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Numerical modeling of the multi-stage Stern–Gerlach experiment by Frisch and Segrè using co-quantum dynamics via the Bloch equation

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Abstract

We numerically study the spin flip in the Frisch–Segrè experiment, the first multi-stage Stern–Gerlach experiment, within the context of the novel co-quantum dynamics (CQD) theory. We model the middle stage responsible for spin rotation by sampling the atoms with the Monte Carlo method and solving the dynamics of the electron and nuclear magnetic moments numerically according to the Bloch equation. The simulation shows that CQD closely reproduces, without using any fitting parameters, the experimental observations reported by Frisch and Segrè in 1933, which have so far lacked theoretical predictions.

Keywords: spin-flip transition, electron spin, Bloch equation, co-quantum dynamics.

(Some figures may appear in colour only in the online journal)

1. Introduction

The Stern–Gerlach (SG) experiment was a crucial benchmark for the early development of quantum mechanics [1, 2] and is still presented in introductory books as evidence of quantization and the existence of the electron spin angular momentum [3–7]. The so-called SG apparatus has been used to illustrate the projection of the quantum wave function onto its eigenstates along the quantization axis, which is given

by the direction of a strong inhomogeneous magnetic field. Despite quantum mechanics being fundamental for explaining physical phenomena in almost any branch of physics, there is no generally accepted theory for how the wave function collapses [8–11].

Recently, a novel theory denoted co-quantum dynamics (CQD) has been proposed to describe the evolution and collapse of electron spins in alkali atoms interacting with an external magnetic field, \mathbf{B} [12, 13]. In CQD, the electron magnetic moment μ_e is termed the principal quantum, whereas the nuclear magnetic moment μ_n is termed the co-quantum. The evolution of both quanta is modeled by the Bloch equation, and the collapse of the principal quantum is treated by adding an induction term. In addition to \mathbf{B} , the magnetic field \mathbf{B}_n generated by the nuclear magnetic moment also acts upon μ_e ; similarly, the magnetic field \mathbf{B}_e generated by the electron magnetic moment acts upon μ_n .

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We apply QCD to model the multi-stage SG experiment conducted by Frisch and Segrè [14, 15]. The combination of SG apparatuses was firstly explored as a gedankenexperiment by Heisenberg [16] and later proposed by Einstein in greater detail to Stern and Ehrenfest in 1928 [17]; further historical remarks can be found in [18, 19] and references therein. Despite the earlier attempts by Phipps and Stern to observe spin flips in a beam of potassium atoms [20], the Frisch–Segrè experiment was the first successful realization [14, 15]. Their apparatus is composed of two SG stages and an intervening stage referred to as the inner rotation chamber. The middle stage is characterized by the presence of a weak but rapidly varying magnetic field that rotates the electron magnetic moment. Despite attempts by Majorana [21] and Rabi [22–24], theoretical descriptions of this experiment deviate from the Frisch–Segrè experimental observation [12, 18]. To date, this divergence remains unresolved by existing theories [18, 19, 25]. However, a closed-form approximation of QCD matches the experimental data with a high coefficient of determination without the use of fitting parameters [12]. The approximation models the dynamics by means of the Schrödinger equation coupled with the QCD concept; this approach has been corroborated numerically [26]. Here, we validate QCD by numerically solving the Bloch equation instead to estimate the fraction of spin flip in the Frisch–Segrè experiment and achieve a high coefficient of determination.

The manuscript is organized as follows. The experimental setup used by Frisch and Segrè is described in section 2. The QCD theory for the experiment is described in section 3. First, we introduce the equations of motion for the electron and nuclear magnetic moments. Second, we present a comprehensive description of all the stages in the Frisch–Segrè experiment with emphasis on the intermediate stage where nonadiabatic rotations of the electron magnetic moment occur. We compare our numerical results with both the experimental observation and the analytical solution reported previously [12]. In section 4, we make final remarks about our findings. In the Appendices, we mathematically derive the approximated external magnetic field (appendix A) and summarize the closed-form analytical formula obtained using QCD (appendix B).

2. Experiment

A schematic of the multi-stage SG apparatus, first constructed by Phipps and Stern [20] and later improved by Frisch and Segrè [14, 15], is shown in figure 1. The experimental setup combines two magnet pairs, SG1 and SG2, which each act as a standard SG apparatus [2, 7, 27]. Between them, a magnetically shielded inner rotation chamber contains a homogeneous remnant magnetic field and a cylindrically symmetric magnetic field generated by a current-carrying wire. The aim of the experiment is to observe spin flips in ground-state alkali atoms due to non-adiabatic rotations in the middle stage.

Alkali atoms are appealing for this experiment since their ground state has a closed shell with only one valence electron

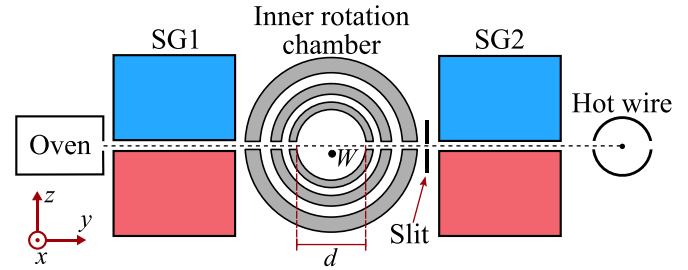


Figure 1. Schematic of the Frisch–Segrè apparatus as in [14, 15]. The atomic beam from the oven is sent to SG1, whose inhomogeneous magnetic field points along the z -axis. The blue color indicates the magnetic south pole, whereas the red color indicates the magnetic north pole. Then, the atomic beam enters the magnetically shielded inner rotation chamber containing a remnant homogeneous magnetic field plus a magnetic field generated by the electric current I_w flowing through a wire W along the $-x$ -direction. A slit post-selects one of the initially aligned branches of the electron magnetic moment. Finally, the atoms travel through SG2, and the fraction of spin flip is measured using a hot wire.

