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Spin flip loss in magnetic confinement of ultracold neutrons for neutron lifetime experiments

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We analyze the spin flip loss for ultracold neutrons in magnetic bottles of the type used in experiments aiming at a precise measurement of the neutron lifetime, extending the one-dimensional field model used previously by Steyerl et al. [Phys. Rev. C 86, 065501 (2012)] to two dimensions for cylindrical multipole fields. We also develop a general analysis applicable to three dimensions. Here we apply it to multipole fields and to the bowl-type field configuration used for the Los Alamos UCNr experiment. In all cases considered the spin flip loss calculated exceeds the Majorana estimate by many orders of magnitude but can be suppressed sufficiently by applying a holding field of appropriate magnitude to allow high-precision neutron lifetime measurements, provided other possible sources of systematic error are under control.

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I. INTRODUCTION

The neutron lifetime \(\tau_n\) is an important parameter in nuclear physics, particle physics, and cosmology. \(\tau_n\) can be combined with the neutron \(\beta\)-decay \((n \to p + e^- + \bar{\nu}_e)\) correlation coefficients to determine the universal weak interaction vector and axial-vector coupling constants whose values allow searches for semileptonic scalar and tensor currents beyond the standard model [1–4]. A \(\tau_n\) of reliable precision is also needed for calculations of the neutrino flux expected from solar and (UCN) (see [11–16] for reviews of cold neutrons or an ensemble of trapped ultracold neutrons). Most common is the counting “survivors” as a function of the holding time. The method involves loading UCNs into a “neutron bottle” and an exactly specified section of the beam while the trapping region is being filled with neutrons from a source. In this technique, the UCNs in one spin state can be stored; those in the other spin state are attracted towards the wall and lost. In the field configurations commonly applied the field increases toward the wall, thus neutrons in the low-field seeking state with spin parallel to \(B\) (i.e., \(\mu\) antiparallel to \(B\)) are stored and should, ideally, experience no losses other than \(\beta\) decay, provided that depolarization, i.e., the spin flip to the opposite spin state, is sufficiently suppressed.

Until recently, UCN depolarization estimates [17,18] have been based on Majorana’s quasiclassical result [19] for a model where a particle with magnetic moment moves with constant velocity vector through an infinitely extended nonuniform magnetic field of specific form. For field parameters as currently used for magnetic UCN storage the probability \(D\) of a spin flip away from the field direction would be of order \(D \sim e^{-10^6}\), thus immeasurably small.

Wall losses can be avoided by confining the UCNs in “magnetic neutron bottles,” utilizing the interaction energy \(-\mu \cdot B\) between the neutron magnetic moment \(\mu = -60.3\) neV/T with a static nonuniform magnetic field \(B\) to establish a closed trapping region. In this scheme, only the neutrons in one spin state can be stored; those in the other spin state are attracted towards the wall and lost. In the field configurations commonly applied the field increases toward the wall, thus neutrons in the low-field seeking state with spin parallel to \(B\) (i.e., \(\mu\) antiparallel to \(B\)) are stored and should, ideally, experience no losses other than \(\beta\) decay, provided that depolarization, i.e., the spin flip to the opposite spin state, is sufficiently suppressed.

In Refs. [21,22] we extended this theory to general orbits with both vertical and horizontal velocity components, using the model of an ideal Halbach magnetic field \(B\) where the magnitude \(B\) only depends on the vertical position. We found that the lateral motion in the plane where the Halbach field rotates is of critical importance. Taking it into account increases the spin flip loss thus calculated by some 10 orders of magnitude to \(D \sim 10^{-20} - 10^{-23}\), which is much larger than the Majorana estimate but still negligible in any actual or projected neutron lifetime experiment.

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The analysis in Refs. [20,21] is based on the following concepts: For the one-dimensional (1D) field model of [21], the potential \(V(z) = gz - \mu B(z)/m = gz + |\mu| B(z)/m\) for the high-field repelled |+\> spin state of a neutron with mass...
m depends only on the vertical \( z \) coordinate. In this model the
neutrons are exposed to a uniform gravitational field \( -g \hat{z} \)
and a nonuniform magnetic field of magnitude \( B(z) \). They
perform an oscillatory motion with turning points (TP) at the
lower and upper horizontal equipotential surfaces (ES) where
\( v_z = 0 \) and the potential is \( V = (E/m) - v_z^2/2 \). Here \( E \)
is the neutron energy; \( v_z \) and \( v_\perp = \sqrt{v_x^2 + v_y^2} \) are the vertical and
horizontal velocity components, respectively. \( v_\perp \) is constant
for the 1D field model.

As the particle moves from one TP to the next, starting out
in a pure \(|\uparrow\rangle\) spin state, its wave component for the \(|\downarrow\rangle\) spin
state increases. It may change over many orders of magnitude
[20,21], peaking at critical points where the field magnitude \( B \)
is small and the vector \( \mathbf{B} \) rotates rapidly in the reference frame
of the moving particle. The spin flip probability is “measured”
only at the next TP where, in the Copenhagen interpretation,
the wave function collapses and UCNs in the \(|\uparrow\rangle\) state return to
the trapping region while the \(|\downarrow\rangle\) projection separates in space
and quickly becomes lost. Conceptually, the “measurement”
could be made by an ideal neutron detector placed just next to
the TP, which would intersect the UCNs in the “wrong” spin
state as they exit the storage space. This “measurement” resets
the UCN wave function to a pure initial \(|\uparrow\rangle\) state for the next
lap where the sequence of wave evolution and collapse at the
following TP is repeated.

## II. OUTLINE

In the present article we extend this approach to the analysis
of depolarization in cylindrical multipole fields such as those
described in Refs. [23–28], where the trapping fields are
generated by Halbach arrays of permanent magnets [24–27]
or, for [23,28] and, earlier [29], by superconducting currents.
For these cylindrical configurations we use a 2D field model
which enables us to obtain a semianalytic expression for the
ensemble-averaged spin flip loss and which can be analyzed
with no need to involve simulations. The results are consistent with
an experimental spin flip probabilities with varying holding field available so far [26].

For the cylindrical \( 2N \) pole we approximate the field in
cylindrical coordinates \( r, \phi, z \) as follows:

\[
\begin{align*}
B_r &= B_{\max}(r/R)^{N-1}\sin(N\phi), \\
B_\phi &= B_{\max}(r/R)^{N-1}\cos(N\phi), \\
|\mathbf{B}| &= B(r) = \sqrt{B_z^2 + B_{\max}(r/R)^{2N-2}},
\end{align*}
\]

(1)

where \( N \geq 2 \), \( \phi \) points along the cylinder axis and the holding
field \( B_z \) is considered constant. \( B_{\max} \) is the trapping field
magnitude at the wall and the radius \( R \) (typically \( \sim 5 \) cm)
is much smaller than the length, which is of order \( 1 \) m. This
justifies the neglect of gravity for horizontal configurations of
this type [23] since the gravitational energy varies little
over the trap radius. To assess the merits of model (1) in
general we have performed 3D simulations including gravity
both for the vertical and the horizontal cylindrical multipole
configurations.

As a second application we extend the previous analysis
[21] of depolarization for a 1D field model of the Los Alamos
UCN\( r \) trap [20,30,31] to the actual field in this magneto-
gravitational trap with its asymmetrically double-curved wall
in the shape of a bowl. As in Ref. [20] we approximate the
field for the curved arrays of permanent magnets by that of
the corresponding infinite planar array tangent to the bowl
surface at the closest point on the bowl surface. We also use
the same expressions for the flat-wall field, dubbed “smooth”
[Eq. (5) of [20]], “one-way ripple” [Eq. (7)] and “two-way
ripple” [Eq. (8)]. The “one-way ripple” takes into account
the finite magnet size and the “two-way ripple” also includes
the effect of iron shims between the magnets, a design feature not
implemented for the current UCN\( r \) system (status of 2016).

