ASSIGNMENT 12: SPIN PRECESSION

E. ARNOLD, M-S. LIU, R. PRABHU & C.S. RICHARDS THE UNIVERSITY OF CAMBRIDGE



SOLENOIDS

INTRODUCTION

In a helium spin-echo experiment, a beam of spin-polarised ³He atoms passes through a magnetic field before being scattered off the sample. The scattered beam then goes through another field before striking the detector. In this tutorial, we will simulate an idealised version of these precession magnetic fields.

PRECESSION FIELD

Generating the magnetic field of produced by a realistic solenoid is a somewhat involved task, and is therefore out of the scope of this tutorial. Instead, we will focus on how to set up an idealised magnetic field without having to consider the geometry of any particular solenoid.

PARAMETERS OF THE SOLENOID

The only properties of our solenoid that we will explicitly define will be its dimensions and its position. For simplicity, we will consider a rectangular solenoid whose symmetry axes align with our coordinate axes, and we will place the centre of the solenoid at the origin. In the tasks we will construct a class the contain properties described. The methods within the class will include the functions that generate our precession magentic fields.

TASK

- 1. Construct a class (which we will call solenoid) with properties described above.
- 2. Write a function that generates a magnetic field with the following features:
 - It should point along the z-axis
 - It should have a uniform magnitude within the solenoid
 - It should have a magnitude equal to 0 outside of the solenoid

3. Write a function that generates a magnetic field with the following features:

- It should point along the z-axis
- It should have a uniform magnitude within the solenoid
- There should be an exponential decay in the magnitude that starts from the two ends of the solenoid
- 4. Write a short script that calls the two functions that you have written, and shows that they work as desired

TIPS

- 1. In addition to the parameters of the solenoid, the solenoid class should have as one (or more) of its properties the set of points at which you wish to evaluate the magnetic field. There are many ways in which you may wish to allow a user to pass these points to the class, but if you are stuck consider how you may use the meshgrid function to help you
- 2. Consider giving your functions the following general structure:
 - Initialise a matrix that will contain the values of the magnetic field at every point that the user is interested in.
 - Use a for loop to run through each point in the matrix and use one or more if statements to check whether each point is inside or outside the solenoid, assigning a value to each point when necessary

SUMMARY

- Helium atoms pass through a magnetic "precession" field before and after striking a sample.
- The nature of the precession fields, particularly their transition time, determines the spin phase the atoms have after leaving the fields
- The analytic magnetic fields for realistic solenoids are difficult to find, and so this tutorial focusses on generating simple, idealised versions.

PREREQUISITES

The chapter Spin Echo from the Theory Handbook.

INTRODUCTION

In previous tutorials, we have considered the scattering of helium-3 atoms from surfaces. These scattered atoms can be detected; thus we have previously discussed how we may interpret the scattering using helium-3 spin-echo spectroscopy (³HeSE). Alongside these tutorials, we have produced models for the diffusion of adsorbates on a surface - which can too be measured with ³HeSE. However, there is a very clear area of the research we have not directed any attention towards: simulating the inner workings of the ³HeSE machine. In this tutorial, we will focus on simulating the spin precession of the atoms in the helium beam while travelling through magnetic fields.

SPIN

Motivation

In the UK, many second year courses cover the so-called "spin" of a particle in good detail. However, many do not. In addition to this, we aim for our package to be suitable for students having completed just one year of university education, and so must introduce the relevent concepts of spin physics here; we hope that this eases the difficulty that may be faced when attempting this tutorial, without overburdening you with information.

Formalism

How do we mathematically describe spin? Suppose that the general state of an object can be written as the state $|\psi\rangle$, which can be decomposed into two parts as

$$|\psi\rangle = |\mathbf{r}, t\rangle |S\rangle$$
.

