Thermodynamic entropy and information entropy change during melting transition of hard-disk system

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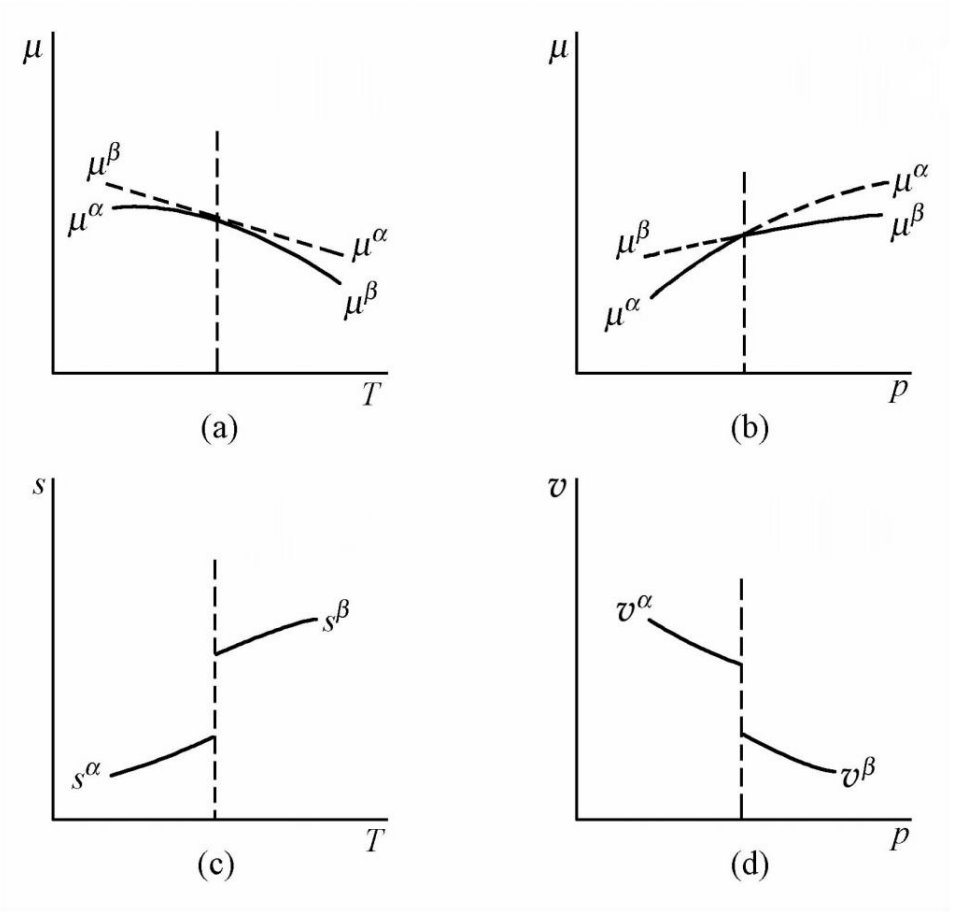
First order phase transition



Gibbs ensemble (NPT):
Minimize chemical potential μ
Derivative of μ is discontinuous

$$s = -\left(\frac{\partial \mu}{\partial T}\right)_p$$

$$v = \left(\frac{\partial \mu}{\partial p}\right)_T$$

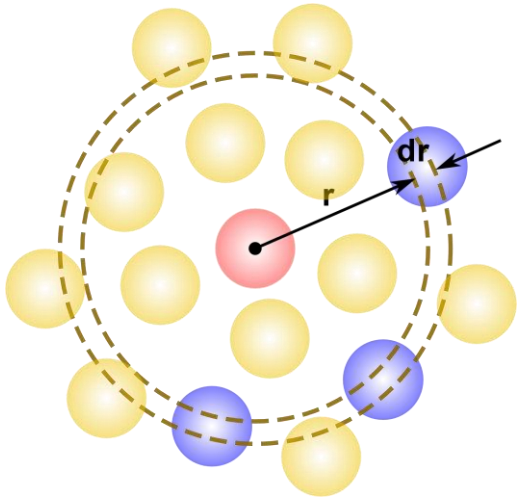
G = U – TS + pV
Hard disk: U = 0
G = -TS + pV
G, p continuous, V jump -> S jump

