Computing the Néel Temperature in Sr_2IrO_4 and $Sr_3Ir_2O_7$

I. SINGLE LAYER

We work with conventions of Neil's notes.

Our initial Hamiltonian is

$$H = J \sum_{\langle i,j \rangle, l} \mathbf{S}_{i,l} \cdot \mathbf{S}_{j,l} + \Gamma \sum_{\langle i,j \rangle, l} S^z_{i,l} S^z_{j,l} + \sum_{\langle i,j \rangle, l} D(-1)^{i_x+j_y} (S^x_{i,l} S^y_{j,l} - S^y_{i,l} S^x_{j,l}) + J_c \sum_{i,l} \mathbf{S}_{i,l} \cdot \mathbf{S}_{i,l+1}, \quad (1)$$

where l is a layer index. I'm ignoring NN and NNN couplings as unimportant. However these are simple to include. For the case of a canted AF, we can rotate the two sublattices of the 2D plane in such a way as to arrive at an isotropic AF Hamiltonian in the plane:

$$H = \tilde{J} \sum_{\langle i,j \rangle, l} \bar{\mathbf{S}}_{i,l} \cdot \bar{\mathbf{S}}_{j,l} + J_c \sum_{i,l} \bar{\mathbf{S}}_{i,l} \cdot \bar{\mathbf{S}}_{j,l+1}, \quad (2)$$

where $\bar{\mathbf{S}}$ are the rotated spins and $\tilde{J} = \sqrt{J^2 + D^2}$.

The spin wave dispersion of such an AF is

$$\begin{aligned} E(k_x, k_y, k_z) &= (J^2(0,0,0) - J^2(k_x, k_y, k_z))^{1/2}; \\ J(k_x, k_y, k_z) &= 2\tilde{J}(\cos(k_x) + \cos(k_y)) + 2J_c \cos(k_z). \end{aligned} \quad (3)$$

The magnetization at site n is then (using Neil's spin wave notations)

$$\begin{aligned} \langle \bar{S}_{x,n} \rangle &= \frac{1}{2} - \langle \bar{a}^\dagger_n \bar{a}_n \rangle = \frac{1}{2} - \frac{1}{V} \sum_k \langle \bar{a}^\dagger_k \bar{a}_k \rangle; \\ &= \frac{1}{2} - \frac{1}{V} \sum_k \Big[\cosh^2(\theta_k) \langle \bar{b}^\dagger_k \bar{b}_k \rangle + \sinh^2(\theta_k) \langle \bar{b}_k \bar{b}^\dagger_k \rangle \Big]; \\ &= \frac{1}{2} - \frac{1}{V} \sum_k \Big[\cosh^2(\theta_k) n_k + \sinh^2(\theta_k)(1 + n_k) \Big]; \\ &= 1 - \frac{1}{V} \sum_k \cosh(2\theta_k)(n_k + \frac{1}{2}) \\ &= 1 - \frac{1}{8\pi^3} \int dk_x dk_y dk_z \frac{4\tilde{J} + 2J_c}{E(\mathbf{k})} \coth \frac{\beta E(\mathbf{k})}{2}. \end{aligned} \quad (4)$$

Here $n_k = (e^{\beta E(\mathbf{k})} - 1)^{-1}$. We define T_N as the temperature for which $\langle \bar{S}_x \rangle = 0$.

The addition of a small interlayer coupling J_c (turning it into a 3D problem) stabilizes the spin wave computation (i.e. rids it of annoying IR singularities which plague spin wave correlators in the ordered phase in 2D, a reflection of the Mermin-Wagner theorem in operation). And from PRB 94 224420 we have an estimate of the interlayer coupling as $J_c = 16\mu eV$. Knowing this will allow us to estimate T_N. While we can do this numerically, for the case when $T_N \ll J/2$, we can reduce the above constraint on T_N to (PRB 55 12318)

$$T_N = \frac{\pi \tilde{J}}{\log(\frac{T_N^2}{4\tilde{J}J_c})}. \tag{5}$$

This same PRB offers improvements on the spin wave T_N (which we can look at if seems desirable – we generically expect this MFT T_N should be too high). However as we are going to use spin waves as well on the bilayer, it might be better to be consistent in approximations.

