(1) **Ferrimagnetism** – A ferrimagnet is a magnetic structure in which there are different types of spins present. Consider a sodium chloride structure in which the A sublattice spins have magnitude $S_A$ and the B sublattice spins have magnitude $S_B$ with $S_B < S_A$ (e.g., $S = 1$ for the A sublattice but $S = \frac{1}{2}$ for the B sublattice). The Hamiltonian is

$$\mathcal{H} = J \sum_{\langle ij \rangle} S_i \cdot S_j + g_A \mu_0 H \sum_{i \in A} S_i^z + g_B \mu_0 H \sum_{j \in B} S_j^z$$

where $J > 0$, so the interactions are antiferromagnetic.

(a) Work out the mean field theory for this model. Assume that the spins on the A and B sublattices fluctuate about the mean values

$$\langle S_A \rangle = m_A \hat{z}, \quad \langle S_B \rangle = m_B \hat{z}$$

and derive a set of coupled mean field equations of the form

$$m_A = F_A(\beta g_A \mu_0 H + \beta J z m_B)$$
$$m_B = F_B(\beta g_B \mu_0 H + \beta J z m_A)$$

where $z$ is the lattice coordination number ($z = 6$ for NaCl) and $F_A(x)$ and $F_B(x)$ are related to Brillouin functions. Show graphically that a solution exists, and fund the criterion for broken symmetry solutions to exist when $H = 0$, i.e., find $T_c$. Then linearize, expanding for small $m_A$, $m_B$, and $H$, and solve for $m_A(T)$ and $m_B(T)$ and the susceptibility

$$\chi(T) = -\frac{1}{2} \frac{\partial}{\partial H}(g_A \mu_0 m_A + g_B \mu_0 m_B)$$

in the region $T > T_c$. Does your $T_c$ depend on the sign of $J$? Why or why not?

We apply the mean field Ansatz $\langle S_i \rangle = m_{A,B}$ and obtain the mean field Hamiltonian

$$\mathcal{H}^{MF} = -\frac{1}{2} N J z m_A \cdot m_B + \sum_{i \in A} (g_A \mu_0 H + zJ m_B) \cdot S_i + \sum_{j \in B} (g_B \mu_0 H + zJ m_A) \cdot S_j.$$ 

Assuming the sublattice magnetizations are collinear, this leads to two coupled mean field equations:

$$m_A(x) = F_{S_A}(\beta g_A \mu_0 H + \beta J z m_B)$$
$$m_B(x) = F_{S_B}(\beta g_B \mu_0 H + \beta J z m_A),$$

where

$$F_S(x) = -S B_S(Sx),$$

and $B_S(x)$ is the Brillouin function,

$$B_S(x) = \left(1 + \frac{1}{2S}\right) \text{ctnh} \left(1 + \frac{1}{2S}\right) x - \frac{1}{2S} \text{ctnh} \frac{x}{2S}.$$
The mean field equations may be solved graphically, as depicted in fig. 1.

Expanding $F_S(x) = -\frac{1}{3}S(S + 1)x + O(x^3)$ for small $x$, and defining the temperatures $k_B T_{A,B} = \frac{1}{2}S_{A,B}(S_{A,B} + 1) zJ$, we obtain the linear equations,

$$m_A - \frac{T_A}{T} m_B = -\frac{g_A \mu_0}{zJ} H$$
$$m_B - \frac{T_B}{T} m_A = -\frac{g_B \mu_0}{zJ} H,$$

with solution

$$m_A = \frac{g_A T_A - g_B T_A T_B \mu_0 H}{T^2 - T_A T_B \frac{zJ}{zJ}}$$
$$m_B = \frac{g_B T_B T - g_A T_A T_B \mu_0 H}{T^2 - T_A T_B \frac{zJ}{zJ}}.$$
The susceptibility is
\[
\chi = \frac{1}{N} \frac{\partial M}{\partial H} = \frac{1}{2} \frac{\partial}{\partial H} (g_A \mu_0 m_A + g_B \mu_0 m_B)
\]
\[
= \frac{1}{T^2 - \frac{2 g_A g_B T}{T_A T_B}} \frac{\mu_0^2}{2 z J},
\]
which diverges at
\[
T_c = \sqrt{T_A T_B} = \sqrt{S_A S_B (S_A + 1)(S_B + 1)} \frac{2 |J|}{3 k_B}.
\]
Note that \( T_c \) does not depend on the sign of \( J \). Note also that the signs of \( m_A \) and \( m_B \) may vary. For example, let \( g_A = g_B \equiv g \) and suppose \( S_A > S_B \). Then \( T_B < \sqrt{T_A T_B} < T_A \) and while \( m_A < 0 \) for all \( T > T_c \), the B sublattice moment changes sign from negative to positive at a temperature \( T_B > T_c \). Finally, note that at high temperatures the susceptibility follows a Curie \( \chi \propto T^{-1} \) behavior.