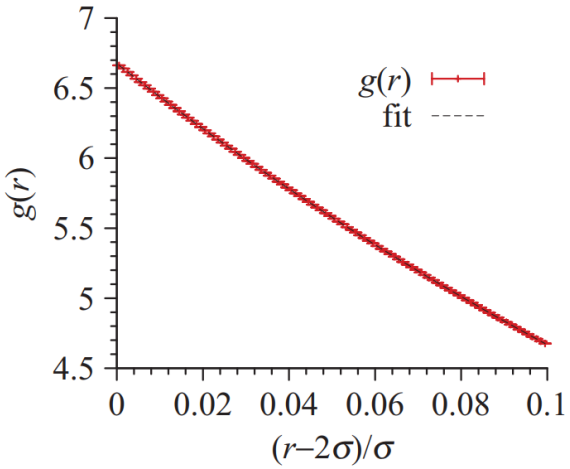
Pair correlation function (radial distribution function)

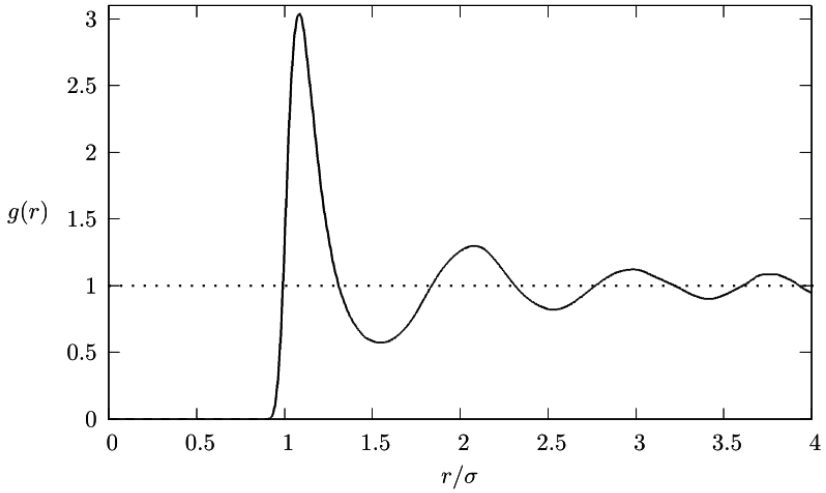
$$g(r) = \frac{L^d}{N^2}\langle \sum_i \sum_{j \neq i} \delta(\vec{r} - \vec{r}_{ij}) \rangle$$

