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% Magnetization transfer test from a third spin to a pair of coupled spins
%
% Florin, 26.01.2022
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
clear all

%spin system
sys.magnet=9.4; %400.228 MHz
sys.isotopes={'1H','1H','1H'};
gamma_H=spin('1H')/(2*pi);

%Zeeman interactions
inter.zeeman.scalar={-0.025 0.025 1}; % delta_niu = 100 Hz
inter.coupling.scalar{1,2}=17.9;
inter.coupling.scalar{3,3}=0;
inter.coordinates={[0 0 0] [0 0 1.74] [0 1.5 0.87]};

%Basis formalism
bas.formalism='sphten-liouv';
bas.approximation='none';

% Relaxation theory
inter.relaxation={'redfield'};
inter.equilibrium='zero';
inter.rlx_keep='labframe';
inter.tau_c={100e-12};

% Spinach housekeeping
spin_system=create(sys,inter);
spin_system=basis(spin_system,bas);

% Generate operators
H=hamiltonian(assume(spin_system,'nmr'),'comm');
R=relaxation(spin_system);
L=H+1i*R;

%Build the initial state
Kx=(state(spin_system,{'L+'},{3},'exact')+...
    state(spin_system,{'L-'},{3},'exact'))/2;

% Control operators
Lz=operator(spin_system,'Lz','1H');
Lx=(operator(spin_system,'L+','1H')+operator(spin_system,'L-','1H'))/2;
Ly=(operator(spin_system,'L+','1H')-operator(spin_system,'L-','1H'))/2i;

%Evolution under Liouvillian
traj_ev=evolution(spin_system,L+2*pi*2000*Lx,[],Kx,0.01,100,'trajectory');

figure(1);
trajan(spin_system,traj_ev,'correlation_order');

figure(2);
trajan(spin_system,traj_ev,'coherence_order');
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