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Cumulants associated with geometric phases

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Abstract – The Berry phase can be obtained by taking the continuous limit of a cyclic product $-\mathrm{Im}\ln\prod_{I=0}^{M-1}\langle\Psi_0(\boldsymbol{\xi}_I)|\Psi_0(\boldsymbol{\xi}_{I+1})\rangle$, resulting in the circuit integral $i\oint \mathrm{d}\boldsymbol{\xi}\cdot\langle\Psi_0(\boldsymbol{\xi})|\nabla_{\boldsymbol{\xi}}|\Psi_0(\boldsymbol{\xi}\rangle$. Considering a parametrized curve $\boldsymbol{\xi}(\chi)$ we show that a set of cumulants can be obtained from the product $\prod_{I=0}^{M-1}\langle\Psi_0(\chi_I)|\Psi_0(\chi_{I+1})\rangle$. The first cumulant corresponds to the Berry phase itself, the others turn out to be the associated spread, skew, kurtosis, etc. The cumulants are shown to be gauge invariant. Then the spread formula from the modern theory of polarization is shown to correspond to the second cumulant of our expansion. It is also shown that the cumulants can be expressed in terms of the expectation value of an operator. An example of the spin-$\frac{1}{2}$ particle in a precessing magnetic field is analyzed.

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Introduction. – The concept of geometric phase was first suggested by Pancharatnam [1] in optics. In 1984 Berry [2] published a paper about phases which arise when a quantum system is brought around an adiabatic cycle. The phase advocated in this paper was overlooked earlier [3] as it was considered part of the arbitrary phase of a quantum wave function. Berry has shown that this is not the case, and that the phase of an adiabatic cycle can be a measurable quantity. Since the publication of Berry's paper this concept was found to be at the core [4,5] of a number of interesting physical effects, including the Aharonov-Bohm effect [6], quantum Hall effect [7], topological insulators [8], dc conductivity [9], or the modern theory of polarization [10,11]. More recently an example of a geometric phase, the Zak phase [12], has been measured in optical waveguides [13] and optical lattices [14].

To derive a Berry phase, one considers a Hamiltonian which depends parametrically on a set of variables. One can then take a discrete set of points in this parameter space, obtain the wave function, and form a cyclic product of the type in eq. (2). The imaginary part of the logarithm of this cyclic product corresponds to the discrete Berry phase. If the discrete points are along a cyclic curve then the continuous limit can be taken, and it corresponds to the well-known circuit integral [2]. The real part of the product is usually not considered, due to the common belief that, as a result of the normalization of the wave function, it is zero, therefore not physically relevant. In this work we show that when the product in eq. (2) associated with an adiabatic cycle is equated to a cumulant expansion and the continuous limit is taken, then a series of physically well-defined quantities result. The quantities are integrals around the adiabatic cycle of the parameter which gives rise to the Berry phase itself. The first-order term corresponds to the Berry phase, the higher-order terms give the associated cumulants. Gauge invariance is demonstrated up to fourth order, but our proof suggests that it holds for higher-order terms as well. Since the Berry phase is usually not written in terms of an operator, the question arises, what distribution do the cumulants correspond to? To answer this we construct an operator via first-order perturbation theory. For the Berry phase, the phase of the wave function along the adiabatic path causes a shift. However, the higher-order cumulants are unaffected by this shift, as is the case for the usual cumlants in probability theory. We then compare our results to those of the modern theory of polarization in which cumulants have been obtained from a generating function approach [15]. We stress that this work addresses the particular case of the single-point Berry phase [15,16]. In particular, we show that the second cumulant obtained from our derivation is identical to the result of Resta and Sorella [17]. We also analyze one of the canonical examples for the Berry phase [2] in light of our findings. Our results show that the cumulants give information about the underlying probability distribution associated with the Berry phase.

General remarks. – The most general way to obtain the Berry phase is to write it in the discrete representation, and then take the continuous limit. Pancharatnam's [1] original derivation is based on considering discrete phase changes. The discrete Berry phase first appeared in 1964, in a paper by Bargmann [18], as a mathematical tool for proving a theorem. The expression which forms the basis of our derivation here has also been used extensively in the case of the path-integral–based representation of geometric phases [19,20].