The theoretical approach is outlined in Sec. III, where we
derive a first-order approximation to the spin flip probability
from the spin-dependent Schrödinger-Pauli equation (SE), and
in Sec. IV where we average these results over the ensemble
of orbits in the field configurations of UCN\( r \) and of multipole
bottles. In Sec. V we derive a higher-order solution of the
spin-dependent SE and show that it deviates very little from
the first-order approximation. These various approaches are
semiclassical since the field \( \mathbf{B}(t) \) acting on the neutron spin
is determined by the classical motion of the particle through
the field. However, the results have been shown [20,21] to
be consistent also with a fully quantum mechanical analysis
starting from the spin and space dependent SE. We show in the
Appendix that this equivalence also holds for our extension to
arbitrary field configurations.

As in Refs. [20,21], we use the Wentzel-Kramers-Brillouin
(WKB) approximation [32] to solve the SE. This is justified
since the spatial variation of field variables is much slower
than the variation of the UCN wave function. The scales are
of order cm for gravity and \( \mathbf{B} \), and of order \( \mu \)m or less for
the wavelength. Thus the wave function for spin state \(|\uparrow\rangle\)
can be expressed in the WKB form except at a TP \( z' = 0 \), where
its amplitude \( 1/\sqrt{k_\perp(z')} \) diverges since the wave number \( k_\perp \)
vanishes. [See Eq. (A12) for details.] Furthermore, due to the
slow variation of field variables their gradients are small
quantities.

## III. SEMICLASSICAL APPROACH

Neutron lifetime experiments based on magnetic storage
require that the spin follows the changes of field direction
along the neutron path for a time much longer than the neutron
lifetime, implying that the probability \( |\alpha(t)|^2 \) for spin \(|\uparrow\rangle\),
parallel to the local field, is always much larger than the small
spin-flipped part \( |\beta(t)|^2 \). Therefore, in order to separate large
terms in the SE [e.g. those in Eq. (6) below] from the small
ones [those in Eq. (7)] it is advantageous to use a reference
system which rotates with the field experienced by the moving
particle. Thus we use the SE for spin \( 1/2 \) with quantization
axis in the local field direction, as in Refs. [20,21]:

\[
\mathcal{H} \frac{d}{dt} [\alpha(t) \chi^+(t) + \beta(t) \chi^-(t)]
= |\mu| B [\alpha(t) \chi^+(t) - \beta(t) \chi^-(t)],
\]

(2)
where the spinors

\[ \chi^+ = \begin{pmatrix} c \\ e_+ s \end{pmatrix} \quad \text{and} \quad \chi^- = \begin{pmatrix} e_- s \\ -c \end{pmatrix} \]  

(3)

are the orthonormal basis vectors corresponding to the spin aligned in the direction of the local magnetic field \( \mathbf{B} \) and opposite to it, respectively. Here \( c = \cos(\theta/2) \), \( s = \sin(\theta/2) \) and \( e_\pm = e^{\pm i \phi} \) are given by the angles \( \theta \) (polar) and \( \phi \) (azimuthal) defining the direction of \( \mathbf{B}(x,y,z) \) at the point \( x(t), y(t), z(t) \) through which the particle passes along its trajectory at time \( t \). For example, for the Los Alamos “bowl” we choose, as in Ref. [20], the fixed Cartesian coordinate system \( x,y,z \), where \( z \) points vertically up, \( y \) (horizontal) and \( z \) define the vertical symmetry plane. In this plane \((x = 0)\) the holding field points in the \( x \)-direction and we refer \( \theta \) and \( \phi \) to this fixed direction: \( \theta = \arccos(B_x/B) \) and \( \phi = \arctan(B_y/B_x) \). Similarly, for the cylindrical multipole field we refer \( \theta \) and \( \phi \) to the direction of the symmetry axis.

In the reference system moving with the particle, \( \theta \) and \( \phi \) depend on \( t \). In Eq. (2) we need the temporal derivatives \( \dot{\chi}^+ (t) \) and \( \dot{\chi}^- (t) \) [21]

\[ \dot{\chi}^+ = A_{pp} \chi^+ + A_{pm} \chi^- \quad \dot{\chi}^- = A_{mp} \chi^+ + A_{mm} \chi^- \]  

(4)

with time dependent coefficients

\[ A_{pp} = \frac{i}{2} \dot{\phi} (1 - \cos \theta), \quad A_{pm} = -\frac{1}{2} e_+ (\dot{\theta} + i \dot{\phi} \sin \theta), \]

\[ A_{mp} = -A_{pm}^*, \quad A_{mm} = A_{pp}^* = -A_{pp}. \]  

(5)

\( A_{mp} \) and \( A_{pp} \) are determined by the time derivatives of the field \( \dot{\theta} \) and \( \dot{\phi} \). These are small quantities as compared to the wave frequency which is given by the Larmor frequency \( \omega_L = 2 |\mu| B / \hbar \). In practical cases, \( |A_{pp}| \) and \( |A_{mp}| \) are \( \sim 10^{-4} \omega_L \) or less even at the field minima. Therefore, we will treat these quantities as small perturbations.

Using Eqs. (3)–(5) in Eq. (2) we obtain for the terms with \( \chi^+ \) in first order

\[ \dot{\alpha} + \frac{i \omega_L}{2} \alpha = 0, \]  

(6)

and for those with \( \chi^- \)

\[ \dot{\beta} - \frac{i \omega_L}{2} \beta = -\alpha A_{pm} = \frac{\alpha}{2} e_+ (\dot{\theta} + i \dot{\phi} \sin \theta). \]  

(7)

In WKB approximation, the solutions of ordinary differential equations (ODEs) (6) and (7) are [20,21]

\[ \alpha(t) = e^{-i \Theta / 2}, \]

(8)

\[ \beta(t) = \frac{i A_{pm}}{\omega_L} e^{-i \Theta / 2} = \frac{i}{2 \omega_L} e_+ (\dot{\theta} + i \dot{\phi} \sin \theta) e^{-i \Theta / 2}, \]  

(9)

where \( \Theta = \int_0^t \omega_L (t') dt' \) is twice the phase angle accumulated since the previous TP. Since \( \alpha \) and \( \beta \) have the same phase factor \( e^{-i \Theta / 2} \), the wave components \( \alpha \) and \( \beta \) propagate between TPs as a unit (they do not run apart). This important feature had also been noted in Ref. [21].

From (9), the probability of finding the neutron in the spin-flipped state along the way to the next TP is

\[ p(t) = |\beta(t)|^2 = \frac{\theta^2(t) + \phi^2(t) \sin^2 \theta(t)}{4 \omega_L^2} = \frac{\Omega^2(t)}{4 \omega_L^2(t)}. \]  

(10)

\( \Omega(t) \) is the frequency of field rotation about an axis normal to the plane defined by \( \mathbf{B} \) and \( \mathbf{B} \) and can be expressed as \( \Omega = |\mathbf{B} \times \mathbf{B}/B^2| \). This form holds since \( \theta^2 + \phi^2 \sin^2 \theta \) is the squared projection of vector \( \mathbf{B} \) at a time interval \( t_i \) from the through of the direction of the unit sphere. For any trajectory we determine the arrival time and the position of the TPs from the condition that the velocity component along the gradient of potential \( V \) vanishes, \( \mathbf{v} \cdot \nabla V = 0 \), since, at a TP, the particle momentarily moves along the ES at a stationary speed.

