Liquid-gas spinodal and the interfacial properties from the lattice gas-fluid isomorphism approach

Kulinskii V. L.

Department for Theoretical Physics,
Odessa National University, Dvoryanskaya 2, 65026 Odessa, Ukraine

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Outline

Empirical facts

- Global cubic character of the binodal of simple liquids;

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- Batchinsky law (Zeno-Line)

PCS

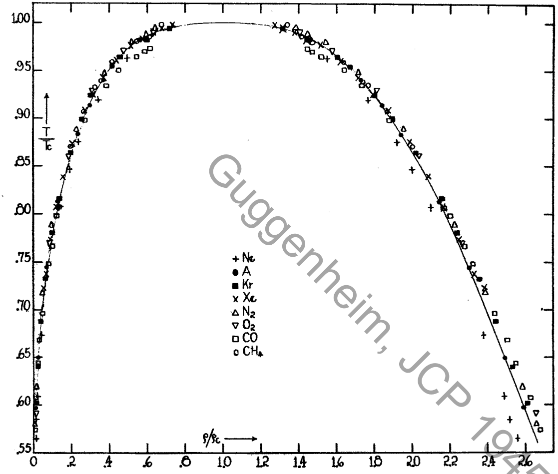
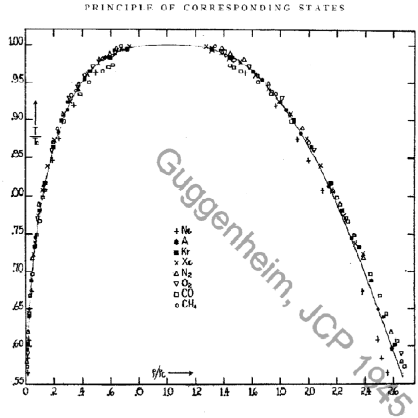

1.00
.95
.90
.85
.80
.75
.70
.65
.60
.55
T/Tc
ρ/ρc
0
.2
.4
.6
.8
1.0
1.2
1.4
1.6
1.8
2.0
2.2
2.4
2.6
+ Ne
● A
■ Kr
× Xe
△ N2
▽ O2
□ CO
o CH4
Guggenheim, JCP 1945

FIG. 2.

PCS and Global cubic character of the binodal



$$\frac{\rho_l}{\rho_c} = 1 + \frac{3}{4}\left(1 - \frac{T}{T_c}\right) + \frac{7}{4}\left(1 - \frac{T}{T_c}\right)^{\frac{1}{3}}$$

$$\frac{\rho_g}{\rho_c} = 1 + \frac{3}{4}\left(1 - \frac{T}{T_c}\right) - \frac{7}{4}\left(1 - \frac{T}{T_c}\right)^{\frac{1}{3}}$$

LRD: Cailletet&Mathias, 1886

Law of Rectilinear Diameter

$$n_d = \frac{n_l + n_g}{2n_c} = 1 + A\,\frac{T_c - T}{T_c}\ .$$

LRD: present time

Liquid–vapor coexistence curves for model potentials 9167

Okumura&Yonezawa, JCP v.113 (2000)

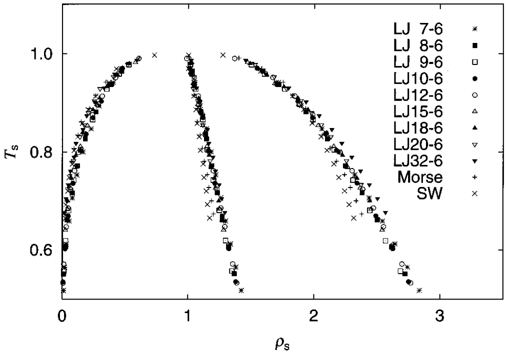


FIG. 8. The liquid–vapor coexistence curves and the diameters in the scaled temperature $T_s = T^*/T_c^*$ – density $\rho_s = \rho^*/\rho_c^*$ plane.

Zeno-Line

$$\mathrm{Z} = \mathrm{P}/(\mathrm{n\,T}) = 1$$

Zeno-Line

$$Z = P/(n\,T) = 1$$

$$Z = \frac{P}{n\,T} = 1 - \frac{2\pi\,n}{3\,T}\int r^3 \frac{\partial\,\Phi(r)}{\partial\,r}\,g_2(r;n,T)\,d\,r\,,$$

g_2 - pair correlation function.