Given a parameter space $\boldsymbol{\xi}$ and some Hamiltonian $H(\boldsymbol{\xi})$ with

$$H(\boldsymbol{\xi})|\Psi_i(\boldsymbol{\xi})\rangle = E_i(\boldsymbol{\xi})|\Psi_i(\boldsymbol{\xi})\rangle, \tag{1}$$

where $|\Psi_i(\boldsymbol{\xi})\rangle(E_i(\boldsymbol{\xi}))$ is an eigenstate (eigenvalue) of the Hamiltonian. Consider a set of M points in this parameter space $\{\boldsymbol{\xi}_I\}$. In this case one can form the quantity

$$\phi = -\mathrm{Im}\ln\prod_{I=0}^{M-1}\langle\Psi_0(\boldsymbol{\xi}_I)|\Psi_0(\boldsymbol{\xi}_{I+1})\rangle, \tag{2}$$

where $\Psi_0(\boldsymbol{\xi}_M) = \Psi_0(\boldsymbol{\xi}_0)$ (cyclic) which is physically well defined since arbitrary phases cancel. In eq. (2) ϕ is formed using the ground state, without loss of generality. If the points $\{\boldsymbol{\xi}_I\}$ are points on a closed curve, one can take the continuous limit and obtain

$$\phi = i\oint \mathrm{d}\boldsymbol{\xi}\cdot\langle\Psi_0(\boldsymbol{\xi})|\nabla_{\boldsymbol{\xi}}|\Psi_0(\boldsymbol{\xi}\rangle. \tag{3}$$

ϕ can be shown to be gauge invariant and is therefore a physically well-defined quantity. If the wave function can be taken to be real, then a nontrivial Berry phase corresponds to $\phi = \pi$ and will only occur if the enclosed region of parameter space is not simply connected. If the wave functions cannot be taken as real then a nontrivial Berry phase can occur even if the parameter space is not simply connected.

Cumulant expansion associated with the Bargmann invariant. – We consider the product in eq. (2) along a cyclic curve. We assume that the curve is parametrized according to a scalar hence the product is $\prod_{I=0}^{M-1}\langle\Psi_0(\chi_I)|\Psi_0(\chi_{I+1})\rangle$. We also assume that the length of the curve is Λ and that χ_I defines an evenly spaced (spacing $\Delta\chi$) grid. We start by equating this product to a cumulant expansion,

$$\left[\prod_{I=0}^{M-1}\langle\Psi_0(\chi_I)|\Psi_0(\chi_{I+1})\rangle\right]^{\Delta\chi} = \exp\left(\sum_{n=1}^{\infty}\frac{(i\Delta\chi)^n}{n!}C_n\right). \tag{4}$$

We now expand both sides and equate like powers of $\Delta\chi$ term by term, mindful of the fact that the left-hand side includes a sum over I. For example, the first-order term will be

$$C_1 = -i\sum_{I=0}^{M-1}\Delta\chi\gamma_1(\chi_I), \tag{5}$$

the second will be

$$C_2 = -\sum_{I=0}^{M-1}\Delta\chi[\gamma_2(\chi_I) - \gamma_1(\chi_I)^2] \tag{6}$$

with $\gamma_i(\chi) = \langle\Psi_0(\chi)|\partial_\chi^i|\Psi_0(\chi)\rangle$. Straightforward algebra and taking the continuous limit ($\Delta\chi \to 0$, $M \to \infty$, Λ fixed) gives

$$\begin{aligned} C_1 &= -i\int_0^\Lambda \mathrm{d}\chi\gamma_1 \\ C_2 &= -\int_0^\Lambda \mathrm{d}\chi[\gamma_2 - \gamma_1^2] \\ C_3 &= i\int_0^\Lambda \mathrm{d}\chi[\gamma_3 - 3\gamma_2\gamma_1 + 2\gamma_1^3] \\ C_4 &= \int_0^\Lambda \mathrm{d}\chi[\gamma_4 - 3\gamma_2^2 - 4\gamma_3\gamma_1 + 12\gamma_1^2\gamma_2 - 6\gamma_1^4] \end{aligned} \tag{7}$$

Note that the limit $\Delta\chi \to 0$ corresponds to both sides of eq. (4) going to unity if all C_i's are finite. This may bring into question the physical relevance of the C_i's. However, the quantity C_1, the Berry phase itself, is already known to have physical relevance, which strongly suggests a similar role for the other C_i's. Note that the definitions of C_i's (eq. (7)) hold as a result of the term-by-term expansion of eq. (4) independent of the fact that both sides of this equation approach unity as $\Delta\chi \to 0$. The physical significance of the C_i's will be made clearer below by casting them in terms of an operator. Note also that the cumulants can also diverge, for example the divergence of the spread of the total position is a sign of metallic conduction [9,15,17,21].