II. BILAYER

Here the Heisenberg Hamiltonian is given by

$$\begin{aligned} H &= \sum_{\langle n,m\rangle,l} \Big(J\mathbf{S}_{n,l}\cdot\mathbf{S}_{m,l} + \Gamma S^z_{n,l}S^z_{m,l}\Big) + \sum_{\langle n,m\rangle,l} D(-1)^{n_x+n_y+l}(S^x_{n,l}S^y_{m,l} - S^y_{n,l}S^x_{m,l}) \\ &+ \sum_n \Big(J_c\mathbf{S}_{n,1}\cdot\mathbf{S}_{n,2} + \Gamma_c S^z_{n,1}S^z_{n,2}\Big) + \sum_n D_c(-1)^{n_x+n_y}(S^x_{n,1}S^y_{n,2} - S^y_{n,1}S^x_{n,2}). \end{aligned} \tag{6}$$

We introduce as in Neil's notes the Holstein-Primakoff bosons, $a_{n,l}$. If we introduce their bonding and anti-bonding counterparts,

$$a_{n,\pm} = \frac{1}{\sqrt{2}}(a_{n,1} \pm a_{n,2}), \tag{7}$$

we can write the Hamiltonian in block diagonal form as

$$H = \sum_k A_k^\dagger \begin{bmatrix} B_{k,+} & C_{k,+} & 0 & 0 \\ C^*_{k,+} & B_{k,+} & 0 & 0 \\ 0 & 0 & B_{k,-} & C_{k,-} \\ 0 & 0 & C^*_{k,-} & B_{k,-} \end{bmatrix} A_k, \tag{8}$$

where $A_k^\dagger = (a^\dagger_{k,+}, a_{-k,+}, a^\dagger_{k,-} a_{-k,-})$. To diagonalize this Hamiltonian we write

$$\begin{aligned} a_{k,\pm} &= \frac{\cosh(\theta_{k,\pm})}{N_{k,\pm}} b_{k,\pm} + \frac{\sinh(\theta_{k,\pm})}{N_{k,\pm}} b^\dagger_{-k,\pm}; \\ a^\dagger_{-k,\pm} &= \frac{\sinh^*(\theta_{k,\pm})}{N_{k,\pm}} b_{k,\pm} + \frac{\cosh^*(\theta_{k,\pm})}{N_{k,\pm}} b^\dagger_{-k,\pm}. \end{aligned} \tag{9}$$

Here the Bogoliubov angle θ_k is complex and so $N_{k,\pm} \neq 1$. We find that the needed angle is given by

$$
\begin{aligned}
\cosh(2\mathrm{Re}\theta_{k,\pm}) &= \frac{B_{k,\pm} + \mathrm{Im}C_{k,\pm}\sin(2\mathrm{Im}\theta_k)}{E_\pm(k)}; \\
\sinh(2\mathrm{Re}\theta_{k,\pm}) &= \frac{-\mathrm{Re}C_{k,\pm}}{E_\pm(k)}; \\
\sin(2\mathrm{Im}\theta_{k,\pm}) &= -\frac{\mathrm{Im}C_{k,\pm}}{B_{k,\pm}}; \\
E_\pm(k) &= (B_{k,\pm}^2 - |C_{k,\pm}|^2)^{1/2}; \\
B_{k,\pm} &= \frac{1}{2}(8J + 8\Gamma + J_c + \Gamma_c) - 4J_2(1 - \cos(k_x)\cos(k_y)) - 4J_3(1 - \gamma_{2k}) - 4J_{2c}(1 \mp \gamma_k); \\
C_{k,\pm} &= \frac{1}{2}(8J\gamma_k \pm J_c) - \frac{i}{2}(8D\gamma_k \pm D_c); \\
\gamma_k &= \frac{1}{2}(\cos(k_x) + \cos(k_y)). \qquad (10)
\end{aligned}
$$

Note that because we are now including next-nearest neighbour couplings, $B_{k,\pm}$ is different for the bonding (+) and anti-bonding (−) bands.

With these relations in hand we can write the magnetization at a given site in the bilayer as

$$
\begin{aligned}
\langle S^z_{n,1}\rangle &= \frac{1}{2} - \frac{1}{2}\sum_{s=\pm}\langle a^\dagger_{n,s}a_{n,s}\rangle \\
&= 1 - \frac{1}{16\pi^2}\int dk_x dk_y \left[\frac{B_{k,+}}{E_+(k)}\coth(\beta E_+(k)) + \frac{B_{k,-}}{E_-(k)}\coth(\beta E_-(k))\right]. \qquad (11)
\end{aligned}
$$

Right now I don't have a simplifed form for this integral. Given the magnons are gapped, it seems that all points in the Brillouin zone will contribute and so the integral has to been done without the simplifications possible in the single layer case. For the choice of parameters, $J = 93/2, J_2 = 11.9/2, J_3 = 14.6/2, J_{2c} = 6.2, \Gamma = 4.4/2, J_c = 25.2, \Gamma_c = 34.3, D = 24.5/2, D_c = 28.1$, I find $T_N = 118$, and for the choice of parameters, $J = 93/2, J_2 = 0, J_3 = 0, J_{2c} = 0, \Gamma = 4.4/2, J_c = 25.2, \Gamma_c = 34.3, D = 24.5/2, D_c = 28.1$, I find $T_N = 237$. All energies/temperatures are given in meV. We can conclude that the exact value of T_N is sensitive to the presence of next and next-next nearest neighbour couplings.