - i\beta_1 \delta t) - \Sigma' u_m(t) \frac{\langle m|\partial H/\partial t|n\rangle}{E_m - E_n}\delta t + \text{higher order terms}, \tag{2}$$

where $(1 - i\beta_1\delta t) \approx \exp(-i\beta_1 \delta t)$ is an arbitrary phase factor which we have retained (β_1 is otherwise taken to be zero in the usual perturbation theory). Such arbitrary phase factors arise at all orders of perturbation theory, but we do not dwell on them here as only the first order is relevant in the adiabatic approximation in which Berry's phase arises. It immediately follows from (2) that

$$\beta_1 = i\langle u_n(t)|\dot{u}_n(t)\rangle. \tag{3}$$

$\int_0^T \beta_1 \mathrm{d}t$ is immediately recognized as Berry's phase, where T is such that $H(0) = H(T)$.

2. Transformation of Hannay angle and Berry phase under a shear transformation and application to the q-harmonic oscillator

Consider a shear transformation that is directly relevant to a number of systems particularly those involving the parametric harmonic oscillator discussed extensively by many authors [4,8,10–17]. Let a Hamiltonian $H(q,p,\mathbf{R}(t))$ describing a system transform to $K(Q,P,\mathbf{R}(t))$ under the application of the following shear transformation (with shear applied in the p-direction)

$$Q = q, \quad P = p - \alpha\frac{\partial G}{\partial q}, \tag{4}$$

where $G(q,\mathbf{R}(t))$ is a function only of q and the external parameters $\mathbf{R}(t)$. The transformation is effected by the following F_2 type generating function

$$F_2(q,P,\mathbf{R}(t)) = qP + \alpha G(q;\mathbf{R}(t)). \tag{5}$$

We now transform $H(q,p,\mathbf{R}(t))$ and $K(Q,P,\mathbf{R}(t))$ to their action-angle counterparts

$$\begin{aligned} H(I,\theta,\mathbf{R}(t)) &= \mathcal{H}(q(I,\theta,\mathbf{R}(t)),p(I,\theta,\mathbf{R}(t)),\mathbf{R}(t)) \\ &\quad + \frac{\partial S^{(0)}}{\partial t}(q(I,\theta,\mathbf{R}(t)),I;\mathbf{R}(t)), \\ K(I,\theta,\mathbf{R}(t)) &= \mathcal{K}(Q(I,\theta,\mathbf{R}(t)),P(I,\theta,\mathbf{R}(t)),\mathbf{R}(t)) \\ &\quad + \frac{\partial S}{\partial t}(Q(I,\theta,\mathbf{R}(t)),I;\mathbf{R}(t)), \end{aligned} \tag{6}$$

where $\mathcal{H}$ and $\mathcal{K}$ are H and K expressed in terms of action angle variables and S and $S^{(0)}$ are F_2 type generating functions. We may write

$$S(Q,I,\mathbf{R}(t)) = S^{(0)}(q,I,\mathbf{R}(t)) - \alpha G(q,\mathbf{R}(t)), \tag{7}$$

so that (7) is consistent with (4) and in the limit $\alpha \to 0, S$ reduces to $S^{(0)}$. It follows from (7) that Hannay angles $\Delta\theta'_h$ and $\Delta\theta_h$ are related as follows

$$\Delta\theta'_h = \Delta\theta_h - \alpha\frac{\partial}{\partial I}\int \langle \mathrm{d}G\rangle, \tag{8}$$

where dG is the 1-form over parameter space. For the quantum case (4) becomes an operator equation and it can be shown that $|q\rangle$ transforms to $\exp(-i\alpha G(q,\mathbf{R}(t)/\hbar)|q\rangle$ [18].