The C_i's other than C_1 appear very similar to the usual cumulants (compare coefficients), provided that we can interpret $-i\partial_\chi$ as an operator and the integral as a proper expectation value. C_1 is known to be gauge invariant, therefore it is natural to ask whether the other C_i's are also gauge invariant. We consider the proof of gauge invariance for C_1. One first alters the phase of the wave function, *i.e.* define

$$|\tilde{\Psi}_0(\chi)\rangle = \exp[i\beta(\chi)]|\Psi_0(\chi)\rangle. \tag{8}$$

Defining

$$\tilde{C}_1 = -i\int_0^\Lambda \mathrm{d}\chi\langle\tilde{\Psi}_0(\chi)|\partial_\chi|\tilde{\Psi}_0(\chi)\rangle, \tag{9}$$

it is easy to show that

$$\tilde{C}_1 - C_1 = \beta(\Lambda) - \beta(0). \tag{10}$$

with $\tilde{\gamma}_1 = \langle\tilde{\Psi}_0(\chi)|\partial_\chi^i|\tilde{\Psi}_0(\chi)\rangle$. Hence the Berry phase of the original wave function differs from the shifted one by the difference of $\beta(\Lambda) - \beta(0)$ which for an adiabatic cycle is $2\pi m$, with m integer. Applying the same procedure to the other cumulants we obtain the following results:

$$\begin{aligned} \tilde{C}_2 - C_2 &= \partial_\chi\beta(\Lambda) - \partial_\chi\beta(0) = 0, \\ \tilde{C}_3 - C_3 &= \partial_\chi^2\beta(\Lambda) - \partial_\chi^2\beta(0) = 0, \\ \tilde{C}_4 - C_4 &= \partial_\chi^3\beta(\Lambda) - \partial_\chi^3\beta(0) = 0, \end{aligned} \tag{11}$$

hence, if the function $\beta(\chi)$ and its derivatives are continuous at the boundaries gauge invariance holds. We have carried out this proof up to fourth order. There appears to be a pattern in eq. (11) suggesting that gauge invariance holds up to any order.

The cumulants derived above can be expressed in terms of expectation values of operators. Consider the expression from perturbation theory

$$\partial_\chi|\Psi_0(\chi)\rangle = \sum_{j\neq 0}|\Psi_j(\chi)\rangle\langle\Psi_j(\chi)|\frac{\partial_\chi H(\chi)}{E_j - E_0}|\Psi_0(\chi)\rangle. \quad (12)$$

Defining the operator $\hat{O}$ as

$$\partial_\chi H(\chi) = i[H(\chi), \hat{O}] \quad (13)$$

it can be shown that the cumulants of this operator correspond to the C_i's derived above, except for the case $i = 1$, the Berry phase itself, for which application of eq. (12) leads to zero. For the Berry phase the expression from perturbation theory (eq. (12)) is not valid since it makes a definite choice about the phase of the wave function for all values of χ. The most general expression is

$$|\Psi(\chi + \Delta\chi)\rangle = e^{i\alpha} \times \left[|\Psi(\chi)\rangle + \sum_{j\neq 0}|\Psi_j(\chi)\rangle\langle\Psi_j(\chi)|\frac{\partial_\chi H(\chi)}{E_j - E_0}|\Psi_0(\chi)\rangle\right], \quad (14)$$

but in standard perturbation theory α is assumed to be zero. This phase difference shifts the first cumulant (the Berry phase), however since it is a mere shift, it leaves the other cumulants unaffected. One can conclude that while the Berry phase itself cannot be expressed in terms of an operator, its associated cumulants can. This statement will be clarified in an example below.

