Effective geometric phases and topological transitions in SO(3) and SU(2) rotations

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Abstract
We address the development of geometric phases in classical and quantum magnetic moments (spin-1/2) precessing in an external magnetic field. We show that nonadiabatic dynamics lead to a topological phase transition determined by a change in the driving field topology. The transition is associated with an effective geometric phase which is identified from the paths of the magnetic moments in a spherical geometry. The topological transition presents close similarities between SO(3) and SU(2) cases but features differences in, e.g. the adiabatic limits of the geometric phases, being 2\pi and \pi in the classical and the quantum case, respectively. We discuss possible experiments where the effective geometric phase would be observable.

Keywords: geometric phase, Berry phase, topology, rotation, magnetism, spin, nonadiabatic

(Some figures may appear in colour only in the online journal)
fields of different relative strength. Spin transport calculations predict that such a transition in the field topology causes a distinct shift in the interference pattern of the conductance in loop-shaped spin-interferometers [23]. However, due to complex nonadiabatic spin dynamics, the topological transition is associated with an emergent effective geometric phase [23] and not with the bare geometric phase that can be calculated from the solid angle that the spin subtends in a roundtrip around the circuit.

Recently, Berry phases have also been extracted using interferometry in superconducting qubit systems [24]. Indeed, a topological transition in such spin-$\frac{1}{2}$ superconducting qubit systems has been observed by measuring the Chern number, a topological invariant that counts the number of degenerate energy eigenvalues inside a closed manifold along which the parameters of the Hamiltonian are swept [25, 26]. Geometric phases have been studied also in the context of nuclear magnetic resonance spectroscopy (NMR) [27] for which a general treatment was developed by Bloch and Siegert [28]. NMR beyond a perturbative regime has been considered in [29, 30].

In the experiments discussed above, the rotating field is usually assumed to be perpendicular to the homogeneous magnetic field [3, 27]. In contrast, here we change the topology of the field using a coplanar arrangement of the homogeneous and rotating field components with arbitrary field strengths. The changing field topology is then associated with nonadiabatic dynamics when a degeneracy is placed along the path of the cycle, leading to emergent effective geometric phases undergoing a smooth but distinct transition.

Here we study the nonadiabatic dynamics of a classical and a quantum mechanical (spin) magnetic moment precessing in a time-dependent magnetic field with varying topology due to the combined action of coplanar, homogeneous and rotating, field components. $\text{U}(1)$ phases do not play any role in the classical dynamics (in contrast to the quantum case) but the Lie algebras of the group $\text{SU}(2)$ of spin rotations and $\text{SO}(3)$ of classical rotations are isomorphic leading to analogous phenomena. Cina demonstrated in a study on spin and classical magnetic moment precessions that \textit{adiabatic} Berry phase factors have a geometric interpretation in terms of rotations [31]. Moreover, $\text{SO}(3)$ has been found to be connected with adiabatic geometric phases in qubit systems [32]. Therefore we expect analogies to emerge also in the nonadiabatic regime and we anticipate comparable topological effects in both cases. Indeed, we show here that precessions of a classical magnetic moment give rise to effective nonadiabatic geometric and dynamic phase angles with an associated topological transition, showing a clear correspondence with those found for spin rotations. The results also provide insights into the origin of the effective geometric phases in quantum systems [23]. We demonstrate that, in the classical case, the effective geometric phase is associated with the dynamics of precessions of the classical magnetic moment in the $S^2$ sphere, much like it was found to be related to the windings of the spin magnetic moment on the Bloch sphere in the quantum case [23]. In the adiabatic limit we recover a Berry phase equal to $2\pi$ for classical rotations which is in contrast to the Berry phase of $\pi$ for spin rotations. We also suggest experimental setups that would demonstrate the discussed effects.