Equations (9) and (10) make use of an approximation which we will discuss in Sec. V in connection with the higher-order solution given in Eqs. (25) and (27). In short, this analysis shows the following features of \( p(t) \): Starting from zero at a TP, \( p(t) \) increases to the value given in Eq. (10) within a short time of order \( \mu s \). Equation (10) holds over the entire remainder, typically \( 0.01–0.1 \) s, of the motion to the next TP where \( p(t) \) is “measured.” Equation (10) shows that the result depends only on the local field variables \( \Omega(t) \) and \( \omega_L(t) \). It does not depend on the path history; from (9), only the phase \(-\theta / 2 \) of \( \beta(t) \) does. [This is similar to the behavior of \( \alpha(t) \) shown in Eq. (8).]

For the sequence of TPs encountered along a neutron path of total duration \( T_{\text{tot}} \) we determine the spin flip rate between consecutive TPs at \( t_{i-1} \) and \( t_i \) by dividing \( p(t_i) \), from (10), by the time interval \( \Delta T_i = t_i - t_{i-1} \). Taking into account the probability \( \Delta T_i/T_{\text{tot}} \) of finding the particle on this path element the spin flip rate for the entire path becomes

\[ 1/\tau_{\text{dep}} = \frac{1}{T_{\text{tot}}} \sum_{i=1}^{n} p(t_i), \]  

(11)

where \( n \) is the number of TPs encountered. Finally, the depolarization rate measured in the experiments is the ensemble average over all paths, which is determined by the source characteristics and by spectral cleaning. We assume an isotropic Maxwell spectrum, thus an energy independent phase space density (PSD). The Boltzmann factor \( e^{-E/k_B T} \) is close to unity since UCN energies \( E \), which are of order \( \lesssim 10^{-7} \) eV, are much lower than \( k_B T \) even for a low trap temperature \( T \). The corresponding velocity dependence of the spectrum is \( f(v) \sim v^2 \) [for \( v \) up to the local trapping limit; from energy conservation, this limit depends on the local potential \( V(x,y,z) \)].

Relation (10) is also obtained in a fully quantum mechanical approach using the space and spin dependent SE in WKB approximation [20,21]. This equivalence holds for any field geometry, as shown in the Appendix.

IV. ENSEMBLE AVERAGE OF SPIN FLIP LOSS

In actual magnetic UCN storage systems it is difficult to make sure that the spectrum is isotropic and fills phase space uniformly up to the trapping limit. In practice this would require the complete removal of UCNs with energies slightly exceeding the limit. These tend to be in quasistable orbits lasting for times of the order of \( \tau_n \), thus affecting
the precision of a measurement of $\tau_{\text{dep}}$. Deviations from the
Maxwell spectrum may also be due to the characteristics of
the UCN source and of UCN transport to the trap but we will
disregard these differences since they are expected to be of
minor importance for the specific loss due to spin flip.

A. 1D field model

For the 1D field model of Ref. [21] the condition of
constant PSD was taken into account as follows: The spin flip
probability was averaged over the vertical velocity component
$v_z$ in the plane $z = z_0$ where the gravitational downward force,
$-mg$, is balanced by the magnetic upward force, $-\mu d|B|/dz$.
$z_0$ is the 1D equivalent of an elliptic fixed point $O$ and $z = z_0$
is the only plane where UCNs of any energy $E$ can reside,
down to $E = 0$ and up to the maximum value for trapping.
(Here and henceforth we set the potential $V = 0$ at $O$ and
assume that there are no other potential minima in the trapping
region; this is the case for the field configurations presently
used or proposed.) For any other height, the lower energy
limit is nonzero. Therefore, to include all possible orbits in the
averaging process we have to choose $z_0$ as the reference height,
and since the statistical distribution of $v_z$ values is uniform
for uniform PSD, the mean depolarization rate is given as the
average of $1/\tau_{\text{dep}}$ as a function of $v_z$.

To analyze the depolarization between consecutive TPs
we start trajectories from a TP, not from the fixed point
$O$; so we have to connect the statistics at $z_0$, which is
given by a uniform distribution of $v_z$, with the distribution
$P(z)$ of launching height $z$ for given $v_z$. $P(z)$ follows from
energy conservation: The potential at the launching point
is $V(z) = v_z^2/2$, thus $(dv_z/dz)dz = v_z dv_z$. Therefore, to
represent constant spacing in velocity space ($\Delta v_z = \text{const.}$)
for orbits launched at height $z$ we have to choose the density
$P(z)$ of launching points proportional to
\[
\frac{1}{\Delta z} = \frac{|dV(z)/dz|}{v_z \Delta v_z} = \left( \frac{|dV(z)/dz|}{\Delta v_z \sqrt{2} \sqrt{V}} \right),
\]
thus
\[
P(z) = \frac{|dV(z)/dz|}{\sqrt{V}},
\]
where we have omitted the irrelevant constant factor
$1/(\Delta v_z \sqrt{2})$. In this form, $P(z)$ is neither normalized nor made
dimensionless. This is not necessary since in the simulations
described below we use von Neumann’s acceptance or rejec-
tion method to implement probability distributions. For this
purpose we only need the relative value $P/P_{\text{max}}$, where $P_{\text{max}}$
is the maximum value of $P$ for the ensemble of trajectories.

B. General 3D field models

Now we adapt this result to arbitrary 3D field models as
are relevant for the Los Alamos bowl [20]. In this system the
asymmetry introduced by the choice of two different radii of
curvature along the rows of Halbach field magnets helps to
randomize the orbits, although fully mixing phase flow cannot
be achieved. To select a representative sample of orbits for
depolarization calculations we assume that most particles with
energy $E$ below the trapping limit will, at some time, be found
at rest. (This would be the case for full phase mixing and
is a reasonable approximation for UCNR. Moreover, for the
argument made below it suffices to assume that, at some time
during storage, the particle is slowed down, by field gradients,
to a small velocity, not necessarily to a full stop.) At the
time of a momentary halt the particle has just reached the ES
$V = E/m = \text{constant}$. It will then be accelerated back into the
region of lower potential in the direction perpendicular to the
ES.

Taking these points as the initial position for simulated
trajectories starting from rest, we make sure that the particle
remains within the volume bounded by the ES with potential
$V = E/m$ (as long as no spin flip to the $|\rangle$ state takes
place.) The statistical distribution of launch points in space
is determined by the following extension of (12) to 3D
gometry: We relate the launching point to the fixed point
$O$ in the same way as for the 1D field model. Equating
the initial energy $E = mv(x,y,z)$ with the kinetic energy at
$O$, $E = mv_0^2/2$, we differentiate $V(x,y,z) = v_0^2/2$. This
gives $\nabla V \cdot ds = |\nabla V| ds = v_0 dV_0$ where we have taken into
account that the path element $ds$ is parallel to the gradient of
$V(x,y,z)$ at the launching point. Furthermore, in the immediate
vicinity of $O$ the potential is constant, thus the spatial density
is stationary. Hence, to satisfy uniformity of PSD the density in
velocity space must be uniform, $\Delta v_0 = \text{constant}$, and we have
to choose the spatial density of launching points proportional to
\[
\frac{1}{\Delta z} = \frac{|\nabla V|}{v_0 \Delta v_0} = \frac{|\nabla V|}{(\Delta v_0 \sqrt{2}) \sqrt{V}}.
\]
As in Eq. (12) we can ignore the constant factor $1/(\Delta v_0 \sqrt{2})$
and define
\[
P(x,y,z) = \frac{|\nabla V(x,y,z)|}{\sqrt{V(x,y,z)}},
\]
as the (non-normalized) probability distribution representing
the number of launch points per unit volume at position
$(x,y,z)$.

