Lattice deformations
and
the order-by-disorder phase transition

The frustrated J1-J2 classical Heisenberg model

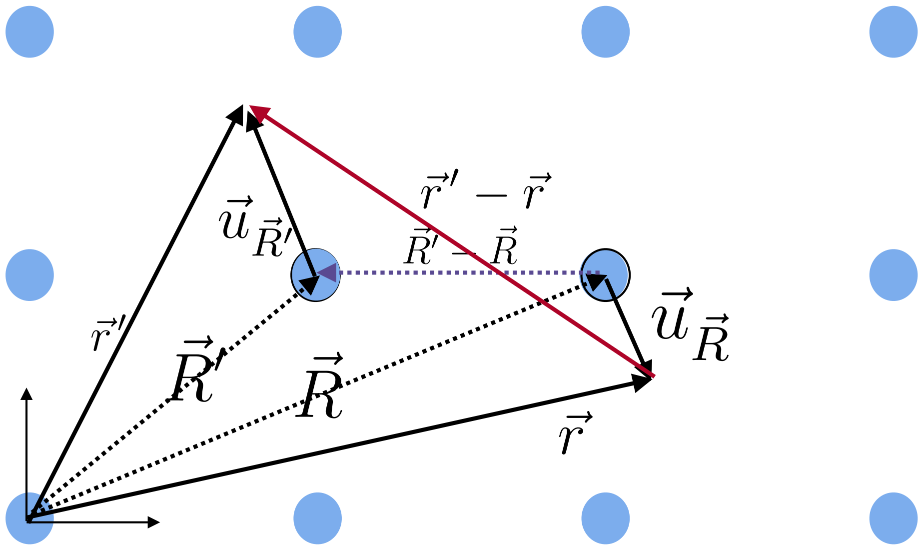
A collaboration with Jens Paaske, Niels Bohr Inst.

$$H = \frac{1}{2} \sum_{\vec{r},\vec{r}\,'} J(\vec{r}\,' - \vec{r}) S^{\alpha}_{\vec{r}} S^{\alpha}_{\vec{r}\,'}$$

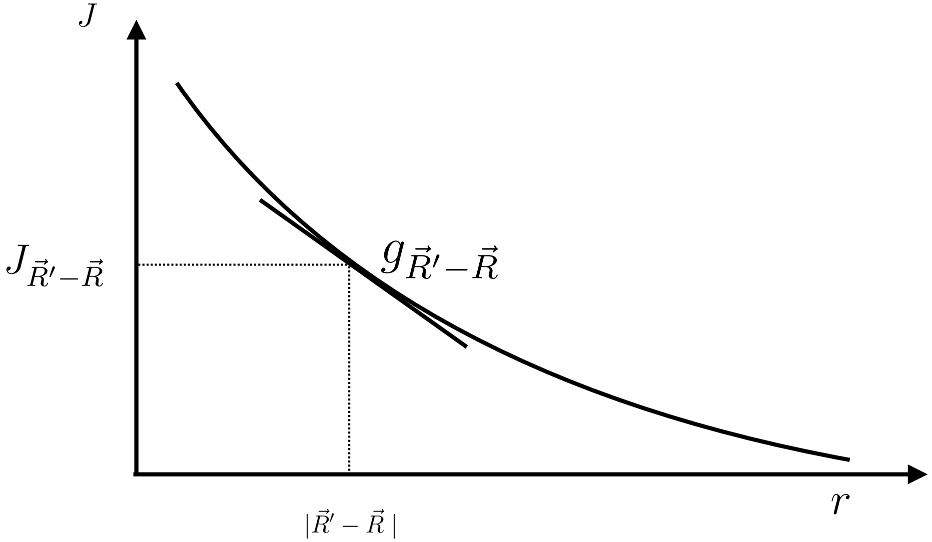
$$J(\vec{r}\,' - \vec{r}) \approx J_{\vec{R}' - \vec{R}} + (\vec{u}_{\vec{R}'} - \vec{u}_{\vec{R}}) \cdot \nabla J_{\vec{R}' - \vec{R}}$$

