Physics 211B : Solution Set #4

[**1**] *Atomic physics* – Consider an ion with a partially filled shell of angular momentum J, and Z additional electrons in filled shells. Show that the ratio of the Curie paramagnetic susceptibility to the Larmor diamagnetic susceptibility is

$$\frac{\chi^{\mathrm{para}}}{\chi^{\mathrm{dia}}} = -\frac{g_{\mathrm{L}}^2 \, J(J+1)}{2Zk_{\mathrm{B}}T} \frac{\hbar^2}{m\langle r^2 \rangle} \ .$$

where g_{L} is the Landé g-factor. Estimate this ratio at room temperature.

Solution: We have derived the expressions

$$\chi^{\mathrm{dia}} = -\frac{Zne^2}{6mc^2} \langle r^2 \rangle$$

and

$$\chi^{\mathrm{para}} = \tfrac{1}{3}n \left(g_{\mathrm{L}}\mu_{\mathrm{B}} \right)^2 \frac{J(J+1)}{k_{\mathrm{B}}T} \ ,$$

where

$$g_{\mathrm{L}} = \tfrac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)} \ ,$$

and where $\mu_{\mathrm{B}} = e\hbar/2mc$ is the Bohr magneton. The ratio is thus

$$\frac{\chi^{\mathrm{para}}}{\chi^{\mathrm{dia}}} = -\frac{g_{\mathrm{L}}^2 \, J(J+1)}{2Zk_{\mathrm{B}}T} \frac{\hbar^2}{m\langle r^2 \rangle} \ .$$

If we assume $\langle r^2 \rangle = a_{\mathrm{B}}^2$, so that $\hbar^2/m\langle r^2 \rangle \simeq 27.2\,\mathrm{eV}$, then with $T = 300\,\mathrm{K}$ (and $k_{\mathrm{B}}T \approx \frac{1}{40}\,\mathrm{eV}$), $g_{\mathrm{L}} = 2$, $J = 2$, and $Z \approx 30$, the ratio is $\chi^{\mathrm{para}}/\chi^{\mathrm{dia}} \approx -450$.

[**2**] *Adiabatic demagnetization* – In an ideal paramagnet, the spins are noninteracting and the Hamiltonian is

$$\mathcal{H} = \sum_{i=1}^{N_{\mathrm{P}}} \gamma_i \, \boldsymbol{J}_i \cdot \boldsymbol{H}$$

where $\gamma_i = g_i\mu_i/\hbar$ and $\boldsymbol{J}_i$ are the gyromagnetic factor and spin operator for the ith paramagnetic ion, and $\boldsymbol{H}$ is the external magnetic field.

(**a**) Show that the free energy $F(H,T)$ can be written as

$$F(H,T) = T\,\Phi(H/T) \ .$$

If an ideal paramagnet is held at temperature T_{i} and field $H_{\mathrm{i}}\,\hat{\boldsymbol{z}}$, and the field H_{i} is *adiabatically* lowered to a value H_{f}, compute the final temperature. This is called "adiabatic demagnetization".

(b) Show that, in an ideal paramagnet, the specific heat at constant field is related to the susceptibility by the equation

$$c_H = T \left(\frac{\partial s}{\partial T} \right)_H = \frac{H^2 \chi}{T} \ .$$

Further assuming all the paramagnetic ions to have spin J, and assuming Curie's law to be valid, this gives

$$c_H = \tfrac{1}{3} n_{\rm p} k_{\rm B} J(J+1) \left(\frac{g\mu_{\rm B} H}{k_{\rm B} T} \right)^2 \ ,$$

where $n_{\rm p}$ is the density of paramagnetic ions. You are invited to compute the temperature T^* below which the specific heat due to lattice vibrations is smaller than the paramagnetic contribution. Recall the Debye result

$$c_V = \tfrac{12}{5} \pi^4 \, n k_{\rm B} \left(\frac{T}{\Theta_{\rm D}} \right)^3 \ ,$$

where $n = 1/\Omega$ is the inverse of the unit cell volume (*i.e.* the density of unit cells) and $\Theta_{\rm D}$ is the Debye temperature. Compile a table of a few of your favorite insulating solids, and tabulate Θ_D and T^* when 1% paramagnetic impurities are present, assuming $J = \frac{5}{2}$.

Solution: The partition function s a product of single-particle partition functions, and is explicitly a function of the ratio H/T:

$$Z = \prod_i \sum_{m=-J_i}^{J_i} e^{-m\gamma_i H/k_{\rm B} T} = Z(H/T) \ .$$

Thus,

$$F = -k_{\rm B} T \ln Z = T \, \Phi(H/T) \ ,$$

where

$$\Phi(x) = -k_{\rm B} \sum_{i=1}^{N_{\rm P}} \ln \left[\frac{\sinh \left((J_i + \tfrac{1}{2}) \gamma_i \, x/k_{\rm B} \right)}{\sinh \left(\gamma_i \, x/2k_{\rm B} \right)} \right] \ .$$

The entropy is

$$S = -\frac{\partial F}{\partial T} = -\Phi(H/T) + \frac{H}{T} \, \Phi'(H/T) \ ,$$

which is itself a function of H/T. Thus, constant S means constant H/T, and

$$\frac{H_{\rm f}}{H_{\rm i}} = \frac{T_{\rm f}}{T_{\rm i}} \qquad \Rightarrow \qquad T_{\rm f} = \frac{H_{\rm f}}{H_{\rm i}} \, T_{\rm i} \ .$$

The heat capacity is

$$C_H = T \left(\frac{\partial S}{\partial T} \right)_H = -x \, \frac{\partial S}{\partial x} = -\Phi''(x) \ ,$$

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with $x = H/T$. The (isothermal) magnetic susceptibility is

$$\chi = -\left(\frac{\partial^2 F}{\partial H^2}\right)_T = -\frac{1}{T}\,\Phi''(x)\;.$$

Thus,

$$C_H = \frac{H^2}{T}\,\chi\;.$$

Next, write

$$C_H = \tfrac{1}{3}n_{\mathrm{p}}\,k_{\mathrm{B}}\,J(J+1)\left(\frac{g_{\mathrm{L}}\mu_{\mathrm{B}}H}{k_{\mathrm{B}}T}\right)^2$$

$$C_V = \tfrac{12}{5}\pi^4\,n\,k_{\mathrm{B}}\left(\frac{T}{\Theta_{\mathrm{D}}}\right)^3$$

and we set $C_H = C_V$ to find T^*. Defining $\Theta_H \equiv g_{\mathrm{L}}\mu_{\mathrm{B}}H/k_{\mathrm{B}}$, we obtain

$$T^* = \frac{1}{\pi}\left[\tfrac{5\pi}{36}\,J(J+1)\,\frac{n_{\mathrm{p}}}{n}\,\Theta_H^2\,\Theta_{\mathrm{D}}^3\right]^{1/5}\;.$$