$$g(r) = \frac{n/p}{2\pi\delta r/V}$$

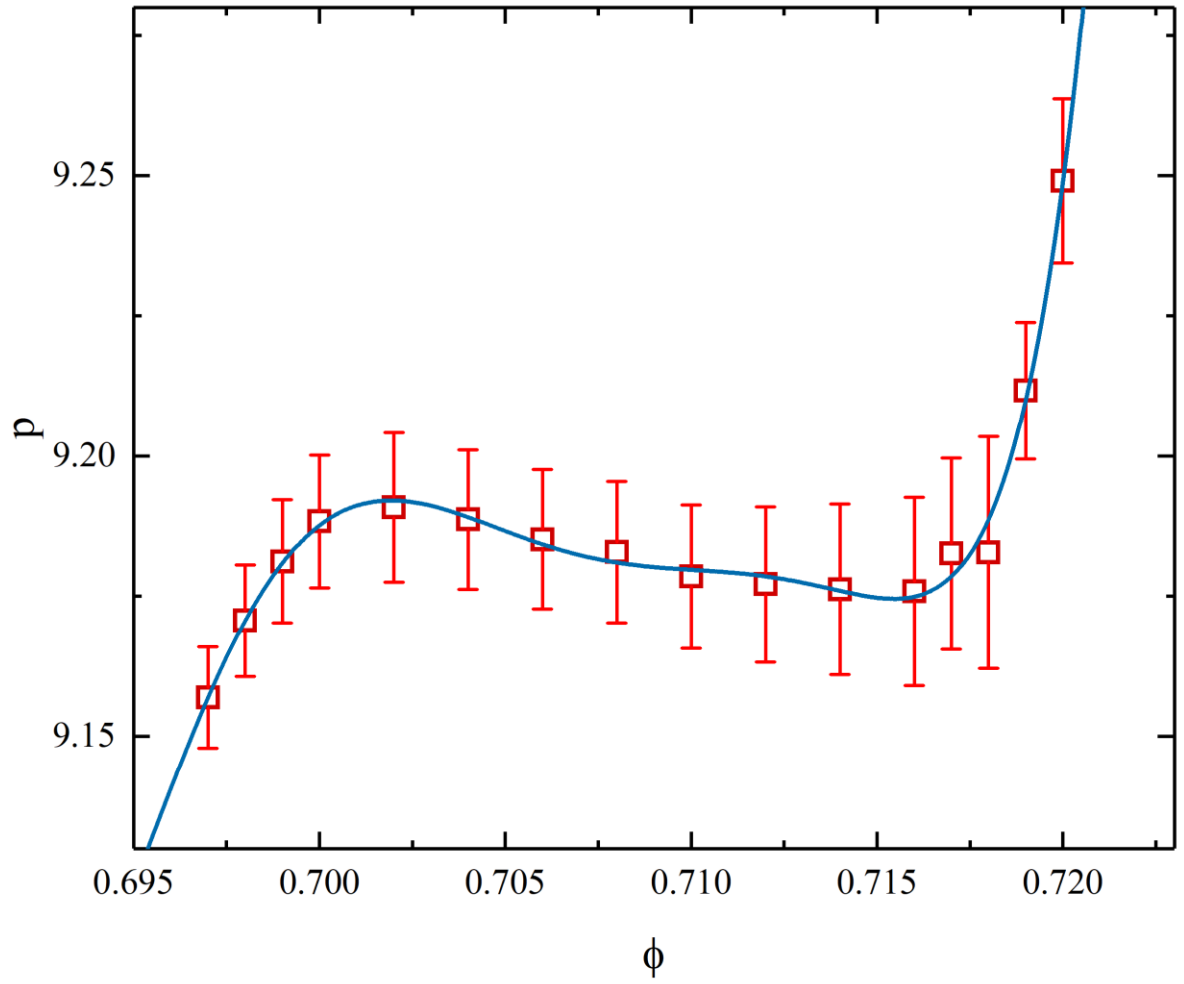
$$\beta p = \frac{N}{V}[1 + 2\phi g(2\sigma^+)]$$



