
Homework - Computational Nanoscience

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Problem.
At roughing temperature ($\beta = 0$):

$$\exp\left(\frac{J_y}{k_B T}\right) = \coth\left(\frac{J_x}{2k_B T}\right)$$

Derive equation:

$$T_R = \frac{J}{k_B \ln\left(1+\sqrt{2}\right)}$$

$\coth(z) = \frac{e^{2z}+1}{e^{2z}-1}$ and we assume $J_x = J_y = J$.

$$\begin{aligned} \exp\left(\frac{J}{k_B T}\right) &= \frac{\exp\left(\frac{J}{k_B T}\right)+1}{\exp\left(\frac{J}{k_B T}\right)-1} \\ x &= \frac{x+1}{x-1} \\ x^2 - 2x - 1 &= 0 \\ x &= 1 \pm \sqrt{2} \end{aligned}$$

with $x = \exp\left(\frac{J}{k_B T}\right)$,
so the solution is $\exp\left(\frac{J}{k_B T}\right) = 1+\sqrt{2}$.
and roughing temperature (when $\beta = 0$) is $T_R = \frac{J}{k_B \ln(1+\sqrt{2})}$