having an orbital angular momentum $\mathbf{L} = 0$. As a consequence, the total angular momentum for the electron of the atom equals the spin \mathbf{S} , with $S = 1/2$, and the spin–orbit coupling vanishes. However, the electron–nuclear spin interaction, also called the hyperfine interaction, arises from the coupling between the nuclear magnetic moment μ_n and the magnetic field generated by the electron magnetic moment μ_e , or equivalently vice versa. The coupling strength depends on the relative orientations of the magnetic moments, which are related to the spin angular momenta as

$$\mu_e = \gamma_e \mathbf{S}, \quad \mu_n = \gamma_n \mathbf{I}, \quad (1)$$

where γ_e is the electron gyromagnetic ratio, γ_n is the nuclear gyromagnetic ratio, and \mathbf{I} is the nuclear spin.

A beam of alkali atoms is easily generated since alkali metals have sufficient vapor pressure at temperatures of only a few hundred degrees Celsius [28, 29]. Let us consider the beam of atoms emerging from an oven and propagating along the y direction as shown in figure 1. The atomic beam first enters SG1, the strong magnetic field ($\mathbf{B}_0 \sim 0.5$ T) along the z -axis defines the quantization axis. The initially isotropically oriented electron magnetic moments are quickly aligned parallel \uparrow or antiparallel \downarrow to the magnetic field direction. The gradient of the magnetic field deflects the atoms into two branches. Despite no branch being physically selected before the inner rotation chamber, in the following description, we track only the branch with magnetic moments parallel to the field [15]. Figure 2 depicts the general behavior of electron magnetic moments through the experimental setup.

Next, the split beam is sent into an inner rotation chamber, which has an innermost diameter d . Despite the shielding from the fringe fields of SG1 and SG2, in the innermost chamber a weak remnant magnetic field \mathbf{B}_r persists, predominantly aligned along the z -axis. A wire with electric current I_w , flowing along the $-x$ direction, is placed at a vertical distance z_a below the selected atomic beam path. Figure 3(a) shows the main elements and the coordinate system inside the chamber.

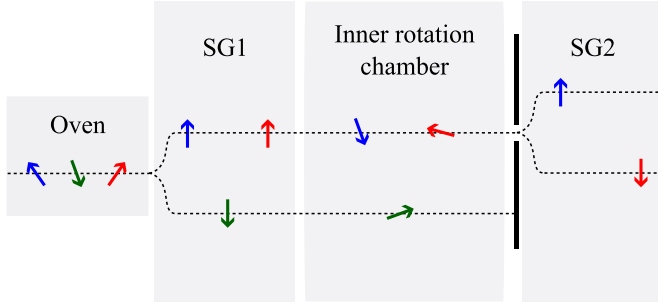


Figure 2. Illustration of three representative electron magnetic moments of atoms traversing the Frisch–Segrè apparatus. At the oven, the electron magnetic moments are randomly oriented, SG1 aligns them to \uparrow and \downarrow with respect to the orientation of the magnetic field. Both branches enter the inner rotation chamber, where the varying magnetic field rotates the electron magnetic moments. The upper branch is selected using a slit, and the atomic beam is sent to SG2 where the electron magnetic moments are again aligned. Finally, both branches are measured to quantify the fraction of spin flip.

For an infinitely long straight wire, the magnetic field generated by the current, $\forall y, z$ in the chamber, is given by

$$\mathbf{B}_w = \frac{\mu_0 I_w}{2\pi [(z+z_a)^2 + y^2]} [(z+z_a)\hat{y} - y\hat{z}], \quad (2)$$

where μ_0 denotes the vacuum permeability. Therefore, the total field in the innermost shielded region is $\mathbf{B} = \mathbf{B}_w + \mathbf{B}_r$. As illustrated in figure 3(b), the magnetic field cancels at the null point (NP), at position $\mathbf{r}_{\text{NP}} = y_{\text{NP}}\hat{y} - z_a\hat{z}$, with

$$y_{\text{NP}} = \frac{\mu_0 I_w}{2\pi B_r}. \quad (3)$$

In the region near the NP, a first-order Taylor expansion around the point $(y_{\text{NP}}, -z_a)$ approximates the magnetic field as a quadrupole (see appendix A for details):

$$\mathbf{B} \xrightarrow[\text{vicinity}]{\text{NP}} \mathbf{B}_q = \frac{2\pi B_r^2}{\mu_0 I_w} [(z+z_a)\hat{y} + (y-y_{\text{NP}})\hat{z}]. \quad (4)$$

After the atom interacts with the field inside the inner rotation chamber, the upper branch is selected using a slit while the lower branch is blocked, as illustrated in figure 2. Frisch and Segrè claimed that placing the slit immediately after instead of before the inner rotation chamber improved the beam quality [14].

Finally, the selected atomic branch enters SG2. This second SG stage again aligns the electron magnetic moment of each atom in parallel \uparrow and antiparallel \downarrow directions with respect to the strong magnetic field \mathbf{B}_0 along the $+z$ -axis. A hot wire records the final distribution of the atoms, which is used to quantify the fraction of spin flip of the electron magnetic moment resulting from the inner rotation chamber. The experiment is repeated with varying wire currents I_w , producing a fraction of spin flip as a function of the current.