$$\nabla J_{\vec{R}' - \vec{R}} = g_{\vec{R}' - \vec{R}} \frac{\vec{R}' - \vec{R}}{|\vec{R}' - \vec{R}\,|}$$

$$g_{\vec{R}' - \vec{R}} = \frac{\partial J}{\partial r}\Big|_{r=|\vec{R}' - \vec{R}\,|}$$



$$\vec{r} = \vec{R} + \vec{u}_{\vec{R}}$$

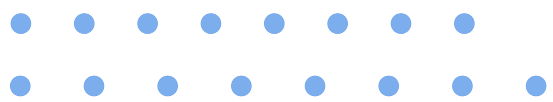


elastic deformation tensor

normal mode amplitude for mode n at wave vector $\vec{k}$.

$$u^i_{\vec{R}} = e^{ij} R^j + \sum_{\vec{k}\neq 0, n} W^i_{\vec{k},n} e^{i\vec{k}\cdot\vec{R}} X_{\vec{k},n}$$

normal mode eigenvector



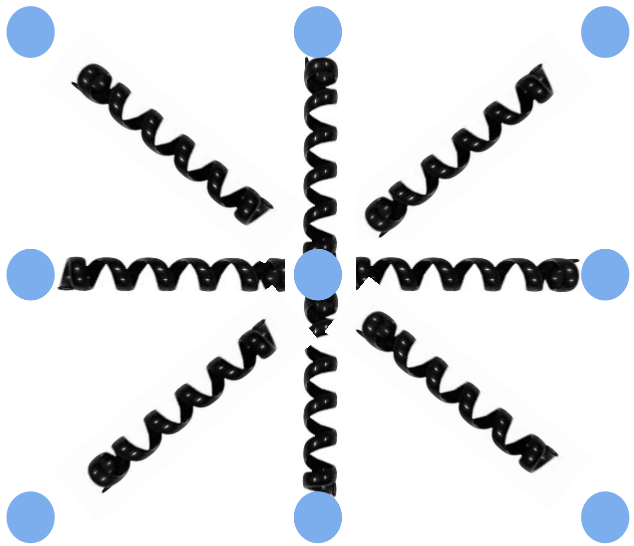
$$H_{latt} = \frac{1}{2} V c_{ij,kl} e^{ij} e^{kl} + \sum_{\vec{k} \neq 0, n} \frac{1}{2} M \omega_{\vec{k},n}^2 \left(|X_{\vec{k},n}|^2 + |P_{\vec{k},n}|^2 \right)$$

$c_{ij,kl}$ is the elastic moduli tensor per unit volume

phonon mode frequencies are given by $\omega_{\vec{k},n}$.

M is the atom mass.

$$D^{ij}_{\vec{k}} = \frac{1}{M}\sum_m \frac{\partial^2 V_{pot}}{\partial r^i_m \partial r^j_n}|_{eq} e^{-i\vec{k}\cdot\left(\vec{R}_m - \vec{R}_n\right)}$$



$$D^{xx}_{\vec{k}} = 2\frac{\alpha_1}{M}\left(1-\cos k_x a\right) + 2\frac{\alpha_2}{M}\left[1-\cos\left(k_x a\right)\cos\left(k_y a\right)\right]$$

$$D^{yy}_{\vec{k}} = 2\frac{\alpha_1}{M}\left(1-\cos k_y a\right) + 2\frac{\alpha_2}{M}\left[1-\cos\left(k_x a\right)\cos\left(k_y a\right)\right]$$

$$D^{xy}_{\vec{k}} = 2\frac{\alpha_2}{M}\sin\left(k_x a\right)\sin\left(k_y a\right) = D^{yx}_{\vec{k}}.$$

$$\frac{MN}{V} D^{ij}_{\vec{k}}|_{\vec{k}\to 0} = \sum_{kl} c_{ik,jl} k^k k^l$$

$$E_{el} = V\frac{1}{2} c_{ij,kl} e^{ij} e^{kl} = V\frac{1}{2} c_{\rho,s} \epsilon^{\rho} \epsilon^{s}$$