Set $J \approx 1$, $g_{\mathrm{L}} \approx 2$, $n_{\mathrm{p}} = 0.01\,n$ and $\Theta_{\mathrm{D}} \approx 500\,\mathrm{K}$. If $H = 1\,\mathrm{kG}$, then $\Theta_H = 0.134\,\mathrm{K}$. For general H, find

$$T^* \simeq 3\,\mathrm{K}\cdot\left(H\,[\mathrm{kG}]\right)^{2/5}\;.$$

[3] *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 $S_{\mathrm{B}} < S_{\mathrm{A}}$ (*e.g.* $S = 1$ for the A sublattice but $S = \frac{1}{2}$ for the B sublattice). The Hamiltonian is

$$\mathcal{H} = J\sum_{\langle ij\rangle} \boldsymbol{S}_i\cdot\boldsymbol{S}_j + g_{\mathrm{A}}\mu_0 H\sum_{i\in\mathrm{A}} S_i^z + g_{\mathrm{B}}\mu_0 H\sum_{j\in\mathrm{B}} S_j^z$$

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

$$\langle\boldsymbol{S}_{\mathrm{A}}\rangle = m_{\mathrm{A}}\,\hat{\boldsymbol{z}}\qquad,\qquad \langle\boldsymbol{S}_{\mathrm{B}}\rangle = m_{\mathrm{B}}\,\hat{\boldsymbol{z}}$$

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

$$m_{\mathrm{A}} = F_{\mathrm{A}}(\beta g_{\mathrm{A}}\mu_0 H + \beta Jzm_{\mathrm{B}})$$
$$m_{\mathrm{B}} = F_{\mathrm{B}}(\beta g_{\mathrm{B}}\mu_0 H + \beta Jzm_{\mathrm{A}})$$

where z is the lattice coordination number ($z = 6$ for NaCl) and $F_{\mathrm{A}}(x)$ and $F_{\mathrm{B}}(x)$ are related to Brillouin functions. Show graphically that a solution exists, and fund the criterion for

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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?

(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 $\big|N\big\rangle$ in which the spins are up on the A sublattice and down on the B sublattice, and choose

<table>
<tr><td align="center">A Sublattice</td><td align="center">B Sublattice</td></tr>
<tr><td>$S^+ = a^\dagger\,(2S_A - a^\dagger a)^{1/2}$</td><td>$S^+ = -(2S_B - b^\dagger b)^{1/2}\,b$</td></tr>
<tr><td>$S^- = (2S_A - a^\dagger a)^{1/2}\,a$</td><td>$S^+ = -b^\dagger\,(2S_B - b^\dagger b)^{1/2}$</td></tr>
<tr><td>$S^z = a^\dagger a - S_A$</td><td>$S^z = S_B - b^\dagger b$</td></tr>
</table>

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

<u>Solution:</u> We apply the mean field *Ansatz* $\langle\boldsymbol{S}_i\rangle = \boldsymbol{m}_{A,B}$ and obtain the mean field Hamiltonian

$$\mathcal{H}^{\mathrm{MF}} = -\tfrac{1}{2}NJzm_A\cdot m_B + \sum_{i\in A}\big(g_A\mu_0\boldsymbol{H} + zJ\boldsymbol{m}_B\big)\cdot\boldsymbol{S}_i + \sum_{j\in B}\big(g_B\mu_0\boldsymbol{H} + zJ\boldsymbol{m}_A\big)\cdot\boldsymbol{S}_j\ .$$

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

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

where

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

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

$$B_S(x) = \big(1 + \tfrac{1}{2S}\big)\operatorname{ctnh}\big(1 + \tfrac{1}{2S}\big)x - \tfrac{1}{2S}\operatorname{ctnh}\tfrac{x}{2S}\ .$$

The mean field equations may be solved graphically, as depicted in fig. 1.

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

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

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

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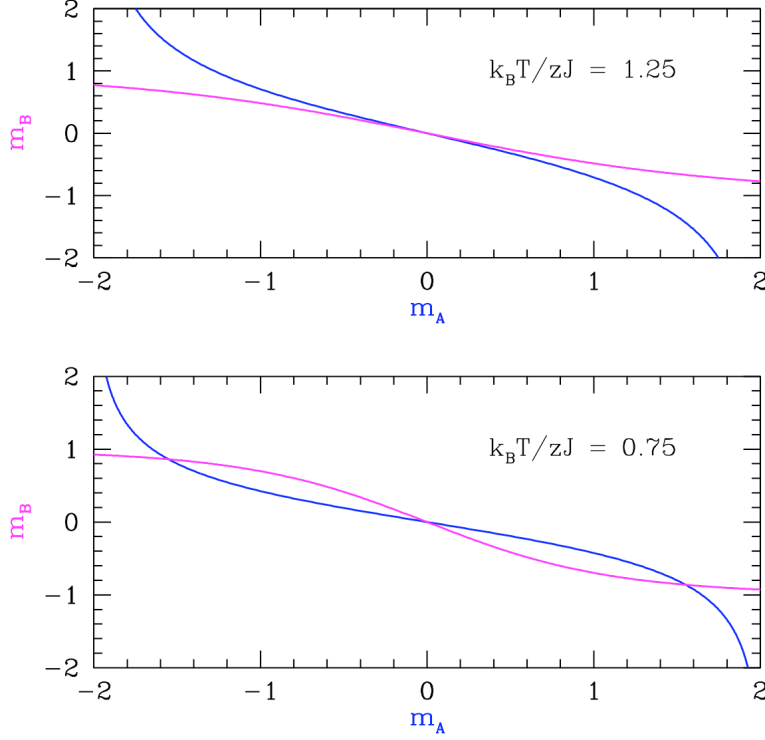
Figure 1: Graphical solution of of mean field equations with $S_A = 1$, $S_B = 2$, $g_A = g_B = 1$, $zJ = 1$, and $H = 0$. Top: $T > T_c$; bottom: $T < T_c$.

with solution

$$m_A = -\frac{g_A T_A T - g_B T_A T_B}{T^2 - T_A T_B} \frac{\mu_0 H}{zJ}$$

$$m_B = -\frac{g_B T_B T - g_A T_A T_B}{T^2 - T_A T_B} \frac{\mu_0 H}{zJ} \ .$$

The susceptibility is

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

$$= \frac{(g_A^2\, T_A + g_B^2\, T_B)T - 2g_A g_B\, T_A T_B}{T^2 - T_A T_B}\frac{\mu_0^2}{2zJ} \ ,$$

which diverges at

$$T_c = \sqrt{T_A T_B} = \sqrt{S_A S_B (S_A + 1)(S_B + 1)}\,\frac{z|J|}{3k_B} \ .$$

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

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at a temperature $T_{\mathrm{B}} > T_{\mathrm{c}}$. Finally, note that at high temperatures the susceptibility follows a Curie $\chi \propto T^{-1}$ behavior.