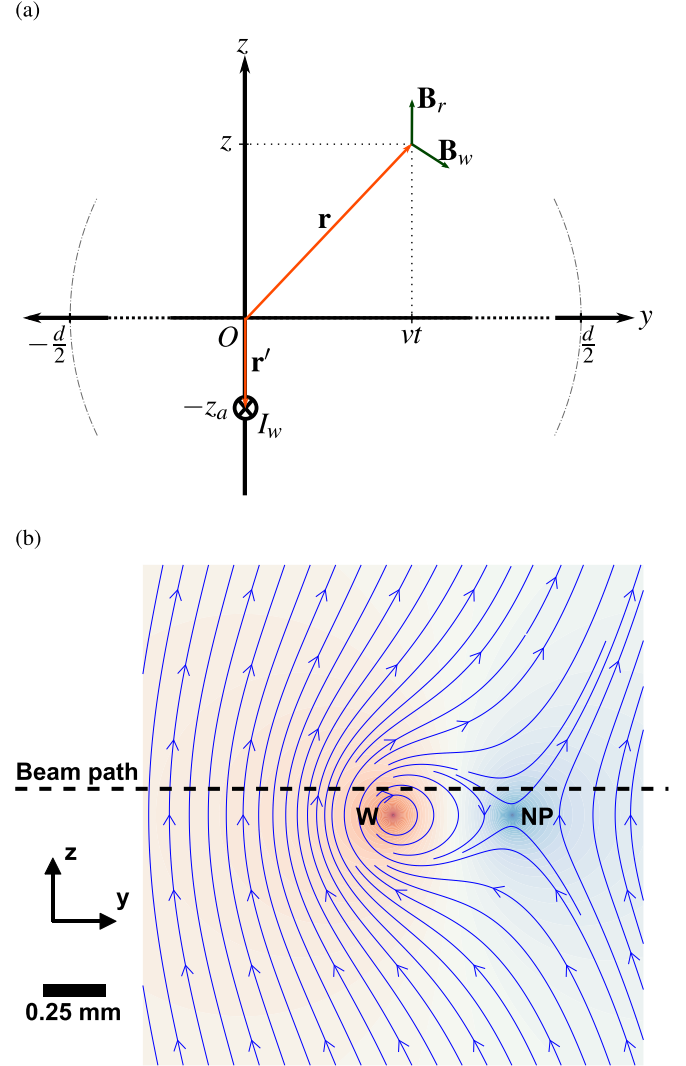


Figure 3. Magnetic field inside the inner rotation chamber. The beam propagates along the y -axis at constant speed v . The top panel shows the Cartesian reference frame, the position of the current-carrying wire (not drawn to scale), and the contributions from the remnant field \mathbf{B}_r and the wire field \mathbf{B}_w to the total magnetic field at position \mathbf{r} . The bottom panel shows the field lines of the total magnetic field with a null point (NP) below the beam path. In this example from the Frisch–Segrè experiment [14], $B_r = 42 \mu\text{T}$, $I_w = 0.02 \text{ A}$, and $z_a = 105 \mu\text{m}$.

3. Theory

Here, we use CQD [12, 13] to describe the multi-stage SG experiment by Frisch and Segrè. The formalism provides a mechanism of collapse of the electron spin in atoms interacting with an external magnetic field based on the combined dynamics of the electron and nuclear magnetic moments (1). CQD postulates that $|\theta_e(t) - \theta_n(t)|$ tends to increase, where θ denotes the polar angles of the electron and nuclear magnetic moments relative to the quantization axis. In addition, the Bloch equation is used to govern the evolution of the magnetic moments in the inner rotation chamber.

3.1. Magnetic moment evolution

The evolution of the magnetic moments in an external magnetic field are described by the Bloch equation [30]:

$$\frac{d\hat{\boldsymbol{\mu}}}{dt} = \gamma \hat{\boldsymbol{\mu}} \times \mathbf{B}, \quad (5)$$

where $\hat{\boldsymbol{\mu}}$ denotes the unit vector of the magnetic moment, γ is the gyromagnetic ratio, and \mathbf{B} is the magnetic flux density. This equation governs an undamped precession of the magnetic moment about the magnetic field \mathbf{B} . While usually considered a classical formalism, the Bloch equation has been recently shown to yield the space-independent von Neumann equation [13].

For the principal quantum μ_e and the co-quantum μ_n , the Bloch equation (5) becomes

$$\frac{d\hat{\boldsymbol{\mu}}_e}{dt} = \gamma_e \hat{\boldsymbol{\mu}}_e \times (\mathbf{B} + \mathbf{B}_n), \quad (6)$$

$$\frac{d\hat{\boldsymbol{\mu}}_n}{dt} = \gamma_n \hat{\boldsymbol{\mu}}_n \times (\mathbf{B} + \mathbf{B}_e), \quad (7)$$

where γ_e and γ_n denote the gyromagnetic ratios of the electron and the nucleus, respectively, and \mathbf{B} the external magnetic field. QCD introduces the $\mu_e - \mu_n$ interaction via each other's torque-averaged magnetic field, given by [12]

$$\mathbf{B}_e = \frac{5\mu_0 \mu_e}{16\pi R^3} \hat{\boldsymbol{\mu}}_e = B_e \hat{\boldsymbol{\mu}}_e, \quad (8)$$

$$\mathbf{B}_n = \frac{5\mu_0 \mu_n}{16\pi R^3} \hat{\boldsymbol{\mu}}_n = B_n \hat{\boldsymbol{\mu}}_n, \quad (9)$$

where R is the van der Waals radius of the atom, and μ_e and μ_n are the magnitudes of the magnetic moments for the electron and the nucleus, respectively.

