Phase-space approach to Berry's phases

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Abstract

We propose a new formula for the adiabatic Berry phase which is based on phase-space formulation of quantum mechanics. This approach sheds a new light into the correspondence between classical and quantum adiabatic phases — both phases are related with the averaging procedure: Hannay's angle with averaging over the classical torus and Berry's phase with averaging over the entire classical phase space with respect to the corresponding Wigner function. Generalizations to the non-abelian Wilczek–Zee case and mixed states are also included.

Geometric Berry phase [1] and its classical analog, so called Hannay angle, [2] (see also [3]) have found numerous applications in various branches of physics (see e.g. [4] and [5]). Recently, it turned out that adiabatic Berry phase plays important role in quantum computation algorithms as a model of a quantum gate in a quantum computer (see e.g. [6, 7]). In this paper we present a new formula for the Berry phase which is based on the phase space formulation of quantum mechanics. This approach sheds a new light into the correspondence between classical and quantum adiabatic phases.

Both Berry's phase and Hannay's angles have been introduced in the context of adiabatic evolution in quantum and classical mechanics, respectively. Let us consider for simplicity a classical system with one degree of freedom and let the corresponding phase space be parameterized by canonical coordinates (q, p). Suppose, that a Hamiltonian $H(q, p; \mathbf{X})$ depends on a set of some external parameters $\mathbf{X}$ from the parameter space $\mathcal{M}$ and that $\mathbf{X}$ are changed adiabatically along a circuit C and come back to their initial values, i.e. $\mathbf{X}(T) = \mathbf{X}(0)$ for some $T > 0$. Now, the classical adiabatic theorem [8] states that the system will evolve on the torus defined by the constant value of the action variable I and the angle variable varies according to

$$\theta(T) = \int_0^T \omega(I; \mathbf{X}(t))dt + \Delta\theta(I; C) \ , \tag{1}$$

where the frequency $\omega(I, X) = \partial H(I; X)/\partial I$ and the additional shift — Hannay angle $\Delta\theta$ — is given by the following integral over an arbitrary two-dimensional region Σ in $\mathcal{M}$ such that $C = \partial\Sigma$

$$\Delta\theta(I; C) = -\frac{\partial}{\partial I} \int\int_{\partial\Sigma=C} F^{\rm c}(I; X) \ , \tag{2}$$

where $F^{\rm c}(I; \mathbf{X})$ denotes the following two-form on $\mathcal{M}$:

$$F^{\rm c}(I; \mathbf{X}) = \langle\, d_{\mathbf{X}}\, p(I; \mathbf{X}) \wedge d_{\mathbf{X}}\, q(I; \mathbf{X}) \,\rangle \ , \tag{3}$$

and $\langle\, f(I)\,\rangle$ denotes the average of $f(I,\theta)$ over the torus I.

Now, let us consider the quantized system defined by $\hat{H}(\mathbf{X})$. Clearly, the quantization $H \to \hat{H}$ is not unique and depends on the ordering of $\hat{q}$ and $\hat{p}$. In what follows we assume the Wigner–Weyl (or symmetric) ordering, i.e. for example $qp \to (\hat{q}\hat{p} + \hat{p}\hat{q})/2$. The quantum adiabatic theorem [9] states that a system originally in an eigenstate $|n;\mathbf{X}(0)\,\rangle$ will remain in the same eigenstate $|n;\mathbf{X}(t)\,\rangle$ with energy $E_n(\mathbf{X}(t))$. Now if the initial state $|\psi(0)\,\rangle$ belongs to the nth eigenspace, then after the circuit C the final state $|\psi(T)\,\rangle$ is given by

$$|\psi(T)\,\rangle = \exp(i\gamma_n(C)) \exp\left(-\frac{i}{\hbar}\int_0^T E_n(\mathbf{X}(t))dt\right) |\psi(0)\,\rangle\ , \tag{4}$$

where the Berry phase reads:

$$\gamma_n(C) = -\int\!\!\int_{\partial\Sigma=C} F_n^{\mathrm{q}}(\mathbf{X})\ , \tag{5}$$

and F_n^{q} (Berry's curvature) denotes the following two-form on $\mathcal{M}$:

$$F_n^{\mathrm{q}}(\mathbf{X}) = \mathrm{Im}\,\langle\, d_{\mathbf{X}}\, n;\mathbf{X}| \wedge |d_{\mathbf{X}}\, n;\mathbf{X}\,\rangle\ . \tag{6}$$