In this expression, $|\mathbf{r}, t\rangle$ is a ket representing the wavefunction of the object, and $|S\rangle$ is a ket representing the spin state of the object. What do we do with this new way of writing the state of the particle? Introducing an operator $\hat{\mathbf{S}}$ to represent the spin observable, then some basic comments can be made. These can be seen by investigating the behaviour of the spin operator on the state of the system; thus writing the action of the spin as:

$$\mathbf{\hat{S}}|\psi\rangle = \mathbf{\hat{S}}(|\mathbf{r},t\rangle|S\rangle),$$

our first comment can be made. The spin of a particle does not depend on the position of the particle; this is no surprise - a fair comparison would be to assert that the charge of a particle does not changed when the position of the particle changes. Therefore the spin of a particle depends on different degrees of freedom: those intrinsic to the particle itself! How is this related to the expression we have written above? If the spin does not depend on spatial degrees of freedom, then the spin operator $|S\rangle$ does not act on the wavefunction's ket. Thus the action of the operator on the state of the object is

$$\hat{\mathbf{S}}|\psi\rangle = |\mathbf{r},t\rangle\hat{\mathbf{S}}|S\rangle$$

(*i.e.* the spin operator acts on the spin state only). The second comment we wish to make is that the spin operator is a vector; it can be written as:

$$\mathbf{\hat{S}} = \hat{S}_x \mathbf{x} + \hat{S}_y \mathbf{y} + \hat{S}_z \mathbf{z},$$

which signals the spin state has spatial components! Note that this is distinct to the spin not having spatial dependence.

Our discussion so far has deviated very little from the most general abstractions we can make. The next steps we take are to make some assumptions about the spin of a particle; assuming that spin has the same behaviour as the angular momentum of a particle, we suggest that:

- 1. Denoting the operator returning the square magnitude of the spin as \hat{S}^2 , the operators \hat{S}^2 and \hat{S}_j are compatible, where j is any component
- 2. If the spin is measured along z, then the eigenvalues of the operator \hat{S}_z are $m_s \hbar$, where m_s is a number from a discrete set of values.
- 3. m_s takes one of two series of values: one is based on integer values in the range $-s \le m_s \le s$; the other is based on half integer values in the range $-s \le m_s \le s$. In both cases, s is a constant that represents the maximum eigenvalue of a measured spin component (divided by \hbar).
- 4. Using this same constant s, the eigenvalues of the square magnitude spin operator \hat{S}^2 are $s(s+1)\hbar^2$.

Following on from the assumptions listed above, the majority of the remainder of the theory is manipulating the mathematics that arises from these assumptions. For the remainder of the discussion in this section, we consider either a helium-3 atom, or an electron. For both of these particles, the value of s is 1/2. Therefore the permitted values of m_s for both particles are +1/2 and -1/2. Note that this has a profound consequence: as the magnitude of the spin along z is always the same in magnitude when observed, and the overall magnitude of the spin is constant, we can assert that the radial component of the spin is also constant in magnitude. Recalling the eigenvalues of the square of the magnitude of the overall spin to be $s(s+1)\hbar^2$, it is evident that for our particles, the magnitude of the overall spin is $\sqrt{3}\hbar/2$. What can we infer from this? The spin of a particle always points at 55° to the z axis.

A Generic Spin State

Consider again that the spin of a particle, when measured along z, always points at 55° to the z axis. Noting that the magnitude is constant, this leads to two packets of particles: one where the number m_s is 1/2, and one where the number m_s is -1/2. These are assigned the labels $|\uparrow\rangle$ and $|\downarrow\rangle$ respectively. If these states form a complete orthonormal basis set, then it is possible to write the spin state $|\chi(t)\rangle$ at a generic time t in the form:

$$|\chi(t)\rangle = \alpha |\uparrow\rangle + \beta |\downarrow\rangle$$

where the coefficients α and β are parameters that may evolve with time. For this spin state to be normalised, the inner product with itself must be unity. This implies that:

$$\langle \chi(t)|\chi(t)\rangle = (\alpha^*\langle\uparrow| + \beta^*\langle\downarrow|)(\alpha|\uparrow\rangle + \beta|\downarrow\rangle);$$

= $|\alpha|^2 + |\beta|^2;$
- 1

Moving from the first to the second line is trivial once it is realised that given the spin states are distinguishable, they are orthogonal. Orthonormality is then assumed from the definition, as the kets represent physical states.

