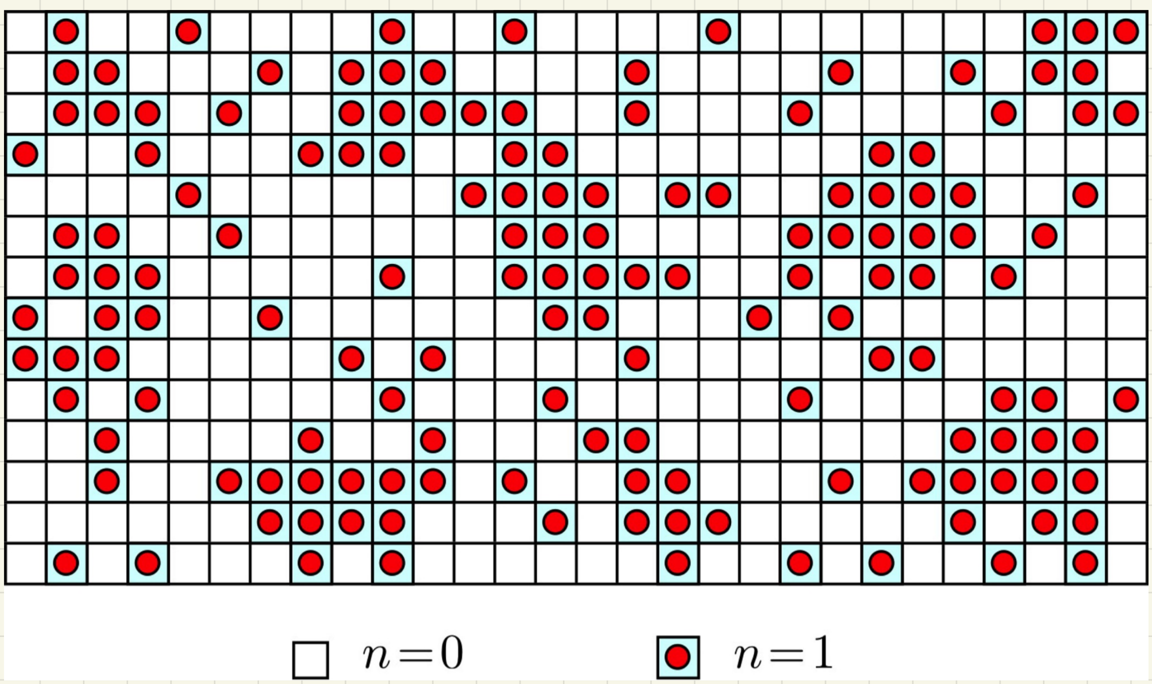
Lattice Gas Model of a Fluid

Recall $\Xi(T,V,\mu) = \sum_{N=0}^{\infty} \frac{e^{N\beta\mu}}{N!} \lambda_T^{-dN} \int \prod_{i=1}^{N} d^d x_i \, e^{-U/k_B T}$

with $U = \sum_{i<j} u(|\vec{x}_i - \vec{x}_j|)$

Lattice gas approximation: divide space into cubic cells of volume a^d where $a \gtrsim$ molecular size



Then $\Xi = \sum_{\{n_{\vec{R}}\}} \prod_{\vec{R}} \zeta^{n_{\vec{R}}} \exp\left(-\frac{1}{2k_B T} \sum_{\vec{R},\vec{R}'} V_{\vec{R}\vec{R}'} \, n_{\vec{R}} n_{\vec{R}'}\right)$

with $\zeta = e^{\beta\mu} \lambda_T^{-d} a^d$ and $V_{\vec{R}\vec{R}'} = u(|\vec{R} - \vec{R}'|)$

Defining $n_{\vec{R}} = \frac{1}{2}(1 + \sigma_{\vec{R}})$ with $\sigma_{\vec{R}} = \pm 1$, and

$$J_{\vec{R}\vec{R}'} \equiv -\frac{1}{4} V_{\vec{R}\vec{R}'} \,, \quad H \equiv \frac{1}{2} k_B T \log z - \frac{1}{4} \sum_{\vec{R}'}{}' \, V_{\vec{R}\vec{R}'} \quad \leftarrow \vec{R}' \neq \vec{R}$$