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 $\{\boldsymbol{R}\}$ and the B sublattice sites at $\{\boldsymbol{R}+\boldsymbol{\delta}\}$. For the NaCl structure, A and B are FCC lattices, and we may take

$$\boldsymbol{a}_1 = a\,(\hat{\boldsymbol{y}} + \hat{\boldsymbol{z}}) \quad , \quad \boldsymbol{a}_2 = a\,(\hat{\boldsymbol{x}} + \hat{\boldsymbol{z}}) \quad , \quad \boldsymbol{a}_3 = a\,(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}}) \quad , \quad \boldsymbol{\delta} = a\,\hat{\boldsymbol{z}} \ ,$$

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

$$\mathcal{H} = \sum_{\boldsymbol{R},\boldsymbol{R}'} \left\{ J_{\mathrm{AA}}\big(|\boldsymbol{R}-\boldsymbol{R}'|\big)\,\boldsymbol{S}_{\mathrm{A}}(\boldsymbol{R})\cdot\boldsymbol{S}_{\mathrm{A}}(\boldsymbol{R}') + J_{\mathrm{BB}}\big(|\boldsymbol{R}-\boldsymbol{R}'|\big)\,\boldsymbol{S}_{\mathrm{B}}(\boldsymbol{R})\cdot\boldsymbol{S}_{\mathrm{B}}(\boldsymbol{R}') \right.$$
$$\left. + J_{\mathrm{AB}}\big(|\boldsymbol{R}-\boldsymbol{R}'-\boldsymbol{\delta}|\big)\,\boldsymbol{S}_{\mathrm{A}}(\boldsymbol{R})\cdot\boldsymbol{S}_{\mathrm{B}}(\boldsymbol{R}') \right\} + \mu_0 H \sum_{\boldsymbol{R}} \left\{ g_{\mathrm{A}}\,S_{\mathrm{A}}^z(\boldsymbol{R}) + g_{\mathrm{B}}\,S_{\mathrm{B}}^z(\boldsymbol{R}) \right\} \ .$$

In our case, $J_{\mathrm{AA}} = J_{\mathrm{BB}} = 0$ and $J_{\mathrm{AB}}\big(|\boldsymbol{R}-\boldsymbol{R}'-\boldsymbol{\delta}|\big) = J\,\delta_{|\boldsymbol{R}-\boldsymbol{R}'-\boldsymbol{\delta}|,a}$, 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 *anisotropic* case, with the field directed along the direction of anisotropy:

$$\mathcal{H} = \sum_{\boldsymbol{R},\boldsymbol{R}'} \left\{ J_{\mathrm{AA}}\big(|\boldsymbol{R}-\boldsymbol{R}'|\big)\left(S_{\mathrm{A}}^x(\boldsymbol{R})\,S_{\mathrm{A}}^x(\boldsymbol{R}') + S_{\mathrm{A}}^y(\boldsymbol{R})\,S_{\mathrm{A}}^y(\boldsymbol{R}')\right) + \Delta_{\mathrm{AA}}\,S_{\mathrm{A}}^z(\boldsymbol{R})\,S_{\mathrm{A}}^z(\boldsymbol{R}') \right)$$
$$+ J_{\mathrm{BB}}\big(|\boldsymbol{R}-\boldsymbol{R}'|\big)\left(S_{\mathrm{B}}^x(\boldsymbol{R})\,S_{\mathrm{B}}^x(\boldsymbol{R}') + S_{\mathrm{B}}^y(\boldsymbol{R})\,S_{\mathrm{B}}^y(\boldsymbol{R}')\right) + \Delta_{\mathrm{BB}}\,S_{\mathrm{B}}^z(\boldsymbol{R})\,S_{\mathrm{B}}^z(\boldsymbol{R}') \right)$$
$$\left. + J_{\mathrm{AB}}\big(|\boldsymbol{R}-\boldsymbol{R}'|\big)\left(S_{\mathrm{A}}^x(\boldsymbol{R})\,S_{\mathrm{B}}^x(\boldsymbol{R}') + S_{\mathrm{A}}^y(\boldsymbol{R})\,S_{\mathrm{B}}^y(\boldsymbol{R}')\right) + \Delta_{\mathrm{AB}}\,S_{\mathrm{A}}^z(\boldsymbol{R})\,S_{\mathrm{B}}^z(\boldsymbol{R}') \right) \right\}$$
$$+ \mu_0 H \sum_{\boldsymbol{R}} \left\{ g_{\mathrm{A}}\,S_{\mathrm{A}}^z(\boldsymbol{R}) + g_{\mathrm{B}}\,S_{\mathrm{B}}^z(\boldsymbol{R}) \right\} \ .$$

Writing $\big[\boldsymbol{S}_i\cdot\boldsymbol{S}_j\big]_\Delta \equiv \frac{1}{2}S_i^+ S_j^- + \frac{1}{2}S_i^- S_j^+ + \Delta\,S_i^z S_j^z$, and expanding the radicals in the Bogoliubov transformation, we obtain

$$\big[\boldsymbol{S}_{\mathrm{A}}(\boldsymbol{R})\cdot\boldsymbol{S}_{\mathrm{A}}(\boldsymbol{R}')\big]_{\Delta_{\mathrm{AA}}} = \Delta_{\mathrm{AA}}\,S_{\mathrm{A}}^2 - \Delta_{\mathrm{AA}}\,S_{\mathrm{A}}\big(a_{\boldsymbol{R}}^\dagger a_{\boldsymbol{R}} + a_{\boldsymbol{R}'}^\dagger a_{\boldsymbol{R}'}\big) + S_{\mathrm{A}}\big(a_{\boldsymbol{R}}^\dagger a_{\boldsymbol{R}'} + a_{\boldsymbol{R}'}^\dagger a_{\boldsymbol{R}}\big) + \ldots$$
$$\big[\boldsymbol{S}_{\mathrm{B}}(\boldsymbol{R})\cdot\boldsymbol{S}_{\mathrm{B}}(\boldsymbol{R}')\big]_{\Delta_{\mathrm{BB}}} = \Delta_{\mathrm{BB}}\,S_{\mathrm{B}}^2 - \Delta_{\mathrm{BB}}\,S_{\mathrm{B}}\big(b_{\boldsymbol{R}}^\dagger b_{\boldsymbol{R}} + b_{\boldsymbol{R}'}^\dagger b_{\boldsymbol{R}'}\big) + S_{\mathrm{B}}\big(b_{\boldsymbol{R}}^\dagger b_{\boldsymbol{R}'} + b_{\boldsymbol{R}'}^\dagger b_{\boldsymbol{R}}\big) + \ldots$$
$$\big[\boldsymbol{S}_{\mathrm{A}}(\boldsymbol{R})\cdot\boldsymbol{S}_{\mathrm{B}}(\boldsymbol{R}')\big]_{\Delta_{\mathrm{AB}}} = -\Delta_{\mathrm{AB}}\,S_{\mathrm{A}}S_{\mathrm{B}} + \Delta_{\mathrm{AB}}\big(S_{\mathrm{B}}\,a_{\boldsymbol{R}}^\dagger a_{\boldsymbol{R}} + S_{\mathrm{A}}\,b_{\boldsymbol{R}}^\dagger b_{\boldsymbol{R}}\big)$$
$$- \sqrt{S_{\mathrm{A}}S_{\mathrm{B}}}\big(a_{\boldsymbol{R}}^\dagger b_{\boldsymbol{R}'}^\dagger + a_{\boldsymbol{R}} b_{\boldsymbol{R}'}\big) + \ldots \ .$$