SPIN PRECESSION

Direction of Spin

Recall that the generic spin state is

$$|\chi(t)\rangle = \alpha |\uparrow\rangle + \beta |\downarrow\rangle.$$

In real cartesian space, does the spin point along a direction? Following through with the mathematics suggests that the answer to this question is yes. Assume that the unit vector representing the direction of the spin is \mathbf{n} . Defining θ as the angle from the vertical and ϕ as the azimuthal angle, then it is clear that the spin points along the direction

$$\mathbf{n} = \sin \theta \cos \phi \mathbf{x} + \sin \theta \sin \phi \mathbf{y} + \cos \theta \mathbf{z}.$$

If α and β can be expressed in terms of these constants, then the direction the spin points in exists. We will now attempt to solve for the coefficients α and β . The solutions are:

$$\alpha = e^{-i\phi/2}\cos(\theta/2);$$

$$\beta = e^{i\phi/2}\sin(\theta/2).$$

Finding these requires the use of more algebra than we wish to use in this document. Therefore we list the results without proof.

Time Evolution Operator

While all of the discussion so far does not account for the origin of spin, it does allow us to start to consider the *time evolution operator* that is central to the understanding of spin precession. The time evolution of any quantum state $|\psi\rangle$ is described by the Schrodinger equation

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = \hat{H} |\psi\rangle.$$

The solution to this is:

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|\psi(0)\rangle,$$

where $e^{-i\hat{H}t/\hbar}$ is known as the time evolution operator. How is this relevant to spin precession? If we know the Hamiltonian, then we can construct the time evolution operator. The Hamiltonian for a spin interacting with a magnetic field is:

$$\hat{H} = -\gamma \hat{\mathbf{S}} \cdot \mathbf{B},$$

where γ is a constant. For a field in the z direction, this gives the coefficients α and β to evolve with time as:

$$\alpha(t) = e^{-i(\phi + \omega_0 t)/2} \cos(\theta/2);$$

$$\beta(t) = e^{-i(\phi + \omega_0 t)/2} \sin(\theta/2).$$

This is best derived with Pauli spin matrices.

TASK

1. Before considering the HeSE experimental setup as a whole, it would be prudent to first write a function to model the precession of atomic spin through a single solenoid. It will be useful to consider not only the central axis but any set of points within the solenoid, as well as a range of atomic speeds. Such a function, called precess() is given in the appendices as a listing.

- (a) Read the function precess() and compare it to the process described in the theory handbook. Note in particular the way in which the lateral points P are used in this function. It is not in fact necessary to consider the location of these points all that is relevant is the magnetic field B along the z-axis at each point modelled. Thus, the choice of coordinate system is irrelevant since the locations and number of points P are all encoded in the field B.
- (b) For all the fields generated in the previous assignment, simulate and plot the variation of the *x*, *y* and *z* spin-components of helium-3 atoms against distance through the solenoid. You may use the following parameters:
 - an initial spin of Si = [0 1 0]',
 - an average speed of $V0=768 \,\mathrm{m \, s^{-1}}$,
 - a range of speeds DV= $0.1 \,\mathrm{m \, s^{-1}}$,
 - a number of considered speeds nV=10,
 - the field B defined only along the central axis,
 - a set of points Z as used in the construction of B.
- (c) Experiment with fields B defined along non-central axes in the solenoid.
- 2. Now we have built up some familiarity with the precess() function, we can move on to considering the arrangement of solenoids used in HeSE experiments. The three main stages of this process are as follows:
 - (a) The atoms pass through the first solenoid and precess, acquiring different phases.
 - (b) The atoms then collide with the surface and change direction. A 'spin rotator field' is used in this stage to compensate for this change in direction by rotating the atomic spins to lie in the new, rotated coordinate system.
 - (c) The atoms pass through the second solenoid which has its field in the opposite direction and acquire an additional phase change that rotates the spin back to its original direction.