We use this method to select random launching points for
simulated orbits in UCNR for the three field models—
“smooth,” “one-way ripple,” and “two-way ripple”—and the
toroidal-shaped holding field coil geometry described in
Ref. [20]. We approximate the latter by a complete (360°),
tightly wound torus, thus neglecting end effects and ripples
for the holding field. Averaging the spin flip rate (11) over
a sample of some 10^3 orbits, each of duration $T_{\text{tot}} = 10$ s
with $n \approx 100$ TPs, for four values of holding field $B_{z_0}$
at the bowl bottom, we obtain the depolarization rate ($1/\tau_{\text{dep}}$)
shown in Table I. The results are consistent, within a factor

<table>
<thead>
<tr>
<th>$B_{z_0}$ (T)</th>
<th>Smooth</th>
<th>One-way ripple</th>
<th>Two-way ripple</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>0.022(1)</td>
<td>0.023(1)</td>
<td>0.024(1)</td>
</tr>
<tr>
<td>0.03</td>
<td>0.32(1)</td>
<td>0.33(1)</td>
<td>0.31(1)</td>
</tr>
<tr>
<td>0.01</td>
<td>1.6(1)</td>
<td>1.7(1)</td>
<td>1.9(1)</td>
</tr>
<tr>
<td>0.001</td>
<td>9.4(1)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
of 2, with those given in Fig. 3 of Ref. [21] for the 1D field model: \(1/\tau_{\text{dep}} \approx 4 \times 10^{-9} \text{ s}^{-1}\) for \(B_{\text{b0}} = 5 \text{ mT}\) and \(1/\tau_{\text{dep}} \approx 5 \times 10^{-11} \text{ s}^{-1}\) for \(B_{\text{b0}} = 50 \text{ mT}\). Figure 1 shows as squares the 1D calculation of [21] and as circles the present 3D calculations for the smooth-field model. In the range \(B_{\text{b0}} \gtrsim 5 \text{ mT}\) the data are represented reasonably well by the proportionality \(1/\tau_{\text{dep}} \sim B_{\text{b0}}^{-2}\) as indicated by the dashed line.

Table I shows that the field ripple has a minor effect on the net depolarization loss. This is plausible since the ripple only affects the immediate vicinity, of order mm, of the wall which contributes little to the spin flip since the adiabatic condition \(\Omega \ll \omega_L\) is well satisfied in the region of high field strength near the wall.

### C. Cylindrical multipole fields

#### 1. Results for the field model of Eq. (1)

We use the field of an ideal cylindrical multipole given in Eq. (1), which does not take into account the deviations induced in the actual designs by the discrete geometry of electric currents [23,28], or by the permanent magnet blocks with constant magnetization within each block in the schemes of Refs. [20,24–27].

Equation (1) neglects gravity and assumes a uniform holding field \(B_{\text{c}}\) in the axial direction. With these simplifications, the field is determined only by the polar coordinates \(r\) and \(\phi\) in the plane perpendicular to the axis. Moreover, the field magnitude \(B\) and the force \(-\mu |B| dB/dr\) acting on a \(\pm\) spin UCN depend only on \(r\). In this central force field the equipotential lines are concentric cylindrical shells. Energy \(E\) and angular momentum \(L_z\) about the symmetry axis are conserved. (For vertical systems, \(L_z\) is conserved also in the presence of gravity as well as for variable \(B_{\text{c}}\), as for end fields, as long as the potential \(V\) remains cylindrically symmetric.)

The orbits of the 2D hexapole \((2N = 6)\) are ellipses. Analytic expressions for the orbits, in terms of elliptic integrals, exist also for the quadrupole \((2N = 4)\), decapole \((2N = 10)\) and for \(2N = 14\) [33]. Alternatively, the radial equation of motion, \(\dot{r} = \sqrt{2[ E - V_{\text{eff}}(r)]/m}\), in the effective potential \(V_{\text{eff}}(r) = V(r) + L_z^2/(2m^2r^2)\) is readily solved numerically for any \(N \geq 2\). There are two apsidal radii, \(r_{\text{min}}\) and \(r_{\text{max}}\), and the orbits are symmetric about the angular positions of these TPs. Therefore, it suffices to analyze only the path section between any consecutive TPs.

We average over all possible orbits confined within the trap radius \(R\) and subject to the requirement of uniform PSD as follows. Choosing the radius \(r_1 < R\) of an ES we consider all orbits which turn around at \(r_1\). Subset \(a\) of these orbits comes from the inside and has \(0 \leq r_{\text{min}} \leq r_1\) and \(r_{\text{max}} = r_1\). The other subset \(b\) of orbits comes from the outside and has \(r_{\text{min}} = r_1\) and \(r_1 \leq r_{\text{max}} < R\). In case \(a\) (b) the region exterior to the storage space for spin \(+\) is the range \(r > r_1\) (\(r < r_1\)). In either case, a spin-flipped UCN entering this “forbidden zone” is attracted toward the high field at the wall and considered as lost.

The classification \(a\) or \(b\) is determined by the peripheral velocity \(v_1\) at \(r_1\): For group \(a\) the range of \(v_1\) is between 0 (for the radial path from or toward the center \(r = 0\), for which the angular momentum is zero) and \(v_1 = \sqrt{r_1} F(r_1)/m\) with centripetal force \(F(r) = m dV/dr_1\). In the latter limit the path is circular with radius \(r_1\). For group \(b\), \(v_1\) ranges from \(v_1\) (circular) to \(v_2\) for the limiting path skirting the wall \((r_{\text{max}}(v_2) = R)\). In each case, the second turning radius and the time \(\Delta t(r_1,v_1)\) it takes from one TP to the next are found numerically from the radial equation of motion.

To determine the statistical weight of a given orbit with one TP at radius \(r_1\) we have to modify the strategy used for the UCNr field. In that case we considered only the sample of orbits where the particle starts from rest at the ES with the highest potential, \(V = E/m\), reached for given energy \(E\).

For the cylindrical multipole field (1) only regular orbits exist and releasing a particle from rest would cover only the subset (of measure zero) of trajectories with angular momentum \(L_z\) with \(\rho < \rho_1\) and \(\rho_1 < 0\). However, field (1) is an idealization and in the physical situations field irregularities such as “ripples” and stray fields in the axial \(\xi\) direction are unavoidable. As far as the statistics of orbits perturbed in this way goes, the following strategy appears justified: For a path turning around at \(r_1\) with peripheral velocity \(v_1\) at \(r_1\) we consider the ES of radius \(\rho\) such that \(V(\rho) = E/m = V(r_1) + v_1^2/2\) and relate the statistical weight for radius \(\rho\) to the uniform phase-space density at \(O\). As in Secs. IV A and IV B we differentiate the energy balance between \(r = \rho\) and \(r = 0\), \(E/m = V(\rho) = v_0^2/2\), and obtain the proportionality

\[
\frac{\Delta v_0}{\Delta \rho} \sim \frac{dV(\rho)/d\rho}{\sqrt{V(\rho)}}. \tag{14}
\]

Multiplying by \(\rho\) to take into account the number of allowed points along the circle with radius \(\rho\), we derive the weighting factor for radius \(\rho\), and therefore also the probability \(P(r_1,v_1)\) for an orbit with apsidal radius \(r_1\) and apsidal
the dependence of ensemble of paths, the overall depolarization rate becomes 

\[ \frac{d\tau}{d\rho} = \rho \frac{dV(\rho)}{d\rho} \sqrt{V(\rho)} \] (15)

where, by definition of \( V(\rho) \) and using (1),

\[ V(\rho) = V(r_1) + v_1^2/2 \]

and

\[ \rho = \rho \left[ \left( |\mu|B_{\text{tr}} + mv_1^2/2 \right)^2 - |\mu|^2B_{\text{tr}}^2 \right]^{1/(2N-2)} \] (16)