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The spin-wave Hamiltonian is then

$$\mathcal{H} = S_{\mathrm{A}} \sum_{\boldsymbol{R},\boldsymbol{R}'} J_{\mathrm{AA}}\big(|\boldsymbol{R} - \boldsymbol{R}'|\big) \Big\{ a_{\boldsymbol{R}}^{\dagger} a_{\boldsymbol{R}'} + a_{\boldsymbol{R}'}^{\dagger} a_{\boldsymbol{R}} - \Delta_{\mathrm{AA}} a_{\boldsymbol{R}}^{\dagger} a_{\boldsymbol{R}} - \Delta_{\mathrm{AA}} a_{\boldsymbol{R}'}^{\dagger} a_{\boldsymbol{R}'} + \Delta_{\mathrm{AA}} S_{\mathrm{A}} \Big\}$$

$$+ S_{\mathrm{B}} \sum_{\boldsymbol{R},\boldsymbol{R}'} J_{\mathrm{BB}}\big(|\boldsymbol{R} - \boldsymbol{R}'|\big) \Big\{ b_{\boldsymbol{R}}^{\dagger} b_{\boldsymbol{R}'} + b_{\boldsymbol{R}'}^{\dagger} b_{\boldsymbol{R}} - \Delta_{\mathrm{BB}} b_{\boldsymbol{R}}^{\dagger} b_{\boldsymbol{R}} - \Delta_{\mathrm{BB}} b_{\boldsymbol{R}'}^{\dagger} b_{\boldsymbol{R}'} + \Delta_{\mathrm{BB}} S_{\mathrm{B}} \Big\}$$

$$+ \sum_{\boldsymbol{R},\boldsymbol{R}'} J_{\mathrm{AB}}\big(|\boldsymbol{R} - \boldsymbol{R}' - \boldsymbol{\delta}|\big) \Big\{ - S_{\mathrm{A}} S_{\mathrm{B}} \big(a_{\boldsymbol{R}}^{\dagger} b_{\boldsymbol{R}'}^{\dagger} + a_{\boldsymbol{R}} b_{\boldsymbol{R}'} \big)$$

$$+ \Delta_{\mathrm{AB}} S_{\mathrm{B}} a_{\boldsymbol{R}}^{\dagger} a_{\boldsymbol{R}} + \Delta_{\mathrm{AB}} S_{\mathrm{A}} b_{\boldsymbol{R}'}^{\dagger} b_{\boldsymbol{R}'} - \Delta_{\mathrm{AB}} S_{\mathrm{A}} S_{\mathrm{B}} \Big\} \ .$$

We now Fourier transform, with

$$a_{\boldsymbol{R}} \equiv \frac{1}{\sqrt{N_{\mathrm{A}}}} \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} a_{\boldsymbol{k}} \qquad , \qquad b_{\boldsymbol{R}} \equiv \frac{1}{\sqrt{N_{\mathrm{B}}}} \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot(\boldsymbol{R}+\boldsymbol{\delta})} a_{\boldsymbol{k}} \ ,$$

and

$$\hat{J}_{\mathrm{AA}}(\boldsymbol{k}) = \sum_{\boldsymbol{R}} J_{\mathrm{AA}}\big(|\boldsymbol{R}|\big) e^{-i\boldsymbol{k}\cdot\boldsymbol{R}}$$

$$\hat{J}_{\mathrm{BB}}(\boldsymbol{k}) = \sum_{\boldsymbol{R}} J_{\mathrm{BB}}\big(|\boldsymbol{R}|\big) e^{-i\boldsymbol{k}\cdot\boldsymbol{R}}$$

$$\hat{J}_{\mathrm{AB}}(\boldsymbol{k}) = \sum_{\boldsymbol{R}} J_{\mathrm{AB}}\big(|\boldsymbol{R} + \boldsymbol{\delta}|\big) e^{-i\boldsymbol{k}\cdot(\boldsymbol{R}+\boldsymbol{\delta})} \ .$$

Here, $N_{\mathrm{A}} = N_{\mathrm{B}} = \frac{1}{2} N$ is half the total number of lattice sites. This leads to

$$\mathcal{H} = E_0 + \sum_{\boldsymbol{k}} \Big\{ \omega_{\mathrm{A}}(\boldsymbol{k}) \, a_{\boldsymbol{k}}^{\dagger} a_{\boldsymbol{k}} + \omega_{\mathrm{B}}(\boldsymbol{k}) \, b_{\boldsymbol{k}}^{\dagger} b_{\boldsymbol{k}} - \nu(\boldsymbol{k}) \, a_{\boldsymbol{k}}^{\dagger} b_{-\boldsymbol{k}}^{\dagger} - \nu^*(\boldsymbol{k}) \, a_{\boldsymbol{k}} b_{-\boldsymbol{k}} \Big\} \ ,$$

with

$$\omega_{\mathrm{A}}(\boldsymbol{k}) = +g_{\mathrm{A}}\mu_0 H + 2S_{\mathrm{A}} \Big(\hat{J}_{\mathrm{AA}}(\boldsymbol{k}) - \Delta_{\mathrm{AA}} \hat{J}_{\mathrm{AA}}(0) \Big) + \Delta_{\mathrm{AB}} S_{\mathrm{B}} \hat{J}_{\mathrm{AB}}(0)$$

$$\omega_{\mathrm{B}}(\boldsymbol{k}) = -g_{\mathrm{B}}\mu_0 H + 2S_{\mathrm{B}} \Big(\hat{J}_{\mathrm{BB}}(\boldsymbol{k}) - \Delta_{\mathrm{BB}} \hat{J}_{\mathrm{BB}}(0) \Big) + \Delta_{\mathrm{AB}} S_{\mathrm{A}} \hat{J}_{\mathrm{AB}}(0)$$

$$\nu(\boldsymbol{k}) = \sqrt{S_{\mathrm{A}} S_{\mathrm{B}}} \, \hat{J}_{\mathrm{AB}}(\boldsymbol{k}) \ .$$