2. Definitions and models

We study the dynamics of a classical magnetic moment and a spin-$\frac{1}{2}$ system in a composite magnetic field

$$\mathbf{H}(t) = \mathbf{H}_0 + \mathbf{H}(t),$$

where $\mathbf{H}_0 = 2\pi \mathbf{H}_0 \mathbf{e}_z$ is an homogeneous field and $\mathbf{H}(t) = 2\pi \mathbf{H}(t) \mathbf{e}_z$ is a time-dependent one with $\omega$ the angular frequency, $\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z$ the unit vectors along $x$, $y$ and $z$ axes, respectively, and $\mathbf{H}_0$ and $\mathbf{H}_1$ the strengths of the corresponding field components. The coplanar field texture (1) undergoes a change in topology from nonrotating ($\mathbf{H}_0 > \mathbf{H}_1$) to rotating ($\mathbf{H}_0 < \mathbf{H}_1$) when the strengths of the field components are equal, $\mathbf{H}_0 = \mathbf{H}_1$, see figure 1.

The magnetic moment dynamics in the classical case is calculated numerically using the Landau–Lifshitz equation [33] (or Bloch equation [34]). We assume in the following that the magnetic moment $\mathbf{M} = \mathbf{M}_0 \mathbf{e}_z + \mathbf{M}_1 \mathbf{e}_z + \mathbf{M}_2 \mathbf{e}_z$ has unit length.

The total effective magnetic field $\mathbf{H}(t)$ then exerts a torque on the magnetic moment giving rise to precessions as described by the equation of motion

![Figure 1](image-url)

**Figure 1.** Magnetic field $\mathbf{H} = 2\pi (\mathbf{H}_0 \mathbf{e}_y + \mathbf{H}_1 (\sin \theta \mathbf{e}_x + \cos \theta \mathbf{e}_y))$ changes topology from rotating (a) to nonrotating (b) as $\mathbf{H}_0$ becomes larger than $\mathbf{H}_1$. \[\text{J. Phys.: Condens. Matter 28 (2016) 166002} \]
\[
\frac{d\mathbf{M}(t)}{dt} = g\mathbf{H}(t) \times \mathbf{M}(t),
\]

where \( g \) is the gyromagnetic ratio that scales the effective field strength. It does not play another role in the calculations of phase components. Therefore we set it equal to one without loss of generality.

The total rotation matrix in a roundtrip \( \theta = 0 \rightarrow 2\pi \), with \( \theta = \omega t \), is then a matrix product of infinitesimal rotations

\[
R = \prod_{m=1}^{n} \begin{pmatrix} 1 & 0 & H_x(\theta_m)\,d\theta \\ 0 & 1 & -H_y(\theta_m)\,d\theta \\ -H_z(\theta_m)\,d\theta & H_x(\theta_m)\,d\theta & 1 \end{pmatrix}
\]

in the limit \( n \rightarrow \infty \). Here, \( d\theta = 2\pi/n \) and \( \theta_m = (m-1)d\theta \).

Unlike in magnetic resonance models, we focus on the acquired phases during a cycle. In this case, by scaling time as \( t' = \omega t \) and the strength of the magnetic fields as \( \mathbf{H} = \mathbf{H}/\omega \), the solution of equation (2) becomes independent of \( \omega \). Therefore we set \( \omega = 1 \) in the following discussion.

We set \( \mathbf{M}(\theta = 0) = \mathbf{M}_i \) and obtain numerically the magnetic moment after a rotation \( \theta = 0 \rightarrow 2\pi \), \( \mathbf{M}_f \). To this end, we fix \( n \) in equation (3) and normalize \( \mathbf{M} \) to unit length after each step. In numerical calculations, \( n \) is of the order of 10,000 and convergence of the results was conveniently checked. From this SO(3) rotation, we define the total phase acquired during the evolution as the angle between the initial and final magnetic moment orientation

\[
\phi_{\text{tot}} = \angle(\mathbf{M}_i, \mathbf{M}_f) = \angle(\mathbf{M}(\theta = 0), \mathbf{M}(\theta = 2\pi)).
\]

In addition, we define the bare dynamic phase \( \phi_d \) as the total rotation angle of the magnetic moment in the driving field. This is equal to the path length that the tip of the magnetic moment vector sweeps on the unit sphere in a cycle

\[
\phi_d = \int |d\mathbf{M}(\theta)|.
\]

Finally, the bare geometric phase \( \phi_{bg} \) is defined via

\[
\phi_{\text{tot}} = \phi_d - \phi_{bg}.
\]

Note the sign defining \( \phi_{bg} \), which is chosen to keep geometric phases predominantly positive in our discussion.