To evaluate \( dV(\rho)/d\rho \) in Eq. (15) we have to take into account the dependence of \( V(\rho) \) and of

\[ \rho = R \left[ mV(r_1) + |\mu|B_{\text{tr}} + mv_1^2/2 \right] - |\mu|^2B_{\text{tr}}^2 \] (17)

[from (16)] on \( r_1 \) and \( v_1 \):

\[ \frac{d\rho}{d\rho} = \partial V(\rho)/\partial r_1 + \partial V(\rho)/\partial v_1 = 2\frac{dV(r_1)/dr_1}{\rho}\] (18)

where we have used \( \partial \rho/\partial v_1 = \{v_1/[dV(r_1)/dr_1]\} \times (\partial \rho/\partial r_1) \) which follows from (17) with the help of \( \partial V(\rho)/\partial r_1 = dV(r_1)/dr_1 \) and \( \partial V(\rho)/\partial v_1 = v_1 \). The result is

\[ P(r_1, v_1) = \frac{m^2B_{\text{tr}}^2(r_1) + |\mu|B_{\text{tr}}(r_1)mv_1^2 + mv_1^2/4}{\left[ |\mu|B_{\text{tr}}(r_1) + mv_1^2/2 \right] \sqrt{|\mu|\left[ B_{\text{tr}}(r_1) - B_{\text{tr}} + mv_1^2/2 \right]}} \] (19)

where \( B_{\text{tr}}(r) = B_{\text{max}}(r/R)^{2N-2} \) and \( B(r) = B_{\text{max}}^2 + B_{\text{tr}}^2 \) are the multipole fields without and with holding field \( B_{\text{tr}} \), respectively, and we omitted the constant factor \( 2(N-1)/\sqrt{m} \).

Weight factor (19) determines how the depolarization rate from (10) is averaged over all paths. At TPs we have \( \theta = 0 \) since \( \theta \) depends only on \( r \) and \( r = 0 \). (Here we measure \( \theta \) from the \( \xi \) axis.) The angular velocity of trapping field rotation experienced by a neutron moving through a TP is \( \phi = (N-1)v_1/r_1 \). Thus, averaging \( p/\Delta T \) from (10) over the ensemble of paths, the overall depolarization rate becomes

\[ \langle 1/\tau_{\text{dep}} \rangle = \frac{(N-1)^2}{\Delta T} \int_0^R d\rho_1 \sin^2 \theta(r_1) \int_0^v d\theta_1 \int_{\rho_1}^{v_1} d\rho_{\text{tr}} P(r_1, v_1) \frac{v_1^2}{\Delta \rho(r_1, v_1)} \] (20)

with Larmor frequency \( \omega_{\text{L}}(r_1) \) at radius \( r_1 \) and normalization constant \( v = \int_0^R d\rho_1 \int_0^{v_1} d\theta_1 \int_{\rho_1}^{v_1} d\rho_{\text{tr}} P(r_1, v_1) \).

Numerical results for a wide range of multipole orders \( 2N \) are shown in Fig. 2 for \( R = 4.7 \) cm and \( B_{\text{max}} = 1.3 \) T. These are typical values for multipole traps; we keep these parameters the same for hypothetical systems where only the multipole order \( 2N \) is varied and use \( B_{\text{tr}} = 0.001, 0.01, \) and 0.1 T for the holding field. To show the behavior of \( 1/\tau_{\text{dep}} \) vs \( N \) more clearly, we have added the half-integral values \( N = 5/2 \) and \( N = 7/2 \) which cannot be realized with magnetic fields.

We include orbits with \( L_z \neq 0 \) as follows. Choosing a random initial position \( Q \) within the trap volume, a particle is
TABLE II. Mean depolarization rate $\langle 1/\tau_{dep} \rangle$ (10^{-9}/s) from 3D simulations for cylindrical multipoles with gravity and end coils included.

<table>
<thead>
<tr>
<th>2N</th>
<th>4</th>
<th>8</th>
<th>20</th>
</tr>
</thead>
<tbody>
<tr>
<td>HOPE, vertical</td>
<td>[4.1(1)]</td>
<td>0.34(1)</td>
<td>[0.78(1)]</td>
</tr>
<tr>
<td>HOPE, horizontal</td>
<td>[0.61(1)]</td>
<td>0.15(1)</td>
<td>[0.89(1)]</td>
</tr>
<tr>
<td>NIST, mark 2</td>
<td>0.43(1)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>NIST, mark 3</td>
<td>0.021(1)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

launched with initial velocity vector $v_1$ tangential to the ES at $Q$ and pointing in a random direction within the launch plane.

To conform to a uniform distribution in velocity space, the endpoint of $v_1$ is uniformly distributed within the area of a disk whose radius is determined by the maximum velocity for particle trajectories confined to the trap volume. This and the following operations correspond to those described for the 2D field model (1) in Sec. IV C 1, but averages over the circular ESs of the latter model are now replaced by averages over ESs of general shape in 3D space. Based on (13), this leads to an approximation for the weight factor $P(r_1,v_1)$ for launch at position $r_1$ and initial velocity $v_1$ and, finally, to the mean depolarization rate $\langle 1/\tau_{dep} \rangle$ by averaging (11) over some $10^5$ orbits, each of duration $T_{tot} = 10$ s with $n \gtrsim 500$ TPs.

We approximate the effect of spectral cleaning in UCN storage experiments by specifying the largest energy $E_{max}$ of stored particles. The calculations of $\langle 1/\tau_{dep} \rangle$ shown in Table II use $E_{max} \approx 0.8$ times the value $|\mu|B_{high}$ for the highest field $B_{high}$ in the trap and are based on the field parameters of the following two designs:

(a) The HOPE octupole magnet [26] has bore radius 4.7 cm and its axis is oriented vertically or horizontally. For the vertical configuration we assume activation of only the bottom solenoid with a maximum axial field of 1.4 T while gravity provides the cap. With both end field solenoids activated in the horizontal configuration, we assume fields of 1.4 T on both ends, separated by a distance of 1.13 m, without activating the long holding field solenoid. The radial confinement field is $B_{max} = 1.3$ T at the trap wall.

(b) Two horizontal loffle type quadrupole magnets have been used at NIST [34,35] (versions mark 2 and mark 3). For mark 2 (mark 3) we use maximal fields of axially 1.4 T (4.0 T) and radially 1.3 T (3.9 T), a trap radius of 5 cm (5 cm), and a separation of 0.4 m (0.76 m) between the centers of the end field solenoids; for mark 2, the latter include “bucking” coils [34,35] causing the axial field to drop off more quickly to a minimum of 0.1 T at the trap center. For mark 3, the minimum field is 0.6 T.

Since the depolarization rates depend only weakly on the details of the field distribution, such as field ripples, we use the smoothed fields and approximate the solenoid fields by their values on the solenoid axis, neglecting the variations of field magnitude and direction over the trap’s cross section. The results are shown in Table II.

For the HOPE-type system we include, in square brackets, also systems with the same geometries and maximum fields but different multipole order 2N. We observe the same tendency as for the 2D calculations of Fig. 2: The depolarization rates for $2N = 4$ and $2N = 20$ are higher than in the intermediate range ($2N \sim 8$). This can be explained by higher field gradients, near the axis for low $N$ and near the wall for high $N$.

As a further general feature, the magnitudes and $N$ dependence of $\langle 1/\tau_{dep} \rangle$ from the 3D simulations in Table II are well approximated by the 2D results from Fig. 2 if we use values of holding field close to their minima: 0.08 T (vertical configuration with $B_{min} = 0.013$ T) and 0.1 T (horizontal with $B_{min} = 0.09$ T) for HOPE [26] and 0.1 T (0.6 T) for NIST mark 2 (mark 3) with $B_{min} \approx 0.1$ T (0.6 T) [34,35].