At present we assume that the eigenstate $|n\rangle$ corresponding to $H(q,p,\mathbf{R}(t))$ also transforms in the same way i.e.

$$|n'\rangle = \exp(-i\alpha G(q,\mathbf{R}(t)/\hbar)|n\rangle, \tag{9}$$

corresponding to $K(Q,P,\mathbf{R}(t))$ (it is shown later in the paper that this is equivalent to the adiabatic approximation). Using (9) and definition of Berry's phase it follows that

$$\gamma_n' = \gamma_n + \frac{\alpha}{\hbar}\int \langle n|\mathrm{d}G|n\rangle. \tag{10}$$

If we find a suitable G for which $\gamma_n' = 0$, then (10) leads to

$$\gamma_n = -\frac{\alpha}{\hbar}\int \langle n|\mathrm{d}G|n\rangle. \tag{11}$$

Equation (11) serves as a useful formula for calculating Berry's phase. We demonstrate this by considering the generalized q-harmonic oscillator [7] for which Soni [8] has calculated Berry's phase in a somewhat different manner. The Hamiltonian for the system is as follows

$$\hat{H} = (1/2)[Z(t)\hat{P}^2 + Y(t)\{\hat{P}\hat{Q} + \hat{Q}\hat{P}\} + X(t)\hat{Q}^2], \tag{12}$$

where $\hat{P}$ and $\hat{Q}$ are the p-momentum and q-position operators respectively, and X, Y, Z are external parameters such that $XZ > Y^2$ and $Z > 0$. For this case $\alpha = 1$ and $G = (Y/2Z)Q^2$ (see eq. (4)). It is easy to see that

$$\hat{Q}^2 = (\hbar/2)([\hat{N}+1] + [\hat{N}]), \tag{13}$$

where $\hat{N}$ is the number operator, whence it immediately follows from (11) that

$$\frac{(\gamma_n)_q}{(\gamma_n)_{cl}} = \frac{[n+1]+[n]}{2n+1}, \tag{14}$$

a result same as that obtained by Soni. Note that the approximation $|n'\rangle = \exp(-i\alpha G/\hbar)|n\rangle$ is equivalent to neglecting terms of power greater than and equal to 2 in the expansion for the energy eigenvalue E_n in Soni's calculation. We examine this approximation in some more detail in the following case of a general unitary transformation.

3. Transformation of eigenstate and Berry's phase under a general unitary transformation

In quantum mechanics, the Hamiltonian H transforms under a unitary transformation $U(t)$ to the Hamiltonian K as under

$$K = UHU^\dagger + i\hbar U^\dagger \dot{U}. \tag{15}$$

Clearly $|\Psi'\rangle = U|\Psi\rangle$. In order to find a relationship between the eigenstates corresponding to K and H, we treat the second term in (15) as a perturbation over the first. Clearly then

$$|n'\rangle = U|n\rangle + \ldots, \tag{16}$$

where we have retained only the zeroeth order wave function corresponding to the unperturbed Hamiltonian $UHU^\dagger$. Higher order terms represented by dots involving derivatives of $U(\mathbf{R}(t))$ are neglected because when substituted in the formula for Berry's phase [1], they lead to higher powers (> 2) of the derivatives of slow parameters $\mathbf{R}(t)$ (which are neglected because of the adiabatic assumption). Equation (16) leads to a general formula the transformation of Berry's phase

$$\gamma_n' = \gamma_n + i \int \langle n|U^\dagger \mathrm{d}U|n\rangle, \tag{17}$$

of which (10) is a special case. We may add here that one can use (15) to write down

$$E_n' = \langle n'|K|n'\rangle = E_n + i\hbar\langle n|U^\dagger \dot{U}|n\rangle, \tag{18}$$

or

$$-\frac{1}{\hbar}\int E_n'(t)\mathrm{d}t = -\frac{1}{\hbar}\int E_n(t)\mathrm{d}t - i\int \langle n|U^\dagger \mathrm{d}U|n\rangle, \tag{19}$$

implying the exact cancellation of change in Berry's phase with the change in dynamical phase.