(b) Work out the spin wave theory and compute the spin wave dispersion. (You should treat the NaCl structure as an FCC lattice with a two element basis.) Assume a classical ground state \( \langle N \rangle \) in which the spins are up on the A sublattice and down on the B sublattice, and choose

\[
\begin{align*}
S_A^+ &= a^\dagger (2 S_A^0 - a a^\dagger)^{1/2} \\
S_A^- &= (2 S_A^0 - a a^\dagger)^{1/2} a \\
S_A^z &= a^\dagger a - S_A
\end{align*}
\]

\[
\begin{align*}
S_B^+ &= -(2 S_B^0 - b b^\dagger)^{1/2} b \\
S_B^- &= -(2 S_B^0 - b b^\dagger)^{1/2} b \\
S_B^z &= S_B - b b^\dagger
\end{align*}
\]

How does the spin wave dispersion behave near \( k = 0 \)? Show that the spectrum crosses over from quadratic to linear when \( |k a| \approx |S_A - S_B|/\sqrt{S_A S_B} \).

Now let’s work out the spin wave theory. Consider a bipartite lattice, i.e. one formed from two interpenetrating Bravais lattices. The A sublattice sites are located at \( \{ R \} \) and the B sublattice sites at \( \{ R + \delta \} \). For the NaCl structure, A and B are FCC lattices, and we may take
\[
\begin{align*}
a_1 &= a (\hat{y} + \hat{z}) \quad a_2 &= a (\hat{x} + \hat{z}) \quad a_3 &= a (\hat{x} + \hat{y}) \quad \delta = a \hat{z}
\end{align*}
\]
where \( a \) is the Na-Cl separation. Immediately, we know our spin-wave spectrum will exhibit two excitation branches. We assume the classical ground state is a Néel state where all of the A sublattice spins are pointing down \( (S^z = -S) \) and all the B sublattice spins are pointing up \( (S^z = +S) \). The most general Hamiltonian which is isotropic in spin-space and composed of bilinear operators is
\[
\mathcal{H} = \sum_{R, R'} \left\{ J_{AA} (|R - R'|) S_A(R) \cdot S_A(R') + J_{BB} (|R - R'|) S_B(R) \cdot S_B(R') \right. \\
+ \left. J_{AB} (|R - R' - \delta|) S_A(R) \cdot S_B(R') \right\} + \mu_0 H \sum_{R} \left\{ g_A S_A^z(R) + g_B S_B^z(R) \right\}.
\]
In our case, \( J_{AA} = J_{BB} = 0 \) and \( J_{AB}(\|R - R' - \delta\|) = J \delta_{\|R-R'\|,0} \), but it is instructive to consider the more general case in which all pairs of spins potentially interact. Even more generally, let’s consider the \textit{anisotropic} case, with the field directed along the direction of anisotropy:

\[
\mathcal{H} = \sum_{R, R'} \left\{ J_{AA} \left( \|R - R'\| \right) \left( S^x_A(R) S^x_A(R') + S^y_A(R) S^y_A(R') \right) + \Delta_{AA} S^z_A(R) S^z_A(R') \right\} \\
+ J_{BB} \left( \|R - R'\| \right) \left( S^x_B(R) S^x_B(R') + S^y_B(R) S^y_B(R') \right) + \Delta_{BB} S^z_B(R) S^z_B(R') \\
+ J_{AB} \left( \|R - R'\| \right) \left( S^x_A(R) S^x_B(R') + S^y_A(R) S^y_B(R') \right) + \Delta_{AB} S^z_A(R) S^z_B(R') \right\} \\
+ \mu_0 H \sum_R \left\{ g_A S^z_A(R) + g_B S^z_B(R) \right\} .
\]

