

### 1. Tensorprodukt

a) Betrachte den folgenden Hamiltonoperator zweier Spin-1/2 im Magnetfeld:

$$H = J\hat{s}_1 \cdot \hat{s}_2 + B(\hat{s}_1^z + \hat{s}_2^z) \quad (1)$$

Dabei ist  $\hat{s} = \frac{1}{2}\vec{\sigma} = \frac{1}{2}(\sigma_x, \sigma_y, \sigma_z)$ , und

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 0 & 1 \\ 0 & -1 \end{pmatrix} \quad (2)$$

sind die Paulimatrizen. Ferner seien  $J > 0$  und  $B \geq 0$ . Schreibe den Hamiltonoperator als Matrix zur Eigenbasis von  $\hat{s}_1^z$  und  $\hat{s}_2^z$   $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$  und bestimme dessen Eigenwerte und -vektoren. Gib den Grundzustand abhängig von  $J$  und  $B$  an.

b) Nimm an, der Gesamtspin  $\hat{S} = \hat{s}_1 + \hat{s}_2$  erfülle die Drehimpulsalgebra (was auch tatsächlich der Fall ist) und es sei  $\hat{S}^\pm = \hat{S}_x \pm i\hat{S}_y$ . Zeige, dass dann  $\hat{S}^2 = \hat{S}_z^2 - \hbar\hat{S}_z + \hat{S}^+\hat{S}^-$  ist.

c) Zeige unter derselben Annahme, dass  $\hat{S}^2 = (\hat{s}_1 + \hat{s}_2)^2$  mit  $H$  und  $\hat{S}_z = \hat{s}_1^z + \hat{s}_2^z$  kommutiert und berechne die normierten Eigenfunktionen  $|S, S_z\rangle$  von  $\hat{S}^2$  und  $\hat{S}_z$  in der Basis  $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$ . Vergleiche mit dem Ergebnis aus a) und begründe.

(Hinweis: Drücke  $\hat{s}_1 \cdot \hat{s}_2$  durch  $\hat{S}^2$  aus.

2. For this exercise and the next one, consider the case of a non-uniform magnetic field. Here, each spin feels a slightly different value of  $B_0$  and thus precesses at a slightly different frequency. In this case, it will be useful for us to consider the net magnetization as the sum of the individual magnetic moments of each proton.

$$\vec{M} = \sum_{i=1}^N \vec{\mu}_i,$$

where each magnetic moment  $\vec{\mu}_i$  is a classical vector of constant magnitude  $e\hbar/2Mc$ , obeying the precession equation

$$\dot{\vec{\mu}}_i = \gamma\vec{\mu}_i \times \vec{B}_i.$$

(Recall that we can do this because of the result of Shankar's Exercise 14.4.1.) Now model the magnetic field at each proton as

$$\vec{B}_i = (B_0 + b_i)\hat{\mathbf{k}},$$

where  $B_0$  is the average field value, and the individual variations  $b_i$  have a mean of zero. In the rotating reference frame, the precession equations then become

$$\dot{\vec{\mu}}_i = \gamma \vec{\mu}_i \times (b_i \hat{\mathbf{k}}_r).$$

Let us consider, as in the last exercise, a system in thermal equilibrium for times  $t < 0$ , with  $\vec{M} = M_0 \hat{\mathbf{k}}$ . This time, however, let's apply a  $90^\circ$  pulse at  $t = 0$ , instead of a  $180^\circ$  pulse, with rotation being about  $\hat{i}_r$  in the rotating reference frame. Just after the  $90^\circ$  pulse, then, the magnetic moment of each proton becomes, in this rotating frame,

$$\vec{\mu}_i(0) = \frac{e\hbar}{2Mc} \hat{j}_r,$$

and hence the magnetization is  $\vec{M}(0) = M_0 \hat{j}_r$ .

Solve the precession equations for the individual moments  $\vec{\mu}_i$  in the rotating frame for times  $t \ll T_1$ , then evaluate the sum to get the net magnetization  $\vec{M}(t)$ . Show that this net magnetization decays due to dephasing with a characteristic timescale

$$\frac{1}{T_2^*} = \gamma \sqrt{\langle b_i^2 \rangle}.$$

*Hint:* What you will get here is a sum of phases, of the form

$$\sum_{n=1}^N e^{i\phi_n}$$

To evaluate this sum, expand each phase as a series, then sum each order in  $\phi$  separately.

$$\begin{aligned} \sum_{n=1}^N e^{i\phi_n} &= \sum_{n=1}^N \left\{ 1 + i\phi_n + \frac{1}{2}(i\phi_n)^2 + \dots \right\} \\ &= N + \sum_{n=1}^N i\phi_n + \frac{1}{2} \sum_{n=1}^N (i\phi_n)^2 + \dots \end{aligned}$$

The series you wind up with will have an (approximate) exponential representation, with a characteristic decay time equal to  $T_2^*$ .

- Now apply a  $180^\circ$  pulse at a much later time  $t = \tau$  when the initial free-induction-decay signal has long since died away, *i.e.*  $\tau > T_2$ . Show that the magnetization will return to its full initial value at time  $t = 2\tau$ , then decay again with the same time constant  $T_2^*$ . This phenomenon is known as *spin echo*.

*Hint:* Replace the x-y plane in the rotating frame with the real and imaginary axes of the complex plane, write the vector  $\vec{\mu}_i$  as a complex number, and express the precession equation in this complex notation. Remember that the  $180^\circ$  pulse essentially rotates all of the spins around the x-axis, in the rotating reference frame, and this will be particularly easy to represent if the complex plane is used to represent the x-y plane. This is the starting point for a lot of NMR dephasing analysis and is widely used in the NMR literature.

If there are several, uncorrelated mechanisms that cause the variation in  $\vec{B}_i$ , then the dephasing rates for each just add to give a total dephasing rate  $T_2^*$ .

$$\frac{1}{T_2^*} = \frac{1}{T_2^A} + \frac{1}{T_2^B} + \dots$$

Some examples of sources of nonuniformity are

- Inhomogeneities in the field of the permanent magnet used to supply the field  $\vec{B}$ , and
- Interactions between individual spins.

If you were doing research, you would probably want to look at the interactions between the spins and be uninterested in the inhomogeneities of the magnet. Because the inhomogeneities in the magnet do not change with time, any dephasing they cause can be recovered using this spin-echo technique. The spin-spin interactions, however, change over time, and the dephasing they cause cannot be recovered by spin-echo.

We may expect the net magnetization, then, to decay immediately following the initial  $90^\circ$  pulse as

$$M(t) \sim M(0)e^{-(t/T_2^*)^2}.$$

This initial decay is known as the *free-induction decay*, or FID. Spin-spin interactions, and other effects, should keep the spin echo signal from returning to its full initial height  $M(0)$ , and the height of the spin echo should decay as well, with a time constant of  $T_2 \gg T_2^*$ .

This provides us with a way of separating the irreversible dephasing time  $T_2$  from the total dephasing time  $T_2^*$ . Because  $T_2$  is intrinsic to the sample and  $T_2^*$  depends on your apparatus, it is usually  $T_2$  that you are interested in.