Neutron and X-ray Scattering
of
Quantum Materials

PHYS-640

Week 7 exercises

1: The energy resolution in a backscattering experiment

The uncertainty on the final energy of the detected neutron is governed by many factors but one large factor is the scattering angle itself. Here we have a closer look at why that is.

(a) Use Bragg's law, $n\lambda_f = 2d_{\text{ana}} \sin\theta_f$, and propagation of errors to find an expression for the relative uncertainty $\frac{\delta\lambda_f}{\lambda_f}$. Here λ_f is the final wavelength of the neutron, d_{ana} is the lattice spacing of the monochromator and $2\theta_f$ is the scattering angle of the neutrons arriving at the detector.

(b) At which scattering angle is $\frac{\delta\lambda_f}{\lambda_f}$ at a minimum and what does that mean for the detector position if you wish a very high energy resolution?

2: The Heisenberg ferromagnetic chain

Consider a Heisenberg ferromagnetic chain with the following spin Hamiltonian:

$$\hat{\mathcal{H}} = \sum_i J\, \mathbf{S}_i \cdot \mathbf{S}_{i+1},$$

where the sum is only over the nearest neighbors distanced a from each other, see Fig. 1(a), and we assume that all spin pairs interact with the same exchange coupling, J.

(a) Use the operators $S^+ = S^x + iS^y$ and $S^- = S^x - iS^y$ to arrive at the following form for the Hamiltonian:

$$\hat{\mathcal{H}} = \sum_i J \left[S_i^z S_{i+1}^z + \frac{1}{2}\left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+\right)\right]$$

(b) The operators S_j^+ and S_j^- have the effect of respectively raising and lowering the spin value at a site j. S_j^z works a bit like a number operator and measures the spin value on site j. Argue that the state with all spins at their maximum value, S, is an eigenstate of the Hamiltonian and determine the eigenvalue.

(c) Let us now consider a state with all spins at their maximum except the one at j which is now lowered to $S-1$, meaning $|j\rangle = |S, S-1, S, ..., S\rangle$. The operators S_j^+ and S_j^- do the following to the state $|j\rangle$:

$$S^+ |j\rangle = \sqrt{2S}\, |j+1\rangle\,, \qquad S^- |j\rangle = \sqrt{2S}\, |j-1\rangle$$

Is $|j\rangle$ an eigenstate of $\hat{\mathcal{H}}$?

(d) Hopefully you found that a spin lowered on a single site is not an eigenstate of $\hat{\mathcal{H}}$. Instead we try the Fourier transform of $|j\rangle$:

$$|q\rangle = \frac{1}{\sqrt{N}} \sum_j e^{i\mathbf{q}\cdot\mathbf{r}_j}\, |j\rangle\,.$$

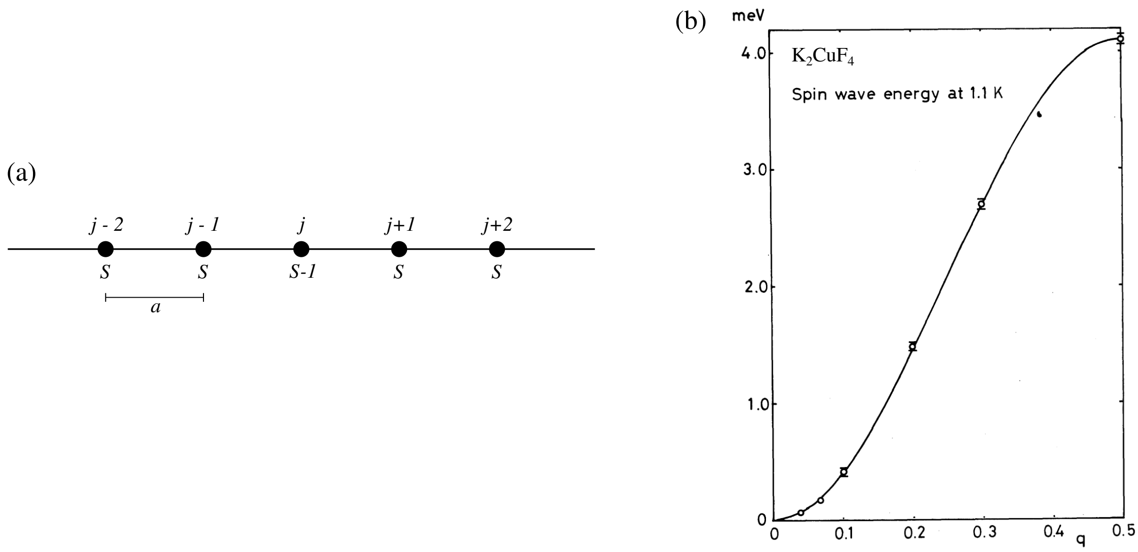

Figure 1: (a) The ferromagnetic chain with spins separated by the distance a and interacting with exhange coupling J. (b) Spinwave spectrum of K_2CuF_4 measured by K. Hirakawa *et al.*, *J. Phys. Soc. Jpn.* **52**, 4220-4230 (1983).

We can also view this as a smearing of the lowered spin over all lattice sites. Evaluate $\hat{\mathcal{H}}\,|q\rangle$ and show that this is indeed an eigenstate of the Hamiltonian with eigenvalue $E = JNS^2 + 2JS\,[\cos(qa) - 1]$.

(e) Plot the spinwave spectrum for a ferromagnetic chain with $S = 2$ and $J = 5$ meV.

(f) The spinwave spectrum of the ferromagnetic chain compound, K_2CuF_4, is shown in Fig. 1(b). What is the value of J in this case?

3: Lattice vibrations in one dimension

Exercise 14.P.1 in the neutron notes.

4: The direct-geometry time-of-flight spectrometer

An inelastic neutron scattering experiment is performed with a $CeCu_6$ single crystal on a time-of-flight spectrometer with direct geometry. The space group of $CeCu_6$ is *Pnma* (orthorhombic) with lattice parameters $a = 5.03$ Å, $b = 8.06$ Å and $c = 10.09$ Å. Suppose the sample is oriented with $(H, 0, 0)$ and $(0, 0, L)$ in the horizontal scattering plane. The incoming energy of the neutrons is $E_i = 8$ meV and the detectors cover a range of scattering angles of $10° - 100°$ in the forward direction.

Calculate the $\mathbf{q}$ coverage for an energy transfer of $E = 0.3$ meV when the crystal is rotated by $90°$ in steps of $1°$.