Writing \([S_i \cdot S_j]_A \equiv \frac{1}{2} S^+_i S^-_j + \frac{1}{2} S^+_j S^-_i + \Delta S^z_i S^z_j\), and expanding the radicals in the Bogoliubov transformation, we obtain

\[
[S_A(R) \cdot S_A(R')]_{\Delta_{AA}} = \Delta_{AA} S^2_A - \Delta_{AA} S_A \left( a_R^\dagger a_R + a_R^\dagger a_R \right) + S_A \left( a_R^\dagger a_R a_R^\dagger a_R + a_R^\dagger a_R a_R \right) + \ldots \\
[S_B(R) \cdot S_B(R')]_{\Delta_{BB}} = \Delta_{BB} S^2_B - \Delta_{BB} S_B \left( b_R^\dagger b_R + b_R^\dagger b_R \right) + S_B \left( b_R^\dagger b_R b_R^\dagger b_R + b_R^\dagger b_R b_R \right) + \ldots \\
[S_A(R) \cdot S_B(R')]_{\Delta_{AB}} = -\Delta_{AB} S_A S_B + \Delta_{AB} \left( S_B a_R^\dagger a_R + S_A b_R^\dagger b_R \right) \\
- \sqrt{S_A S_B} \left( a_R^\dagger b_R^\dagger + a_R b_R \right) + \ldots .
\]

The spin-wave Hamiltonian is then

\[
\mathcal{H} = S_A \sum_{R, R'} J_{AA} \left( \|R - R'\| \right) \left\{ a_R^\dagger a_R^\dagger a_R + a_R^\dagger a_R^\dagger a_R - \Delta_{AA} a_R^\dagger a_R a_R - \Delta_{AA} a_R^\dagger a_R a_R \right\}
\\
+ S_B \sum_{R, R'} J_{BB} \left( \|R - R'\| \right) \left\{ b_R^\dagger b_R^\dagger b_R + b_R^\dagger b_R^\dagger b_R - \Delta_{BB} b_R^\dagger b_R b_R - \Delta_{BB} b_R^\dagger b_R b_R \right\}
\\
+ \sum_{R, R'} J_{AB} \left( \|R - R' - \delta\| \right) \left\{ - S_A S_B \left( a_R^\dagger b_R^\dagger + a_R b_R \right) \\
+ \Delta_{AB} S_B a_R^\dagger a_R + \Delta_{AB} S_A b_R^\dagger b_R - \Delta_{AB} S_A S_B \right\} .
\]

We now Fourier transform, with

\[
a_R \equiv \frac{1}{\sqrt{N_A}} \sum_k e^{i k \cdot R} a_k \quad , \quad b_R \equiv \frac{1}{\sqrt{N_B}} \sum_k e^{i k \cdot (R + \delta)} a_k \quad ,
\]

and

\[
\mathbf{J}_{AA}(R) = \sum_R J_{AA}(\|R\|) e^{-i k \cdot R} \\
\mathbf{J}_{BB}(R) = \sum_R J_{BB}(\|R\|) e^{-i k \cdot R} \\
\mathbf{J}_{AB}(R) = \sum_R J_{AB}(\|R + \delta\|) e^{-i k \cdot (R + \delta)} .
\]
Here, \(N_A = N_B = \frac{1}{2}N\) is half the total number of lattice sites. This leads to

\[
\mathcal{H} = E_0 + \sum_k \left\{ \omega_A(k) a_k^\dagger a_k + \omega_B(k) b_k^\dagger b_k - \nu(k) a_k^\dagger b_k - \nu^*(k) a_k b_k^\dagger \right\}
\]

with

\[
\omega_A(k) = +g_A\mu_0 H + 2S_A \left( \hat{J}_{AA}(k) - \Delta_{AA} \right) + \Delta_{AB} S_B \hat{J}_{AB}(k)
\]

\[
\omega_B(k) = -g_B\mu_0 H + 2S_B \left( \hat{J}_{BB}(k) - \Delta_{BB} \right)
\]

\[
\nu(k) = \sqrt{S_A S_B} \hat{J}_{AB}(k)
\]

Note that \(\hat{J}_{AA}(k)\) and \(\hat{J}_{BB}(k)\) are both real, but not necessarily \(\hat{J}_{AB}(k)\). All three satisfy \(\hat{J}(-k) = \hat{J}^*(k)\), since they are Fourier transforms of real functions \(J(R)\).\(^1\)

OK, now we do the Bogoliubov thang, and write

\[
a_k = u_k \alpha_k + v_k^* \beta^\dagger_{-k} \quad \quad \quad b_{-k} = u_k \beta_{-k} + v_k^* \alpha^\dagger_k
\]

\[
a_k^\dagger = u_k^* \alpha_k^\dagger + v_k \beta_{-k} \quad \quad \quad b_{-k}^\dagger = u_k^* \beta_{-k}^\dagger + v_k \alpha_k
\]

This preserves the bosonic commutation relations:

\[
[a_k, \alpha_{k'}^\dagger] = [\beta_k, \beta_{k'}^\dagger] = [a_k^\dagger, a_{k'}] = [b_k, b_{k'}^\dagger] = \delta_{kk'}
\]

\[
[a_k, \alpha_{k'}^\dagger] = [\alpha_k, \beta_{k'}^\dagger] = [a_k^\dagger, b_{k'}] = [a_{k'}^\dagger, b_k] = 0
\]