Finally, $\langle 1/\tau_{dep} \rangle$ approximately scales like $B_r^{-2}$. A similar increase of $\langle 1/\tau_{dep} \rangle$ with decreasing holding field is also seen for UCN $\tau$, as shown by the dashed line in Fig. 1. As an application of scaling in an experiment, we could deliberately lower the holding field to enhance the depolarization loss to a measurable level to verify that the loss for the actual field is negligible.

V. A HIGHER-ORDER SOLUTION

In this section we compare the first-order approximation for the spin-dependent SE, Eqs. (6) and (7), with a higher-order approach where we retain all the terms with $A_{pm}$ and $A_{pp}$ [given in Eq. (5)], which arose from the transformation to the reference system rotating with the field:

$$\dot{\alpha} + i\frac{\omega_L}{2}\alpha = -A_{pp}\alpha + A^*_{pm}\beta,$$

$$\dot{\beta} - i\frac{\omega_L}{2}\beta = -A_{pm}\alpha + A_{pp}\beta. \quad (21)$$

The coupled first-order ODEs (21) and (22) can be solved by direct numerical integration with initial conditions $\alpha(0) = 1$, $\beta(0) = 0$ for a particle starting in the $|\pm\rangle$ state at $t = 0$.

Alternatively, we can use the perturbation approach developed in Ref. [36] for searches for a permanent electric dipole (EDM) of the neutron, to solve the SE for spin 1/2 to second order of small perturbations. In the EDM case the UCN spin state is perturbed by magnetic field inhomogeneities and a strong static electric field. In Eqs. (21) and (22) the perturbations are the terms on the right-hand side, which are much smaller than those on the left.

To facilitate comparison with [36] we define $\Sigma_{pp}(t) = -2iA_{pp}(t)$ (real-valued), $\Sigma(t) = -2iA_{pm}(t)$ (complex), $\omega_1(t) = \omega_L(t) + \Sigma_{pp}(t)$, and $\theta_1(t) = \int_0^t\omega_1(t')dt'$. In practical cases, $\Sigma_{pp}$ is at least $10^4$ times smaller than $\omega_1L$; thus $\omega_1$ is very close to $\omega_L$.

The transformations $\alpha(t) = u(t)e^{-i\theta_1(t)/2}$, $\beta(t) = w(t)e^{i\theta_1(t)/2}$ turn Eqs. (21) and (22) into

$$i\dot{u}(t) = \frac{1}{2}\Sigma^*(t)u(t)e^{i\theta_1(t)}, \quad i\dot{w}(t) = \frac{1}{2}\Sigma(t)w(t)e^{-i\theta_1(t)}. \quad (23)$$

These coupled ODEs for $u$ and $w$ have the same form as Eqs. (7) for $\alpha_1$ and $\beta_1$ in Ref. [36]. The only difference is the arguments of the exponential functions. In Ref. [36], the SE
was transformed into the reference frame rotating at constant frequency $\omega_0$ for constant applied Larmor field. In the present case, $\omega_0(t)$ can be an arbitrary function of $t$; thus the phase factor $e^{\pm i\omega_0 t}$ is replaced by $e^{\pm i\beta(t)}$.

We combine the two first-order ODEs (23) into the single second-order ODE for $u(t)$:

$$u(t) - \left(i\omega_0(t) + \frac{\Sigma^*(t)}{\Sigma(t)}\right)u(t) = -\frac{1}{4}[\Sigma(t)]^2u(t),$$

(24)

which has the same form as Eq. (8) of [36] with $\omega_0$ in the first term of the expression in brackets replaced by $\omega_0(t)$. This additional time dependence does not affect the method of solving (24) since the second term is time dependent in either case. The initial conditions, $u(0) = 1$ and $u(0) = 0$, are the same as for the EDM case with initial spin up [$\alpha_r(0) = 1$, $\beta_r(0) = 0$].

Following the steps (11) to (18) of [36], we derive

$$w(t) = \frac{2i\xi(t)}{\Sigma(t)}e^{-i\theta_1(t)} = -\frac{i}{2}[\Sigma(t) - \Sigma(0)],$$

(25)

where $\Sigma(t) = \int dt e^{-i\theta_1(t)} \Sigma(t')$.

The initial value, $w(0) = 0$ at $t = 0$, satisfies the required initial condition $\beta(0) = 0$. As $t$ increases, the integral in Eq. (25) rapidly increases on a time scale of order $t_{\text{min}} = 1/\omega_0(0) \approx 1/\omega_L(0)$. In practical applications this is a very short time since the Larmor frequency $\omega_L$ is large everywhere inside the trap volume, even at the field minimum where $B$ is the holding field. For $B(0) = 0.01$ T, $t_{\text{min}} = \pi \hbar/|u|\Sigma(0) \approx 3 \mu$s.

For times $t > t_{\text{min}}$ it is advantageous to change the integration variable in Eq. (25) from $t'$ to $\Theta_1$, with $dt' = d\Theta_1/\omega_1$, and to integrate by parts:

$$w(t) = \frac{\left[\Sigma(t)e^{-i\theta_1(t)}\right]_0^t}{2\omega_1} - \frac{1}{2} \int_0^t dt' e^{-i\theta_1(t')} \frac{d}{dt'} \left[\Sigma(t')/\omega_1(t')\right].$$

(26)

We did not employ the WKB approximation to derive Eq. (26) but its use enables us to evaluate it analytically. We neglect the last term in Eq. (26) since the field variable $\Sigma/\omega_1$ varies slowly on the wavelength scale and get, with (5),

$$\beta(t) = w(t)e^{i\theta_1(t)/2} = \frac{\Sigma(t)e^{-i\theta_1(t)/2}}{2\omega_1(t)} = \frac{i}{2\omega_1(t)} e^{+i\theta(t) + i\theta(t)} e^{-i\theta_1(t)/2}.$$  

(27)

In Eq. (27) we have set the integration constant from the lower limit $t = 0$ of the first term in Eq. (26) equal to zero, and an equivalent approximation had also been made in deriving the first-order solution (9) which differs from (27) only by the replacement of $\omega_0$ by $\omega_L$. The detailed justification in Ref. [21], below Eq. (28), can be summarized as follows. Equations (9) and (27) are semiclassical since the SE is solved for the time dependent field $B(t)$ determined from the classical equations of motion. A fully quantum mechanical treatment requires the solution of the spin and space dependent SE as in Refs. [20,21] and in the Appendix. In this quantum analysis the exact solution for the wave function near a TP involves the Airy functions and the TP is blurred into a nonzero region (typically of order $\mu$s). So is the starting time at a TP. Thus, the initial value of the first term in Eq. (26), at $t_0 \approx 0$, which is $e^{-i\theta_1(t_0)} \approx e^{-i\theta_1(t_0)}$, should be averaged over the rapidly varying phase $\omega_1(0)$, with the result $e^{-i\theta_1(t_0)} = 0$. This holds except for the initial few micrometers of the path subsequent to a TP.

Outside of this region we have, from (27) and (5),

$$|\beta(t)|^2 = |w(t)|^2 = \frac{|\Sigma(t)|^2}{4\omega_1^2(t)} = \left|\frac{A_{\text{pm}}(t)}{\omega^2_1(t)}\right| = \frac{\Omega^2(t)}{4\omega_1^2(t)}.$$  

(28)

Equation (28) agrees with the first-order solution (10) if we replace $\omega_L$ by $\omega_1$. As we have seen, in practical cases the difference between $\omega_L$ and $\omega_1$ is negligible.