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

OK, now we do the Bogoliubov thang, and write

$$a_{\boldsymbol{k}} = u_{\boldsymbol{k}} \alpha_{\boldsymbol{k}} + v_{\boldsymbol{k}}^* \beta_{-\boldsymbol{k}}^{\dagger} \qquad\qquad b_{-\boldsymbol{k}} = u_{\boldsymbol{k}} \beta_{-\boldsymbol{k}} + v_{\boldsymbol{k}}^* \alpha_{\boldsymbol{k}}^{\dagger}$$

$$a_{\boldsymbol{k}}^{\dagger} = u_{\boldsymbol{k}}^* \alpha_{\boldsymbol{k}}^{\dagger} + v_{\boldsymbol{k}} \beta_{-\boldsymbol{k}} \qquad\qquad b_{-\boldsymbol{k}}^{\dagger} = u_{\boldsymbol{k}}^* \beta_{-\boldsymbol{k}}^{\dagger} + v_{\boldsymbol{k}} \alpha_{\boldsymbol{k}} \ .$$

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[1]For the NaCl structure, $\hat{J}_{\mathrm{AB}}(\boldsymbol{k})$ as defined is real.

This preserves the bosonic commutation relations:

$$[\alpha_{\mathbf{k}}, \alpha_{\mathbf{k}'}^{\dagger}] = [\beta_{\mathbf{k}}, \beta_{\mathbf{k}'}^{\dagger}] = [a_{\mathbf{k}}, a_{\mathbf{k}'}^{\dagger}] = [b_{\mathbf{k}}, b_{\mathbf{k}'}^{\dagger}] = \delta_{\mathbf{k}\mathbf{k}'}$$

$$[\alpha_{\mathbf{k}}, \beta_{\mathbf{k}'}] = [\alpha_{\mathbf{k}}, \beta_{\mathbf{k}'}^{\dagger}] = [a_{\mathbf{k}}, b_{\mathbf{k}'}] = [a_{\mathbf{k}}, b_{\mathbf{k}'}^{\dagger}] = 0 \ .$$

Substituting into $\mathcal{H}$, we find $\mathcal{H} = \sum_{\mathbf{k}} \mathcal{H}_{\mathbf{k}}$, with

$$
\begin{aligned}
\mathcal{H}_{\mathbf{k}} = {} & \left\{ \omega_{\mathrm{A}}(\mathbf{k}) \left| u_{\mathbf{k}} \right|^2 + \omega_{\mathrm{B}}(\mathbf{k}) \left| v_{\mathbf{k}} \right|^2 - \nu(\mathbf{k}) \, u_{\mathbf{k}} \, v_{\mathbf{k}}^* - \nu^*(\mathbf{k}) \, u_{\mathbf{k}}^* \, v_{\mathbf{k}} \right\} \alpha_{\mathbf{k}}^{\dagger} \, \alpha_{\mathbf{k}} \\
& + \left\{ \omega_{\mathrm{A}}(\mathbf{k}) \left| v_{\mathbf{k}} \right|^2 + \omega_{\mathrm{B}}(\mathbf{k}) \left| u_{\mathbf{k}} \right|^2 - \nu(\mathbf{k}) \, u_{\mathbf{k}} \, v_{\mathbf{k}}^* - \nu^*(\mathbf{k}) \, u_{\mathbf{k}}^* \, v_{\mathbf{k}} \right\} \beta_{-\mathbf{k}}^{\dagger} \, \beta_{-\mathbf{k}} \\
& + \left\{ \left(\omega_{\mathrm{A}}(\mathbf{k}) + \omega_{\mathrm{B}}(\mathbf{k}) \right) u_{\mathbf{k}} \, v_{\mathbf{k}} - \nu(\mathbf{k}) \, u_{\mathbf{k}}^2 - \nu^*(\mathbf{k}) \, v_{\mathbf{k}}^2 \right\} \alpha_{\mathbf{k}} \, \beta_{-\mathbf{k}} \\
& + \left\{ \left(\omega_{\mathrm{A}}(\mathbf{k}) + \omega_{\mathrm{B}}(\mathbf{k}) \right) u_{\mathbf{k}}^* \, v_{\mathbf{k}}^* - \nu^*(\mathbf{k}) \, u_{\mathbf{k}}^{*\,2} - \nu(\mathbf{k}) \, v_{\mathbf{k}}^{*\,2} \right\} \alpha_{\mathbf{k}}^{\dagger} \, \beta_{-\mathbf{k}}^{\dagger} + \mathrm{const.}
\end{aligned}
$$

We now write $\nu(\mathbf{k}) \equiv |\nu(\mathbf{k})| \, e^{i\varphi(\mathbf{k})}$ and use the freedom to choose $\{u_{\mathbf{k}}, v_{\mathbf{k}}\}$ to eliminate the $\alpha_{\mathbf{k}} \, \beta_{-\mathbf{k}}$ and $\alpha_{\mathbf{k}}^{\dagger} \, \beta_{-\mathbf{k}}^{\dagger}$ terms in $\mathcal{H}_{\mathbf{k}}$:

$$u_{\mathbf{k}} = \cosh \theta_{\mathbf{k}} \, e^{-i\varphi(\mathbf{k})/2}$$

$$v_{\mathbf{k}} = \sinh \theta_{\mathbf{k}} \, e^{+i\varphi(\mathbf{k})/2} \ ,$$

where

$$\tanh 2\theta_{\mathbf{k}} = \frac{2 \left| \nu(\mathbf{k}) \right|}{\omega_{\mathrm{A}}(\mathbf{k}) + \omega_{\mathrm{B}}(\mathbf{k})} \ .$$

This leads to the dispersions

$$E_{+}(\mathbf{k}) = +\omega_{-}(\mathbf{k}) + \sqrt{\omega_{+}^2(\mathbf{k}) - \nu^2(\mathbf{k})}$$

$$E_{-}(\mathbf{k}) = -\omega_{-}(\mathbf{k}) + \sqrt{\omega_{+}^2(\mathbf{k}) - \nu^2(\mathbf{k})} \ ,$$

where

$$\omega_{\pm}(\mathbf{k}) \equiv \tfrac{1}{2} \left\{ \omega_{\mathrm{A}}(\mathbf{k}) \pm \omega_{\mathrm{B}}(\mathbf{k}) \right\} \ ,$$

and where $E_{+}(\mathbf{k})$ is the α-boson dispersion, and $E_{-}(\mathbf{k})$ is the β-boson dispersion:

$$\mathcal{H} = \sum_{\mathbf{k}} \left\{ E_{+}(\mathbf{k}) \, \alpha_{\mathbf{k}}^{\dagger} \, \alpha_{\mathbf{k}} + E_{-}(\mathbf{k}) \, \beta_{\mathbf{k}}^{\dagger} \, \beta_{\mathbf{k}} \right\} \ .$$