Substituting into \(\mathcal{H}\), we find \(\mathcal{H} = \sum_k \mathcal{H}_k\) with

\[
\mathcal{H}_k = \left\{ \omega_A(k) |u_k|^2 + \omega_B(k) |v_k|^2 - \nu(k) u_k v_k^* - \nu^*(k) u_k^* v_k \right\} \alpha_k^\dagger \alpha_k
\]

\[
+ \left\{ \omega_A(k) |v_k|^2 + \omega_B(k) |u_k|^2 - \nu(k) u_k^* v_k - \nu^*(k) u_k v_k^* \right\} \beta_{-k}^\dagger \beta_{-k}
\]

\[
+ \left\{ (\omega_A(k) + \omega_B(k)) u_k v_k - \nu(k) u_k^2 - \nu^*(k) v_k^2 \right\} \alpha_k \beta_{-k}
\]

\[
+ \left\{ (\omega_A(k) + \omega_B(k)) u_k^* v_k^* - \nu^*(k) u_k^2 - \nu(k) v_k^2 \right\} \alpha_k^\dagger \beta_{-k}^\dagger + \text{const.}
\]

We now write \(\nu(k) \equiv |\nu(k)| e^{i\varphi(k)}\) and use the freedom to choose \(\{u_k, v_k\}\) to eliminate the \(\alpha_k \beta_{-k}\) and \(\alpha_k^\dagger \beta_{-k}^\dagger\) terms in \(\mathcal{H}_k\):

\[
u_k = \cosh \theta_k e^{-i\varphi(k)/2}
\]

\[
v_k = \sinh \theta_k e^{+i\varphi(k)/2}
\]

where

\[
\tanh 2\theta_k = \frac{2 |\nu(k)|}{\omega_A(k) + \omega_B(k)}
\]

\(^1\)For the NaCl structure, \(\hat{J}_{AB}(k)\) as defined is real.
This leads to the dispersions

\[ E_+(k) = +\omega_-(k) + \sqrt{\omega_+^2(k) - \nu^2(k)} \]

\[ E_-(k) = -\omega_-(k) + \sqrt{\omega_+^2(k) - \nu^2(k)} \]

where

\[ \omega_\pm(k) \equiv \frac{1}{2} \left\{ \omega_A(k) \pm \omega_B(k) \right\} \]

and where \( E_+(k) \) is the \( \alpha \)-boson dispersion, and \( E_-(k) \) is the \( \beta \)-boson dispersion:

\[ \mathcal{H} = \sum_k \left\{ E_+(k) \alpha_k \alpha_k^\dagger + E_-(k) \beta_k \beta_k^\dagger \right\} \]

Let’s check our dispersion in some simple cases. For the NaCl structure, we take \( J_{AA}(R) = J_{BB}(R) = 0 \) and \( \delta J_{AB}(R + \delta) = \delta |R + \delta|a \). Then

\[ \delta J_{AB}(k) = 2J \left( \cos k_x a + \cos k_y a + \cos k_z a \right) \]

In order for the spin-wave Hamiltonian to be stable, we must have \( E_{\alpha,\beta}(k) \geq 0 \) for all \( k \) in the Brillouin zone. Otherwise, the ground state energy can be lowered by adding \( \alpha \) or \( \beta \) excitations, and at the level of the spin-wave Hamiltonian there is nothing to prevent us from adding an infinite number of such excitations (i.e. there is no spin-wave repulsion) in order to keep lowering the energy. At the zone center, the energy gap is \( E_g(H = 0) = r \delta J_{AB}(0) \), where

\[ r = \frac{1}{2} \sqrt{(S_A + S_B)^2 - 4S_A S_B} - \frac{1}{2} |S_A - S_B| \Delta_{AB} \]