Figure 3 shows the time-dependence of spin flip probability $|\beta(t)|^2$ for a particle released from rest at an arbitrary position in UCNr, here $(x,y,z) = (-0.1,0.2,0.3)$ m, calculated in three ways: (a) The analytic results from Eqs. (10) and (28) (solid curve), and the numerical solutions (b) of differential Eq. (9) (dashed) and (c) of ODEs (21) and (22) (dot-dashed). These three curves closely agree except within short time intervals $t_{\text{min}} \lesssim 10 \mu$s subsequent to passage through TPs at nonzero velocity, such as the TPs marked by the arrows. The deviations (not shown in Fig. 3) are due to the reset to $\beta = 0$ at a TP. They are shown in detail in Fig. 4 for a UCN moving away from a TP at $(x,y,z) = (-0.1,0.2,0.2)$ m at initial velocity $2$ m/s tangential to the local ES. As expected from Eq. (26), $|\beta|^2$ jumps, within a few Larmor periods ($\lesssim 10 \mu$s), from 0 to the
We confirm and generalize the earlier conclusions of [20,21] relating to “Majorana spin flip at zeros of the magnetic field.” Magnetic UCN traps avoid locations of vanishing field by applying a holding field $B_h$ perpendicular to the trapping field. For typical values of $B_h$ we calculate spin flip probabilities which are greater, by many orders of magnitude, than the Majorana prediction [19] which had been derived for fast particles moving in an infinitely extended field rather than the slow UCNs trapped in fields of finite extent. For the magnetic traps investigated we have found an approximate power law behavior of spin flip loss rate as a function of $B_h$, $(1/\tau_{dep}) \sim B_h^{-2}$ (see Figs. 1 and 2), to be compared with the exponential behavior, $\sim e^{-\pi \xi^2}$ with adiabaticity parameter $\xi = \omega_L/\Omega$, for the Majorana case [19].

Numerical results for the depolarization rate $(1/\tau_{dep})$ are summarized in Table I and Fig. 1 for UCN$\tau$ and in Table II and Fig. 2 for cylindrical multipole fields as for the HOPE and NIST systems. We find good agreement between the analytical calculations for simplified low-dimensional model fields (1D for UCN$\tau$ in Ref. [21] and 2D for multipoles in the present Sec. IV C 1) and the more elaborate simulations for 3D field models closer to fields used in experiments. As shown in Fig. 1, $(1/\tau_{dep})$ strongly depends on $B_h$ and less pronouncedly on multipole order $2N$. For the design fields of HOPE (in horizontal or vertical configuration without activating the long holding field solenoid) we obtained $(1/\tau_{dep}) \sim 10^{-10}$/s. The corresponding values for NIST (mark 3) are $(1/\tau_{dep}) \sim 10^{-11}$/s (see Table II) and $\sim 10^{-9}$/s for UCN$\tau$ with $B_h = 0.01$ T (see Table I).

We conclude that $B_h$ can always be increased to a strength that renders spin flip losses negligible compared to other possible sources of systematic error in precision neutron lifetime experiments, foremost that due to marginal trapping. (We leave aside the more fundamental question raised in Ref. [37] whether or not neutron lifetime values derived from storage experiments should indeed be identical to those from beam-type experiments).

VI. SUMMARY AND CONCLUSIONS

The spin flip loss in magnetic storage of UCNs in the Los Alamos UCN$\tau$ permanent magnet trap had been analyzed theoretically in Ref. [20] for neutrons on a specific vertical path, and in Ref. [21] for arbitrary motion. In the latter work we used a 1D model for the trapping field. In the present article we have extended this analysis to arbitrary orbits in arbitrary fields in 3D space and report calculations of mean spin flip rates for the UCN$\tau$ system and for multipole fields such as the cylindrical octupole of the HOPE project [25,26] and the Ioffe-type quadrupole trapping fields of [23,34,35]. In all cases relevant to magnetic UCN storage we have established agreement between the semiclassical approach, solving the spin-dependent SE for the time-dependent field seen by the particle in a classical orbit, and a fully quantum mechanical analysis based on the space and spin dependent SE solved in WKB approximation. The relative difference between a first-order treatment (in Sec. III) and a higher-order analysis (in Sec. V) of depolarization in the semiclassical framework is at most on the order of $10^{-4}$ in practical applications.

ACKNOWLEDGMENTS

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APPENDIX: QUANTUM ANALYSIS

The space and spin dependent wave function $\Psi$ for a neutron with energy $E$ moving in a gravito-magnetic trapping field satisfies the SE

$$E \Psi = \left[ -\frac{\hbar^2}{2m} \nabla^2 + mgz + |\mu| \sigma \cdot B(x,y,z) \right] \Psi,$$

(A1)

where $\Psi = \alpha^{(3)}(x,y,z) \chi^+ + \beta^{(3)}(x,y,z) \chi^-$ and $\sigma_x$, $\sigma_y$, and $\sigma_z$ are Pauli matrices. Superscript (3) indicates that $\alpha^{(3)}(x,y,z)$, for the spin-up wave (relative to the local magnetic field direction), and $\beta^{(3)}(x,y,z)$, for the spin-down wave, are functions of the three spatial coordinates.

The derivatives of $\chi^+$ and $\chi^-$ with respect to $j = x,y,z$ are of the same form as the temporal derivatives (4). In terms
of the spin angles $\theta$ and $\phi$ and of $e_{\pm} = e^{\pm i \phi}$ as defined below Eq. (3) we have
\[ \chi_j^+ = \frac{i}{2} \phi_j (1 - \cos \theta) \chi^+ - \frac{1}{2} e_+ (\theta_j + i \phi_j \sin \theta) \chi^-, \quad (A2) \]
\[ \chi_j^- = \frac{1}{2} e_-(\theta_j - i \phi_j \sin \theta) \chi^+ - \frac{i}{2} \phi_j (1 - \cos \theta) \chi^-, \quad (A3) \]
where the subscript $j$ denotes partial differentiation.

Keeping only the dominant contributions, as in Eqs. (6) and (7), the Laplacian in Eq. (A1) reads
\[ \nabla^2 \psi = \left( \alpha_{xx}^{(3)} + \alpha_{yy}^{(3)} + \alpha_{zz}^{(3)} \right) \chi^+ + \left( \beta_{xx}^{(3)} + \beta_{yy}^{(3)} + \beta_{zz}^{(3)} \right) \chi^- - e_+ \sum_{j=1}^3 \alpha_j^{(3)} (\theta_j + i \phi_j \sin \theta) \chi^-. \quad (A4) \]

Thus, in WKB approximation the spatial wave functions satisfy
\[ \nabla^2 \alpha^{(3)} + k_1^2 \alpha^{(3)} = 0, \quad (A5) \]
\[ \nabla^2 \beta^{(3)} + k_1^2 \beta^{(3)} = e_+ \sum_{j=x,y,z} \alpha_j^{(3)} (\theta_j + i \phi_j \sin \theta), \quad (A6) \]
where
\[ k_1^2(x,y,z) = \frac{2m}{\hbar^2} [E - mgz \mp |\mu| B(x,y,z)]. \quad (A7) \]

are the squared local wave numbers for the (+) and (-) spin state, respectively.

Now we consider a UCN with spin (+) starting at time $t = 0$ at a TP and arriving at $t = \Delta T$ at the next TP which we label $U$. At $U$ the UCN momentarily moves along the local ES at constant speed and we introduce a local Cartesian system of coordinates centered at $U$ with $x'$ and $y'$ in the plane of this ES. $\mathbf{z}'$ points away from the direction into which the UCN is reflected. Coordinate system $x'$, $y'$, $z'$ is defined for the narrow space where the ESs can be considered flat (over a region commensurate with the UCN wavelength) and parallel to one another.

