Quantum Geometric Phases in Deformable Extended Objects

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Abstract. We show that quantum particles may acquire geometrical phases when the curves they are constrained to live on undergo cyclic deformations.

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1. INTRODUCTION

The standard setup of quantum geometrical phases involves a hamiltonian H that depends on external parameters ξ^A, $H = H(\xi)$, which trace out a loop C in ξ-space. The adiabatic theorem states that if the system starts in an eigenstate $|n\rangle$ of H, and the ξ's change slowly enough, then time evolution consists in locking onto the instantaneous eigenstate of H, with a phase that, apart from the dynamical "energy times time" contribution, includes a term that only depends on C [1, 2]. The effect was anticipated in [3] and further explored in [4, 5], before Berry's formulation. An elegant description, due to Simon [6], uses a $U(1)$ bundle over ξ-space, and the holonomy of the parallel-transport law for the phase dictated by Schroedinger's equation.

We study, in this work, the problem of a quantum particle, which is constrained to move along a space curve, via a harmonic oscillator confining potential in the plane normal to the curve, in the presence of cyclic deformations of the curve. It is a known result that, under these conditions, the 1D hamiltonian that governs the motion along the curve, involves the curvature κ and torsion τ of the curve, which can therefore be thought of as external parameters, living in an infinite dimensional parameter space. By writing the time-dependent Schroedinger equation in the coordinate system adapted to the curve an additional term is produced, coming from the transformation of the time derivative, which depends not only on the shape of the curve but, also, on its velocity field — its role is to account for the inertial forces felt in the adapted frame. Inclusion of this term results in an effective 1D hamiltonian that is defined on the tangent bundle of the space of parameters — we use standard time-dependent perturbation theory to compute the geometric phase in this case.

The structure of this short communication is as follows: in section 2 we review the basics of geometric phases, and the confining potential approach to constrained quantum dynamics. Then, in section 3, we explain the peculiarity of the case at hand (or, at least, of our approach to it) and derive *ab initio* a formula for a suitably defined geometric phase, illustrating the general results with the example of a deformed circle.

2. GEOMETRIC PHASES AND CONSTRAINED DYNAMICS

2.1. Geometric phases

We consider a hamiltonian $H(\xi(t))$, where the parameters $\xi^A(t)$ trace out a loop C in ξ-space, starting and finishing at the origin, at times $t=0$ and $t=T$ respectively. The system described by H is assumed to be, at $t=0$, in a nondegenerate eigenstate $|n,\xi(0)\rangle \equiv |n\rangle$ of $H(\xi(0)) \equiv H$, with energy $E_n(\xi(0)) \equiv E_n$,

$$|\psi(0)\rangle = |n\rangle \qquad\qquad H|n\rangle = E_n|n\rangle\,. \tag{1}$$

The adiabatic theorem states that if the change of the ξ's is slow enough, in the time scale set by the energy difference of neighboring eigenstates, then the system "follows" the hamiltonian, and its state is, up to a possible phase factor, the instantaneous eigenstate $|n,\xi(t)\rangle$ of $H(\xi(t))$,

$$|\psi(t)\rangle = e^{i\delta_n(t)}|n,\xi(t)\rangle\,, \tag{2}$$

where $H(\xi(t))|n,\xi(t)\rangle = E_n(\xi(t))|n,\xi(t)\rangle$. Substitution of (2) in the time dependent Schroedinger equation shows that $\delta_n(t) = -\alpha_n(t) + \gamma_n(t)$, where the phase $\alpha_n(t) = \int_0^t d\tau\, E_n(\xi(\tau))$ is the expected dynamical one, and

$$\gamma_n(t) = i\int_0^t d\tau\,\langle n,\xi(\tau)|\frac{d}{d\tau}|n,\xi(\tau)\rangle = i\int_{\xi_0}^{\xi_t} d\xi^A\langle n,\xi|\partial_{\xi^A}|n,\xi\rangle\,, \tag{3}$$

is the geometrical phase — the latter form shows that it is time reparametrization invariant, and defines a connection in a $U(1)$ bundle over ξ-space. Using Stokes theorem, one finds that, upon completing the excursion along C, the system acquires a geometrical phase $\gamma_n(C)$ given by

$$\gamma_n(C) = \frac{1}{2}\int_S d\xi^A d\xi^B K_{AB}^{(n)}\,, \qquad\qquad K_{AB}^{(n)} \equiv -2\,\mathrm{Im}(\partial_A\langle n,\xi|)(\partial_B|n,\xi\rangle)\,, \tag{4}$$

where $K_{AB}^{(n)}$ are the components of the curvature associated with the above connection, and S is any two-dimensional patch with C as its boundary (see [1, 6, 2, 7]).