The gap vanishes when \( r = 0 \), which occurs at the isotropic point \( \Delta_{AB} = 1 \). For \( \Delta_{AB} < 1 \), \( E_g(H = 0) < 0 \) and the spectrum is unstable. Precisely at \( \Delta_{AB} = 1 \), the spectrum is unstable in an infinitesimal field. The system would prefer to enter the spin flop phase, in which the spins lie predominantly in the \( x - y \) plane with some small component parallel to the \( z \)-axis. If we further restrict \( \Delta_{AB} = 1 \), then the spin-wave dispersion for \( H = 0 \) becomes

\[ E_\pm(k) = \pm \frac{1}{2} (S_B - S_A) \delta J_{AB}(0) + \frac{1}{2} \delta J_{AB}(0) \sqrt{(S_A - S_B)^2 + S_A S_B k^2 R^2 + \mathcal{O}(k^4)} \]

where

\[ R^2 = \frac{\sum_R R^2 J_{AB}(R)}{d \sum_R J_{AB}(R)} \]

with \( d \) the dimension of space. For the NaCl structure, \( R_e = a/\sqrt{3} \). If both \( S_A \) and \( S_B \) are large, but their difference is of order unity, then a separation of scales develops. For \( k \ll |S_A - S_B|/\sqrt{S_A S_B} \), the low-lying spin-wave branch disperses quadratically, as in the case of the ferromagnet. For \( |S_A - S_B|/\sqrt{S_A S_B} \ll k \ll \pi/a \), the dispersion is linear, as in the case of the antiferromagnet. At very long wavelengths, then, the ferrimagnet behaves as a ferromagnet, with a net spin \( |S_A - S_B| \) per unit cell. At somewhat longer wavelengths
(but still large compared with the lattice spacing), this quadratic dispersion crosses over to a linear one, typical of an antiferromagnet.

(2) In real solids crystal field effects often lead to anisotropic spin-spin interactions. Consider the anisotropic Heisenberg antiferromagnet in a uniform magnetic field,

$$\mathcal{H} = J \sum_{\langle ij \rangle} (S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z) + h \sum_i S_i^z$$

where the field is parallel to the direction of anisotropy. Assume $\delta \geq 0$ and a bipartite lattice.

(a) Think first about classical spins. In a small external field, show that if the anisotropy $\Delta$ is not too large that the lowest energy configuration has the spins on the two sublattices lying predominantly in the $(x, y)$ plane and antiparallel, with a small parallel component along the direction of the field. This is called a canted, or ‘spin-flop’ structure. What is the angle $\theta_c$ by which the spins cant out of the $(x, y)$ plane? What do I mean by not too large? (You may assume that the lowest energy configuration is a two sublattice structure, rather than something nasty like a four sublattice structure or an incommensurate one.)

We start by assuming a two-sublattice structure in which the spins lie in the $x-z$ plane. (Any two-sublattice structure is necessarily coplanar.) Let the A sublattice spins point in the direction $(\theta = \theta_A, \phi = 0)$ and the B sublattice spins point in the direction $(\theta = \theta_B, \phi = \pi)$. The classical energy per bond is then

$$\varepsilon(\theta_A, \theta_B) = -JS^2 \sin \theta_A \sin \theta_B + JS^2 \Delta \cos \theta_A \cos \theta_B - \frac{hS_z}{z} (\cos \theta_A + \cos \theta_B)$$

Note that in computing the energy per bond, we must account for the fact that for each site there are $\frac{1}{2}z$ bonds, where $z$ is the coordination number. The total number of bonds is thus $N_{\text{bonds}} = \frac{1}{2}Nz$, where $N$ is the number of sites. Note also the competition between $\Delta$ and $h$. Large $\Delta$ makes the spins antialign along $\hat{z}$, while large $h$ prefers alignment along $\hat{z}$.

Let us first assume $\theta_A = \theta_B = \theta_c$ and determine $\theta_c$. Let $\varepsilon(\theta_A, \theta_B) \equiv \varepsilon(\theta_A, \theta_B)/JS^2$:

$$\varepsilon(\theta_c) \equiv \varepsilon(\theta_A = \theta_c, \theta_B = \theta_c) = -\sin^2 \theta_c + \Delta \cos^2 \theta_c - \frac{2h}{zSJ} \cos \theta_c$$

$$\frac{\partial \varepsilon}{\partial \theta_c} = \sin \theta_c \cdot \left\{ 2(1 + \Delta) \cos \theta_c - \frac{2h}{zSJ} \right\}$$

Thus, the extrema of $\varepsilon(\theta_c)$ occur at $\sin \theta_c = 0$ and at

$$\cos \theta_c = \frac{h}{zSJ(1 + \Delta)}$$

The latter solution is present only when $\Delta > \frac{|h|}{zSJ} - 1$. The energy of this state is

$$\varepsilon = -\left\{ 1 + \frac{1}{1 + \Delta} \left( \frac{h}{zSJ} \right)^2 \right\}$$
per bond.