The orientations of the magnetic moments in \mathbb{R}^3 are conveniently described using spherical coordinates. With the polar and azimuthal angles, θ_e and ϕ_e for μ_e and θ_n and ϕ_n for μ_n , we write the unit vectors as

$$\hat{\boldsymbol{\mu}}_e = \begin{pmatrix} \sin(\theta_e) \cos(\phi_e) \\ \sin(\theta_e) \sin(\phi_e) \\ \cos(\theta_e) \end{pmatrix}, \quad (10)$$

$$\hat{\boldsymbol{\mu}}_n = \begin{pmatrix} \sin(\theta_n) \cos(\phi_n) \\ \sin(\theta_n) \sin(\phi_n) \\ \cos(\theta_n) \end{pmatrix}. \quad (11)$$

Meanwhile, the external field is written as

$$\mathbf{B} = \begin{pmatrix} B_x \\ B_y \\ B_z \end{pmatrix}. \quad (12)$$

Finally, substituting (8)–(12) into (6) and (7), we obtain a set of differential equations determining the evolution of the unit vectors of μ_e and μ_n :

$$\begin{aligned} \dot{\theta}_e = & -\gamma_e [B_y \cos(\phi_e) - B_x \sin(\phi_e) \\ & + B_n \sin(\theta_n) \sin(\phi_n - \phi_e)], \end{aligned} \quad (13a)$$

Table 1. Values for potassium-39 [31–35].

| ³⁹ K | | |
|------------------|------------|---|
| | Property | Value |
| Atom | R | 275pm |
| Valence electron | S | $\frac{1}{2}$ |
| | μ_e | $9.2847677043(28) \times 10^{-24} \text{ JT}^{-1}$ |
| | γ_e | $-1.76085963023(53) \times 10^{11} \text{ rad (sT)}^{-1}$ |
| Nucleus | I | $\frac{3}{2}$ |
| | μ_n | $1.97723(4) \times 10^{-27} \text{ JT}^{-1}$ |
| | γ_n | $1.2500612(3) \times 10^7 \text{ rad (sT)}^{-1}$ |

$$\begin{aligned} \dot{\phi}_e = & -\gamma_e [B_z + B_n \cos(\theta_n) - \cot(\theta_e) [B_x \cos(\phi_e) \\ & + B_y \sin(\phi_e) + B_n \sin(\theta_n) \cos(\phi_e - \phi_n)]] , \end{aligned} \quad (13b)$$

$$\begin{aligned} \dot{\theta}_n = & -\gamma_n [B_y \cos(\phi_n) - B_x \sin(\phi_n) \\ & + B_e \sin(\theta_e) \sin(\phi_e - \phi_n)] , \end{aligned} \quad (13c)$$

$$\begin{aligned} \dot{\phi}_n = & -\gamma_n [B_z + B_e \cos(\theta_e) - \cot(\theta_n) [B_x \cos(\phi_n) \\ & + B_y \sin(\phi_n) + B_e \sin(\theta_e) \cos(\phi_e - \phi_n)]] . \end{aligned} \quad (13d)$$

Given the dynamical equations for the electron and nuclear magnetic moments of a single atom, we model their evolution in the inner rotation chamber of the Frisch–Segrè experiment.

3.2. Multi-stage SG experiment by Frisch and Segrè

In the Frisch–Segrè experiment, neutral potassium-39 atoms (³⁹K) with an electron configuration of [Ar] 4s¹ were used. The valence electron in its ground state is fully specified in the Russell-Saunders notation as 4²S_{1/2}. Table 1 lists the values of the van der Waals radius, spins, magnetic moments, and gyromagnetic ratios for the ³⁹K atom. Accordingly, we compute the magnitudes of the magnetic fields generated by the electron and nuclear magnetic moments from (8) and (9):

$$B_e = 55.80626722(2) \text{ mT}, \quad (14a)$$

$$B_n = 11.8842(3) \text{ } \mu\text{T} . \quad (14b)$$

3.2.1. Oven. First, heating ³⁹K atoms in an oven with a small opening produces an effusive beam of non-interacting thermal atoms. We define the y-axis along the beam as shown in figure 1.

The initial orientations of both the electron and nuclear magnetic moments of a single traveling atom are isotropically distributed. Therefore, their angular probability density functions are respectively

$$p_{e,\text{oven}}(\theta_{e,\text{oven}}, \phi_{e,\text{oven}}) = \frac{1}{4\pi},$$

$$p_{n,\text{oven}}(\theta_{n,\text{oven}}, \phi_{n,\text{oven}}) = \frac{1}{4\pi} .$$

To implement a Monte Carlo simulation, the polar and azimuthal angles are numerically generated from independent realizations of

$$\theta_{e,\text{oven}} = 2 \arcsin \left(\sqrt{\zeta_1} \right), \quad \phi_{e,\text{oven}} = 2\pi \zeta_2, \quad (15a)$$

$$\theta_{n,\text{oven}} = 2 \arcsin \left(\sqrt{\zeta_3} \right), \quad \phi_{n,\text{oven}} = 2\pi \zeta_4, \quad (15b)$$

with ζ_j , $j = 1, \dots, 4$, being random numbers uniformly sampled from zero to one.