Zeno-Line

$$Z = 1 \Rightarrow \int r^3 \frac{\partial \Phi(r)}{\partial r} g_2(r; n, T) \, d\, r = 0$$

Condition:

$$g_2(r; n, T) = 0$$

defines “ideal-gas“ states (line $n = 0$ included trivially)

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Complete configurational order

$n = n_B$ - dense packing $\Rightarrow$ $g_2 = 0$

Batchinsky law

$$P(n,T) = \frac{n\,T}{1 - n\,b} - a\,n^2$$

Zeno-Line

$$P(n,T) = \frac{n\,T}{1-n\,b} - a\,n^2$$

$$\frac{P(n,T)}{n\,T} = \frac{1}{1-n\,b} - a\,\frac{n}{T} = 0$$

Batchinsky law

$$\frac{P(n,T)}{n\,T} = \frac{1}{1-n\,b} - a\,\frac{n}{T} = 0$$

$$\frac{P(n,T)}{n\,T} = 1 \Rightarrow \frac{n}{n_B} + \frac{T}{T_B} = 1\,, \quad n_B = 1/b\,, T_B = a/b$$

Batchinsky law

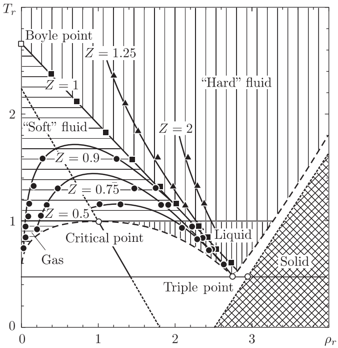

Figure : Simple fluid phase diagram (methane), $\tilde{T} = T/T_c$, $\tilde{n} = n/n_c$, $Z = P/(n\,T) = 1$ - Zeno-Line. States $Z > 1$ "hard fluid", $Z < 1$ "soft fluid" (Ben-Amotz&Herschbach, 1990).

Triangle of Liquid-Gas States

Characteristic properties (E. Apfelbaum and V. Vorob'ev)

- ZL is the tangent to the binodal in $n = n_B\,,\quad T \to 0$
- "Median"

$$\frac{n}{n_B/2} + \frac{T}{T_B} = 1$$

at "low" temperatures is close to the (rectilinear) diameter

Simplest fluid - Ising model (lattice gas)

$$H = -J \sum_{\langle ij \rangle} n_i n_j - \mu \sum_i n_i \,, \quad n_i = 0, 1$$

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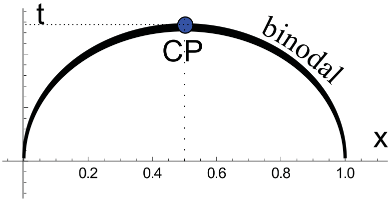

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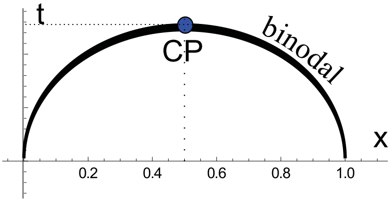


Order parameter $x = \langle n_i \rangle$ - lattice density.

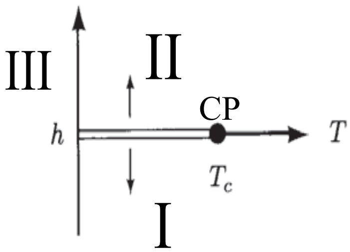
Liquid vs. Gas

J.D. van der Waals, Nobel lecture, 1910

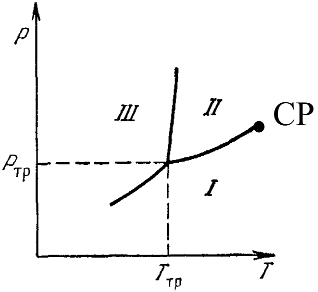
... Thus I conceived the idea that there is no essential difference between the gaseous and the liquid state of matter - that the factors which, apart from the motion of the molecules, act to determine the pressure must be regarded as quantitatively different when the density changes and perhaps also when the temperature changes, but that they must be the very factors which exercise their influence throughout. And so the idea of continuity occurred to me ...