Spin dynamics is calculated in a similar manner using the spin Hamiltonian \( \mathbf{H}_S = \mathbf{H}(\theta) \cdot \mathbf{\sigma} \), where \( \mathbf{\sigma} \) is the vector of Pauli matrices. Here, \( \mathbf{H} = (H_x, H_y) \) are parameters of the Hamiltonian during a cycle. The Hamiltonian features a degeneracy point at \( \mathbf{H} = \mathbf{0} \), which for \( H_y \) \( \geq H_x \) moves outside the path swept by the parameters during a cycle, marking a change in topology (figure 1). For an arbitrary normalized initial spin-\( \frac{1}{2} \) spinor \( \psi_i \), the final state after a roundtrip around the circuit can be calculated by applying the propagator \( n \) times:

\[
\psi_f = \prod_{m=1}^{n} \exp(i\mathbf{H}(\theta_m) \cdot \mathbf{\sigma} \,d\theta)\psi_i,
\]

where \( \theta_m = (m-1)d\theta \) and \( d\theta = 2\pi/n \), with \( n \rightarrow \infty \). We take \( n \) finite but large (of the order of 5000) and check convergence of the numerical solution. The total U(1) phase change \( \phi_{\text{tot}} \) is obtained directly from the phase acquired in the state evolution. Besides, the bare spin dynamic phase is calculated from

\[
\phi_{\text{ad}} = \int_0^{2\pi} \langle \psi | i\mathbf{H}_S | \psi \rangle d\theta.
\]

From this, the bare spin geometric phase is extracted from the difference between \( \phi_{\text{ad}} \) and \( \phi_{\text{tot}} \) as in equation (6).

### 3. Geometric phases for SO(3)

Geometric phases have been associated with adiabatic [1] and nonadiabatic [2] cyclic evolution. Recently, the emergence of an effective geometric phase has been reported in loop-shaped spin interferometers far from the adiabatic regime [23]. This effective geometric phase was found to be related to a topological transition in the quantum conductance occurring at \( H_0 = H_{1} \), and it was explained in terms of the winding parity of the eigenstates around the poles of the Bloch sphere.

In contrast to the smooth behavior displayed by the effective geometric phase, the bare geometric and dynamics phases showed complex correlated patterns close to the topological transition.

Here we show that an analogous effective geometric phase can be also identified when SO(3) rotations of classical magnetic moments are considered. We first study the evolution of a classical magnetic moment initially oriented along the \( x \)-axis, \( \mathbf{M}_i = e_x \), perpendicular to the driving field at \( \theta = 0 \), as a result of applying the rotation matrix (3). Due to precession, the magnetic moment acquires SO(3) phases which can be evaluated as detailed in the previous section. Cosines of the total phase \( \phi_{\text{tot}} \) and the bare dynamic phase \( \phi_d \) in a roundtrip in the field are shown in figures 2(a) and (b). When the rotating field component \( H_y \) is absent, the magnetic moment precesses uniformly and the resulting total phase is equal to the dynamic phase \( \phi_{\text{tot}} = \phi_d = 2\pi H_0 \) according to equations (4) and (5). Precessions give rise to oscillations shown close to the vertical axis of figure 2(a). These are analogous to the Zeeman oscillations (U(1) phase rotation) in the case of spin transport in mesoscopic loops [23]. When both field components are finite the evolution of the magnetic moment is complex. The dynamic phase \( \phi_d \) in figure 2(b) displays a rich texture due to nonadiabatic dynamics. The bare geometric phase \( \phi_{bg} = \phi_d - \phi_{\text{tot}} \), not depicted here, shows a complementary complexity. Still, the total phase has a smooth behaviour and we note a distinct phase shift close to the critical line \( H_0 = H_1 \) (see figure 2(a)). We associate this phenomenon with a change in the topology of the driving field and an emerging effective classical geometric phase in the following.