3.2.2. SG apparatus 1. Emerging from the oven, the atoms enter an SG apparatus consisting of an inhomogeneous magnetic field with a strong gradient along the z -axis, as illustrated in figure 1. Usually, the amplitude of the magnetic field is $B_0 \sim 0.5 \text{ T}$; thus, $B_0 > B_e \gg B_n$. For such a strong field, μ_e and μ_n couple more strongly to the external magnetic field than to each other, and can be considered as independently precessing with Larmor frequencies ω_e and ω_n , for electron and nuclear magnetic moments, respectively, about the external field direction. From the values in table 1, the ratio between the nuclear and electron Larmor frequencies $\omega_n/\omega_e \approx 7 \times 10^{-5}$. In consequence, while the flight time guarantees the collapse of the electron magnetic moment, it is too short for the nuclear magnetic moment to collapse [12].

Therefore, the electron magnetic moments of the single atoms, initially isotropically distributed, split into two branches with well-defined opposite alignments along the z -axis. We characterize the two orientations of the aligned μ_e by setting $\theta_{e,i} = 0$ and $\theta_{e,i} = \pi$ in (10), respectively, as illustrated in figure 2. Meanwhile, since μ_n does not collapse, CQD assumes that θ_n does not vary significantly during the flight. At the end of the SG1 stage, as a consequence of the splitting of the atomic beam, the μ_n orientation in each of the branches is redistributed according to an anisotropic probability density function [12]. For the branch with μ_e parallel to the quantization axis,

$$p_n(\theta, \phi) = 2p_{n,\text{oven}}(\theta_{n,\text{oven}}, \phi_{n,\text{oven}}) \times \int_0^{2\pi} d\phi_e \int_0^{\theta_n} d\theta_e \sin(\theta_e) p_{e,\text{oven}}(\theta_e, \phi_e). \quad (16)$$

Similarly, for the branch with μ_e antiparallel to the quantization axis,

$$p_n(\theta, \phi) = 2p_{n,\text{oven}}(\theta_{n,\text{oven}}, \phi_{n,\text{oven}}) \times \int_0^{2\pi} d\phi_e \int_{\theta_n}^{\pi} d\theta_e \sin(\theta_e) p_{e,\text{oven}}(\theta_e, \phi_e). \quad (17)$$

Hence, the directional angles of the nuclear magnetic moment at the end of SG1 are distributed according to the following probability functions:

$$p_n(\theta_{n,i}, \phi_{n,i}) = \begin{cases} \frac{1}{2\pi} \sin^2 \left(\frac{\theta_{n,i}}{2} \right) & \text{if } \theta_{e,i} = 0, \\ \frac{1}{2\pi} \cos^2 \left(\frac{\theta_{n,i}}{2} \right) & \text{if } \theta_{e,i} = \pi. \end{cases} \quad (18)$$

3.2.3. Inner rotation chamber. The inner rotation chamber consists of three hollow iron shielding spheres. Without shielding, the fringe field was $\sim 0.4 \text{ T}$; with shielding, the measured remnant field along the $+z$ -axis was reported to be $B_r = 42 \mu\text{T}$ [14]. Inside the chamber, an electric current I_w flowing through a wire produces a spatially varying magnetic field (2), resulting in the total field shown in figure 3(b).

We select the branch of the atomic beam with μ_e aligned to the $+z$ -axis according to the original experiment [15], i.e. $\theta_{e,i} = 0$, as shown in figure 2. Therefore, the probability density function (18) becomes

$$p_n(\theta_{n,i}, \phi_{n,i}) = \frac{1}{2\pi} \sin^2 \left(\theta_{n,i}/2 \right). \quad (19)$$

To continue the Monte Carlo simulation, the polar and azimuthal angles $(\theta_{n,i}, \phi_{n,i})$ are sampled from the above anisotropic probability density function:

$$\theta_{n,i} = 2 \arcsin \left(\zeta_1^{1/4} \right), \quad \phi_{n,i} = 2\pi \zeta_2, \quad (20)$$

where ζ_1 and ζ_2 are two independent random numbers sampled uniformly from zero to one.

Each atom in the beam propagates with velocity $\mathbf{v} = v\hat{\mathbf{y}}$, and we approximate the motion to be rectilinear and uniform such that its position on the propagation axis is $y = vt$. The atom is simulated from $-d/2$ to $d/2$ as shown in figure 3(a). Here, $v = 800 \text{ m s}^{-1}$ and $d = 16.3 \text{ mm}$ [14]. Therefore, the time in the inner rotation chamber $t \in [-10.2 \mu\text{s}, 10.2 \mu\text{s}]$. The total external magnetic field along the y -axis varies according to

$$\mathbf{B} = \frac{\mu_0 I_w}{2\pi \left[z_a^2 + (vt)^2 \right]} \left[z_a \hat{\mathbf{y}} - vt \hat{\mathbf{z}} \right] + B_r \hat{\mathbf{z}}. \quad (21)$$

The wire is positioned along the x -axis at a distance $z_a = 105 \mu\text{m}$ below the beam path. The electric current I_w varies from 0.01 A to 0.5 A [14, 15].

It is known that a time-dependent magnetic field can rotate the magnetic moment of the electron [21, 24, 36, 37]. To determine whether the process is adiabatic or non-adiabatic, we compute the so-called adiabaticity parameter k , defined as the ratio between the absolute values of the Larmor frequency ω_e and the rotational speed of the total magnetic field in the yz plane Ω_B [21]

$$k = \left| \frac{\omega_e}{\Omega_B} \right| = \left| \frac{\gamma_e B}{\frac{d}{dt} [\arctan(B_z/B_y)]} \right|. \quad (22)$$

If $\omega_e \gg \Omega_B$ ($k \gg 1$), μ_e is able to follow the changing orientation of the magnetic field, and the rotation is said to be adiabatic. Otherwise, μ_e may be unable to follow the changing orientation of the magnetic field; if so, the rotation is said to be non-adiabatic.

