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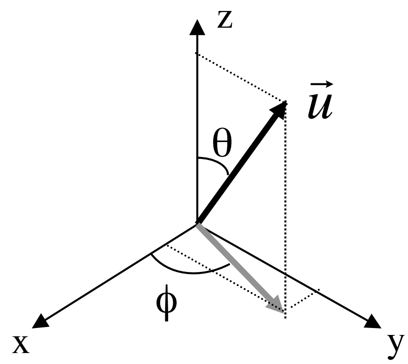
Problem Set #4

Rad 226



1. Pure versus mixed states

Consider the kets corresponding to the following four collections of spin-1/2 nuclei.

$$|s_1\rangle = \tfrac{1}{\sqrt{2}}\left(|+\rangle + |-\rangle\right)$$

$$|s_2\rangle = \begin{cases} |+\rangle \text{ with probability 0.5} \\ |-\rangle \text{ with probability 0.5} \end{cases}$$

$$|s_3\rangle = \tfrac{1}{\sqrt{3}}\left(|s_x\rangle + |s_y\rangle\right)$$

$$|s_4\rangle = \begin{cases} |s_x\rangle \text{ with probability 0.5} \\ |s_y\rangle \text{ with probability 0.5} \end{cases}$$

where $|+\rangle$ and $|-\rangle$ are spin states oriented along the $+z$ and $-z$ directions, and $|s_x\rangle$ and $|s_y\rangle$ are spin states oriented along the $+x$ and $+y$ directions,

a. For each of the four systems, calculate the corresponding density matrix $\underline{\sigma}$ in the $\{|+\rangle, |-\rangle\}$ basis. Which systems are in a pure versus mixed state?

b. For each of the four systems, calculate $\mathrm{Tr}\{\underline{\sigma}^2\}$. If $\mathrm{Tr}\{\underline{\sigma}^2\}$ is considered as a measure of the information content of the system, what do these results say about pure versus mixed state system.

c. For each of the four systems compute $\overline{\langle \hat{M}_x \rangle}$, $\overline{\langle \hat{M}_y \rangle}$, and $\overline{\langle \hat{M}_z \rangle}$.

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2. Transition Operators

Using the $\{|+\rangle,|-\rangle\}$ basis, the transition operators for a spin-1/2 system are defined as:

$$\hat{T}_{++} = |+\rangle\langle+|$$
$$\hat{T}_{+-} = |+\rangle\langle-|$$
$$\hat{T}_{-+} = |-\rangle\langle+|$$
$$\hat{T}_{--} = |-\rangle\langle-|$$

Find the relationship between the Liouville basis sets $\left\{\hat{T}_{++},\hat{T}_{+-},\hat{T}_{-+},\hat{T}_{--}\right\}$ and $\left\{\hat{I}^2,\hat{I}_x,\hat{I}_y,\hat{I}_z\right\}$.

Note: $\hat{I}^2 = \hat{I}_x\hat{I}_x + \hat{I}_y\hat{I}_y + \hat{I}_z\hat{I}_z$.

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3. The Spin Lattice Disconnect

In general, the complete Hamiltonian for a nuclear spin system is

$$\hat{H} = \hat{H}_l + \hat{H}_s + \hat{H}_i$$

- $\hat{H}_l$: Terms only involving the lattice (mass, velocity, etc.)
- $\hat{H}_s$: Terms only involving spin (e.g. magnetic moment)
- $\hat{H}_i$: Interaction terms coupling spin and lattice variables.

If we assume that the interaction term is small, i.e. spin variables have no effect on lattice variables and vice versa, then

$$\hat{H} \approx \hat{H}_l + \hat{H}_s.$$

Given $\hat{\rho}_l$ and $\hat{\sigma}$ are the density operators for lattice and spin systems respectively, find an equation for the density operator of the full system.

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4. **Polarization and the Boltzmann Distribution.**

Fill in the missing entries in the Table below that lists the thermal equilibrium polarization (%) obtained by systems of ^{1}H nuclei, ^{13}C nuclei, and unpaired electrons e^- placed in a 3T magnetic field under a variety of different temperatures.

Temperature	^{1}H	^{13}C	e^-
$310K$	?	?	?
$4K$	?	?	?
$1K$	?	?	?
$?K$	25%	?	?

What conclusions can you draw regarding the feasibility of using low temperatures as a means to increase the SNR for in vivo studies?