Figure 3 illustrates the magnetic moment dynamics at a fixed total phase \( \phi_{\text{tot}} = \frac{2\pi}{n} \), corresponding to paths starting at the ‘north’ pole of the sphere and ending in the ‘south’ pole, for different field topologies. Notice that lines of constant total phase \( \phi_{\text{tot}} \) equal to a half-integer multiple of \( 2\pi \) are easily identified in the \( H_1 - H_0 \) plane as those where \( \cos(\phi_{\text{tot}}) = -1 \) (see, e.g. the dotted line in figure 2(a)). These lines stretch from the \( H_0 \) axis to the \( H_1 \) axis. Along them, \( \phi_{\text{tot}} \) can be directly

\[ 4 \cos(\phi_{\text{tot}}) \] determines \( \phi_{\text{tot}} \) only up to modulo of \( \pi \).
calculated since $\phi_{\text{ad}} = \phi_0 = 2\pi H_0$ at the $H_0$ axis. In our case, when $H_0 = 1.5$ and $H_1 = 0$, the tip of the magnetic moment describes a great circle with length $1.5 \times 2\pi$, equal to the dynamical phase at this point. As we approach the $H_1$ axis, the total rotation angle increases and so does the dynamical phase, which is equal to $\phi_0 = 2.20 \times 2\pi$ at $H_0 = 0$, $H_1 = 2.32$ (figure 3(c)). This angle $\phi_0$ is slightly less than $H_1 \times 2\pi$ due to nonadiabatic effects. In view of equation (6), it is evident that the increase of the total rotation angle is also associated with an increase in the bare geometric phase.

Close to the critical line $H_0 = H_1$ the magnetic field is weak and it changes direction rapidly at $\theta = \pi$. The magnetic moment cannot reorient fast enough causing it to lose the perpendicular orientation with respect to the magnetic field. This is manifested as an increase in nonadiabaticity, quantified here by $|\cos(\angle(M, H))|$, averaged over a cycle of the field (figure 2(c)). Values close to zero indicate approximately adiabatic evolution. Nonadiabatic features are apparent close to the critical line in figure 2(c), causing the complex patterns in the dynamic phase in figure 2(b). However, we find that the evolution is approximately adiabatic when the total phase is a half-integer times $2\pi$, and this approximation improves with field strength, see e.g. the dotted line corresponding to $\phi_{\text{tot}} = 4.5 \times 2\pi$ in figure 2(c). We use this fact to extract the effective geometric phase.

First, we introduce the adiabatic dynamic phase in a closed path, $\phi_{\text{ad}}$, as the phase acquired in an homogeneous field of strength $H_{\text{ave}} = \int_0^{2\pi} d\theta |H|/2\pi$, which is the average field in a roundtrip. An explicit calculation gives

$$
\phi_{\text{ad}} = \sqrt{H_0^2 + H_1^2} \int_0^{2\pi} d\theta \sqrt{1 + 2H_0 H_1/(H_0^2 + H_1^2)} \cos \theta = 2(H_1 + H_0) \left[ E(\pi/4, \mathcal{H}) + E(3\pi/4, \mathcal{H}) \right],
$$

(9)

where $\mathcal{H} = 4H_1 H_0/(H_1 + H_0)^2$, and $E(\varphi, m)$ are elliptic integrals of the 2nd kind. Notice that $\phi_{\text{ad}}$ may be understood as a sort of a smooth component of the bare dynamic phase $\phi_0$. Figure 2(a) clearly shows quasi-adiabatic characteristics in the form of wavefronts at constant adiabatic dynamic phase (dashed lines).

We now define the effective geometric phase as the difference between the adiabatic dynamic phase and the total phase...
\[ \phi_g = \phi_{ad} - \phi_{tot}. \]  

Figure 4(a) shows \( \phi_g \) as a function of the angle \( \tan^{-1} H_1/H_0 \) in the \( H_1 - H_0 \) plane. Two limits are clearly distinguished: \( \phi_g \to 0 \) for \( H_0 \gg H_1 \) while \( \phi_g \to 2\pi \) when \( H_1 \gg H_0 \). These limits correspond to the classical SO(3) adiabatic Berry phases for the two different field topologies shown in figure 1. It is worth noting that, despite the abrupt change in the field topology, the effective geometric phase undergoes a smooth transition that nevertheless features a step-like behaviour in the limit of high fields. Similar results have been found in the case of spin magnetic moments for loop-shaped interferometers [23]. This effect is therefore an SO(3) counterpart of the Lyanda-Geller’s topological transition of the geometric phase for spin rotations [22], but involves an effective geometric phase instead of the bare geometric phase, and displays a smooth transition instead of an abrupt change [22].