The total magnetic field experienced by μ_e includes the torque-averaged magnetic field generated by the nucleus (9) as indicated in (6). However, the time-dependent nature of

$\mathbf{B}_n(\theta_n(t), \phi_n(t))$ does not allow us to write a closed form for k . By neglecting \mathbf{B}_n , the adiabaticity parameter becomes

$$k = \left| \frac{\gamma_e \mu_0 I_w}{2\pi z_a v} \frac{\sqrt{(vt)^2 + z_a^2}}{\left(1 - \frac{4\pi B_r vt}{\mu_0 I_w}\right)} \times \left[1 - \frac{4\pi B_r vt}{\mu_0 I_w} + \left(\frac{2\pi B_r}{\mu_0 I_w}\right)^2 \left((vt)^2 + z_a^2\right) \right]^{3/2} \right|. \quad (23)$$

Figure 4 shows the variation of k around the center of the cavity computed from (23) for a set of representative electric currents I_w .

We note that in the vicinity of the wire position ($t=0$) and before the atoms reach the NP at time

$$t_{\text{NP}} = \frac{y_{\text{NP}}}{v} = \frac{\mu_0 I_w}{2\pi v B_r}, \quad (24)$$

the adiabaticity parameter is much greater than unity at the peaks. Accordingly, as the z component of the magnetic field changes its orientation (see figure 3(b)), the electron magnetic moment follows the varying \mathbf{B} -field adiabatically. Therefore, the electron magnetic moment flips adiabatically, $\theta_e : 0 \mapsto \pi$, in this region. In comparison, Majorana stated that the flip is due to the orientation reversal of the quadrupole field along the flight path [21]. For simplicity, we ignore the contribution from the nucleus (14b) to k ; this approximation is justified since its weaker field does not significantly affect the magnitudes of the adiabatic peaks in figure 4.

Then, the electron magnetic moment is rotated non-adiabatically around the corresponding trough (at times when $k \lesssim 1$) in figure 4, which is near the NP. We make use of the quadrupole approximation for the magnetic field to describe this effect around the NP, \mathbf{B}_q in (4), rewritten for the beam path as

$$B_x = 0, \quad (25a)$$

$$B_y = \frac{2\pi B_r^2}{\mu_0 I_w} z_a, \quad (25b)$$

$$B_z = \frac{2\pi B_r^2}{\mu_0 I_w} v(t - t_{\text{NP}}). \quad (25c)$$

The resulting system of coupled differential equations is reduced to

$$\dot{\theta}_e = -\gamma_e \left[B_y \cos(\phi_e) + B_n \sin(\theta_n) \sin(\phi_n - \phi_e) \right], \quad (26a)$$

$$\dot{\phi}_e = -\gamma_e \left[B_z + B_n \cos(\theta_n) - \cot(\theta_e) \left[B_y \sin(\phi_e) + B_n \sin(\theta_n) \cos(\phi_e - \phi_n) \right] \right], \quad (26b)$$

$$\dot{\theta}_n = 0, \quad (26c)$$

$$\dot{\phi}_n = -\gamma_n \left[B_z + B_e \cos(\theta_e) - \cot(\theta_n) \left[B_y \sin(\phi_n) + B_e \sin(\theta_e) \cos(\phi_e - \phi_n) \right] \right]. \quad (26d)$$

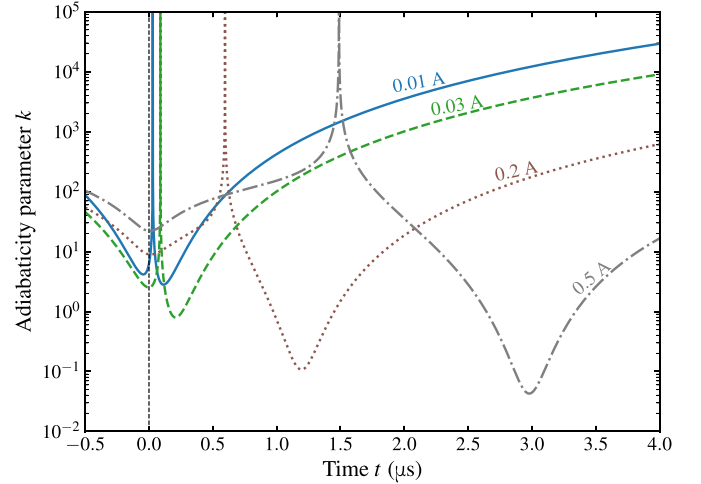


Figure 4. Adiabaticity parameter k along the beam path for various electric currents. Adiabatic rotation of the electron magnetic moment occurs around the peak ($k \gg 1$), whereas non-adiabatic rotation happens around the trough (near the null point t_{NP} of the magnetic field). The vertical black dashed line indicates the time when the atom is above the wire ($t=0$).

Note that we have imposed the condition $\dot{\theta}_n = 0$ since the postulates of the CQD theory require small variations of the polar angle of the nuclear magnetic moment. This condition corresponds to the selection rule for nuclear spin transitions $\Delta m_I = 0$ [12, 38].

To solve the above differential equations, we sample the initial orientation of μ_n from (20) and sample $\phi_{e,i}$ uniformly, in a way similar to (15a), while setting $\theta_{e,i} = \pi$. The concurrence of two vastly different time scales, $\omega_n/\omega_e \approx 7 \times 10^{-5}$, for the dynamics of $\hat{\mu}_e$ and $\hat{\mu}_n$, leads to stiffness prone to numerical instability [39, 40]. We chose the Radau methods [41, 42] implemented in Julia [43, 44] to solve the differential equations (26) numerically. Our source code is posted online [45]. An alternative approach, to avoid the stiffness, approximates the nuclear Larmor frequency as a constant and accelerates the solution using a variable transformation [26].