2.2. The confining potential approach to constrained dynamics

A quantum particle is forced to live on a space curve by means of an attractive parabolic potential W in the plane normal to the curve — the corresponding hamiltonian is taken to be $H_E = -\frac{1}{2}(\partial_x^2 + \partial_y^2 + \partial_z^2) + W_E(x,y,z)$, where (x,y,z) are cartesian coordinates in 3D euclidean space, and $W_E(x,y,z)$ is, in general, a complicated function of its arguments. Following the presentation in [8], we introduce adapted coordinates (s,α,β), where s is arclength along the curve, with corresponding unit vector $\partial_s \equiv \mathbf{t}$, and $\eta\alpha$, $\eta\beta$ are distances along the normal $\mathbf{n}$ and binormal $\mathbf{b}$ of the curve. The length parameter η appears in the confining potential $W(\alpha,\beta) = W_E(x^i(s,\alpha,\beta)) = (\alpha^2+\beta^2)/(2\eta^2)$ and controls the penetration depth of the particle in the ambient 3D space. Taking $\eta \ll \kappa^{-1}$ guarantees that the adapted frame is well defined in the region where the particle penetrates with appreciable probability. We assume that $\kappa(s) \neq 0$. The hamiltonian for the particle in the adapted frame is

$$H_c = -\frac{1}{2\sqrt{|G|}}\partial_a\big(G^{ab}\sqrt{|G|}\big)\partial_b + W(\alpha,\beta)\,, \tag{5}$$

where a, b range over the adapted coordinates, G_{ab} is the euclidean metric in the adapted coordinates, G^{ab} its inverse, and $G = (1-\eta\alpha\kappa)^2$ its determinant. The fact that W does not depend on s means that the tangential motion is classically free. In the adapted frame inner products between state vectors involve the nontrivial measure $\sqrt{G}$, which we opt to absorb in a redefinition of the wavefunction, $\Phi \to \Psi = G^{1/4}\Phi$. The latter must be accompanied by a similarity transformation of the hamiltonian,

$$H_c \to \tilde{H}_c = G^{1/4} H_c G^{-1/4} = \frac{1}{\eta^2} H_{-2} + H_0 + \mathscr{O}(\eta)\,, \tag{6}$$

where

$$H_{-2} = -\frac{1}{2}(\partial_\alpha^2 + \partial_\beta^2) + \frac{1}{2}(\alpha^2+\beta^2)\,, \qquad H_0 = -\frac{1}{2}(\partial_s - \tau L)^2 - \frac{\kappa^2}{8}\,, \tag{7}$$

and $L = \alpha\partial_\beta - \beta\partial_\alpha$ is the (antihermitean) generator of rotations in the normal plane. It is clear that $\tilde{H}_c$ eigenstates, $\tilde{H}_c\Psi = \tilde{E}_c\Psi$, can be sought in the factorized form $\Psi(s,\alpha,\beta) = \chi(\alpha,\beta)\psi(s)$, with $\chi(\alpha,\beta)$ a simultaneous eigenket of H_{-2} and L,

$$H_{-2}\chi_\sigma^{(n)} = (n+1)\chi_\sigma^{(n)}\,, \qquad L\chi_\sigma^{(n)} = i\sigma\chi_\sigma^{(n)}\,. \tag{8}$$

The hamiltonian H that the 1D wavefunction $\psi(s)$ sees then is [9] ($\psi' \equiv \partial_s\psi$, *etc.*)

$$H\psi = -\frac{1}{2}\psi''_\sigma + i\sigma\tau\psi'_\sigma + \frac{1}{2}\left(i\sigma\tau' + \sigma^2\tau^2 - \frac{1}{4}\kappa^2\right)\psi_\sigma = E_\sigma\psi_\sigma\,, \tag{9}$$

and the total energy $\tilde{E}_c$ of the state Ψ is given by $\tilde{E}_c = \eta^{-2}(n+1) + E_\sigma$.

3. DEFORMATIONS

3.1. Time dependent perturbation theory

In this section we consider the case of a curve that is cyclically deformed in time, and would like to identify the associated perturbation hamiltonian. Our ultimate aim is to compute the geometric phase accumulated during one cycle of the perturbation, and we will have to resort to time dependent perturbation theory for that. It will prove convenient to develop first a general formula for the phase, so that we can later decide which terms in the perturbation hamiltonian are relevant to our purposes. We consider the time-dependent Schroedinger equation ($\dot\psi \equiv \partial_t \psi$, *etc.*)

$$\dot\psi(t) = -i\big(H + \lambda V(t)\big)\psi(t)\,, \tag{10}$$

where H does not depend on time and λ is small. Putting $\psi(t) = e^{-iHt}U(t)\psi(0)$, (10) gives

$$\dot U(t) = -i\lambda \tilde V(t) U(t)\,, \tag{11}$$

where $\tilde V \equiv e^{iHt}V(t)e^{-iHt}$. Integration and iteration results in

$$U(t) = 1 - i\lambda \int_0^t dt_1 \tilde V(t_1) - \lambda^2 \int_0^t dt_1 \int_0^{t_1} dt_2 \tilde V(t_1)\tilde V(t_2) + \mathscr{O}(\lambda^3)\,. \tag{12}$$