The evolution of the classical magnetic moment is in general nonadiabatic close to the critical line. However, exactly at the critical line \( H_0 = H_1 \) the total field changes slowly and reverses its direction at \( \theta = \pi \). This causes a cusp in the path of the magnetic moment in figure 3(b). Adiabaticity is then enhanced and an effective geometric phase \( \phi_g = \pi/2 \) is obtained in the limit of high fields5 (see figure 4(b)).

The bare geometric phase in the classical SO(3) case is related to the geometry of the path described by the tip of the classical magnetic moment on the sphere \( S^2 \). This is also approximately true for the effective geometric phase along the lines where \( \phi_{tot} \) is a half-integer due to nearly adiabatic evolution (i.e. using \( \phi_g \approx \phi_{ad} \) and equation (10)). Therefore, at fixed half-integer total phase, the increase in the length of this path (the total rotation angle) is associated with a change in \( \phi_g \) (see the paths in figures 3(a)–(c) and the calculated effective geometric phases in figure 4(a)). The smooth shift in the cosine of the total phase close to the critical line \( H_0 = H_1 \) (solid line) features a shift in the interference peak positions close to the critical line \( H_0 = H_1 \). The lower and upper dashed red lines indicate where the adiabatic dynamic phase \( \phi_{ad} \) (equation (9)) is \( 4.5 \times 2\pi \) and \( 5.5 \times 2\pi \), respectively.

5 This is incidentally the same value as for SU(2) spin rotations at the critical line [22]. However, SU(2) spin dynamics at the critical line displays a \( 4\pi \) periodicity in \( \theta \) ([22]), and the reversal of the field direction at \( \theta = \pi \) is associated with a band transition.
field in the spin-rotation model of equation (7) was associated with the Rashba spin-orbit interaction strength in semiconductor quantum wells. Here we examine the symmetries of the interference pattern in this spin-$\frac{1}{2}$ system and compare it with the classical SO(3) case.

Figure 5 shows the interference pattern for SU(2) spin precessions in the loop configuration. More precisely, we calculate the interference of waves from

$$\frac{1}{2}|\psi_i + \psi_f|^2 = 1 + \frac{1}{2}(\psi_i^\dagger \psi_f + \psi_f^\dagger \psi_i),$$

(11)

where $\psi_i$ denotes an arbitrary normalized initial spin orientation and $\psi_f$ is the spinor after one cycle around the loop, calculated using the method detailed in [23] together with equation (7). This calculation corresponds to a weakly coupled loop where multiple windings around the loop can be neglected. We obtain results recalling adiabatic spin dynamics in a nonadiabatic scenario, giving rise to wavefronts at approximately constant adiabatic dynamic phase (equation (9)). At the critical line, the total probability amplitude remains finite due to complex nonadiabatic spin dynamics and a topological transition is visible. We find a close similarity in how the topological transitions emerge for both SU(2) spin rotations and classical SO(3) rotations (see figure 2(a)).

A detailed analysis of the results reveals that the interference pattern obtained from equation (11), depicted in figure 5, is independent of the initial spin orientation and phase (SU(2) × U(1) symmetry), which contrasts with the classical SO(3) case where the total phase producing the corresponding interference pattern (figure 2(a)) depends on the initial magnetic moment orientation. This is due to the existence of an additional U(1) symmetry only present in the quantum mechanical case. Despite this, we find that decomposition of the total quantum phase in the bare dynamic and geometric contributions actually depends on $\psi_i$. As an example, consider the oscillations along the $H_0$ axis in figure 5 and the associated phases. Here, an initial spin orientation parallel to the horizontal axis has no geometrical contribution, which however is present for an initial perpendicular orientation due to precessions.

5. Periodic states

In the classical case, differences between effective and bare geometric phases become apparent when we consider the evolution of eigenstates after a full cycle of the total magnetic field (Floquet states). We use the fact that the total phase change in a full cycle of SO(3) vanishes for eigenstates (up to integer multiple of $2\pi$) which, using equation (6), means that bare dynamic and geometric phases are equal (modulo $2\pi$). In the following, we study eigenstates of SO(3) rotations and show a topology-related shift in the calculated bare geometric phase associated with the effective geometric phase.