If the collision involved any momentum/energy transfer with the surface, the spins would be altered and wouldn't rotate back to their original direction, producing a measurable change. We

- wish to model the elastic and specular case where no such transfer occurs. The code for this is given in the appendices. Try to understand how it functions before you attempt the next task.
- We now have a complete code that simulates the precession of atomic spins across a range of speeds and transverse positions for a given magnetic field.
 - (a) For a variety of fields, plot the variation in spin components as a function of distance through the solenoid along the central axis for different speeds (*i.e.* separately plot each of the three matrices Spins(1,i0,:,:), Spins(2,i0,:,:) and Spins(3,i0,:,:) against the vector Disps where i0 is the index in B corresponding to the central axis). Try this both with and without a spin rotator field. What is different about the range of output spins for each speed in each case? How does this vary if you assume the spin field provides uniform rotation for all speeds rather than a slight variance as it does in practice? Why is this variance not significant in HeSE experiments? Why might that not be the case if the entire wavelength intensity matrix is to be measured?
 - (b) Repeat the above, but instead of plotting the curves for different speeds, try plotting them for the same speed along different axes.
- 4. Suppose that in a given experiment we choose to measure only outgoing atoms whose spins lie along the *y*-axis ([0 1 0]). In the previous assignment we generated two key magnetic fields of interest for the solenoids: a field with a fast transition and a field with a slow transition.
 - By plotting bar charts of the *y*-component of the spin against both speed and the distance of axes from the centre, observe how the speed of the solenoid field transition affects the spread of spin components. Which is most suitable for the HeSE apparatus?

SUMMARY

In this tutorial, you should have learned how the spin of a helium-3 particle precesses in the magnetic fields of a helium-3 spin-echo spectrometer.