Using semiclassical analysis Berry shown [3] that

$$\Delta\theta(I;C) = -\hbar\frac{\partial\gamma_n(C)}{\partial I} = -\frac{\partial\gamma_n(C)}{\partial n}\ , \tag{7}$$

where n is considered as a continuous variable according to Bohr–Sommerfeld quantization rule $I = \hbar(n+\mu)$, with μ being the Maslov index.

Both two-forms $F^{\mathrm{c}}(I;\mathbf{X})$ and $F_n^{\mathrm{q}}(\mathbf{X})$ live in the parameter space $\mathcal{M}$. Clearly, they are defined by very different objects: 'classical form' $F^{\mathrm{c}}(I;\mathbf{X})$ uses phase-space quantities $q(I,\theta;\mathbf{X})$ and $p(I,\theta;\mathbf{X})$ whereas 'quantum form' $F_n^{\mathrm{q}}(\mathbf{X})$ is defined in terms of Hilbert space eigenvectors $|n;\mathbf{X}\,\rangle$. There is, however, equivalent formulation of quantum mechanics which uses objects defined on the classical phase space only [10]. There is a direct relation — well known Wigner–Weyl correspondence — between functions $F = F(q,p)$ on the classical phase space and self-adjoint operators $\hat{F}$ in the system Hilbert space. If $|\psi\,\rangle$ is the state vector, then

$$\langle\,\psi|\hat{F}|\psi\,\rangle = \int W_\psi(q,p)F(q,p)\,dqdp\ , \tag{8}$$

where $W_\psi = W_\psi(q,p)$ is a Wigner function corresponding to $|\psi\,\rangle$. Moreover, this formulation is perfectly suited to semiclassical analysis. It is well known that Wigner function corresponding to the eigenstate $|n\,\rangle$ of the Hamiltonian $\hat{H}$ depends only on I and not on θ, i.e. $W_n(q,p) = W_n(I)$. In the classical limit, i.e. $\hbar \to 0, n \to \infty$ such that $n\hbar$ is constant and equals I_0, the Wigner function W_n is concentrated on the torus I_0

$$W_n(I) \ \longrightarrow\ \frac{1}{2\pi}\,\delta(I - I_0)\ . \tag{9}$$

If the quantum system depends upon external parameters $\mathbf{X}$ which evolve adiabatically then W_n is adiabatically constant, or, using the language of the classical adiabatic theorem, W_n

defines an adiabatic invariant. Now, since Berry's curvature F_n is a measurable quantity it may be expressed according to

$$F_n^{\rm q} = \int W_n(I)\,\text{`classical quantity'}\,dI\ . \tag{10}$$

Clearly, this 'classical quantity' has to be related with the 'classical two-form' $F^{\rm c}$. Moreover, in the classical limit $F_n^{\rm q}$ and its classical counterpart $F^{\rm c}$ have to be related according to (7), that is,

$$F_n^{\rm q}(\mathbf{X}) = -\frac{1}{\hbar}\,F^{\rm c}(I;\mathbf{X})\ . \tag{11}$$

The natural choice is therefore

$$F_n^{\rm q}(\mathbf{X}) = -2\pi\int W_n(I)F^{\rm c}(I;\mathbf{X})\,dI\ . \tag{12}$$