$$C = \begin{pmatrix} \alpha_1 + \alpha_2 & \alpha_2 & 0 \\ \alpha_2 & \alpha_1 + \alpha_2 & 0 \\ 0 & 0 & \alpha_2 \end{pmatrix}$$

$$= \frac{V}{2}\left[\alpha_1 \left(\frac{-\epsilon^{xx} + \epsilon^{yy}}{\sqrt{2}}\right)^2 + \alpha_2 \left(\epsilon^{xy}\right)^2 + (\alpha_1 + 2\alpha_2) \left(\frac{\epsilon^{xx} + \epsilon^{yy}}{\sqrt{2}}\right)^2\right] = \frac{V}{2} \mu_k \tilde{\epsilon}_k^2$$

Classical spins are unit vectors

$$|\vec{S}_{\vec{r}}| \;=\; 1$$

$$\delta\left(|\vec{S}_{\vec{r}}| - 1\right) = \int_{-\infty}^{\infty} \frac{\beta d\lambda_{\vec{r}}}{\pi}\; e^{-i\beta\lambda_{\vec{r}}\left(\vec{S}_{\vec{r}}\cdot\vec{S}_{\vec{r}}-1\right)}$$

$$\lambda_{\vec{q}} = (-i)\Delta\delta_{\vec{q},0} + \lambda_{\vec{q}}\left(1 - \delta_{\vec{q},0}\right)$$

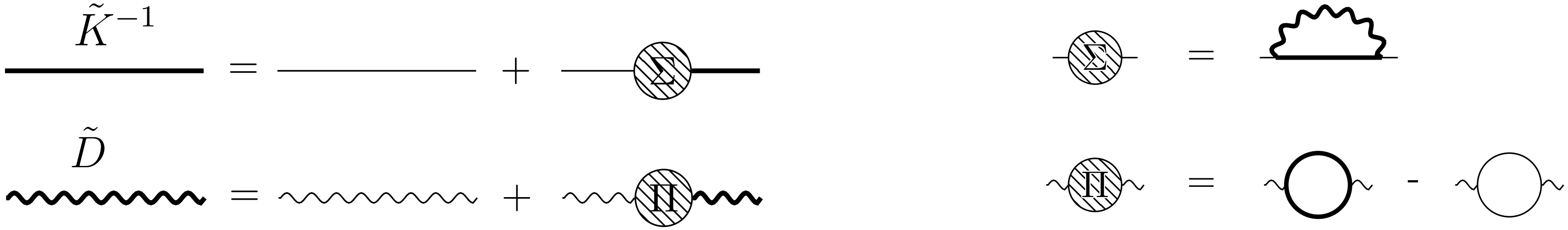
Partition function

$$Z = \int D\Delta D\tilde{\epsilon} D\lambda DX DS \; e^{-S}$$

$$S = \sum_{\vec{q},\vec{q}'} S^{\alpha *}_{\vec{q}} \left(\overbrace{\left(J_{\vec{q}} + \Delta + g_{\vec{q},k}\tilde{\epsilon}_k\right)\delta_{\vec{q},\vec{q}'}}^{\mathbf{K}} - (-i)\left[\Gamma^{n\,\vec{q}-\vec{q}'}_{\vec{q},\,\vec{q}'} X_{\vec{q}-\vec{q}',n} + \lambda_{\vec{q}-\vec{q}'}\right]\right) S^{\alpha}_{\vec{q}'}$$

$$- \beta V \Delta + \frac{\beta V}{2}\mu_k \tilde{\epsilon}^2_k + \frac{\beta}{2}\sum_{\vec{k},n}\left(|X_{\vec{k},n}|^2 + |P_{\vec{k},n}|^2\right)$$

$$\Gamma^{n\,\vec{q}-\vec{q}'}_{\vec{q},\,\vec{q}'} = \frac{2i}{\sqrt{NM}} \sum_{\vec{R}} g_{\vec{R}} \; \frac{R^i}{|\vec{R}|} \frac{W^i_{\vec{q}-\vec{q}',n}}{\omega_{\vec{q}-\vec{q}',n}} \left(e^{i\vec{q}\cdot\vec{R}} - e^{i\vec{q}'\cdot\vec{R}}\right)$$