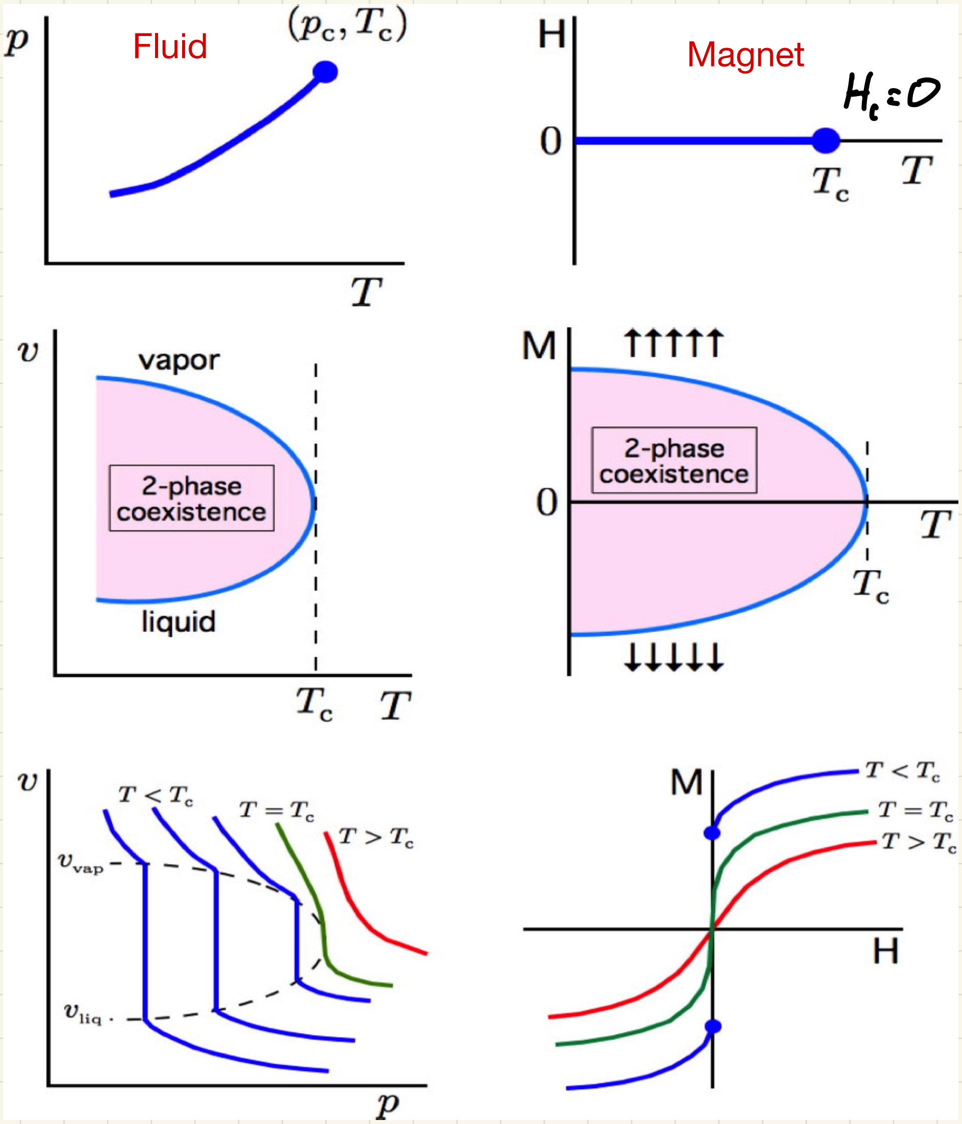
$$E_0 \equiv \frac{1}{8} \sum_{\vec{R} \neq \vec{R}'} V_{\vec{R}\vec{R}'}$$

we arrive at

$$\Xi = \mathrm{Tr}\, e^{-\beta \hat{H}_{LG}}$$

with $$\hat{H}_{LG} = -\frac{1}{2} \sum_{\vec{R},\vec{R}'} J_{\vec{R},\vec{R}'} \sigma_{\vec{R}} \sigma_{\vec{R}'} - H \sum_{\vec{R}} \sigma_{\vec{R}} + E_0$$

which is the Ising model in an external field.



$$\kappa_T = -\frac{1}{v} \frac{\partial v}{\partial p}\bigg|_T$$

isothermal compressibility

$$\chi_T = \frac{\partial m}{\partial H}\bigg|_T$$

isothermal susceptibility

$N_c = \#$ sites, $N = \frac{1}{2}(M + N_c) = \#$ occupied $(n_{\vec{R}} = 1)$ sites

Magnetization density: $m = \frac{1}{N_c} \sum_{\vec{R}} \langle \sigma_{\vec{R}} \rangle$ order parameter

In the vicinity of a critical point,

$$m(T, H_c) \propto (T_c - T)_+^{\beta}, \quad \chi(T, H_c) \propto |T - T_c|^{-\gamma}$$

$$C_M(T, H_c) \propto |T - T_c|^{-\alpha}, \quad m(T_c, H) \propto \pm |H|^{1/\delta}$$

Exponent equalities: $\alpha + 2\beta + \gamma = 2$ (Rushbrooke)

$\beta + \gamma = \beta\delta$ (Griffiths)

(there are others)

Correlations: $C(\vec{r}, T, H) = r^{-(d-2+\eta)} \phi(r/\xi, H/\xi_H)$

where $\xi(T) \propto |T - T_c|^{-\nu}$ and $\xi_H(T) \propto |T - T_c|^{\Delta}$ with

$$\Delta = \beta\delta, \quad (2-\eta)\nu = \gamma, \quad d\nu = 2 - \alpha$$

(hyperscaling)