Example. As an example let us consider a generalized harmonic oscillator [3] defined by

$$H(q,p;\mathbf{X}) = \frac{1}{2}\left(Xq^2 + 2Yqp + Zp^2\right)\ , \tag{13}$$

where the parameters $\mathbf{X} = (X,Y,Z) \in \mathbb{R}^3$ satisfy $XZ > Y^2$ (this condition implies that the above system describes oscillatory motion round elliptic contours in the two-dimensional phase space $\mathbb{R}^2$). One shows [3]

$$F^{\rm c}(I;\mathbf{X}) = -\frac{I}{4\omega^3}\left(XdY\wedge dZ + YdZ\wedge dX + ZdX\wedge dY\right)\ , \tag{14}$$

with the frequency of the quasi-periodic motion $\omega = \sqrt{XZ-Y^2}$. The quantized system (according to the Wigner–Weyl correspondence) is given by

$$\hat{H}(\mathbf{X}) = \frac{1}{2}\left(X\hat{q}^2 + Y(\hat{q}\hat{p}+\hat{p}\hat{q}) + Z\hat{p}^2\right)\ . \tag{15}$$

The eigen-equation $\hat{H}\psi_n = E_n\psi_n$ is solved by the following normalized eigenfunctions:

$$\psi_n(q;\mathbf{X}) = \sqrt{\alpha}\,\chi_n\left(\alpha q\right)\,\exp\left(\frac{-iYq^2}{2Z\hbar}\right)\ ,$$

where $\alpha = \sqrt{\omega/Z\hbar}$, and $\chi_n(\xi) = N_n e^{-\xi^2/2}H_n(\xi)$, with H_n being the nth Hermite polynomial and the normalization constant $N_n = (2^n n!\sqrt{\pi})^{-1/2}$. Energy levels are given by the standard formula $E_n = \hbar\omega(n+1/2)$. The corresponding Wigner function $W_n(q,p;\mathbf{X})$ reads as follows

$$\begin{aligned} W_n(q,p;\mathbf{X}) &= \frac{1}{\pi\hbar}\int_{-\infty}^{\infty} ds\,\overline{\psi}_n(q+s;\mathbf{X})\psi_n(q-s;\mathbf{X})\,e^{2ips/\hbar} \\ &= \frac{\alpha}{\pi\hbar}\int_{-\infty}^{\infty} ds\,\overline{\chi}_n\left(\alpha(q+s)\right)\chi_n\left(\alpha(q-s)\right)\,e^{2i[(p+Yq/Z)s]/\hbar} \\ &= W_n^{\rm osc}(q,\tilde{p})\ , \end{aligned} \tag{16}$$

where $W_n^{\rm osc}$ is the nth Wigner function corresponding to the standard harmonic oscillator

$$H^{\rm osc}(q,\tilde{p}) = \frac{1}{2}\left(Z\tilde{p}^2 + \frac{\omega^2}{Z}q^2\right) \ , \tag{17}$$

with $\tilde{p} = p + Yq/Z$. Clearly, the $\mathbf{X}$–dependent canonical transformation $(q,p) \longrightarrow (q,\tilde{p})$ transforms (13) into (17). Now, $W^{\rm osc}$ is given by the well known formula (see e.g. [10])

$$W_n(I) = W_n^{\rm osc}(q,\tilde{p}) = \frac{(-1)^n}{\pi\hbar}\, e^{-2I/\hbar} L_n(4I/\hbar) \ , \tag{18}$$

where $I = H^{\rm osc}/\omega$ is the action variable and L_n denotes the nth Laguerre polynomial. Finally, using

$$\int_0^\infty W_n(I) I \, dI = \frac{n+\frac{1}{2}}{2\pi} \ ,$$

one finds the following formula for the Berry curvature

$$\begin{aligned} F_n^{\rm q}(\mathbf{X}) &= -\frac{n+\frac{1}{2}}{I}\, F^{\rm c}(I;\mathbf{X}) \\ &= \frac{n+\frac{1}{2}}{4\omega^3}\left(XdY\wedge dZ + YdZ\wedge dX + ZX\wedge dY\right) \ , \end{aligned} \tag{19}$$

in perfect agreement with [3].