Self-consistent equations:

$$\tilde{K}_{\vec{q}} = J_{\vec{q}} + \Delta + \tilde{\epsilon}_k g_{\vec{q},k} - \Sigma_{\vec{q}}$$

$$\tilde{D}_{\vec{q}}^{-1mm'} = \frac{N_s}{2} \sum_{\vec{k}} \tilde{K}_{\vec{k}}^{-1} \Gamma^{m\,-\vec{q}}_{\vec{k},\vec{k}+\vec{q}} \tilde{K}_{\vec{k}+\vec{q}}^{-1} \Gamma^{m'\,\vec{q}}_{\vec{k}+\vec{q},\vec{k}} + \beta \delta_{m'm}(1 - \delta_{m,0})$$

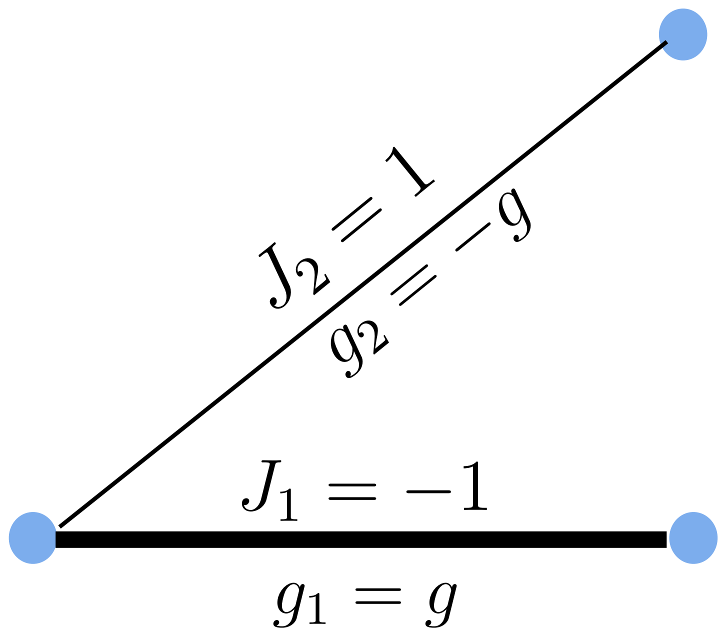
$$\Sigma_{\vec{k}} = (-i)^2 \sum_{\vec{q}} \Gamma^{m\,-\vec{q}}_{\vec{k},\vec{k}+\vec{q}} \tilde{K}_{\vec{k}+\vec{q}}^{-1} \Gamma^{m'\,\vec{q}}_{\vec{k}+\vec{q},\vec{k}} \tilde{D}_{\vec{q}}^{m'm}$$

