Dynamical structure factor for two spins

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1 Definition

We have two classical spins ($\mathbf{s}_1, \mathbf{s}_2 \in \mathbb{R}^3$, $|s_i|^2 = 1$), spaced out by a distance L. The semiclassical time evolution is given by:

$$\begin{cases} \frac{\mathrm{d}\mathbf{s}_1}{\mathrm{d}t} & = -J\mathbf{s}_1 \times \mathbf{s}_2 \\ \frac{\mathrm{d}\mathbf{s}_2}{\mathrm{d}t} & = -J\mathbf{s}_2 \times \mathbf{s}_1 \end{cases} \tag{1}$$

The goal is to compute the **dynamical structure factor**, that is:

$$S(Q,t) = \langle s_{\text{-Q}}(0) \cdot s_{\text{Q}}(t) \rangle \tag{2}$$

, defining $\mathbf{s}_Q(t) = \mathbf{s}_1(t) + \mathbf{s}_2(t)e^{-iQL}$.

2 Solution for the equations of motion

We can see that the magnetization $\mathbf{M} := \mathbf{s}_1 + \mathbf{s}_2$ is conserved. Thus, replacing $\mathbf{s}_2 = \mathbf{M} - \mathbf{s}_1$ in the first equation, we get:

$$\frac{\mathrm{d}\mathbf{s}_1}{\mathrm{d}t} = -J\mathbf{s}_1 \times (\mathbf{M} - \mathbf{s}_1) = -J\mathbf{s}_1 \times \mathbf{M} \tag{3}$$

This can be solved, projecting $\mathbf{s}_1$ onto $\mathbf{M}$:

$$\mathbf{s}_1 = (\mathbf{s}_1 \cdot \hat{\mathbf{M}})\hat{\mathbf{M}} + \Big(\mathbf{s}_1 - (\mathbf{s}_1 \cdot \hat{\mathbf{M}})\hat{\mathbf{M}}\Big) := \mathbf{s}_\parallel + \mathbf{s}_\perp \tag{4}$$

yielding the following equations:

$$\begin{cases} \frac{\mathrm{d}\mathbf{s}_\parallel}{\mathrm{d}t} & = \mathbf{0} \\ \frac{\mathrm{d}\mathbf{s}_\perp}{\mathrm{d}t} & = -J\mathbf{s}_\perp \times \mathbf{M} \end{cases} \tag{5}$$

which can be solved exactly, with $\omega := J|M|$, and $\hat{\mathbf{M}} = \mathbf{M}/|M|$:

$$\begin{cases} \mathbf{s}_\parallel(t) & = \mathbf{s}_\parallel(0) \\ \mathbf{s}_\perp(t) & = \cos(\omega t)\mathbf{s}_\perp(0) + \sin(\omega t)\hat{\mathbf{M}} \times \mathbf{s}_\perp(0) \end{cases} \tag{6}$$

3 Computing the dynamical structure factor

For readability, (0) is dropped.

$$\begin{aligned} S(Q,t) &= \langle \mathbf{s}_{-Q} \cdot \mathbf{s}_Q(t) \rangle \\ &= \langle \mathbf{s}_1 \cdot \mathbf{s}_1(t) \rangle + \langle \mathbf{s}_2 \cdot \mathbf{s}_2(t) \rangle + \langle \mathbf{s}_2 \cdot \mathbf{s}_1(t) \rangle e^{iQL} + \langle \mathbf{s}_2 \cdot \mathbf{s}_1(t) \rangle e^{-iQL} \\ &= 2\left(\langle \mathbf{s}_1 \cdot \mathbf{s}_1(t) \rangle + \cos(QL)\langle \mathbf{s}_2 \cdot \mathbf{s}_1(t) \rangle\right) \end{aligned} \tag{7}$$

The last line is obtained as the system is left unchanged under the inversion $\mathbf{s}_1 \leftrightarrow \mathbf{s}_2$.