APPENDIX

PRECESS.M

```
1 function [Sf] = precess(Si, Z, V, B)
 2 % precondition: Si = initial spin of all atoms at each of the na
         different speeds and different points P
                    Z = the set of points along the axis of the
 3
   %
        solenoid
 4
    %
                    B = matrix of the magnetic field at each point (
        P,Z) in the solenoid
 5 %
                    V0 = average speed of incident atoms
 6
   %
                    DV = fractional spread in speeds of incident
        atoms
 7 %
                    na = number of atoms considered
 8
   %
 9
    % postcondition: Sf = set of final spins for each speed and
        lateral point P
10 %
11
12
13
        % set up dynamic variables of system
14
15
16
        % number of Z-points within solenoid
17
        nZ = length(Z);
        nP = size(B,2);
18
19
        nV = length(V);
20
21
        % produce a linearly-varying set of speeds for each atom in
            the given range
22
        tmp(:,1,1) = V;
        % repeat this over the extent of the beam, i.e. constant
23
            speed since particles are uncharged
24
        V = repmat(tmp(:,1,1), [1 nP nZ]);
25
        % calculate the time taken for each atom to travel each
26
            considered distance \Rightarrow function t(d)
27
        t = zeros(size(V));
        t(:,1,:) = reshape(repmat(Z', [nV 1]), [nV 1 nZ])./V(:,1,:);
28
29
        % repeat this over the extent of the beam, i.e. constant
            speed since particles are uncharged
30
        t = repmat(t(:,1,:), [1 nP 1]);
31
32
        % differentiate t(Z) once wrt. Z to obtain the time interval
             dt taken to travel between each considered distance
            along the length
33
        dt=diff(t,1,3);
        dt(:,:,end+1)=dt(:,:,end);
34
```

```
35
        % normalise spin to get initial orientation (unit vector):
36
        % initial spins should all have the same magnitude...
37
        Simag = sqrt(sum(Si(:,1).^2, 1));
38
39
        % ...but possibly different directions for each speed
40
41
        Sidir=Si./(sqrt(sum(Si.^2))+eps);
42
43
44
45
46
47
48
49
50
51
52
        % calculate Larmor frequency
53
54
55
        % gyromagnetic ratio for helium 3
56
        gamma=2.0378e8; %rad/sec;
57
        % calculate Larmor frequency for atoms of all speeds b/c
58
            independent of speed
59
        w=gamma*sqrt(sum(B.^2,1));
60
61
        % magnitude of B
62
        Bmag=sqrt(sum((B.^2),1));
63
        % normalise B since we only needed the magnitude for the
64
            Larmor frequency (eps rounds to the nearest floating-
            point number)
65
        Bdir=B./(eps+repmat(Bmag, [3 1 1]));
66
67
68
69
70
71
72
73
74
75
76
77
        % precess spin vectors of atoms along the length of the
78
79
        % rotation matrix for precessing spin at point in the
80
            solenoid
81
        R=zeros(3,3,nP,nZ);
82
        \% final spin direction for each atom
83
84
        spinvec1=zeros(3,nP,nZ,nV);
85
        % matrix of *change* in precession angle in travelling
86
            between each considered distance, for each atom
        dphimat=repmat(w, [nV 1 1]).*dt;
87
88
89
        % for each velocity iV...
```

```
for iV=1:nV
 90
 91
             % change in angle phi in each step along the length for
 92
             dphi = (dphimat(iV,:,:));
 93
 94
             % calculate the rotation matrix for atoms of speed V(iV)
                  that acts on the spin at each point for every step
                 along the solenoid
95
             R(1,1,:,:)=(Bdir(1,:,:).^2).*(1-cos(dphi))+cos(dphi);
 96
 97
             R(1,2,:,:)=(Bdir(1,:,:).*Bdir(2,:,:)).*(1-cos(dphi))-
                 Bdir(3,:,:).*sin(dphi);
 98
             R(1,3,:,:)=(Bdir(1,:,:).*Bdir(3,:,:)).*(1-cos(dphi))+
                 Bdir(2,:,:).*sin(dphi);
99
100
             R(2,1,:,:)=(Bdir(1,:,:).*Bdir(2,:,:)).*(1-cos(dphi))+
101
                 Bdir(3,:,:).*sin(dphi);
102
             R(2,2,:,:)=(Bdir(2,:,:).^2).*(1-cos(dphi))+cos(dphi);
103
             R(2,3,:,:)=(Bdir(2,:,:).*Bdir(3,:,:)).*(1-cos(dphi))-
                 Bdir(1,:,:).*sin(dphi);
104
105
106
             R(3,1,:,:)=(Bdir(1,:,:).*Bdir(3,:,:)).*(1-cos(dphi))-
                 Bdir(2,:,:).*sin(dphi);
107
             R(3,2,:,:)=(Bdir(2,:,:).*Bdir(3,:,:)).*(1-cos(dphi))+
                 Bdir(1,:,:).*sin(dphi);
108
             R(3,3,:,:)=(Bdir(3,:,:).^2).*(1-cos(dphi))+cos(dphi);
109
110
             % initial spin for velocity iV at Z-point Z(iZ=1)=0
             spinvec1(:,:,1,iV)=Sidir(:,:,iV);
111
112
113
             % for points iP at each further step Z(iZ) along the
                 length, apply the corresponding rotation operator
114
             for iP = 1:nP
                 for iZ=2:nZ
115
                     spinvec1(:,iP,iZ,iV)=R(:,:,iP,iZ)*spinvec1(:,iP,
116
                          iZ-1,iV);
117
                 end
118
             end
119
         end
120
121
         % output spin, making sure dimensions are correct (so no
             squeezing of 1-dim axes)
         Sf = Simag .* reshape(spinvec1, [3 nP nZ nV]);
122
123
     end
```

MAIN.M

The first step is to initialise the variable parameters of the incident atoms (3-He atoms are assumed so the gyromagnetic ratio is not initialised here)

```
7
    % maximum fractional difference of atom speeds from average
 9
    DV=0.1;
10
   % number of velocities simulated at each point
11
12
    nV=20;
13
14
   % initialise vector of velocities
15
    V = linspace(V0-(V0*DV), V0+(V0*DV), nV);
16
17
    % initial spin polarisation (parallel to the y-axis)
18
    spin=[0 1 0]'; Smag = sum(spin.^2);
19
   % scattering angle at surface
20
21
    sctAngle = pi/4;
22
23
   %-
24
```