Polarization, current and their spreads. – We now consider the Berry phase corresponding to the polarization from the modern theory [10,11,15,17,22–24]. In this theory an expression for the spread of a Berry phase associated quantity has been suggested, and we now show that it is equivalent to C_2/Λ.

Resta showed that the expectation value of the position over some wave function $|\Psi_0\rangle$ of a system with unit cell dimension L can be written as

$$\langle X\rangle = -\frac{1}{\Delta K}\mathrm{Im}\ln\langle\Psi_0|e^{-i\Delta K\hat{X}}|\Psi_0\rangle, \quad (15)$$

where $\Delta K = 2\pi/(N_k L)$, N_k denotes an integer, $\hat{X} = \sum_j \hat{x}_j$ is the sum of the positions of all particles. The spread in position ($\sigma_X^2 = \langle X^2\rangle - \langle X\rangle^2$) can be written as

$$\sigma_X^2 = -\frac{2}{\Delta K^2}\mathrm{Re}\ln\langle\Psi_0|e^{-i\Delta K\hat{X}}|\Psi_0\rangle, \quad (16)$$

The operator $e^{i\Delta K\hat{X}}$ is the total momentum shift operator which, as has been shown elsewhere [25,26] has the property that for a state $|\Psi_0(K)\rangle$ with particular crystal momentum K defined as

$$\Psi_0(k_1 + K, k_2 + K, \ldots), \quad (17)$$

it holds that

$$e^{-i\Delta K\hat{X}}|\Psi_0(K)\rangle = |\Psi_0(K + \Delta K)\rangle, \quad (18)$$

in other words it shifts the crystal momentum by ΔK. To use the shift operator we first write

$$\sigma_X^2 = -\frac{2}{N_k\Delta K^2}\mathrm{Re}\ln\langle\Psi_0|e^{-i\Delta K\hat{X}}|\Psi_0\rangle^{N_k}. \quad (19)$$

We associate the state $|\Psi_0\rangle$ with a particular crystal momentum K_0,

$$|\Psi_0\rangle = |\Psi_0(K_0)\rangle. \quad (20)$$

Using the total momentum shift the scalar product can be rewritten as

$$\begin{aligned}\langle\Psi_0(K_0)|e^{-i\Delta K\hat{X}}|\Psi_0(K_0)\rangle &= \langle\Psi_0(K_0)|\Psi_0(K_1)\rangle \\ &= \langle\Psi_0(K_I)|\Psi_0(K_{I+1})\rangle, \quad (21)\end{aligned}$$

where $K_{I+1} = K_I + \Delta K$. To show the last equation one applies the Hermitian conjugate of the total momentum shift to $\langle\Psi_0(K_0)|$ I times and the total momentum shift operator to $|\Psi_0(K_0)\rangle$ $I + 1$ times and forms the scalar product. Thus we can also write

$$\langle\Psi_0(K_0)|e^{-i\Delta K\hat{X}}|\Psi_0(K_0)\rangle^{N_k} = \prod_{I=0}^{N_k-1}\langle\Psi_0(K_I)|\Psi_0(K_{I+1})\rangle. \quad (22)$$

The points K_I form an evenly spaced grid with spacing ΔK in the Brillouin zone. Using this result the spread can be rewritten as

$$\sigma_X^2 = -\frac{2}{N_k\Delta K^2}\sum_{I=0}^{N_k}\mathrm{Re}\ln\langle\Psi_0(K_I)|\Psi_0(K_{I+1})\rangle, \quad (23)$$

We now expand the scalar product up to second order as

$$\begin{aligned}\langle\Psi_0(K_I)|\Psi_0(K_{I+1})\rangle &= 1 + \Delta K\langle\Psi_0(K_I)|\partial_K|\Psi_0(K_I)\rangle \\ &\quad + \frac{\Delta K^2}{2}\langle\Psi_0(K_I)|\partial_K^2|\Psi_0(K_I)\rangle. \quad (24)\end{aligned}$$

The subsequent expansion of the logarithm and keeping all terms up to second order in ΔK results in a first-order term of the form

$$\frac{N_k L^2}{2\pi^2}\mathrm{Re}\sum_{I=0}^{N_k-1}\Delta K\langle\Psi_0(K_I)|\partial_K|\Psi_0(K_I)\rangle. \quad (25)$$