Both terms can be evaluated separately:

$$\begin{aligned}
\langle \mathbf{s}_1 \cdot \mathbf{s}_1(t) \rangle &= \langle (\mathbf{s}_\parallel + \mathbf{s}_\perp) \cdot (\mathbf{s}_\parallel + \mathbf{s}_\perp \cos(\omega t) + \hat{\mathbf{M}} \times \mathbf{s}_\perp \sin(\omega t)) \rangle \\
&= \langle \mathbf{s}_\parallel^2 + \mathbf{s}_\perp^2 \cos(\omega t) \rangle \\
\langle \mathbf{s}_2 \cdot \mathbf{s}_1(t) \rangle &= \langle \mathbf{M} \cdot \mathbf{s}_1(t) \rangle - \langle \mathbf{s}_1 \cdot \mathbf{s}_1(t) \rangle \\
&= \langle \mathbf{M} \cdot \mathbf{s}_\parallel \rangle - \langle \mathbf{s}_\parallel^2 + \mathbf{s}_\perp^2 \cos(\omega t) \rangle
\end{aligned} \tag{8}$$

Average integrals

Without loss of generality, one can assume that $\mathbf{s}_1 = \hat{\mathbf{z}}$. We can use a spherical coordinates parameterization:

$$\langle \dots \rangle = \frac{1}{4\pi} \int_0^\pi \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi \dots \tag{9}$$

In these coordinates, $\mathbf{s}_2$ and $\mathbf{M}$ are written as:

$$\mathbf{s}_2 = \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix}, \ \mathbf{M} = \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ 1+\cos\theta \end{pmatrix} \tag{10}$$

One can see that

$$\langle M^2 \rangle = \langle (1+\cos\theta)^2 + \sin\theta^2 \rangle = 2\langle 1+\cos\theta \rangle = 2 \tag{11}$$

Thus:

$$\begin{aligned}
\langle \mathbf{M} \cdot \mathbf{s}_\parallel \rangle &= \langle \frac{(\hat{\mathbf{z}} \cdot \mathbf{M})}{M^2} \mathbf{M} \cdot \mathbf{M} \rangle \\
&= \langle \frac{1+\cos\theta}{M^2} M^2 \rangle \\
&= \langle 1+\cos\theta \rangle \\
&= 1
\end{aligned} \tag{12}$$

$$\begin{aligned}
\langle \mathbf{s}_\parallel \cdot \mathbf{s}_\parallel \rangle &= \langle \frac{(\hat{\mathbf{z}} \cdot \mathbf{M})}{M^2} \mathbf{M} \cdot \frac{(\hat{\mathbf{z}} \cdot \mathbf{M})}{M^2} \mathbf{M} \rangle \\
&= \langle \frac{(1+\cos\theta)^2}{M^4} M^2 \rangle \\
&= \langle \frac{(1+\cos\theta)^2}{2(1+\cos\theta)} \rangle \\
&= \frac{1}{2} \langle 1+\cos\theta \rangle = \frac{1}{2}
\end{aligned} \tag{13}$$

$$\begin{aligned}
\langle \mathbf{s}_\perp \cdot \mathbf{s}_\perp \rangle &= \langle \mathbf{s}_1 \cdot \mathbf{s}_1 \rangle - \langle \mathbf{s}_\parallel \cdot \mathbf{s}_\parallel \rangle \\
&= 1 - \frac{1}{2} = \frac{1}{2}
\end{aligned} \tag{14}$$

Putting everything together

$$\begin{aligned}
\langle \mathbf{s}_1 \cdot \mathbf{s}_1(t) \rangle &= \langle \mathbf{s}_\parallel^2 + \mathbf{s}_\perp^2 \cos(\omega t) \rangle \\
&= \frac{1}{2} \left(1 + \cos(\omega t)\ \right) \\
\langle \mathbf{s}_2 \cdot \mathbf{s}_1(t) \rangle &= \langle \mathbf{M} \cdot \mathbf{s}_\parallel \rangle - \langle \mathbf{s}_\parallel^2 + \mathbf{s}_\perp^2 \cos(\omega t) \rangle \\
&= 1 - \frac{1}{2} \left(1 + \cos(\omega t)\right) \\
&= \frac{1}{2} \left(1 - \cos(\omega t)\right)
\end{aligned} \tag{15}$$