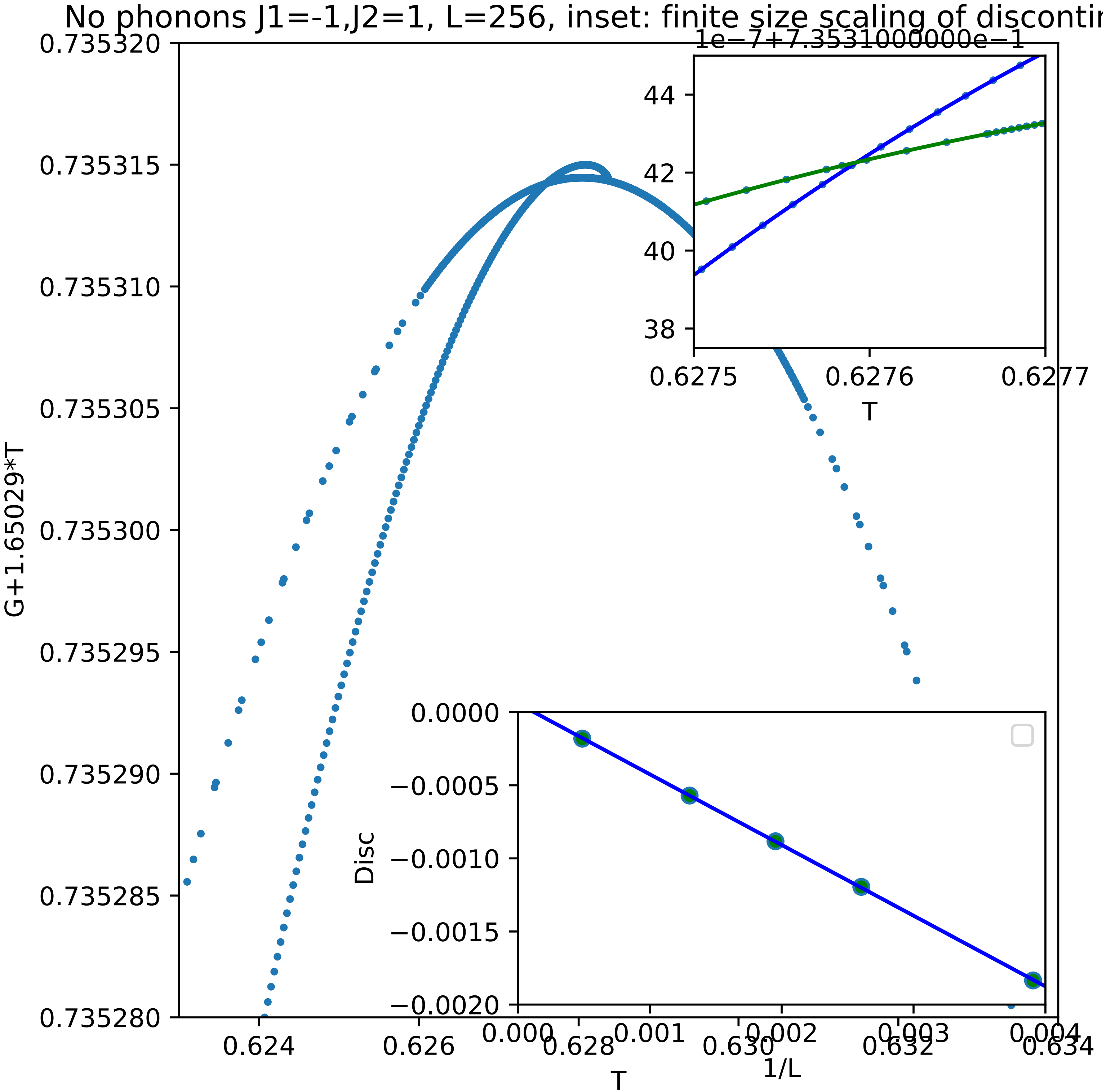
Saddle-point equations:

$$\beta = \frac{N_s}{V} \sum_{\vec{q}} \tilde{K}_{\vec{q}}^{-1} \qquad \beta \tilde{\epsilon}_k = -\frac{N_s}{2V\mu_k} \sum_{\vec{q}} \tilde{K}_{\vec{q}}^{-1} g_{\vec{q},k}$$