To assess stability, we’ll need the second derivatives,

\[
\frac{\partial^2 e}{\partial \theta_A^2} \bigg|_{\theta_A^c = \theta_c} = \frac{\partial^2 e}{\partial \theta_B^2} \bigg|_{\theta_B^c = \theta_c} = \sin^2 \theta_c - \Delta \cos^2 \theta_c + \frac{h}{z S J} \cos \theta_c
\]

\[
\frac{\partial^2 e}{\partial \theta_A \partial \theta_B} \bigg|_{\theta_A^c = \theta_c, \theta_B^c = \theta_c} = -\cos^2 \theta_c + \Delta \sin^2 \theta_c ,
\]

from which we obtain the eigenvalues of the Hessian matrix,

\[
\lambda_+ = (1 + \Delta)(1 - 2 \cos^2 \theta_c) + \frac{h}{z S J} \cos \theta_c
\]

\[
= (1 + \Delta) \left\{ 1 - \left( \frac{h}{z S J (1 + \Delta)} \right)^2 \right\}
\]

\[
\lambda_- = (1 - \Delta) + \frac{h}{z S J} \cos \theta_c
\]

\[
= \frac{1}{1 + \Delta} \left\{ 1 - \Delta^2 + \left( \frac{h}{z S J} \right)^2 \right\} .
\]

Assuming \( \Delta > 0 \), we have that \( \lambda_+ > 0 \) requires

\[
\Delta > \frac{|h|}{z S J} - 1 ,
\]

which is equivalent to \( \cos^2 \theta_c < 1 \), and \( \lambda_- > 0 \) requires

\[
\Delta < \sqrt{1 + \left( \frac{h}{z S J} \right)^2} .
\]

This is the meaning of “not too large.”

The other extrema occur when \( \sin \theta_c = 0 \), i.e. \( \theta_c = 0 \) and \( \theta_c = \pi \). The eigenvalues of the Hessian at these points are:

\[
\theta_c = 0 : \quad \lambda_+ = -(1 + \Delta) + \frac{h}{z S J}
\]

\[
\lambda_- = 1 - \Delta + \frac{h}{z S J}
\]

\[
\theta_c = \pi \quad \lambda_+ = -(1 + \Delta) - \frac{h}{z S J}
\]

\[
\lambda_- = 1 - \Delta - \frac{h}{z S J} .
\]

Without loss of generality we may assume \( h \geq 0 \), in which case the \( \theta_c = \pi \) solution is always unstable. This is obvious, since the spins are anti-aligned with the field. For \( \theta_c = 0 \),
the solution is stable provided $\Delta < (h/zJS) - 1$. For general $h$, the stability condition is $\Delta < |h|/zJS - 1$. The other possibility is that $\Delta$ is so large that neither of these solutions is stable, in which case we suspect $\theta_A = 0$ and $\theta_B = \pi$ or vice versa.

Thus, for $h < zJS(1 + \Delta)$, the solution with $\theta_c = \cos^{-1} \left( \frac{h}{zJS(1 + \Delta)} \right)$ is stable. The Hessian matrix in this case is

$$
\begin{pmatrix}
\frac{\partial^2 e}{\partial \theta_A^2} & \frac{\partial^2 e}{\partial \theta_A \partial \theta_B} \\
\frac{\partial^2 e}{\partial \theta_B \partial \theta_A} & \frac{\partial^2 e}{\partial \theta_B^2}
\end{pmatrix}_{\theta_A=0, \theta_B=\pi} = \begin{pmatrix}
\Delta + \frac{h}{zSJ} & 1 \\
1 & \Delta - \frac{h}{zSJ}
\end{pmatrix}
$$

whose eigenvalues are

$$
\lambda_{\pm} = \Delta \pm \sqrt{1 + \left( \frac{h}{zSJ} \right)^2}.
$$

Thus, this configuration is stable only if

$$
\Delta > \sqrt{1 + \left( \frac{h}{zSJ} \right)^2}.
$$

(b) Now work out the quantum spin wave theory. To do this, you’ll have to rotate the quantization axes of the spins to their classical directions. This means taking

$$
S^x \rightarrow \cos \theta S^x + \sin \theta S^z \\
S^y \rightarrow S^y \\
S^z \rightarrow -\sin \theta S^x + \cos \theta S^z
$$

with $\theta = \pm \theta_0$, depending on the sublattice in question. How is $\theta_0$ related to $\theta_c$ above? This may seem like a pain in the neck, but really it isn’t so bad. Besides, you shouldn’t complain so much. And stand up straight – you’re slouching. And brush your teeth.