We then turn to initialising the parameters of the apparatus, in particular the solenoids. We additionally define a meshgrid of lateral points inside the solenoid, with the understanding that incident atom trajectories will not colinear, rather they will be spread approximately uniformly over a circular area within the solenoid. In principle, this code allows for a meshgrid of any shape so long as the magnetic field for the solenoid is defined at each point on it.

```
25
26
    % solenoid parameters
27
28
   % length of solenoid /m
29
30
   L = 0.005;
32 % width/height of rectangular solenoid /m
33 Lx = 0.05;
34
   Ly = 0.05;
35
36
37
38
39
40
41
   % solenoid dimensions of interest
42
43
44
45
   % SETUP:
46
47
   % length of the region of interest (symmetrical about solenoid)
    Zmax = 5/4*L;
48
49
50
  % number of Z-points to simulate
51
   nZ = 750;
52
53
  % maximum allowed beam radius
54
55 a = min(Lx, Ly)/2;
56
   % number of radii to simulate
57
```

```
58
    nr = 5;
59
60
    % number of angles to simulate -- in range [0,2*pi)
61
    ntheta = 8;
62
63
64
65
   % CALCULATION:
66
    % initialise vector of Z-points
67
68
    Z = linspace(0,Zmax,nZ)';
69
    % calculate spacing between Z-points (we wish to keep this
70
        consistent throughout the simulation
71
    dZ = Z(2)-Z(1);
72
73
74
    % set of radii around central beam in range [0,a)
    r = linspace(0,a,nr+1); r(end) = [];
75
76
77
78
   % set of angles around central beam in range [0,2*pi)
79
    theta = linspace(0,2*pi,ntheta+1); theta(end) = [];
80
81
82
83
    % meshgrid of all lateral points on the beamline/cylinder of
        atoms (the meshgrid here isn't actually important, just each
         meshgrid index corresponds to the field value in B at the
        same index (see below)
84
    [R, Theta] = meshgrid(r, theta);
85
    nP = numel(R); % number of points in meshgrid
86
87
88
89
90
   % extract Cartesian grid for use with Solenoid class
    X = reshape(R.*cos(Theta), [nP 1]); Y = reshape(R.*sin(Theta), [
        nP 1]);
92
93
```

Having defined the solenoid parameters, we now either import a field from another file or create one. Below we define both a simple uniform field along the *z*-axis as well as a field directed along the central *z*-axis with its magnitude given by Gaussian disitribution across the distance from the centre. This should demonstrate the required format of the field variable B. Note that in this code there are several calls to functions in the Solenoid class which are commented-out for use in the questions in this exercise.

```
102
103
     [Bx,By] = s.box_xy();
104
    % FAST Z-TRANSITION:
105
106
    %Bz = s.box_z();
107
108 % SLOW Z-TRANSITION:
109 % the smoothing length is chosen to maximise smoothing over the
        considered region Z
110 Bz = s.smoothstep_z((Z(end) - L)/2);
111
112 % APPLY RADIAL DECAY OF FIELD STRENGTH:
113 % the standard deviation is chosen to be a third of the radius
         of the solenoid so that the field strength is close to zero
         at the edges
114 %radial_decay_const = 3 * 1/(2*(min(Lx,Ly)/2)^2);
115 %for ij = 1:nP
116 %
         for k = 1:nZ
             Bz(ij,k) = Bz(ij,k) * exp(-(X(ij)^2)*radial_decay_const
117 %
          - (Y(ij)^2)*radial_decay_const);
118 %
          end
119
     %end
120
121 % intialise set of vectors for B-field at each point along the
        length
122 B=zeros([3 nP nZ]);
123 B(1,:,:) = Bx; B(2,:,:) = By; B(3,:,:) = Bz;
124
125
     B = 0.15 .* B;
126
127
128
```

The final step of initialisation is to initialise the parameters of the spin rotator field, as well as the distances between components of the apparatus. In the given code there are three options for the spin rotator field.

```
129
130
     % spin rotator field parameters
131
132
133 % this variable is: - 0 if there is no spin rotator field
134 %
                        - 1 if the spin rotation is ideal (i.e.
         uniform rotation for all speeds)
135
                         - 2 if the spin rotator field is (fast-
         transitioning) uniform (i.e. rotation depends on speed)
136
     spinRotator = 2;
137
    % distance from end of each solenoid to the spin rotator field
138
139
    rotBDist= 0.05;
140
141 % length of the spin rotator field
142 rotBLen = 0.05;
143
144
145
```