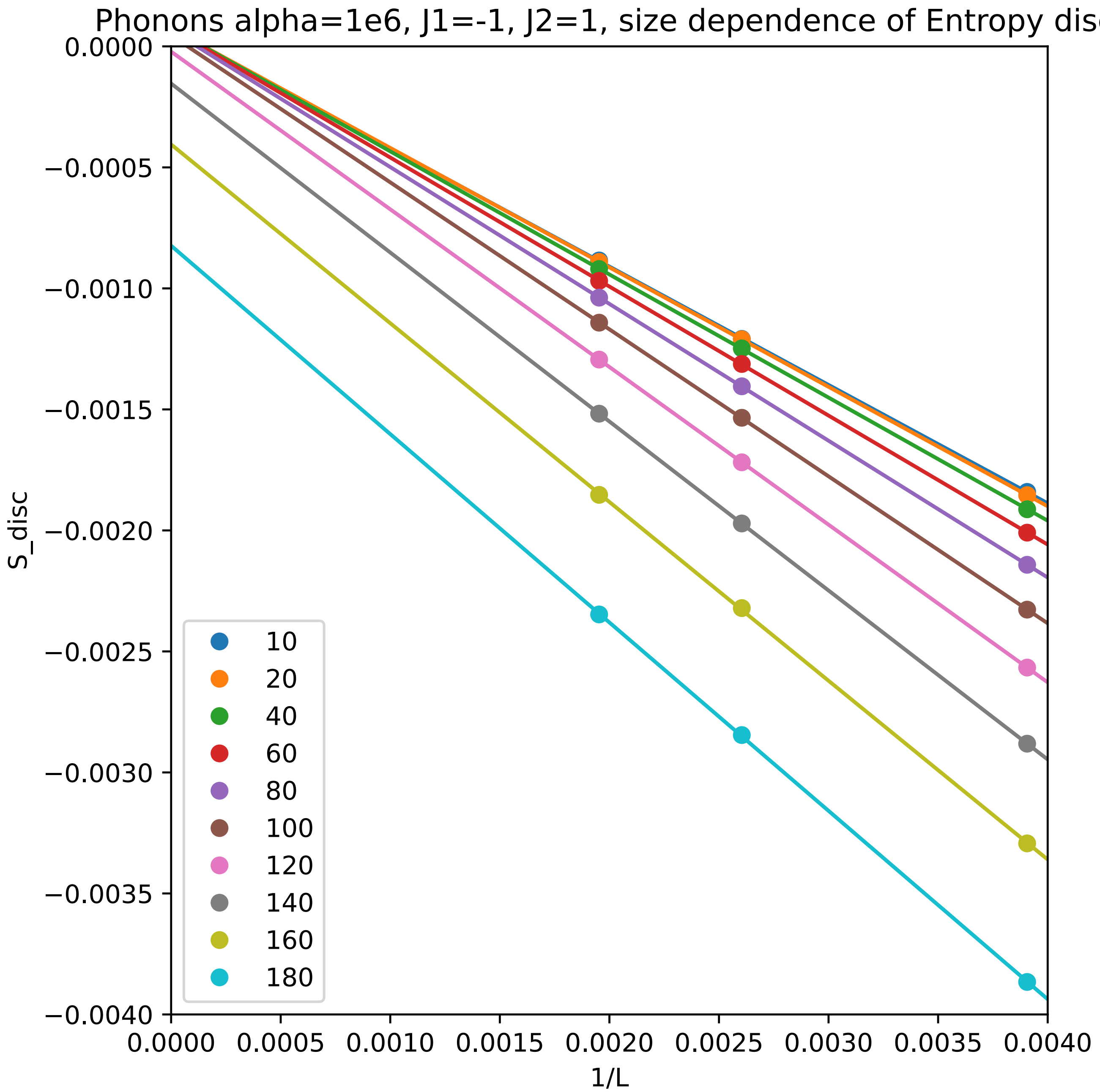
Gibbs free energy density

$$\frac{G}{V} = -\Delta + \frac{1}{2}\mu_k \tilde{\epsilon}_k^2 + \frac{N_s}{2\beta V}\sum_{\vec{q}} \ln \tilde{K}_{\vec{q}} + \frac{1}{2\beta V}\sum_{\vec{q}} \mathrm{tr}\ln\left(\tilde{D}_{\vec{q}}^{-1}\right) + \frac{N_s}{2\beta V}\sum_{\vec{q}}\left(\tilde{K}_{\vec{q}}^{-1}\Sigma_{\vec{q}}\right) + \cdots$$