Assume the system starts, at $t = 0$, in an eigenstate $|n\rangle$ of H, $H|n\rangle = E_n|n\rangle$, and $V(0) = V(T) = 0$. The (assumed) adiabatic nature of the perturbation guarantees then that $\psi(T) = e^{-iHT}U(T)|n\rangle$ will be proportional to $|n\rangle$, by a phase factor given by

$$\langle n|\psi(T)\rangle = e^{-iE_nT}\langle n|U(T)|n\rangle\,, \tag{13}$$

or, substituting from (12),

$$e^{iE_nT}\langle n|\psi(T)\rangle = 1 - i\lambda \int_0^T dt_1 V_{nn}(t_1) - \lambda^2 \sum_k \int_0^T dt_1 \int_0^{t_1} dt_2\, e^{iE_{nk}(t_1-t_2)} V_{nk}(t_1) V_{kn}(t_2)\,, \tag{14}$$

where $E_{nk} \equiv E_n - E_k$, $V_{nk}(t_1) \equiv \langle n|V(t_1)|k\rangle$, and higher order terms have been neglected. The quadratic term above contains information about the geometric phase, as well as second order and the square of first order corrections to the energy. A detailed treatment of this integral is deferred to a lengthier publication, currently in progress. For the moment we consider the case of two parameters ξ and ζ, and assume, as it will turn out to be the case below, that the perturbation hamiltonian depends not only on their values but also on those of their time derivatives, $\lambda V(t) = \xi(t)V_\xi + \dot\xi(t)V_{\dot\xi} + \zeta(t)V_\zeta + \dot\zeta(t)V_{\dot\zeta}$, where V_ξ, $V_{\dot\xi}$, *etc.*, are time independent operators. Then we consider driving the system around a circle in the ξ-ζ plane, $\xi = \lambda(\cos\omega t - 1)$, $\zeta = \lambda \sin\omega t$, with $\omega \ll E_{nk}$, for all k, as adiabaticity demands (notice that in the limit $\omega \to 0$ the condition $V(0) = V(T) = 0$ assumed above is satisfied). Having fixed the time dependence of V, the double integral in (14) may be performed (with $T = 2\pi/\omega$), and the result expanded in powers of ω, giving

$$e^{iE_nT}\langle n|\psi(T)\rangle = -\lambda^2\, 2\pi i \sum_{k\neq n} E_{nk}^{-2}\left(\mathrm{Im}\left(V_{\xi\,nk}V_{\zeta\,kn}\right) + E_{nk}\,\mathrm{Re}\left(V_{\xi\,nk}V_{\dot\zeta\,kn} - V_{\dot\xi\,nk}V_{\zeta\,kn}\right)\right) + \ldots \tag{15}$$

where the omited terms depend on ω. The above, ω-independent, contribution to the phase we identify as (i times) the geometric phase. Dividing by the area $\pi\lambda^2$ of the circle traced out in the ξ-ζ plane, we find for the curvature

$$K_{\xi\zeta} = -2\sum_{k\neq n} E_{nk}^{-2}\left(\mathrm{Im}\left(V_{\xi\,nk}V_{\zeta\,kn}\right) + E_{nk}\,\mathrm{Re}\left(V_{\xi\,nk}V_{\dot\zeta\,kn} - V_{\dot\xi\,nk}V_{\zeta\,kn}\right)\right)\,. \tag{16}$$

The problem has been reduced now to the identification of the shape-dependent V_ξ and the velocity-dependent $V_{\dot{\xi}}$.

3.2. Shape dependent perturbations

An infinitesimal deformation of a curve $\mathbf{r}(s)$ can be described by a vector field $\mathbf{v}(s)$ defined over the curve, which specifies the velocity of each of its points under the deformation. To simplify a bit the analysis, we will concentrate on an important class of such vector fields, given by the *locally arclength preserving* (LAP) ones, which satisfy $\mathbf{t}\cdot\mathbf{v}' = 0$. In terms of adapted frame components, $\mathbf{v} = v^t\,\mathbf{t} + v^n\,\mathbf{n} + v^b\,\mathbf{b}$, the LAP condition becomes $v^{t\,\prime} - \kappa v^n = 0$. Consider now an infinitesimal LAP deformation of the form $\mathbf{r} \to \mathbf{r} + \xi\,\mathbf{v}$ with $\xi \ll 1$. Such a deformation brings along changes in the curvature and torsion, $\kappa \to \kappa + \xi\kappa_\xi$, $\tau \to \tau + \xi\tau_\xi$ (the detailed expressions are not particularly illuminating), so that the hamiltonian H in (9) becomes ξ-dependent, $H(\xi) = H + \xi H_\xi$, with

$$H_\xi = i\sigma\tau_\xi\partial_s + \frac{1}{2}\big(i\sigma\tau_\xi' + 2\sigma^2\tau\tau_\xi - \frac{1}{2}\kappa\kappa_\xi\big) \qquad (17)$$

in the role of a shape-dependent perturbation.