In the continuum limit ($N_k \to \infty$) the sum turns into the integral which gives the standard Berry phase, but since this integral is purely imaginary it will not contribute to the spread. The final result for the spread is

$$\sigma_X^2 = \frac{L}{2\pi}\sum_{I=0}^{N_k-1}\Delta K\sigma_X^2(K_I) = \frac{L}{2\pi}\int_{-\pi/L}^{\pi/L}\mathrm{d}K\sigma_X^2(K), \quad (26)$$

where

$$\sigma_X^2(K) = -\langle\Psi_0(K)|\partial_K^2|\Psi_0(K)\rangle + \langle\Psi_0(K)|\partial_K|\Psi_0(K)\rangle^2. \tag{27}$$

Equation (26) is actually the average of the spread over the Brillouin zone. One can think of $i\partial_K$ as a "heuristic position operator" [27], and the quantity $\sigma_X^2(K)$ as the spread for a wave function with crystal momentum K. This spread of the position operator, derived by different means, has also been obtained by Marzari and Vanderbilt [28]. One can also start from the expression for the spread of the total current [29]

$$\sigma_K^2 = -\frac{2}{\Delta X^2}\mathrm{Re}\ln\langle\Psi_0|e^{-i\Delta X\hat{K}}|\Psi_0\rangle, \tag{28}$$

and apply exactly the same steps as in the case of the total position. This derivation results in

$$\sigma_K^2 = -\frac{1}{L}\int_0^L \mathrm{d}X[\langle\Psi_0(X)|\partial_X^2|\Psi_0(X)\rangle - \langle\Psi_0(X)|\partial_X|\Psi_0(X)\rangle^2]. \tag{29}$$

Example: spin-$\frac{1}{2}$ particle in a precessing magnetic field. – We now calculate the cumulants up to fourth order for one of the canonical examples for the Berry phase [2], a spin-$\frac{1}{2}$ particle in a precessing magnetic field. The Hamiltonian is given by

$$\hat{H}(t) = -\mu\mathbf{B}(t)\cdot\boldsymbol{\sigma}, \tag{30}$$

where $\boldsymbol{\sigma}$ are the Pauli matrices, and $\mathbf{B}(t)$ denotes the magnetic field,

$$\mathbf{B}(t) = \begin{bmatrix}\sin\theta\cos\phi\\ \sin\theta\sin\phi\\ \cos\theta\end{bmatrix}. \tag{31}$$

The z-component of the field is fixed, the projection on the (x, y)-plane is performing rotation, *i.e.* $\phi = \omega t$. We can proceed to evaluate the Berry phase and the associated cumulants by defining an adiabatic cycle in which ϕ rotates from zero to 2π. Using one of the eigenstates

$$|n_-(t)\rangle = \begin{bmatrix}-\sin\left(\frac{\theta}{2}\right)\\ e^{i\phi}\cos\left(\frac{\theta}{2}\right)\end{bmatrix}. \tag{32}$$

The associated cumulants (divided by 2π) evaluate to

$$\begin{aligned} C_1 &= \cos^2\left(\tfrac{\theta}{2}\right),\\ C_2 &= \left[\cos^2\left(\tfrac{\theta}{2}\right) - \cos^4\left(\tfrac{\theta}{2}\right)\right],\\ C_3 &= \left[\cos^2\left(\tfrac{\theta}{2}\right) - 3\cos^4\left(\tfrac{\theta}{2}\right) + 2\cos^6\left(\tfrac{\theta}{2}\right)\right],\\ C_4 &= \left[\cos^2\left(\tfrac{\theta}{2}\right) - 7\cos^4\left(\tfrac{\theta}{2}\right) + 12\cos^6\left(\tfrac{\theta}{2}\right) - 6\cos^8\left(\tfrac{\theta}{2}\right)\right]. \end{aligned} \tag{33}$$

Figure 1 shows the cumulants as a function of the angle θ. C_1, the Berry phase associated with a spin-$\frac{1}{2}$ particle in a precessing magnetic field, is a well-known result. The spread is zero when the Berry phase is zero or π. The skew changes sign halfway between zero and π and the kurtosis also varies in sign as a function of the angle θ.