Thus the dynamical structure factor is given by:

$$S(Q,t) = (1+\cos\omega t) + \cos qL(1-\cos\omega t) \tag{16}$$

4 Actually...

This derivation is wrong, for two different reasons:

- it holds for an uniform distribution, yet the system should obey the Boltzmann distribution
- it assumes the frequency ω is independent of the state, yet it depends on M, so should be averaged accordingly.

The first problem can be mitigated by simply checking the code without any Monte Carlo step, hence sampling from the uniform distribution.

For the second problem, it is more subtle: the answer we get is clearly wrong. The variation of the frequency induces a phase shift that gets bigger as time goes: it decays. With some handwavy calculation it seems gaussian.

5 Structure factor for multiple unit cells

Assuming multiple unit cells, yet with no coupling between these:

$$\mathbf{s}_{\mathbf{q}}(t) = \sum_{\mathbf{R}} e^{-i\mathbf{q}\cdot\mathbf{R}} \left(s_{1\mathbf{R}}(t) + e^{-i\mathbf{q}\cdot\mathbf{r}_2} s_{2\mathbf{R}}(t)\right)$$

$$\begin{aligned}
S(\mathbf{q},t) &= \sum_{\mathbf{R},\mathbf{R}'} e^{i\mathbf{q}\cdot(\mathbf{R}-\mathbf{R}')} \langle(\mathbf{s}_{1\mathbf{R}}\cdot\mathbf{s}_{1\mathbf{R}}(t) + \mathbf{s}_{2\mathbf{R}}\cdot\mathbf{s}_{2\mathbf{R}}(t) + e^{i\mathbf{q}\cdot\mathbf{r}_2}\mathbf{s}_{2\mathbf{R}}\cdot\mathbf{s}_{1\mathbf{R}}(t) + e^{-i\mathbf{q}\cdot\mathbf{r}_2}\mathbf{s}_{1\mathbf{R}}\cdot\mathbf{s}_{2\mathbf{R}}(t))\rangle \\
&= 2N\langle\mathbf{s}_1\cdot\mathbf{s}_1(t)\rangle + 2N\cos(\mathbf{q}\cdot\mathbf{r}_2)\langle\mathbf{s}_2\cdot\mathbf{s}_1(t)\rangle \\
&= 2N\left(\frac{1}{2} + \langle s_\perp^2\cos\omega t\rangle + \cos(\mathbf{q}\mathbf{r}_2)\left(\frac{1}{2} - \langle s_\perp^2\cos\omega t\rangle\right)\right) \\
&= 2N\left(\frac{1}{2}\left(1+\cos(\mathbf{q}\mathbf{r}_2)\right) + \langle s_\perp^2\cos\omega t\rangle\left(1-\cos(\mathbf{q}\mathbf{r}_2)\right)\right)
\end{aligned} \tag{17}$$

as $\langle\mathbf{s}_{i\mathbf{R}}\cdot\mathbf{s}_{j\mathbf{R}'}\rangle = \delta_{\mathbf{R}\mathbf{R}'}\langle s_i\cdot s_j(t)\rangle$.

I don't think that $\langle s_\perp^2\cos(\omega t)\rangle$ can be computed analytically. However, we know that:

- for $t=0$, this is equal to $\langle s_\perp^2\rangle = \frac{1}{2}$
- for $t\to\infty$, this should vanish (because all the cosines go with a random phase shift, hence averaging to zero I think ?)

Thus:

$$\frac{S(\mathbf{q},t\to\infty)}{S(\mathbf{q},t=0)} = \frac{1}{2}\left(1+\cos(\mathbf{q}\cdot\mathbf{r}_2)\right) \tag{18}$$