Figure 5 shows the characteristic dynamics of θ_e inside the inner rotation chamber for a representative set of currents. To facilitate comparison, we introduce $\Delta t = t - t_{\text{NP}}$, such that the time $\Delta t = 0$ at the current-dependent NP (24). The dynamics are characterized by an oscillatory behavior; the polar angle θ_e varies rapidly in the vicinity of the NP ($\Delta t = 0$) due to strong non-adiabatic rotation. From the simulations in figure 5, we observe that the effective interaction duration depends on the electric current—higher currents prolong interaction time—which is also evident in figure 4. CQD estimated the effective interaction time for null-point rotations to be $t_{\text{int}} = \pi \frac{z_a}{v} \approx 0.4 \mu\text{s}$ [12].

Then, the oscillations are damped due to the increasing adiabaticity parameter for $\Delta t > 0$. However, since θ_e has not asymptotically converged to a definite value, we numerically approximate its final value $\theta_{e,f}$ by averaging the oscillations over the last $2 \mu\text{s}$.

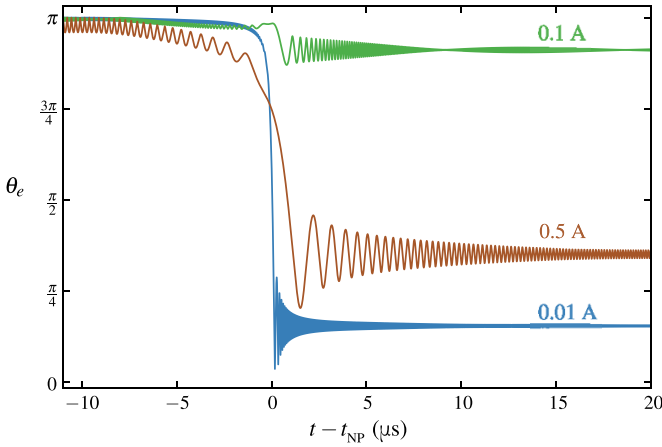


Figure 5. Dynamics of θ_e for different electric currents I_w . The initial conditions are $\theta_{e,i} = \pi$ and $\phi_{e,i} = 0$ for the electron magnetic moment, whilst $\theta_{n,i} = \frac{5}{8}\pi$ and $\phi_{n,i} = \frac{11}{10}\pi$ for the nuclear magnetic moment.

3.2.4. SG apparatus 2. After traveling through the inner rotation chamber, the atom enters the second SG apparatus as shown in figure 1. The strong magnetic field along the z -axis realigns the electron magnetic moment. The final orientation $\theta_{e,f} \mapsto \theta_{e,D}$ follows the branching condition postulated by the CQD theory [12]:

$$\theta_{e,D} = \begin{cases} 0 & \text{if } \theta_{e,f} < \theta_{n,f}, \\ \pi & \text{if } \theta_{e,f} > \theta_{n,f}. \end{cases} \quad (27)$$

Therefore, the measured polar angle $\theta_{e,D}$ takes on either 0 or π .

3.2.5. Fraction of spin flip. The spin flip corresponds to those atoms with $\theta_{e,D} = \pi$, as depicted in figure 2. We numerically solved the Bloch equations for $N = 15\,000$ atoms for each current I_w . Thus, the fraction of spin flip, for a given I_w , is computed using

$$W_{\text{num}} = \frac{1}{N} \sum_{j=1}^N [\theta_{e,D}^{(j)} = \pi], \quad (28)$$

where j denotes the j th-atom sampled and $[P]$ is the Iverson bracket, which is defined to take on the value 1 when the statement P is true and 0 otherwise.

Figure 6 shows the resulting fraction of spin flip obtained from the numerical simulation in comparison with the experimental results reported by Frisch and Segrè [14]. In addition, the closed-form analytical prediction from the CQD theory is included (see appendix B) [12].

The coefficient of determination for our numerical simulation is $R_{\text{num}}^2 = 0.945$, an alternative numerical solution that approximates the interaction with the nuclear magnetic moment and performs a variable transformation to avoid stiffness [26] yield $R_{\text{alt}} = 0.950$, and the closed-form analytical solution obtained in [12] gives $R_{\text{ana}}^2 = 0.962$. The statistical errors associated with the numerical results are

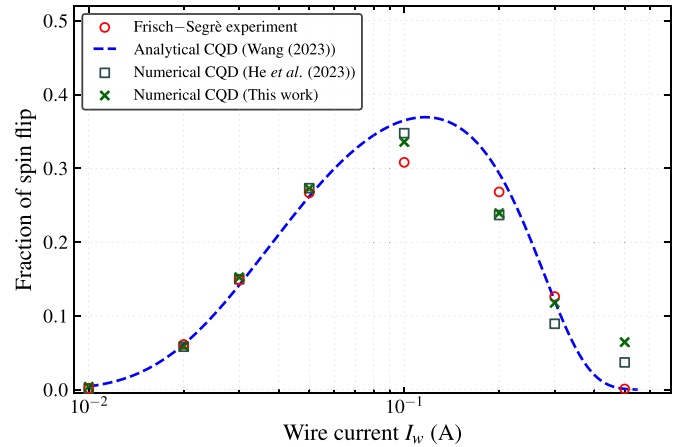


Figure 6. Fraction of spin flip for the multi-stage Stern–Gerlach experiment by Frisch and Segrè. The red circles are the original experimental data [14], the blue dashed line is the closed-form analytical solution from CQD [12], the gray squares show the numerical CQD solution solved via the Schrödinger equation [26], and the green crosses are the result from the numerical CQD solution obtained here.

smaller than the symbol size in figure 6. The mismatch observed at high currents is attributed to the numerical stiffness of the differential equations, which worsens with increasing effective interaction time. Nevertheless, these results show a close agreement of CQD with the experimental data [14], which has not yet been achieved using standard quantum mechanical treatments [25].