3.3. Velocity dependent perturbations: the effect of inertial forces

In the previous section we saw how the change to the frame adapted to the curve, and the subsequent similarity transformation by the square root of the measure, leads to the simplified form (6) of the hamiltonian. However, if the above change of coordinates is time dependent, as is the case when the space curve is being deformed, an additional term arises that should be added to $\tilde{H}_c$, coming from the transformation of the time derivative in the time dependent Schroedinger equation. Indeed, under the change of coordinates $(t,x^1,x^2,x^3) \to (t',y^1,y^2,y^3)$, with $t' = t$ and $y^i = y^i(x;\xi(t))$, the time derivative transforms as $\partial_t = \partial_{t'} + \dot{\xi}(\partial y^i/\partial\xi)\partial_{y^i}$, where we have assumed that the time dependence is through a parameter $\xi(t)$. The quantities $u^i = -\partial y^i/\partial\xi$ are the adapted frame components of the velocity of a point with fixed adapted coordinates y^i, as seen in the ambient cartesian frame, and can be computed in terms of the velocity field $\mathbf{v}(s)$ of the curve itself. One then effects the similarity transformation $u \to \tilde{u} \equiv G^{1/4}uG^{-1/4}$ to find the time dependent Schroedinger equation obeyed by the rescaled wavefunction Ψ,

$$\partial_{t'}\Psi = -i\left(\tilde{H}_c + \xi H_\xi + i\dot{\xi}\tilde{u}\right)\Psi \qquad (18)$$

where, in H_ξ, σ should be replaced by $-iL$ (there is in fact an extra term $G^{1/4}\partial_{t'}G^{-1/4}$ showing up but it can be shown to not contribute to the curvature).

3.4. An example: deformed circular loop

Take as undeformed curve a circle, with $\kappa(s) = 1$ and $\tau(s) = 0$. For the normal plane wavefunctions we choose the states $\chi_\pm^{(1)} \equiv |\pm\rangle = (|10\rangle \pm i|01\rangle)/\sqrt{2}$, with H_{-2} eigenvalue 2 and $L|\pm\rangle = \pm|\pm\rangle$. Eq. (9) then becomes

$$-\frac{1}{2}\psi_\sigma'' - \frac{1}{8}\psi_\sigma = E_\sigma \psi_\sigma\,, \tag{19}$$

with solutions $\psi_\sigma^{(m)}(s) = e^{ims}/\sqrt{2\pi}$, and eigenvalues $E_\sigma^{(m)} = (4m^2 - 1)/8$, $m = 0, \pm 1, \pm 2, \ldots$ Consequently, all but the ground state, are doubly degenerate (apart from the $\sigma = \pm 1$ degeneracy, common to all states). The corresponding rescaled 3D states are then $\Psi_\pm^{(1,m)} = \chi_\pm^{(1)} \psi_\pm^{(m)}$ with

$$\chi_\pm^{(1)} = \rho e^{-\rho^2/2} e^{\pm i\phi}/\sqrt{\pi}\,, \qquad E_\pm^{(1,m)} = \frac{2}{\eta^2} + \frac{4m^2-1}{8} \tag{20}$$

(ρ, ϕ denote the standard polar coordinates in the normal plane). We assume the particle to be in the ground state, $m = 0$, and consider the two-parameter deformation, in the adapted frame, $\tilde{\mathbf{r}}(s) = (0,-1,0) + \xi\,(p^{-1}\sin ps, \cos ps, 0) + \zeta\,(0,0,\cos ps)$, $p = 1, 2, \ldots$, for which we find

$$H_\xi = \frac{1}{4}(p^2-1)\cos(ps) \qquad H_\zeta = \frac{i}{2}\sigma p(p^2-1)\big(2\sin(ps)\partial_s + p\cos(ps)\big)$$
$$H_{\dot\xi} = ip^{-1}\sin(ps)\partial_s + \frac{i}{2}\cos(ps) \qquad H_{\dot\zeta} = \sigma p^2\cos(ps)\,,$$

so that the sum in (16) only receives contributions from $k = \pm p$, leading to the expression $K_{\xi\zeta} = -\sigma(p^2-1)^2/2p^2$ for the curvature, which coincides with the result of [10], for $p = 2$ (notice the difference in the definition of K by a factor of 2).

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