We will perform the spin-wave analysis for the case

$$
\frac{|h|}{zSJ} - 1 < \Delta < \sqrt{1 + \left( \frac{h}{zSJ} \right)^2}.
$$

We begin the analysis by rotating they spins in each sublattice by an angle $\pm \theta$ in the $x - z$ plane. Thus,

$$
S^x(\theta) = \cos \theta S^x + \sin \theta S^z \\
S^y(\theta) = S^y \\
S^z(\theta) = -\sin \theta S^x + \cos \theta S^z.
$$
In terms of the $S^\pm$ operators,
\[
S^+ (\theta) = \frac{1}{2} (\cos \theta + 1) S^+ + \frac{1}{2} (\cos \theta - 1) S^- + \sin \theta S^z
\]
\[
S^- (\theta) = \frac{1}{2} (\cos \theta - 1) S^+ + \frac{1}{2} (\cos \theta + 1) S^- + \sin \theta S^z
\]
\[
S^z (\theta) = -\frac{1}{2} \sin \theta S^+ - \frac{1}{2} \sin \theta S^- + \cos \theta S^z .
\]

The Holstein-Primakoff transformation is given by
\[
S^+ = a^\dagger (2S - a^\dagger a)^{1/2} , \quad S^- = (2S - a^\dagger a)^{1/2} a , \quad S^z = a^\dagger a - S ,
\]
in which case we have
\[
S^+ (\theta) = \sqrt{\frac{S}{2}} (\cos \theta + 1) a^\dagger + \sqrt{\frac{S}{2}} (\cos \theta - 1) a + \sin \theta (a^\dagger a - S) + \ldots
\]
\[
S^- (\theta) = \sqrt{\frac{S}{2}} (\cos \theta - 1) a^\dagger + \sqrt{\frac{S}{2}} (\cos \theta + 1) a + \sin \theta (a^\dagger a - S) + \ldots
\]
\[
S^z (\theta) = -\sqrt{\frac{S}{2}} \sin \theta a^\dagger - \sqrt{\frac{S}{2}} \sin \theta a + \cos \theta (S - a^\dagger a) + \ldots ,
\]
where the $\ldots$ stands for terms of higher order in the expansion of $(2S - a^\dagger a)^{1/2}$. The Hamiltonian may be written as a sum over links,
\[
\mathcal{H} = J \sum_{\langle ij \rangle} \mathcal{H}_{ij} ,
\]
where
\[
\mathcal{H}_{ij} = \frac{1}{2} S_{ij}^+ S_{ij}^- + \frac{1}{2} S_{ij}^+ S_{ij}^- + S_{ij}^z S_{ij}^z - \frac{h}{zJ} (S_{ij}^z + S_{ij}^z) .
\]
We assume that $i \in A$ and $j \in B$. Remembering that the spins are rotated by $\pm \theta$ on alternate sublattices, we obtain
\[
\mathcal{H}_{ij} = (\cos^2 \theta - \sin^2 \theta) (a_i^\dagger a_i - S) (a_j^\dagger a_j - S)
\]
\[
+ \sqrt{\frac{S}{2}} (1 + \Delta) \sin \theta \cos \theta \left\{ (a_i^\dagger a_i - S) (a_j + a_j^\dagger) - (a_j^\dagger a_j - S) (a_i - a_i^\dagger) \right\}
\]
\[
+ \frac{1}{2} S \cos^2 \theta \left( a_i^\dagger + a_i^\dagger a_j a_j + a_j^\dagger (a_j + a_j^\dagger) - \frac{1}{2} S (a_i - a_i^\dagger) (a_j - a_j^\dagger) \right)
\]
\[
+ \frac{h}{zJ} \sqrt{\frac{S}{2}} \sin \theta (a_i - a_i^\dagger - a_j + a_j^\dagger) - \frac{h}{zJ} \cos \theta (a_i^\dagger a_i + a_j^\dagger a_j - 2S) .
\]

The spin-wave Hamiltonian is obtained by dropping terms which contain more than two boson operators:
\[
\mathcal{H}_{ij} = S \left\{ (\sin^2 \theta - \Delta \cos^2 \theta) - \frac{h}{zJS} \cos \theta \right\} (a_i^\dagger a_i + a_j^\dagger a_j)
\]
\[
+ \frac{1}{2} S \cos^2 \theta - \Delta \sin^2 \theta) (a_i + a_i^\dagger) (a_j + a_j^\dagger) - \frac{1}{2} S (a_i - a_i^\dagger) (a_j - a_j^\dagger)
\]
\[
+ \frac{1}{\sqrt{2}} S^{3/2} \sin \theta \left\{ (1 + \Delta) \cos \theta + \frac{h}{zSJ} \right\} (a_i + a_j^\dagger - a_j - a_j^\dagger)
\]
\[
+ S^2 \left\{ \Delta \cos^2 \theta - \sin^2 \theta + \frac{2h}{zJS} \cos \theta \right\} .
\]
The third line above contains bare $a$ and $a^\dagger$ operators, and is also formally of order $S^{3/2}$. We can eliminate it by choosing $\theta$ such that

$$\cos \theta = -\frac{1}{1+\Delta} \frac{h}{zSJ} .$$

Note the minus sign, which is due to the fact that the vacuum state $|0\rangle$ for the bosons, prior to rotation, is directed along $-\hat{z}$.