Having defined the necessary parameters, we may now turn to simulating the apparatus. We begin by simulating the precession in

the first solenoid. We store the spins as a function of distance travelled through the apparatus in the matrix Spins and store those distances in the vector Disps. Note also that we choose to record a short period of propagation before reaching the solenoid to later produce graphics that are easier to understand.

```
146
147
     % first solenoid
148
149
    % propagate short distance up to solenoid
150
151
     Spins = repmat(spin, [1 nP 5 nV]);
152
     Disps = [-0.01:0.002:-0.002]';
153
154
     % initial spins are the same for all axes and speeds
155
     Si = repmat(spin, [1 nP nV]);
156
157
     % precess spin through first solenoid
158
     Sf1 = precess(Si, Z, V, B);
159
    % update stored spins/distances
160
161
     Spins = cat(3, Spins, Sf1);
     Disps = cat(1, Disps, Z);
162
163
164
    % continue propagating up to SR field
     numStepsTorotB = rotBDist/dZ - 1;
165
     Disps = cat(1, Disps, linspace(Disps(end)+dZ, Disps(end)+
166
         rotBDist, numStepsTorotB)');
167
     Spins = cat(3, Spins, repmat(Spins(:,:,end,:), [1 1
         numStepsTorotB 1]));
168
169
170
```

Having propagated through the first solenoid, we then apply the spin rotator (SR) field. In the case of spinRotator==1 we assume an 'ideal' SR field that rotates atoms of all speeds uniformly through the total scattering angle (to compensate for the change in direction at scatter).

```
171
172 % spin rotator field
173 %-
174 % Rotates spin about the x-axis through sctAngle rad without
         affecting trajectory (roughly the same for all speeds
175
176
     Nsr = rotBLen/dZ - 1;
     Zsr = linspace(Disps(end)+dZ, Disps(end)+rotBLen, Nsr)';
177
178
179
     if spinRotator == 1
         % for an ideal uniform rotation for all speeds...
180
181
         % define small rotation for each step along axis
182
183
         RotMsr = [1 0 0; 0 cos(sctAngle/Nsr) -sin(sctAngle/Nsr); 0
             sin(sctAngle/Nsr) cos(sctAngle/Nsr)];
184
185
         % initialise temporary spin variable
186
         Sfsr = zeros([3 nP Nsr nV]);
187
```

```
188
         % first rotation
         for iP = 1:nP
189
190
             Sfsr(:,iP,1,:) = RotMsr * squeeze(Spins(:,iP,end,:));
191
192
193
         % iteratively rotate through small angle until sctAngle rad
             in total
194
         for iV=2:Nsr
195
             for iP = 1:nP
                 Sfsr(:,iP,iV,:) = RotMsr * squeeze(Sfsr(:,iP,iV-1,:)
196
197
198
         end
199
200
         % update stored spins
201
         Spins = cat(3, Spins, Sfsr);
```

If instead spinRotator==2, we apply a uniform field along the x-axis which causes precession in the y-z plane as desired. However, as shown in the theoretical background this will cause atoms of different speeds to precess by different total amounts. The average precession angle is given by:

$$\langle \phi \rangle = \frac{\gamma B \ell}{\langle v \rangle},$$

as confirmed in the theoretical background. Thus, it is possible to choose a field strength that gives an average precession angle equal to the scattering angle. Whilst there will be a spread in the precession angle, for different atoms, this is rather small and becomes negligible when the intensity of a particular spin component is measured in a spin-echo experiment.

```
202
     elseif spinRotator == 2
203
         % for a (fast-transitioning) uniform SR field with variance
             in rotation for diff speeds...
204
205
         % CREATE SR FIELD:
206
         % intialise set of vectors for B-field at each point along
             the length
         Bsr = zeros([3 nP length(Zsr)]);
207
208
209
         % for each point along the length...
210
         Bsr(1,:,:) = ones([1 nP, length(Zsr)]);
211
         % gyromagnetic ratio for helium 3
212
213
         gamma=2.0378e8; %rad/sec;
214
         % scale B-field for phi=sctAngle/Nsr -> <phi>=l*gamma*B/<v>
215
216
         Bsr = sctAngle*V0/(rotBLen*gamma) .* Bsr;
217
218
         % PRECESS SPIN THROUGH FIELD
219
         Sfsr = precess(Spins(:,:,end,:), Zsr, V, Bsr);
220
221
         % update stored spins
222
         Spins = cat(3, Spins, Sfsr);
```

