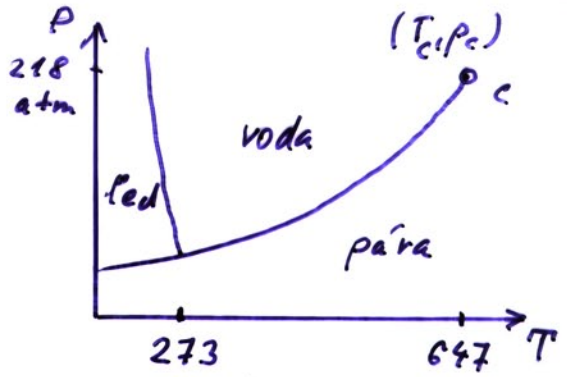
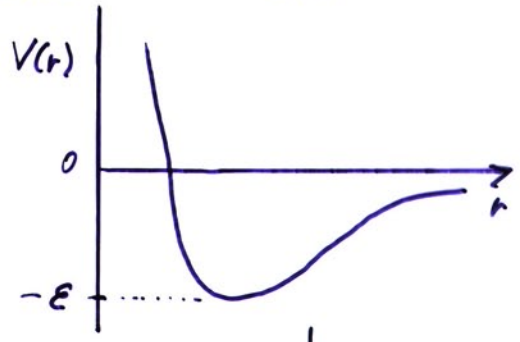
FÁZOVÝ PŘECHOD KAPALINA – PÁRA

parametr uspořádání:
hustota ρ



- nejjednodušší spojitý model
  Lennard – Jones

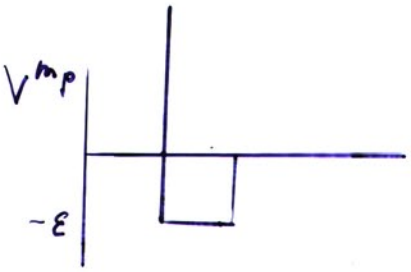
$$V^{(LJ)}(r) = 4\varepsilon\left[\left(\frac{r_0}{r}\right)^{12} - \left(\frac{r_0}{r}\right)^{6}\right]$$



potenciální energie:

$$E = \sum_{IJ} V(\vec{r}_I - \vec{r}_J)$$

- mřížový plyn
  rozdělme prostor na



$\square \leftarrow i$ $\quad n_i = \begin{cases} 0 \\ 1 \end{cases}$ i $\quad V_{ij}^{(mp)} = \begin{cases} \infty & i=j \\ -\varepsilon & i,j \text{ sousedi} \\ 0 & \text{ostatní} \end{cases}$

$$E^{(mp)} = -\sum_{\langle ij\rangle} \varepsilon n_i n_j, \quad N = \sum_i n_i, \quad \rho = \frac{1}{L^d} N$$

grand kanonická partiční suma

$$Z = \sum_{\{n_i\}} \exp\left\{\beta\varepsilon \sum_{\langle ij\rangle} n_i n_j - \mu \sum_i n_i\right\}$$

při $n_i = \frac{s_i + 1}{2}$ ekvivalentní Isingově modelu

$$E^{(mp)} - \mu N = -\frac{\varepsilon}{4}\sum_{\langle ij\rangle} s_i s_j - \sum_i \left(\frac{\mu}{2} + \frac{\varepsilon}{4} c\right) s_i - \frac{L^d}{2}\left(\mu + \frac{\varepsilon}{4} c\right)$$

c .... konektivita = počet nejbližších sousedů

$$J = \frac{\varepsilon}{4}, \quad h = \frac{\mu}{2} + \frac{\varepsilon c}{4}, \quad M = 2\rho - 1$$

Kritické exponenty pro Isingův model

exponent	střední pole	2 d Ising	3d Ising
α	nespojitost	0	0.119± 0.006
β	1/2	1/8	0.326± 0.004
γ	1	7/4	1.239± 0.003
δ	3	15	5
η	1/2	1	0.627± 0.002
ν	0	1/4	0.024± 0.007

Srovnání: kritický bod kapalina/para

Landau-Ginzburg model 3d Ising exper. data

	$\phi^4, d = 3$	Ising, $d = 3$	Fluid
α	0.110 ± 0.005	0.119 ± 0.006	0.101 − 0.116
β	0.325 ± 0.002	0.326 ± 0.004	0.316 − 0.327
γ	1.241 ± 0.002	1.239 ± 0.003	1.23 − 1.25
η	0.032 ± 0.005	0.024 ± 0.007	−
ν	0.630 ± 0.002	0.627 ± 0.002	0.625 ± 0.006

Srovnání: magnetický kritický bod

Landau-Ginzburg model exper. data Heisenbergův model

	$\phi^4, D = 3, d = 3$	Ni	Heisenberg. $d = 3$
α	−0.115 ± 0.009	0.04 ± 0.12	− 0.14
β	0.368 ± 0.004	0.358 ± 0.003	0.3
γ	1.390 ± 0.010	1.33 ± 0.02	1.43
ν	0.710 ± 0.007	0.64 ± 0.10	0.7

Kritické exponenty pro Isingův model

exponent	střední pole	2 d - Onsager	3d rozvoj vysoké T
α	nespojitost	0	0.119± 0.006
β	1/2	1/8	0.326± 0.004
γ	1	7/4	1.239± 0.003
δ	3	15	5
η	1/2	1	0.024± 0.007
ν	0	1/4	0.627± 0.002

Srovnání Isingův model vs. experiment

exponent	IM - 3d	exper. data - Ni	exper. data fluid
α	0.119± 0.006	0.04± 0.12	0.101 - 0.116
β	0.326± 0.004	0.358± 0.003	0.316 - 0.327
γ	1.239± 0.003	1.33± 0.02	1.23 - 1.25
ν	0.627± 0.002	0.64± 0.1	0.625 ± 0.006