The classical eigenstates describe periodic states, and they are given by the solutions of the equation $R\mathbf{M}(0) = \mathbf{M}(0)$, where $R$ is the matrix governing the classical rotations defined in equation (3). The bare geometric phase $\phi_{bg}$ (modulo $2\pi$) for SO(3) eigenstates is shown in the left panel of figure 6. It features a complex structure close to the critical line which contrast with the smooth behavior outside this region. The wide regions of nearly constant bare geometric phase close to the $H_0$ and $H_1$ axes resemble a topological phase shift related to the emerging effective geometric phase. In particular, close to the horizontal axis the effective geometric phase coincides with the adiabatic Berry phase, i.e. $2\pi$. The bare geometric phase for SU(2) spin eigenstates, obtained from equation (7), displays an analogous structure (right panel of figure 6; see also [23]), with the adiabatic Berry phase equal to $\pi$ in this case.

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6 In [23], only periodic spin eigenstates were considered. Here, on the contrary, we present results corresponding to the interference of an arbitrary spinor before and after coming across the loop.

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Figure 6. The bare geometric phase $\phi_{bg}$ modulo $2\pi$ displays a topological phase shift across the critical line (solid lines) both for SO(3) (left) and SU(2) (right) eigenstates. The geometric phase at $H_1 = 0$ vanishes and the values in the limit of high $H_1$ and $H_0 \ll H_1$ are $2\pi$ and $\pi$ for SO(3) and SU(2), respectively, matching the adiabatic Berry phases. Close to the critical line, precessions give a large bare geometric phase leading to the complex patterns in the figures. The adiabatic dynamic phase $\phi_{ad} = 4 \times 2\pi$ at the dashed lines.
Figure 7. Averaged absolute value of the projection of the driving field to the corresponding magnetic moment $\mathbf{M}$ eigenstates (left) and spin $\mathbf{s}$ eigenstates (right). The field and magnetic moment (spin) orientations are approximately parallel for $H_0 \gg H_1 \gg 1$ and $H_1 \gg H_0 \gg 1$. Close to the critical line the angle is close to $90^\circ$ and dynamics are dominated by precessions. The adiabatic dynamic phase $\phi_{ad} = 4 \times 2\pi$ at the dashed lines.

Left panel of figure 7 shows $|\cos(\angle(\mathbf{M}, \mathbf{H}))|$ averaged over a cycle. These results demonstrate that close to the critical line the eigenstate is almost perpendicular to the driving field. This favours precessions, which give rise to large dynamic and geometric $SO(3)$ phases resulting in the complex pattern shown in the left panel of figure 6. In contrast, far from this region the eigenstates are approximately parallel to the driving field. We find analogous dynamics for $SU(2)$ spin eigenstates (right panel of figure 7), displaying a double frequency pattern due to spin evolution on the Bloch sphere. Spin precessions close to the critical line give a large bare geometric phase which is the dominating contribution to the total phase.

6. Discussion and outlook

We have shown that an effective geometric phase emerges in classical systems where the topology of the driving field changes. The effective geometric phase is analogous to that found in quantum spin-$\frac{1}{2}$ systems. These results are therefore very general. In addition, they are linked to the properties of the $SO(3)$ group of rotations [32]. The difference between the values obtained for the effective geometric phase in the adiabatic limit ($2\pi$ and $\pi$ in the classical and quantum cases, respectively) is related to the fact that $SO(3)$ is doubly connected while $SU(2)$ is simply connected. Despite the abrupt change in the field topology, the effective geometric phase shows a smooth but distinct transition close to the critical line of the phase boundary due to nonadiabatic effects, both in the quantum as well as in the classical case.

Applications of the theory would require a method to measure the resulting phases, e.g. via interference, resonance or a direct measurement of the magnetic moment orientation. In the case of spin rotations applications may include electron spin phases in mesoscopic spin systems or nuclear magnetic resonance experiments. Topological transitions of the effective geometric phases could be probed also in spins other than $\frac{1}{2}$ such as bosons [35], spin-$\frac{3}{2}$ of holes [36] or nuclei in nuclear quadrupole resonance spectroscopy (NQR) [37, 38]. Classical systems could include macrospins in ferromagnetic resonance experiments and JPB acknowledge support from project No. FIS2014-53385-P (MINECO, Spain) with FEDER funds.

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