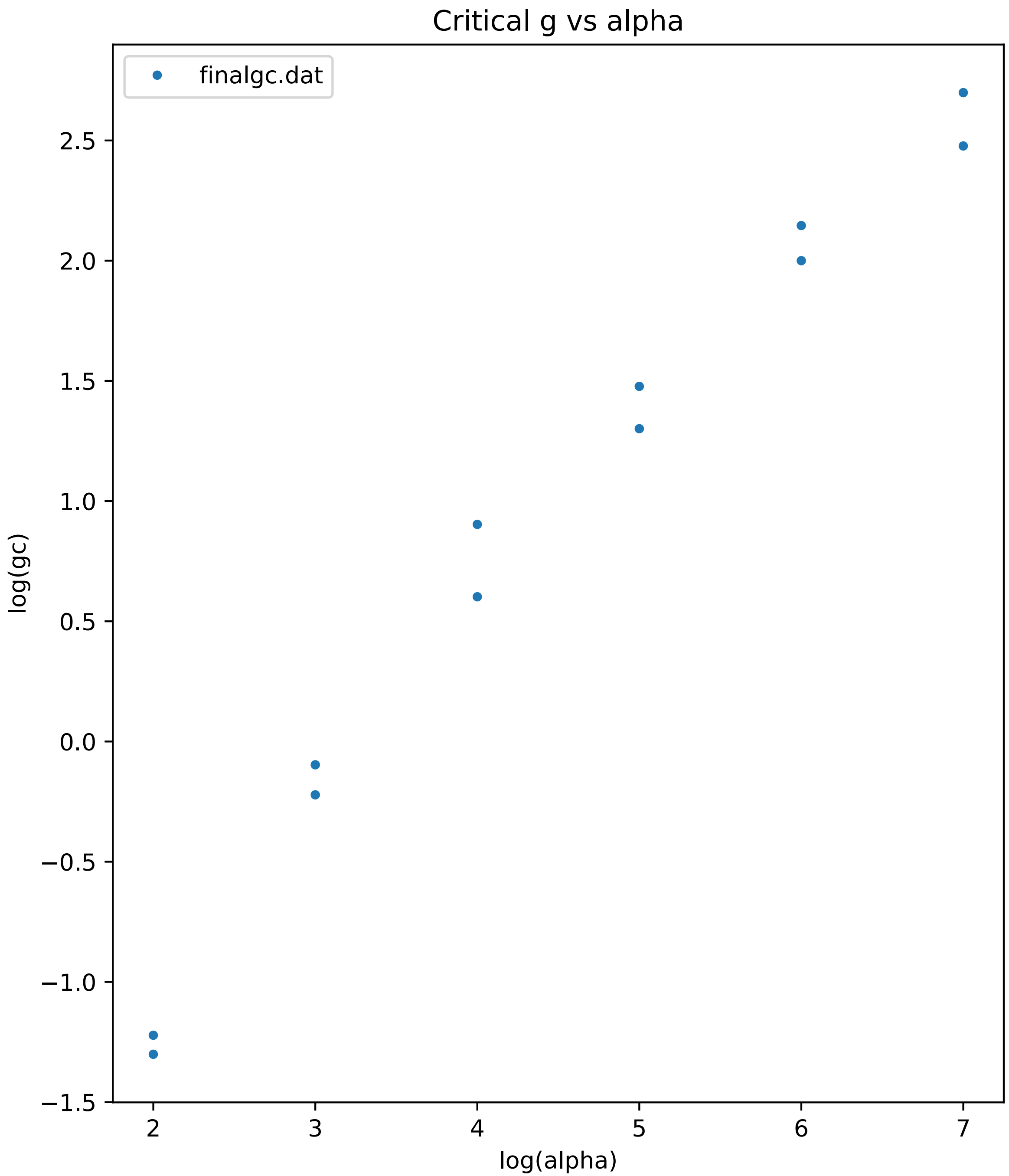




No phonons J1=-1,J2=1, L=256, inset: finite size scaling of disconti
G+1.65029*T
0.735320
0.735315
0.735310
0.735305
0.735300
0.735295
0.735290
0.735285
0.735280
0.624
0.626
0.628
0.630
0.632
0.634
T
1e−7+7.3531000000e−1
44
42
40
38
0.6275
0.6276
0.6277
T
0.0000
−0.0005
−0.0010
−0.0015
−0.0020
Disc
0.000
0.001
0.002
0.003
0.004
1/L



Phonons alpha=1e6, J1=-1, J2=1, size dependence of Entropy dis
S_disc
1/L
0.0000
−0.0005
−0.0010
−0.0015
−0.0020
−0.0025
−0.0030
−0.0035
−0.0040
0.0000
0.0005
0.0010
0.0015
0.0020
0.0025
0.0030
0.0035
0.0040
10
20
40
60
80
100
120
140
160
180


Critical g vs alpha
finalgc.dat
log(gc)
log(alpha)
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
2
3
4
5
6
7