4. Conclusions

We used CQD to numerically model the Frisch–Segrè experiment without using any fitting parameters. The numerical problem is stiff because of the two vastly different characteristic time scales [12]. The solver of the differential equations must be carefully chosen and validated. We described all the stages of the experiment, with emphasis on the inner rotation chamber where nonadiabatic rotations take place. Using the Monte Carlo method, we sampled the spatial orientations of the electron and nuclear magnetic moments of the atoms in the atomic beam. Our findings show that the fraction of spin flip obtained by means of CQD, with no additional approximations, closely reproduces the reported experimental results, with a coefficient of determination of $R_{\text{num}}^2 = 0.945$. The obtained results have not been explained by standard quantum mechanical approaches [25], despite attempts by Majorana [21, 36, 37] and Rabi [22–24], whose theoretical formulae deviate from the experimental results.

Hence, this work supports CQD as a model for both the evolution and the collapse of the electron spin in atoms in the presence of external magnetic fields. Some other reported experiments involving multi-stage SG experiments [46, 47] could be explored using the present formalism. Notwithstanding, we hope that this work will encourage further experiments to verify CQD.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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Appendix A. Approximation to quadrupole field

The total magnetic field inside the inner rotation chamber, $\mathbf{B} = \mathbf{B}_w + \mathbf{B}_r$, can be approximated as an ideal quadrupole field. The Taylor expansion of \mathbf{B} in the yz plane around the NP ($y_{\text{NP}}, -z_a$) reads

$$\begin{aligned} \mathbf{B} = & \mathbf{B} \Big|_{\text{NP}} + \frac{\partial \mathbf{B}}{\partial y} \Big|_{\text{NP}} (y - y_{\text{NP}}) + \frac{\partial \mathbf{B}}{\partial z} \Big|_{\text{NP}} (z + z_a) \\ & + \frac{1}{2} \frac{\partial^2 \mathbf{B}}{\partial y^2} \Big|_{\text{NP}} (y - y_{\text{NP}})^2 + \frac{1}{2} \frac{\partial^2 \mathbf{B}}{\partial z^2} \Big|_{\text{NP}} (z + z_a)^2 \\ & + \frac{\partial \mathbf{B}}{\partial y \partial z} \Big|_{\text{NP}} (y - y_{\text{NP}})(z + z_a) + \dots \end{aligned} \quad (\text{A1})$$

Up to the first order, for the hyperbolic field approximation, the coefficients are

$$\mathbf{B} \Big|_{\text{NP}} = 0, \quad (\text{A2a})$$

$$\frac{\partial \mathbf{B}}{\partial y} \Big|_{\text{NP}} = \frac{2\pi B_r^2}{\mu_0 I_w} \hat{z}, \quad (\text{A2b})$$

$$\frac{\partial \mathbf{B}}{\partial z} \Big|_{\text{NP}} = \frac{2\pi B_r^2}{\mu_0 I_w} \hat{y}. \quad (\text{A2c})$$

Substituting (A2) into (A1), the quadrupole magnetic field can be written as

$$\mathbf{B}_q = \frac{2\pi B_r^2}{\mu_0 I_w} (z + z_a) \hat{y} + \frac{2\pi B_r^2}{\mu_0 I_w} (y - y_{\text{NP}}) \hat{z}. \quad (\text{A3})$$

This corresponds to the magnetic field in (4).

Appendix B. Closed-form solution of the CQD theory

Using the CQD theory, it is possible to derive a closed-form formula for the probability of spin flip in the inner rotation chamber in the presence of the quadrupole magnetic field and the nuclear magnetic moment as we described for the experiment conducted by Frisch and Segrè [12].

In terms of the parameters of the experiment, the fraction of spin flip, shown as the blue dashed line in figure 6, is given by

$$\mathcal{W}_{\text{ana}}(I_w) = \exp \left[-\sqrt{\left(\frac{c_{r0}}{I_w}\right)^2 + c_{rs}^2 - c_{rr} I_w^3} \right], \quad (\text{B1})$$

where

$$c_{r0} = |\gamma_e| \frac{2\pi^2 z_a^2}{\mu_0 v} (B_r + B_n \cos(\langle \theta_n \rangle))^2, \quad (\text{B2a})$$

$$c_{rs} = |\gamma_e| \frac{\pi z_a}{v} B_n \sin(\langle \theta_n \rangle), \quad (\text{B2b})$$

$$c_{rr} = \frac{\mu_0^3 \gamma_e^2 \gamma_n}{32\pi v^3} \frac{B_e (B_n \sin(\langle \theta_n \rangle))^5}{(B_r + B_n \cos(\langle \theta_n \rangle))^6}. \quad (\text{B2c})$$

The coefficients represent three physical effects identified in the solution, i.e. null-point rotation, rotation saturation, and resonant rotation, respectively. The mean polar angle of the nuclear magnetic moment is computed from the probability density function (19) as follows:

$$\langle \theta_n \rangle = \int d\theta_n d\phi_n \sin(\theta_n) p_n(\theta_n, \phi_n) = \frac{5}{8}\pi. \quad (\text{B3})$$

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