4. A proof of total angle invariance

We now show that just as the total phase arg $\langle\psi(0)|\psi(T)\rangle$ is trivially invariant under a unitary transformation U such that $U(0) = U(T)$, the proof of the invariance of the total angle is equally simple. Consider canonically related Hamiltonians $H(q, p, \mathbf{R}(t))$ and $K(Q, P, \mathbf{R}(t))$ which transform (under appropriate canonical transformations) to the action angle Hamiltonians $H'(I, \theta, \mathbf{R}(t))$ and $K'(I', \theta', \mathbf{R}(t))$ respectively. It is easy to argue that the actions $I = \int p\mathrm{d}q$ and $I' = \int P\mathrm{d}Q$ are equal and $\theta' = \theta + f(\mathbf{R}(t))$, where $f(\mathbf{R}(t))$ is an arbitrary function and is of no consequence. Since $H'(I, \theta, \mathbf{R}(t))$ and $K'(I, \theta, \mathbf{R}(t))$ must also be canonically related, we relate them by an F_4 type of generating function (which has arguments as P, p for a transformation from (q, p) to (Q, P)) i.e.

$$H' = K' + \frac{\partial F_4}{\partial t}(I, \mathbf{R}(t)). \tag{20}$$

It is obvious from the above that

$$\int \frac{\partial H'}{\partial I}\mathrm{d}t = \int \frac{\partial K'}{\partial I}\mathrm{d}t, \tag{21}$$

i.e. the total angle is conserved. Having proved total angle invariance, we now turn our attention to the general transformation for the Hannay angle. Relating the Hamiltonians $H(q, p, \mathbf{R}(t))$ and $K(Q, P, \mathbf{R}(t))$ by an F_2 type generating function and utilizing total angle invariance we arrive at the following

$$\Delta\theta_h' - \Delta\theta_h = -\frac{\partial}{\partial I}\int \langle \mathrm{d}F_2\rangle. \tag{22}$$

5. Semiclassical treatment

To arrive at semiclassical formulae, we replace the quantum expectation value $\langle n|\mathrm{d}G|n\rangle$ in (10) and (11) by $\langle \mathrm{d}G\rangle$ an average over the 'fast' angles so that we get

$$\gamma_n' = \gamma_n + (1/\hbar)\int \langle \mathrm{d}G\rangle, \tag{23}$$

$$\gamma_n = -(1/\hbar)\int \langle \mathrm{d}G(0)\rangle, \tag{24}$$

where $G(0)$ is such that $\gamma_n' = 0$. The above formula, as mentioned earlier, was surmised by Biswas and used by BS for calculating Berry's phase for a few typical systems (note that there is no difference between $\langle \mathrm{d}G\rangle$ and $\langle \mathrm{d}F_2\rangle$ for all the examples considered by BS). If Hanny angle $\Delta\theta_h'$ is also zero for the above gauge, we get from (22)

$$\Delta\theta_h = -\frac{\partial}{\partial I}\int \langle \mathrm{d}G(0)\rangle. \tag{25}$$

Thus by relating Berry's phase γ_n and Hannay's angle to a common generating function $G(0)$ in (24) and (25), we arrive at the well-known semiclassical relation of Berry

$$\Delta\theta_h = -\partial\gamma_n/\partial n. \tag{26}$$

Validity of (26) is of course dependent on our being able to find a gauge for which $\Delta\theta\,'_h$ and γ_n' simultaneously vanish.

We now investigate whether semiclassical formulae (23) and (24) are valid for the shear transformation only or any general canonical transformation. We now consider a transformation of the kind

$$Q = q + \frac{\partial G}{\partial p}(q,p,\mathbf{R}),$$
$$p = P + \frac{\partial G}{\partial q}(q,p,\mathbf{R}), \tag{27}$$

for which the corresponding unitary transformation is $U = \exp(-iG(q,p,\mathbf{R}(t))/\hbar)$ [18] (where q and p are operators). Using this in (17) one can verify that we do not get formulae of the kind (10) (and hence (23)) for any arbitrary choice of G. However for $G(q,p,\mathbf{R}(t))$ that effects a translation of the form $P = p+a$ and $Q = q+b$ (where a and b are constants), we do get (10) (hence (23) and (24)). In all the examples considered by BS, they have taken either the shear transformation or translation and that is why their method works.

6. Conclusions

To conclude, we have accomplished the following tasks in this paper. We have derived transformation formulae for Berry's phase (Hannay's angle) under unitary(canonical) transformations thereby also deriving useful formulae for the same in terms of a unitary operator/generating function. The special role of the shear transformation is discussed. It is shown that the formula of Biswas for the Berry phase in terms of the generating function is valid for the shear transformation (as well as a translation) and does not hold for a general transformation. We have also given a simpler and more elegant proof of total angle invariance than hitherto available.

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