Let's check our dispersion in some simple cases. For the NaCl structure, we take $J_{\mathrm{AA}}(\mathbf{R}) = J_{\mathrm{BB}}(\mathbf{R}) = 0$ and $\hat{J}_{\mathrm{AB}}(\mathbf{R} + \boldsymbol{\delta}) = \delta_{|\mathbf{R}+\boldsymbol{\delta}|, a}$. Then

$$\hat{J}_{\mathrm{AB}}(\mathbf{k}) = 2J \left(\cos k_x a + \cos k_y a + \cos k_z a \right) \ .$$

In order for the spin-wave Hamiltonian to be stable, we must have $E_{\alpha,\beta}(\boldsymbol{k}) \geq 0$ for all $\boldsymbol{k}$ in the Brillouin zone. Otherwise, the ground state energy can be lowered by adding α or β 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 $E_{\mathrm{g}}(H = 0) = r\,\hat{J}_{\mathrm{AB}}(0)$, where

$$r = \tfrac{1}{2}\sqrt{(S_{\mathrm{A}} + S_{\mathrm{B}})^2\,\Delta_{\mathrm{AB}}^2 - 4S_{\mathrm{A}}S_{\mathrm{B}}} - \tfrac{1}{2}\big|S_{\mathrm{A}} - S_{\mathrm{B}}\big|\,\Delta_{\mathrm{AB}} \ .$$

The gap vanishes when $r = 0$, which occurs at the isotropic point $\Delta_{\mathrm{AB}} = 1$. For $\Delta_{\mathrm{AB}} < 1$, $E_{\mathrm{g}}(H = 0) < 0$ and the spectrum is unstable. Precisely at $\Delta_{\mathrm{AB}} = 1$, 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 $\Delta_{\mathrm{AB}} = 1$, then the spin-wave dispersion for $H = 0$ becomes

$$E_{\pm}(\boldsymbol{k}) = \pm\tfrac{1}{2}(S_{\mathrm{B}} - S_{\mathrm{A}})\,\hat{J}_{\mathrm{AB}}(0) + \tfrac{1}{2}\hat{J}_{\mathrm{AB}}(0)\,\sqrt{(S_{\mathrm{A}} - S_{\mathrm{B}})^2 + S_{\mathrm{A}}S_{\mathrm{B}}\,k^2 R_*^2} + \mathcal{O}(k^4) \ ,$$

where

$$R_*^2 \equiv \frac{\sum_{\boldsymbol{R}}\boldsymbol{R}^2\,J_{\mathrm{AB}}(\boldsymbol{R})}{d\sum_{\boldsymbol{R}}J_{\mathrm{AB}}(\boldsymbol{R})} \ ,$$

with d the dimension of space. For the NaCl structure, $R_* = a/\sqrt{3}$. If both S_{A} and S_{B} are large, but their difference is of order unity, then a separation of scales develops. For $k \ll |S_{\mathrm{A}} - S_{\mathrm{B}}|/\sqrt{S_{\mathrm{A}}S_{\mathrm{B}}}$, the low-lying spin-wave branch disperses quadratically, as in the case of the ferromagnet. For $|S_{\mathrm{A}} - S_{\mathrm{B}}|/\sqrt{S_{\mathrm{A}}S_{\mathrm{B}}} \ll k \ll \pi/a$, the dispersion is linear, as in the case of the antiferromagnet. At very long wavelengths, then, the ferrimagnet behaves as a *ferro*magnet, with a net spin $|S_{\mathrm{A}} - S_{\mathrm{B}}|$ 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.

[4] *Thinking about singlets* – Consider the antiferromagnetic Heisenberg model on a bipartite lattice:

$$\mathcal{H} = J\sum_{\langle ij\rangle}\boldsymbol{S}_i \cdot \boldsymbol{S}_j$$

where $J > 0$ and the sum is over the bonds of the lattice.

(a) Break up the lattice into a dimer covering. There are exponentially many such dimer coverings, *i.e.* the number grows as $e^{\alpha N}$ where N is the number of lattice sites. Think about tiling a chessboard with with dominoes. The analysis of this problem was performed by H. N. V. Temperley and M. E. Fisher, *Phil. Mag.* **6**, 1061 (1961). Denote one sublattice as A and the other as B. You are to develop a mean field theory of interacting dimers in the presence of a self-consistent staggered field

$$\langle\boldsymbol{S}_{\mathrm{A}}\rangle = -\langle\boldsymbol{S}_{\mathrm{B}}\rangle \equiv m\hat{\boldsymbol{z}} \ .$$

The mean field Hamiltonian then breks up into a sum over dimer Hamiltonians

$$\mathcal{H}_{\mathrm{dimer}} = J\boldsymbol{S}_{\mathrm{A}} \cdot \boldsymbol{S}_{\mathrm{B}} + (z - 1)J\langle\boldsymbol{S}_{\mathrm{B}}\rangle \cdot \boldsymbol{S}_{\mathrm{A}} + (z - 1)J\langle\boldsymbol{S}_{\mathrm{A}}\rangle \cdot \boldsymbol{S}_{\mathrm{B}}$$
$$= J\boldsymbol{S}_{\mathrm{A}} \cdot \boldsymbol{S}_{\mathrm{B}} - H_{\mathrm{s}}\left(S_{\mathrm{A}}^z - S_{\mathrm{B}}^z\right)$$

where the effective staggered field is $H_{\rm s} = (z - 1)Jm$, and z is the lattice coordination number. Find the eigenvalues of the dimer Hamiltonian when $S = \frac{1}{2}$.

(b) Define $x = 2h/J$. What is the self-consistent equation for x when $T = 0$? Under what conditions is there a nontrivial solution? What then is the self-consistent staggered magnetization? How does it compare with the result of spin-wave theory?

<u>**Solution:**</u> The mean field Hamiltonian,

$$\mathcal{H} = J\, \boldsymbol{S}_{\rm A} \cdot \boldsymbol{S}_{\rm B} - H_{\rm s}\left(S_{\rm A}^z - S_{\rm B}^z\right),$$

is written in matrix form (for $S = \frac{1}{2}$) as

$$
\mathcal{H} =
\overbrace{\phantom{\begin{pmatrix} \frac14 J & 0 \end{pmatrix}}}^{\displaystyle |\uparrow\uparrow\rangle \quad |\uparrow\downarrow\rangle}
\overbrace{\phantom{\begin{pmatrix} 0 & 0 \end{pmatrix}}}^{\displaystyle |\downarrow\uparrow\rangle \quad |\downarrow\downarrow\rangle}
\begin{pmatrix}
\frac14 J & 0 & 0 & 0 \\
0 & -\frac14 J - H_{\rm s} & \frac12 J & 0 \\
0 & \frac12 J & \frac14 J + H_{\rm s} & 0 \\
0 & 0 & 0 & \frac14 J
\end{pmatrix}.
$$