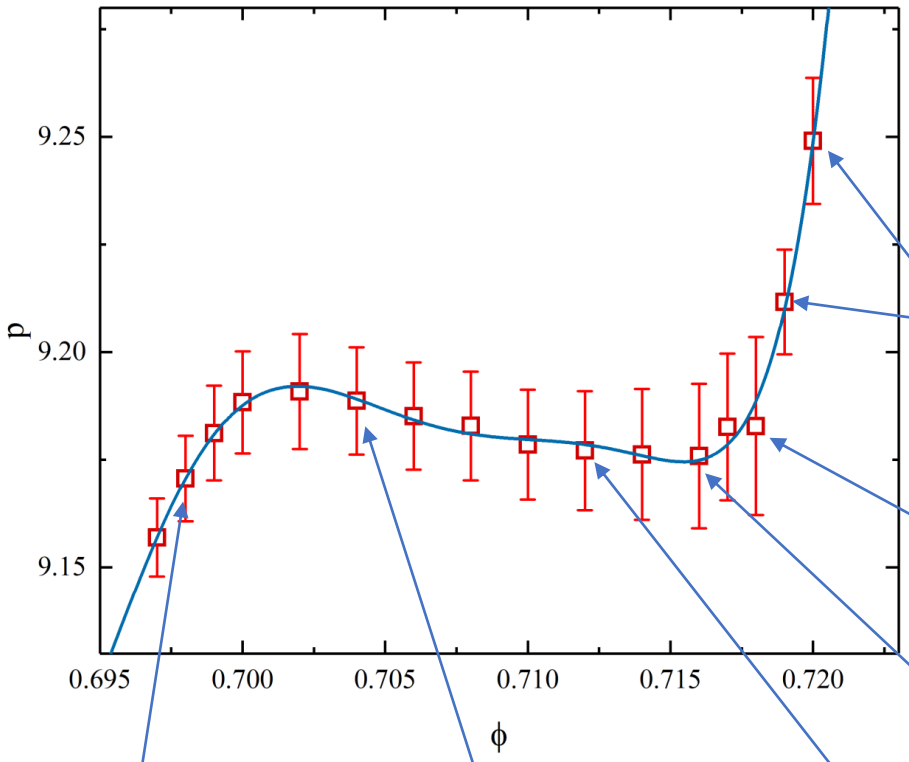




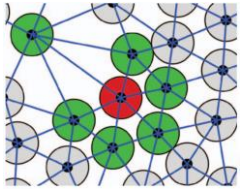
Equation of states

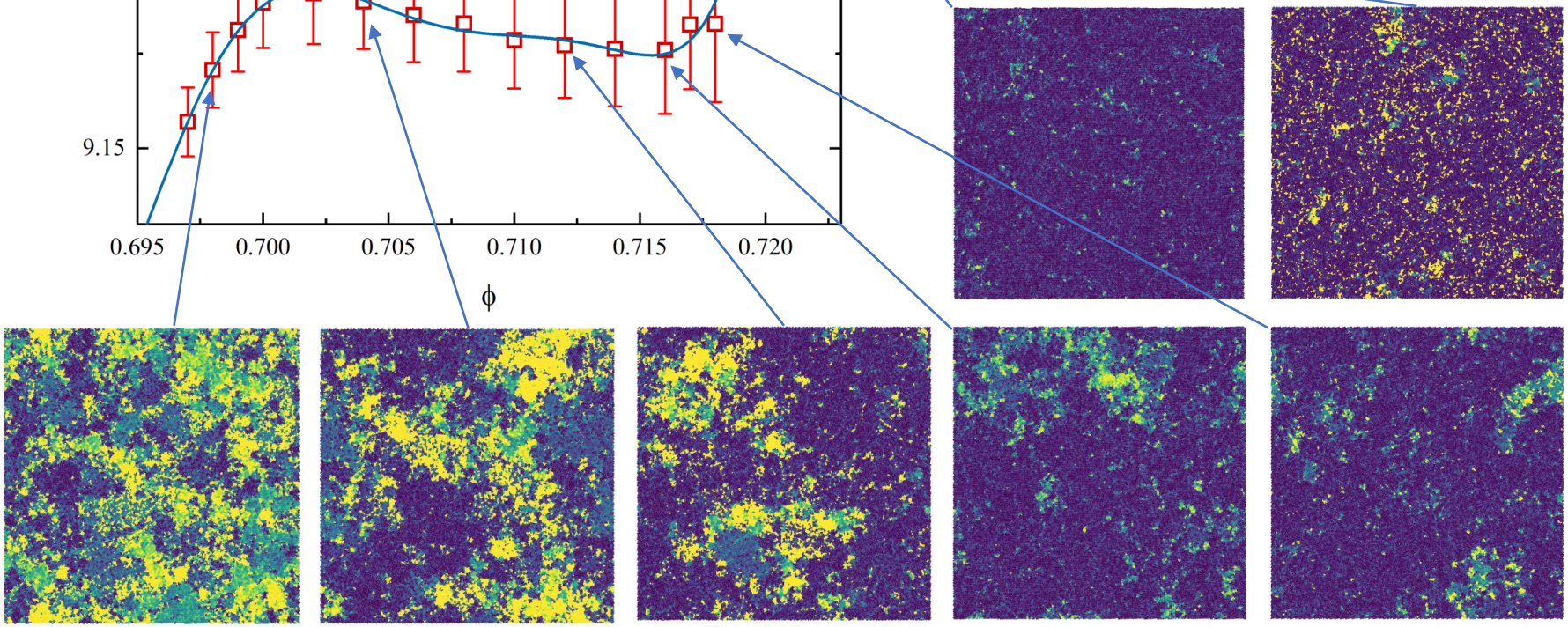


Hexatic (orientational) Order Parameter



$$\Psi_{j,6} = \frac{1}{6}\sum_{k=1}^{6} e^{i\,6\phi_{j,k}}$$





Information entropy

Shannon entropy <-> information content & order

Computable Information Density:

$$\mathrm{CID} \equiv \frac{\mathcal{L}(x)}{L}$$

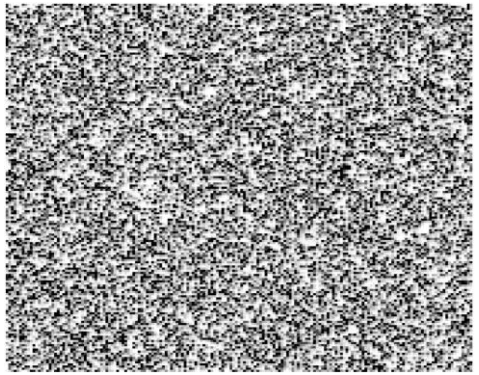
$\mathcal{L}(x)$ is the total binary code length of the compressed sequence, and L is the length of the original sequence x