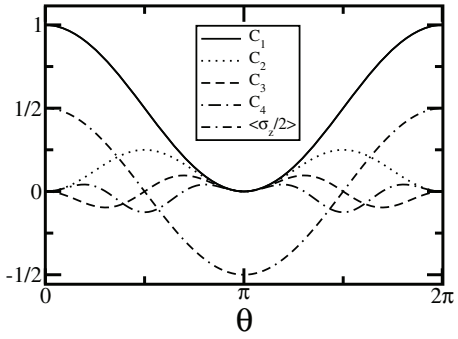


Fig. 1: Cumulants of a spin-$\frac{1}{2}$ particle in a precessing field.

The operator $\hat{O}$ for this example can easily be shown to be the Pauli matrix $\frac{\sigma_z}{2}$. The first-order cumulant is given by

$$\left\langle\frac{\sigma_z}{2}\right\rangle = \sin^2\left(\frac{\theta}{2}\right) - \cos^2\left(\frac{\theta}{2}\right); \tag{34}$$

in other words it is merely shifted compared to the Berry phase. The higher-order cumulants are identical to those in eqs. (33). In the operator representation of the Berry phase the meaning of the first and second cumulants is rendered more clear. For the value of θ for which $\langle\sigma_z/2\rangle$ is either $\pm\frac{1}{2}$ the spread is zero. Indeed those are the maximum and minimum values the operator σ_z can take, hence the spread must be zero. It is obvious from these results that the cumulants derived from the Bargmann invariant give information about the probability distribution of the operator associated with the Berry phase.

Measurement of C_i's. – While it has been shown that C_i's are physically well defined, their measurement may not be trivial. The operator may not exist or be easily written down. In this case one can proceed as follows. Define

$$\begin{aligned} \mathbf{\Pi} &= \prod_{I=0}^{M-1}\langle\Psi_0(\chi_I)|\Psi_0(\chi_{I+1})\rangle,\\ \mathbf{\Pi}^{(o)} &= \prod_{I=0}^{M/2-1}\langle\Psi_0(\chi_{2I+1})|\Psi_0(\chi_{2I+3})\rangle,\\ \mathbf{\Pi}^{(e)} &= \prod_{I=0}^{M/2-1}\langle\Psi_0(\chi_{2I})|\Psi_0(\chi_{2I+2})\rangle. \end{aligned} \tag{35}$$

Using these definitions one can show that

$$\begin{aligned} C_3 &\approx \frac{2}{\Delta\chi^2}\mathrm{Im}\ln\left[\frac{(\mathbf{\Pi}^{(o)}\mathbf{\Pi}^{(e)})^{\frac{1}{2}}}{\mathbf{\Pi}}\right] + O(\Delta\chi^3),\\ C_4 &\approx \frac{4}{\Delta\chi^3}\mathrm{Re}\ln\left[\frac{(\mathbf{\Pi}^{(o)}\mathbf{\Pi}^{(e)})^{\frac{1}{4}}}{\mathbf{\Pi}}\right] + O(\Delta\chi^3). \end{aligned} \tag{36}$$

Conclusions. – In this paper it was shown that there exists a cumulant expansion associated with the Berry phase. The starting point was the Bargmann invariant, which gives rise to the discrete Berry phase. It was shown

how a cumulant expansion associated with the Berry phase can be obtained from the Bargmann invariant. Up to fourth order it was demonstrated that the cumulants are gauge invariant. It was also shown that the cumulants derived can also be related to corresponding expectation values of a particular operator. Since, in the modern theory of polarization, an expression for the second cumulant (spread or variance) is already in use, as a consistency check, equivalence between that and the spread resulting from the cumulant expansion presented here was shown. The cumulants were calculated for the spin-$\frac{1}{2}$ particle in a precessing magnetic field. The results indicate that the cumulants aid in reconstructing the underlying distribution from which the Berry phase arises.

We also note that while the ideas above may not be straightforward to apply to all Berry phases (it depends on the ease with which a cyclic curve is parametrized), it is straightforward for two very important cases: the TKNN invariant [7] and the topological invariant in the Drude weight [9]. The Berry phase associated with these quantities arises from a circuit integral around a rectangle.

* * *

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