Clearly the states $\left|\,\uparrow\uparrow\,\right\rangle$ and $\left|\,\downarrow\downarrow\,\right\rangle$ are eigenstates of $\mathcal{H}$ with eigenvalues $\frac14 J$. The other two eigenvalues are easily found to be

$$\lambda_{\pm} = -\tfrac14 J \pm \sqrt{H_{\rm s}^2 + \tfrac14 J^2}\,,$$

The ground state eigenvector is then

$$\left|\,\Psi_0\,\right\rangle = \alpha\,\left|\,\uparrow\downarrow\,\right\rangle + \beta\,\left|\,\downarrow\uparrow\,\right\rangle,$$

with

$$\frac{\beta}{\alpha} = x - \sqrt{1 + x^2}\,,$$

with $x = 2H_{\rm s}/J$. The staggered moment is then

$$m = \left\langle S_{\rm A}^z \right\rangle = \frac{1}{2}\frac{|\alpha|^2 - |\beta|^2}{|\alpha|^2 + |\beta|^2} = \frac{x}{2\sqrt{1 + x^2}}\,.$$

Since $m = \frac{1}{2}x/(z - 1)$, we have $\sqrt{1 + x^2} = (z - 1)$, or

$$m = \frac{\sqrt{z(z - 2)}}{2(z - 1)}$$

for the staggered magnetization. For $z = 4$ (square lattice) we find $m = \frac{\sqrt{2}}{3} \simeq 0.471$, which is 94% of the full moment $S = \frac{1}{2}$. Spin wave theory gives $m \simeq S - 0.19 \simeq 0.31$, which is only 62% of the full moment for $S = 4$.

[5] *Let's all do the spin flop* – In real solids crystal field effects often lead to anisotropic spin-spin interactions. Consider the anisotropic Heisenberg antiferromagnet in a uniform magnetic field,

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

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 Δ 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 θ_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.)

(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

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

with $\theta = \pm\theta_0$, depending on the sublattice in question. How is θ_0 related to θ_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.

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

Solution: 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 let the B sublattice spins point in the direction $(\theta = \theta_B, \phi = 0)$. The classical energy per bond is then

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

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 Δ and h. Large Δ 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 θ_c. Let $e(\theta_A, \theta_B) \equiv \varepsilon(\theta_A, \theta_B)/JS^2$:

$$e(\theta_c) \equiv e(\theta_A = \theta_c, \theta_B = \theta_c)$$
$$= -\sin^2\theta_c + \Delta\cos^2\theta_c - \frac{2h}{zSJ}\cos\theta_c$$
$$\frac{\partial e}{\partial \theta_c} = \sin\theta_c \cdot \left\{2(1 + \Delta)\cos\theta_c - \frac{2h}{zSJ}\right\}.$$

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

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

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

$$e = -\left\{ 1 + \frac{1}{1+\Delta} \left(\frac{h}{zSJ} \right)^2 \right\}$$

per bond.

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

$$\left. \frac{\partial^2 e}{\partial \theta_A^2} \right|_{\substack{\theta_A = \theta_c \\ \theta_B = \theta_c}} = \left. \frac{\partial^2 e}{\partial \theta_B^2} \right|_{\substack{\theta_A = \theta_c \\ \theta_B = \theta_c}} = \sin^2\theta_c - \Delta \cos^2\theta_c + \frac{h}{zSJ} \cos\theta_c$$

$$\left. \frac{\partial^2 e}{\partial \theta_A \partial \theta_B} \right|_{\substack{\theta_A = \theta_c \\ \theta_B = \theta_c}} = -\cos^2\theta_c + \Delta \sin^2\theta_c ,$$

from which we obtain the eigenvalues of the Hessian matrix,

$$\lambda_+ = (1+\Delta)(1 - 2\cos^2\theta_c) + \frac{h}{zSJ} \cos\theta_c$$

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

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

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

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

$$\Delta > \frac{|h|}{zSJ} - 1 ,$$

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

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

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:

$$\theta_c = 0 : \qquad \lambda_+ = -(1+\Delta) + \frac{h}{zSJ}$$

$$\lambda_- = 1 - \Delta + \frac{h}{zSJ}$$

$$\theta_c = \pi \qquad \lambda_+ = -(1+\Delta) - \frac{h}{zSJ}$$

$$\lambda_- = 1 - \Delta - \frac{h}{zSJ} .$$

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 Δ 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 $\theta_c = \cos^{-1}(h/zJS(1 + \Delta))$ is stable. The Hessian matrix in this case is

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

whose eigenvalues are

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

Thus, this configuration is stable only if

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

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,

$$
\begin{aligned}
S^x(\theta) &= \cos\theta \, S^x + \sin\theta \, S^z \\
S^y(\theta) &= S^y \\
S^z(\theta) &= -\sin\theta \, S^x + \cos\theta \, S^z \ .
\end{aligned}
$$

In terms of the $S^\pm$ operators,

$$
\begin{aligned}
S^+(\theta) &= \tfrac{1}{2}(\cos\theta + 1) \, S^+ + \tfrac{1}{2}(\cos\theta - 1) \, S^- + \sin\theta \, S^z \\
S^-(\theta) &= \tfrac{1}{2}(\cos\theta - 1) \, S^+ + \tfrac{1}{2}(\cos\theta + 1) \, S^- + \sin\theta \, S^z \\
S^z(\theta) &= -\tfrac{1}{2}\sin\theta \, S^+ - \tfrac{1}{2}\sin\theta \, S^- + \cos\theta \, S^z \ .
\end{aligned}
$$

The Holstein-Primakoff transformation is given by

$$
S^+ = a^\dagger \, (2S - a^\dagger a)^{1/2} \quad , \quad S^- = (2S - a^\dagger a)^{1/2} \, a \quad , \quad S^z = a^\dagger a - S \ ,
$$

in which case we have

$$S^+(\theta) = \sqrt{\tfrac{S}{2}}\,(\cos\theta + 1)\,a^\dagger + \sqrt{\tfrac{S}{2}}\,(\cos\theta - 1)\,a + \sin\theta\,(a^\dagger a - S) + \ldots$$

$$S^-(\theta) = \sqrt{\tfrac{S}{2}}\,(\cos\theta - 1)\,a^\dagger + \sqrt{\tfrac{S}{2}}\,(\cos\theta + 1)\,a + \sin\theta\,(a^\dagger a - S) + \ldots$$

$$S^z(\theta) = -\sqrt{\tfrac{S}{2}}\,\sin\theta\,a^\dagger - \sqrt{\tfrac{S}{2}}\,\sin\theta\,a + \cos\theta\,(S - a^\dagger a) + \ldots\,,$$

where the ... 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

$$\mathcal{H}_{ij} = \tfrac{1}{2}\,S_i^+\,S_j^- + \tfrac{1}{2}\,S_i^-\,S_j^+ + S_i^z\,S_j^z - \frac{h}{zJ}\,(S_i^z + S_j^z)\,.$$