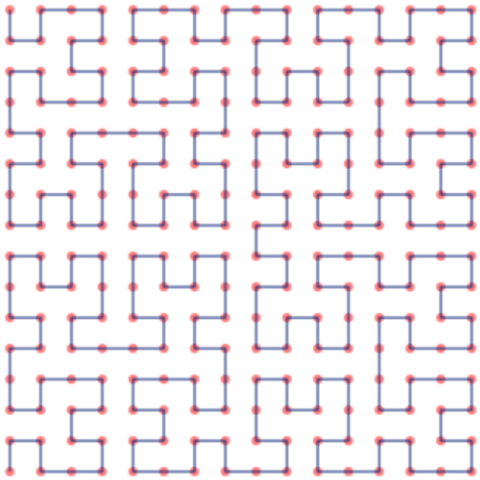
LZ77 encoding :

$$\mathcal{L}_{LZ77}(x) \approx C\log C + 2C\log\frac{L}{C}$$

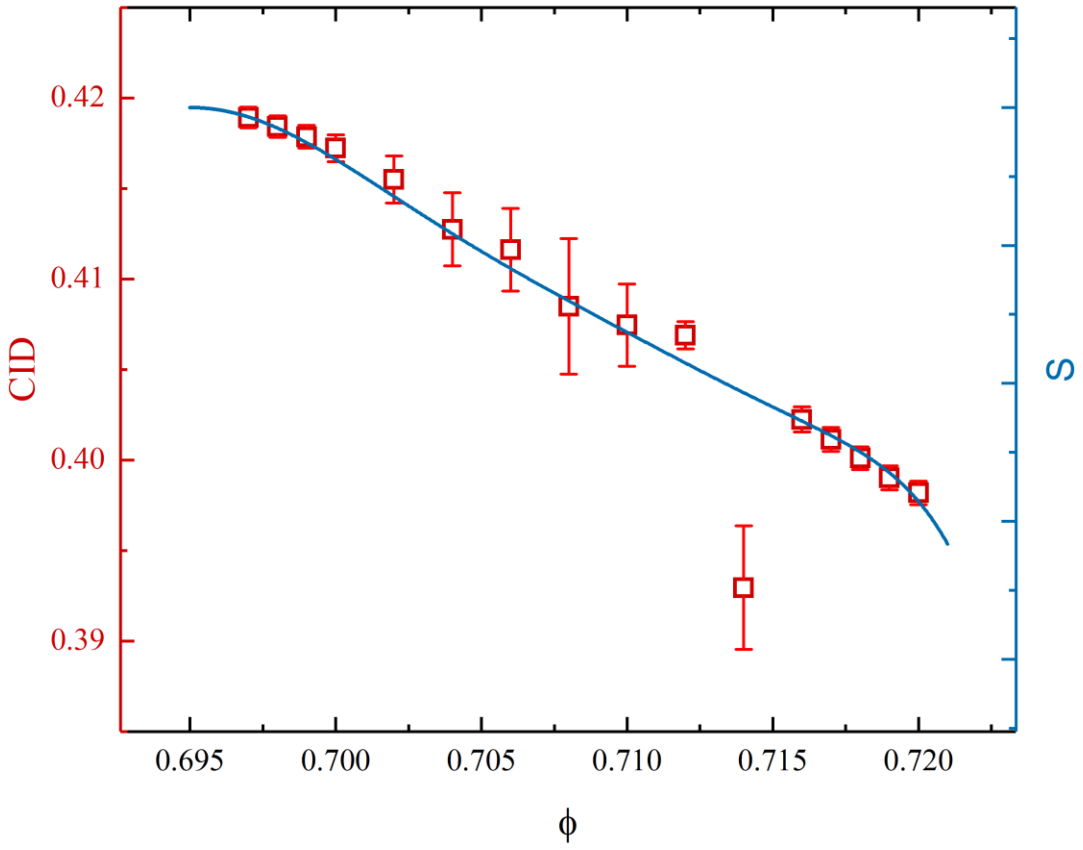
C is the number of the longest previous factor, L is the length of the original sequence.