Finally, if spinPrecession takes any other value then no SR field is applied at all:

```
223
     else
224
         % for no SR field at all...
225
226
         % update stored spins
         Spins = cat(3, Spins, repmat(Spins(:,:,end,:), [1 1 Nsr 1]))
227
228
     end
229
230
     % update stored distances
231
     Disps = cat(1, Disps, Zsr);
232
233
234
```

It is now necessary to resolve the spins of atoms into a new rotated basis since the direction of travel changes on scatter at the surface. This can be trivially achieved with a rotation matrix. (unfortunately, the the lack of support for higher-dimensional matrix products in Matlab demands the use of a cumbersome for-loop):

```
235
236
     % resolve Sf into new direction ready for second solenoid
237
238
239
    % rotation matrix between two bases
     RotM = [1 0 0; 0 cos(sctAngle) sin(sctAngle); 0 -sin(sctAngle)
240
         cos(sctAngle)];
241
     % rotate frame for final spins
242
243
     Sfrot = zeros(size(Spins(:,:,end,:)));
     for iP = 1:nP
244
245
         Sfrot(:,iP,:) = RotM * squeeze(Spins(:,iP,end,:));
246
247
     % continue propagating up to next solenoid
248
     Disps = cat(1, Disps, linspace(Disps(end)+dZ, Disps(end)+
249
         rotBDist, numStepsTorotB)');
250
     Spins = cat(3, Spins, repmat(Spins(:,:,end,:), [1 1
         numStepsTorotB 1]));
251
252
253
```

Having rotated into the new basis, we can simply apply the precession code for the second solenoid. Note that the magnetic field is in the opposite direction!

For measurement, since the polarising filters are aligned with respect to the initial direction of travel, we must rotate the pecessed

spins back to the original basis with an inveres rotation matrix:

```
263
264
    % resolve Sf2 back
265
266
267
    % rotate frame back to original basis
268
    Sf2 = zeros(size(Sf2rot));
     for iP=1:nP
269
270
         for iV=1:nV
271
             Sf2(:,iP,:,iV) = RotM \ squeeze(Sf2rot(:,iP,:,iV));
272
         end
273
     end
274
275
     % update stored spins/distances
     Spins = cat(3, Spins, Sf2);
276
277
     Disps = cat(1,Disps,Disps(end)+dZ+Z);
279
    % propagate short distance after solenoid
280 Spins = cat(3, Spins, repmat(Spins(:,:,end,:), [1 1 5 1]));
281 Disps = cat(1, Disps, [Disps(end)+0.002:0.002:Disps(end)+0.01]')
282
283
284
```

It may then be desirable to plot curves of spin components against distance through the apparatus for different speeds/trajectories. An example is given below for plots of curves for different speeds, all along the central axis:

```
1
   % plot graphs of spin for diff speeds on central axis
 2
 3
 4
 5
    figure();
 6
    % lateral point we wish to plot components for (central axis)
 7
    iP = 1;
 8
10
   % plot x-component of spin against distance through solenoid
11
    subplot(3,1,1);
    plot(Disps, squeeze(Spins(1,iP,:,:)));
12
   title('$x$ component'); xlim([Disps(1) Disps(end)]); ylim([-Smag
         Smag]);
14
  % plot y-component of spin against distance through solenoid
15
    subplot(3,1,2);
    plot(Disps, squeeze(Spins(2,iP,:,:)));
17
    title('$y$ component'); xlim([Disps(1) Disps(end)]); ylim([-Smag
         Smag]);
19
   % plot z-component of spin against distance through solenoid
20
    subplot(3,1,3);
    plot(Disps, squeeze(Spins(3,iP,:,:)));
22
   title('$z$ component'); xlim([Disps(1) Disps(end)]); ylim([-Smag
23
         Smag]);
24
25
26
```