Since the $\alpha^{(3)}$ and $\beta^{(3)}$ constituents of the wave function move as a unit the wave numbers $k_x'$ and $k_y'$ are the same for both. Thus we put
\[ \alpha^{(3)}(x',y',z') = \alpha(z') e^{ik_{x'}x'\hat{\mathbf{x}} + ik_{y'}y'\hat{\mathbf{y}}}, \]
\[ \beta^{(3)}(x',y',z') = \beta(z') e^{ik_{x'}x'\hat{\mathbf{x}} + ik_{y'}y'\hat{\mathbf{y}}}. \quad (A8) \]
As in Ref. [21], $e_+ = e^{i \theta}$ can be interpreted as a Bloch-wave modulation due to the field rotation.

Substituting (A8) in Eqs. (A5) and (A6) we obtain
\[ \frac{d^2 \alpha(z')}{dz'^2} + k_1^2 \alpha(z') = 0 \quad (A9) \]
and
\[ \left[ \frac{d^2 \beta(z')}{dz'^2} + k_1^2 \beta(z') \right] e^{ik_{x'}x'\hat{\mathbf{x}} + ik_{y'}y'\hat{\mathbf{y}}} = \sum_{j=x,y,z} \alpha_j^{(3)}(x',y',z') (\theta_j + i \phi_j \sin \theta), \quad (A10) \]
where the wave numbers for the $z'$ direction are given by
\[ k_{x}^2 = k_{x}'^2 - k_{y}'^2, \quad (A11) \]
with $k_{x}'^2$ defined in Eq. (A7). Among the components of $k_x'$ and $k_y'$, the $z'$ component $k_z'(z')$ plays a special role. Even within the narrow space where the primed system of coordinates has been defined, $k_z'$ is not constant. It becomes zero at the TP $z' = 0$ and, in this semiclassical picture, is only defined for $z' \ll 0$.

In WKB approximation the solution of (A9) is
\[ \alpha(z') = \frac{1}{\sqrt{k_1(z')}} e^{X_z'(z')}, \quad (A12) \]
with $X_z'(z') = \int z' k_z'(u) du$. (The exact quantum solution in form of an Airy function has no singularity at $z' = 0$ and decays exponentially in the classically forbidden zone $z' > 0$.)

To solve (A10) we substitute the WKB approximation for the partial derivatives on the right-hand side, $\alpha_{x'}^{(3)} = i k_{x'} \alpha^{(3)}$, $\alpha_{y'}^{(3)} = i k_{y'} \alpha^{(3)}$, $\alpha_{z'}^{(3)} = i k_{z'}(z') \alpha^{(3)}$, and implement the total time derivative in the form $d/dt = v_x(\partial/\partial x') + v_y(\partial/\partial y') + v_z(\partial/\partial z')$ with velocity $\mathbf{v} = (\hbar/m) \mathbf{k}_x$. Employing also (A12), (A10) becomes
\[ \frac{d^2 \beta(z')}{dz'^2} + k_1^2 \beta(z') = \frac{m}{\hbar} \frac{i}{\sqrt{k_1(z')}} (\theta + i \phi \sin \theta) e^{X_z'(z')}. \quad (A13) \]

The solution of (A13) has been outlined in Refs. [20,21]. The phase factor for the wave function $\beta(z')$ is the same as for $\alpha(z')$: $e^{X_z'(z')}$. Therefore, in WKB approximation we have $d^2 \beta(z')/dz'^2 = -k_1^2 (z') \beta(z')$ and the solution of (A13) becomes
\[ \beta(z') = \frac{m}{\hbar} \frac{i}{\sqrt{k_1(z')}} \frac{\dot{\theta} + i \phi \sin \theta}{k_1^2(z')} e^{X_z'(z')} \quad (A14) \]

The depolarization loss measured at TP $U$ is given by the probability current for spin-flipped UCNs,
\[ j_-(z') = -\frac{\hbar}{m} \text{Re} \left[ i \beta^*(z') \left( \frac{d \beta}{dz'} \right) \right], \quad (A15) \]
leaving the storage space at $z' = 0$ in the positive $z'$ direction. With (A14) this current is
\[ j_-(z') = \frac{m}{\hbar} \frac{\dot{\theta}^2 + \dot{\phi}^2 \sin^2 \theta}{k_1^2(z')^2 - k_{x'}^2(z')^2} = \frac{\hbar}{m} \frac{\Omega^2}{4\omega_L^2}, \quad (A16) \]

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evaluated at $z' = 0$ (i.e., for the field variables $\Omega$ and $\omega_L$ at the particle position at time $t = \Delta T$). In the last step of (A16) we have used the Larmor frequency $\omega_L = \hbar (k^2 L^2 - k^2_0^2)/(2m)$.

To evaluate the spin flip loss rate $1/\tau_{dep}$ between the consecutive TPs we divide the current (A16) by the number $N$ of (+) spin UCNs moving between the TPs in a channel with unit cross section centered at the trajectory. The cross section of this channel is measured parallel to the ES at every point along the path. The $N$ particles within this volume contribute to loss current (A16), their decay rate $-N$ equaling $j_-(0)$.

Denoting the wave number perpendicular to the ESs traversed along the way by $k'_s(t)$ and using the WKB form $|a(t)|^2 = 1/k'_s(t)$ as the particle density we have

$$N = \int_{\Delta T} |a(t)|^2 d(\text{volume}) = \int_0^{\Delta T} \frac{\hbar k'_s(t)}{m} dt = \frac{\hbar}{m} \Delta T. \quad (A17)$$

As for the 1D field model of [21], $N$ is given directly by the travel time $\Delta T$. Using (A16), the depolarization rate becomes

$$1/\tau_{dep} = -N/\dot{N} = m \frac{j_-(0)}{\hbar \cdot \Delta T} = \frac{\Omega^2}{4 \omega_L^2 \Delta T}. \quad (A18)$$

evaluated for the field at the endpoint $U$. This agrees with the semiclassical result $1/\tau_{dep} = p(\Delta T)/\Delta T$ with $p(t)$ given by Eq. (10). Generalizing this result to arbitrary time $t$ in the range $t_{min} < t \leq \Delta T$ (with $t_{min}$ of order $\mu$s), we choose the UCN position at $t$ as the center of reference system $x', y', z'$, with $z'$ normal to the local ES, and use (A14) and (A15) to obtain the identity

$$\frac{m}{\hbar} j_-(t) = \frac{\Omega^2(t)}{4 \omega_L^2(t)} = p(t). \quad (A19)$$

This shows that the semiclassical and the quantum approaches to depolarization are equivalent, with $p(t)$ directly corresponding to $m/\hbar$ times the probability current $j_-(t)$.

There is an open question of interpretation: In the derivation of (A13) we used a total time derivative in the form $\dot{f} = v_x(\partial f/\partial x') + v_y(\partial f/\partial y') + v_z(\partial f/\partial z')$ with velocity $v$ referring to the particle’s motion along its classical path. In this sense, the quantum approach of this appendix does involve classical concepts. Use of the WKB method is not the only approximation made.

A similar caveat applies to the possibility of going to higher-order approximations in this quantum approach. In the semiclassical analysis we were allowed to add, in Eqs. (21) and (22), terms such as $A_{ppB}$ which are of second order and had been neglected in the first-order Eqs. (6) and (7). However, adding the corresponding second-order contributions in the quantum treatment would require that we also add the second-order quantities neglected in the WKB approximation used to derive the ODEs (A5) and (A6). These would be replaced by coupled nonlinear PDEs of high complexity. At this stage the semiclassical and quantum approaches clearly diverge.