Image -> data sequence: Hilbert curve





CID & thermodynamic entropy

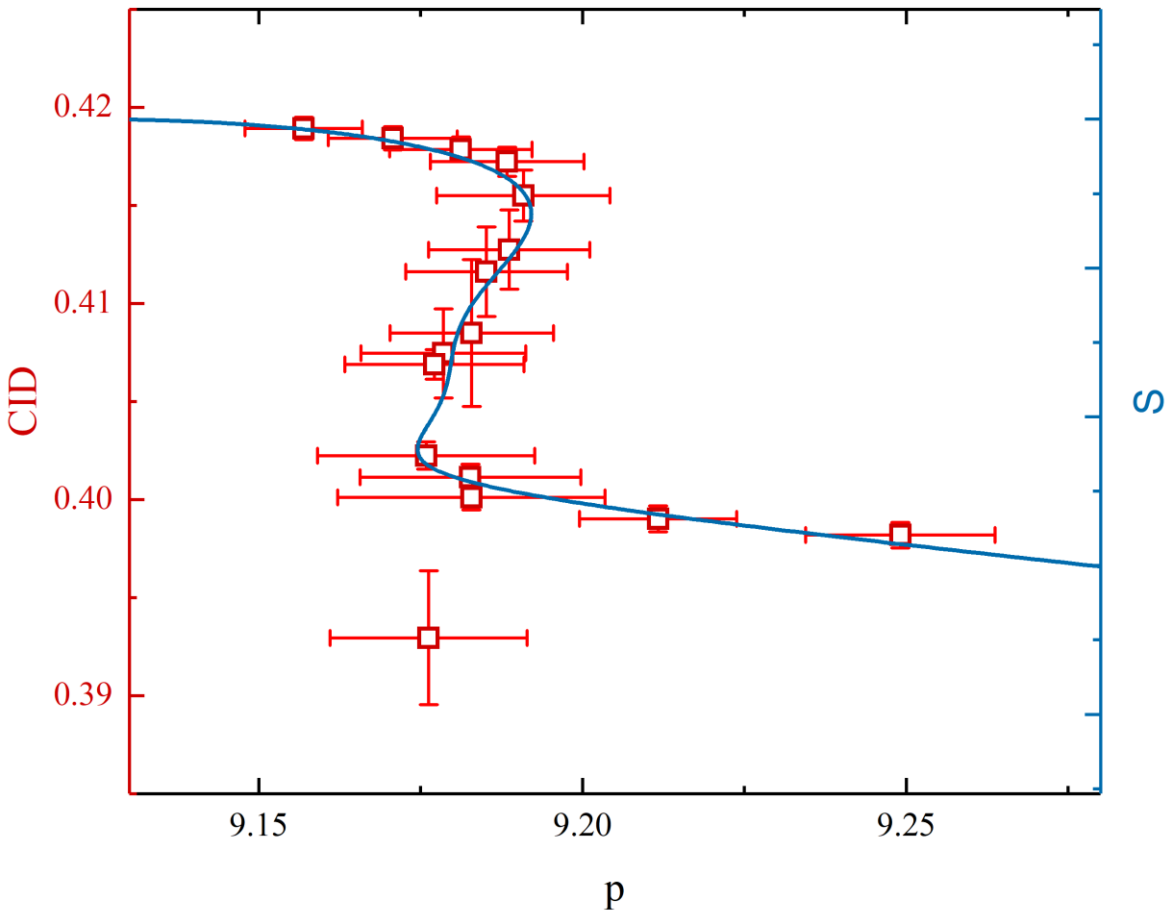


CID: from image compression

S: from integrating the equation of states

$$p = -\left(\frac{\partial F}{\partial V}\right)_{T,N} \quad \rightarrow \quad F \propto -S$$

Discontinuity of entropy in Gibbs ensemble



$\phi \rightarrow p$: NPT & NVT ensembles are equivalent in thermodynamic limit

Next steps

Discover the effect of coarse graining grid size Δ on the calculation of CID, try to find the relation between Δ and the mapping coefficients from CID to thermodynamic entropy.

Go larger systems, N>=1024^2.

Gibbs ensemble, constant pressure Monte Carlo.

Systems with soft interacting potential, melting along temperature coordinate with fixing density.