We assume that $i \in A$ and $j \in B$. Remembering that the spins are rotated by $\pm\theta$ on alternate sublattices, we obtain

$$\begin{aligned}
\mathcal{H}_{ij} =\ & (\Delta\cos^2\theta - \sin^2\theta)\,(a_i^\dagger a_i - S)\,(a_j^\dagger a_j - S) \\
& + \sqrt{\tfrac{S}{2}}\,(1 + \Delta)\,\sin\theta\cos\theta\left\{(a_i^\dagger a_i - S)\,(a_j + a_j^\dagger) - (a_j^\dagger a_j - S)\,(a_i + a_i^\dagger)\right\} \\
& + \tfrac{1}{2}S\,(\cos^2\theta - \Delta\sin^2\theta)\,(a_i + a_i^\dagger)\,(a_j + a_j^\dagger) - \tfrac{1}{2}S\,(a_i - a_i^\dagger)\,(a_j - a_j^\dagger) \\
& + \frac{h}{zJ}\,\sqrt{\tfrac{S}{2}}\,\sin\theta\,(a_i + a_i^\dagger - a_j - a_j^\dagger) - \frac{h}{zJ}\,\cos\theta\,(a_i^\dagger a_i + a_j^\dagger a_j - 2S)\,.
\end{aligned}$$

The spin-wave Hamiltonian is obtained by dropping terms which contain more than two boson operators:

$$\begin{aligned}
\mathcal{H}_{ij} =\ & S\left\{(\sin^2\theta - \Delta\cos^2\theta) - \frac{h}{zJS}\,\cos\theta\right\}(a_i^\dagger a_i + a_j^\dagger a_j) \\
& + \tfrac{1}{2}S\,(\cos^2\theta - \Delta\sin^2\theta)\,(a_i + a_i^\dagger)\,(a_j + a_j^\dagger) - \tfrac{1}{2}S\,(a_i - a_i^\dagger)\,(a_j - a_j^\dagger) \\
& + \tfrac{1}{\sqrt{2}}\,S^{3/2}\,\sin\theta\left\{(1 + \Delta)\cos\theta + \frac{h}{zSJ}\right\}(a_i + a_i^\dagger - a_j - a_j^\dagger) \\
& + S^2\left\{\Delta\cos^2\theta - \sin^2\theta + \frac{2h}{zSJ}\,\cos\theta\right\}.
\end{aligned}$$

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 θ 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 $-\hat{\boldsymbol{z}}$.

We next substitute for θ and obtain the bond Hamiltonian

$$\mathcal{H}_{ij} = \tfrac{1}{2} S \left\{ \frac{1}{1+\Delta} \left(\frac{h}{zSJ} \right)^2 - \Delta - 1 \right\} (a_i \, a_j + a_i^\dagger \, a_j^\dagger)$$

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

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

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

$$\sum_{\langle ij \rangle} (a_i^\dagger a_i + a_j^\dagger a_j) = \tfrac{1}{2} z \sum_{\boldsymbol{k}} (a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}} + a_{-\boldsymbol{k}}^\dagger a_{-\boldsymbol{k}})$$

$$\sum_{\langle ij \rangle} (a_i a_j + a_i^\dagger a_j^\dagger) = \tfrac{1}{2} z \sum_{\boldsymbol{k}} \gamma_{\boldsymbol{k}} \, (a_{\boldsymbol{k}} a_{-\boldsymbol{k}} + a_{\boldsymbol{k}}^\dagger a_{-\boldsymbol{k}}^\dagger)$$

$$\sum_{\langle ij \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) = \tfrac{1}{2} z \sum_{\boldsymbol{k}} \gamma_{\boldsymbol{k}} \, (a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}} + a_{-\boldsymbol{k}}^\dagger a_{-\boldsymbol{k}}) \ ,$$

where

$$\gamma_{\boldsymbol{k}} = \frac{1}{z} \sum_{\boldsymbol{\delta}} e^{i \boldsymbol{k} \cdot \boldsymbol{\delta}}$$

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

$$\mathcal{H} = \tfrac{1}{2} J S^2 \sum_{\boldsymbol{k}} \left\{ \omega_{\boldsymbol{k}} \, (a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}} + a_{-\boldsymbol{k}}^\dagger a_{-\boldsymbol{k}}) + \nu_{\boldsymbol{k}} \, (a_{\boldsymbol{k}} a_{-\boldsymbol{k}} + a_{\boldsymbol{k}}^\dagger a_{-\boldsymbol{k}}^\dagger) \right\} ,$$

with

$$\omega_{\boldsymbol{k}} = 1 + \gamma_{\boldsymbol{k}} - \tfrac{1}{2} r \, \gamma_{\boldsymbol{k}}$$

$$\nu_{\boldsymbol{k}} = \tfrac{1}{2} r \, \gamma_{\boldsymbol{k}}$$

$$r \equiv 1 + \Delta - \frac{1}{1+\Delta} \left(\frac{h}{zSJ} \right)^2 .$$

We now invoke the Bogoliubov transformation,

$$a_{\boldsymbol{k}} = \cosh \beta_{\boldsymbol{k}} \, \alpha_{\boldsymbol{k}} - \sinh \beta_{\boldsymbol{k}} \, \alpha_{-\boldsymbol{k}}^\dagger$$

$$a_{-\boldsymbol{k}} = \cosh \beta_{\boldsymbol{k}} \, \alpha_{-\boldsymbol{k}} - \sinh \beta_{\boldsymbol{k}} \, \alpha_{\boldsymbol{k}}^\dagger \ ,$$

with

$$\tanh(2\beta_{\boldsymbol{k}}) = \frac{\nu_{\boldsymbol{k}}}{\omega_{\boldsymbol{k}}}$$

to obtain the spin-wave Hamiltonian

$$\mathcal{H} = JS^2 \sum_{\boldsymbol{k}} E_{\boldsymbol{k}} \, a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}} + \tfrac{1}{2} JS^2 \sum_{\boldsymbol{k}} (E_{\boldsymbol{k}} - \omega_{\boldsymbol{k}}) \ ,$$

with

$$E_{\boldsymbol{k}} = \sqrt{\omega_{\boldsymbol{k}}^2 - \nu_{\boldsymbol{k}}^2} = \sqrt{(1 + \gamma_{\boldsymbol{k}})(1 + \gamma_{\boldsymbol{k}} - r\,\gamma_{\boldsymbol{k}})} \ .$$

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

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

$$r = 0 \quad \Rightarrow \quad \Delta = \frac{|h|}{zSJ} - 1$$

$$r = 2 \quad \Rightarrow \quad \Delta = \sqrt{1 + \left(\frac{h}{zSJ}\right)^2} \ .$$