We next substitute for $\theta$ and obtain the bond Hamiltonian

$$H_{ij} = \frac{1}{2} S \left\{ \frac{1}{1+\Delta} \left( \frac{h}{zSJ} \right)^2 - \Delta - 1 \right\} (a_i a_j + a_i^\dagger a_j^\dagger)$$

$$+ \frac{1}{2} S \left\{ \frac{1}{1+\Delta} \left( \frac{h}{zSJ} \right)^2 - \Delta + 1 \right\} (a_i^\dagger a_j + a_j^\dagger a_i)$$

$$+ S (a_i^\dagger a_i + a_j^\dagger a_j) - S^2 \left\{ 1 + \frac{1}{1+\Delta} \left( \frac{h}{zSJ} \right)^2 \right\} .$$

Note that the last term is the classical ground state energy. Fourier transforming,

$$\sum_{(ij)} (a_i^\dagger a_i + a_j^\dagger a_j) = \frac{1}{2z} \sum_k (a_k^\dagger a_k + a_{-k}^\dagger a_{-k})$$

$$\sum_{(ij)} (a_i a_j + a_i^\dagger a_j^\dagger) = \frac{1}{2z} \sum_k \gamma_k (a_k a_{-k} + a_{-k}^\dagger a_k^\dagger)$$

$$\sum_{(ij)} (a_i^\dagger a_j + a_j^\dagger a_i) = \frac{1}{2z} \sum_k \gamma_k (a_{-k}^\dagger a_k + a_{-k} a_k^\dagger)$$

where

$$\gamma_k = \frac{1}{z} \sum_{\delta} e^{ik\cdot\delta}$$

is a sum over nearest neighbor vectors $\delta$. On the square lattice, we have $\gamma_k = \frac{1}{2} \{ \cos(k_x a) + \cos(k_y a) \}$. We then obtain

$$\mathcal{H} = \frac{1}{2} JS^2 \sum_k \left\{ \omega_k (a_k^\dagger a_k + a_{-k}^\dagger a_{-k}) + \nu_k (a_k a_{-k} + a_{-k}^\dagger a_k^\dagger) \right\} ,$$

with

$$\omega_k = 1 + \gamma_k - \frac{1}{2} r \gamma_k$$

$$\nu_k = \frac{1}{2} r \gamma_k$$

$$r = 1 + \Delta - \frac{1}{1+\Delta} \left( \frac{h}{zSJ} \right)^2 .$$
We now invoke the Bogoliubov transformation,

\[ a_k = \cosh \beta_k \alpha_k - \sinh \beta_k \alpha_k^\dagger \]
\[ a_{-k} = \cosh \beta_k \alpha_{-k} - \sinh \beta_k \alpha_{-k}^\dagger, \]

with

\[ \tanh(2\beta_k) = \frac{\nu_k}{\omega_k} \]

to obtain the spin-wave Hamiltonian

\[ \mathcal{H} = JS^2 \sum_k E_k a_k^\dagger a_k + \frac{1}{2} JS^2 \sum_k (E_k - \omega_k) \]

with

\[ E_k = \sqrt{\omega_k^2 - \nu_k^2} = \sqrt{(1 + \gamma_k) (1 + \gamma_k - r \gamma_k)} \]

The second (constant) term in \( \mathcal{H} \) is the shift of the ground state energy due to quantum fluctuations. This term is negative, since \( E_k \leq \omega_k \).

(c) Compute the spin wave dispersion and find under what conditions the theory is unstable.

The spin-wave theory is stable provided \( E_k \) is real and nonnegative for all \( k \). Since \( \gamma_k \in [-1, 1] \), we have instabilities at \( r = 0 \) (zone corner, \( \gamma_k = -1 \)) and at \( r = 2 \) (zone center, \( \gamma_k = +1 \)). These are precisely the classical instabilities we found earlier:

\[ r = 0 \quad \Rightarrow \quad \Delta = \frac{|h|}{zSJ} - 1 \]
\[ r = 2 \quad \Rightarrow \quad \Delta = \sqrt{1 + \left( \frac{h}{zSJ} \right)^2}. \]