Our basic formula (12) may be generalized in two evident ways: if the classical integrable system has N degrees of freedom then the corresponding Berry curvature reads:

$$F_n^{\rm q}(\mathbf{X}) = -(2\pi)^N \int\!\ldots\!\int W_n(\mathbf{I}) F^{\rm c}(\mathbf{I};\mathbf{X})\, d\mathbf{I} \ , \tag{20}$$

with

$$F^{\rm c}(\mathbf{I};\mathbf{X}) = \sum_{k=1}^{N} \langle\, d_{\mathbf{X}}\, p_k(\mathbf{I};\mathbf{X}) \wedge d_{\mathbf{X}}\, q_k(\mathbf{I};\mathbf{X}) \,\rangle \ , \tag{21}$$

where now one averages over N-dimensional torus $\mathbf{I} = (I_1,\ldots,I_N)$. The second generalization corresponds to the non-abelian case developed by Wilczek and Zee [11]. Suppose that nth eigenvalue is N times degenerate and let $|n,a;\mathbf{X}\,\rangle$ $(a = 1,\ldots,N)$ span the corresponding N-dimensional eigenspace. Then the Wilczek–Zee curvature is given by the following formula

$$F_{n;ab}^{\rm WZ}(\mathbf{X}) = -2\pi \int W_{n;ab}(I) F^{\rm c}(I;\mathbf{X})\, dI \ , \tag{22}$$

with $W_{n;ab}$ being the following 'Wigner matrix'

$$W_{n;ab}(q,p;\mathbf{X}) = \frac{1}{\pi\hbar}\int_{-\infty}^{\infty} ds\, \langle\, n,a;\mathbf{X}|q+s\,\rangle\langle\, q-s|n,b;\mathbf{X}\,\rangle\, e^{2ips/\hbar} \ . \tag{23}$$

Clearly, $W_{n;ab}$ is hermitian and hence $iF_n^{\rm WZ} \in u(N)$. Now, changing $|n,a;\mathbf{X}\,\rangle$ to $|\widetilde{n,a};\mathbf{X}\,\rangle = \sum_b U_{ab}(\mathbf{X})|n,b;\mathbf{X}\,\rangle$, with $U(\mathbf{X}) \in U(N)$, one finds

$$\widetilde{F}_n^{\rm WZ}(\mathbf{X}) = U(\mathbf{X}) F_n^{\rm WZ}(\mathbf{X}) U^\dagger(\mathbf{X}) \ , \tag{24}$$

that is, tensorial rule for the gauge transformation of F_n^{WZ}. Finally, the formula (12) suggests the following generalization for the adiabatic evolution of mixed states. Suppose that ρ is a density operator such that the corresponding Wigner function $W_\rho = W_\rho(I)$ is adiabatically constant. Following Sjöqvist et. al. [12] one defines a phase of $\rho(T)$ with respect to ρ as $\phi = \arg \mathrm{Tr}[U(t)\rho]$. Now, ϕ may be recovered from space-phase quantities as follows:

$$\phi = \int\int_{\partial\Sigma=C} F_\rho(\mathbf{X}) \ , \tag{25}$$

where the two-form $F_\rho(\mathbf{X})$ on the parameter space $\mathcal{M}$ is defined by

$$F_\rho(\mathbf{X}) = -2\pi \int W_\rho(I) F^{\mathrm{c}}(I;\mathbf{X})\, dI \ . \tag{26}$$

Clearly, if the stationary (in the adiabatic limit) state ρ is pure, then necessarily $\rho = |n;\mathbf{X}\rangle\langle n;\mathbf{X}|$ and (26) reduces to (12).

Acknowledgments: This work was partially supported by the Polish Ministry of Scientific Research and Information Technology under the grant No PBZ-MIN-008/P03/2003.

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