Liquid vs. Gas

Ising model



Fluid



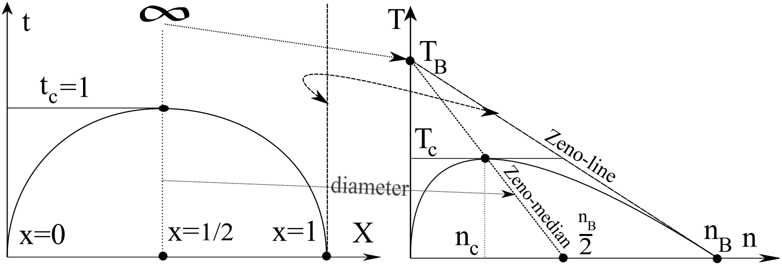


Figure : Correspondence between the linear elements of the phase diagrams. Zeno-Line and Zeno-median are shown. The latter coincides with the rectilinear diameter.

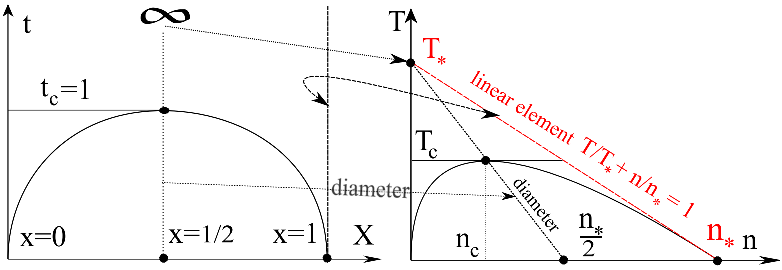


Figure : Correspondence between the linear elements of the phase diagrams. Zeno-line, generally, is not linear and we introduce the linear element $T/T_* + n/n_* = 1$

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$$\text{Zeno-Line} \quad x = 1 \Leftrightarrow \quad \frac{n}{n_*} + \frac{T}{T_*} = 1\,.$$

$$n/n_* = \frac{x}{1 + a\,t}\,, \quad T/T_* = \frac{a\,t}{1 + a\,t}\,, \quad a = \frac{T_c}{T_B - T_c}\,.$$

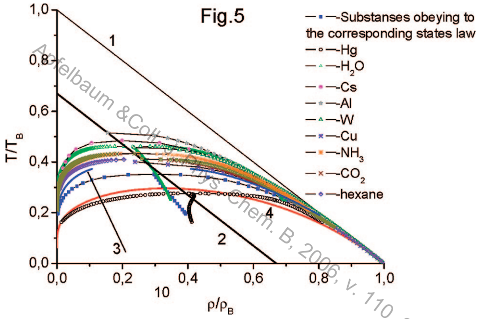
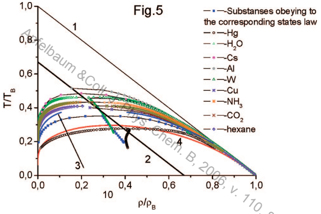


Figure 5. Dependence of the temperature and density along the phase coexistence curves on parameters reduced to the Zeno-line parameters for the different model systems and substances: (line 1) $Z = 1$ line, (line 2) critical points line, (line 3) Lennard-Jones numerical modeling of ref 11, (line 4) according to the van der Waals equation. The symbols correspond to the different substances. We have added the average diameter for Hg, water, and substances satisfying the corresponding states law.



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$$T_c = T_* \frac{z}{1+z}\,, \quad n_c = \frac{n_*}{2(1+a)}\,.$$

Line of the critical points for the substances with z fixed:

$$\frac{n_c}{n_B} + \frac{T_c}{T_B} = \frac{2z+1}{2\,(\,1+z\,)}$$

Global isomorphism

$$n = n_* \frac{x}{1 + a\,t}\,, \qquad T = T_* \frac{a\,t}{1 + a\,t}\,,$$

$$x = \frac{n}{n_*}\left(1 - T/T_*\right), \qquad t = \frac{1}{a}\,\frac{T/T_*}{1 - T/T_*}$$

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- thermodynamic similarity class parameter. For 3D LJ $a = 1/2$.

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$$T/T_* + n/n_* = 1 \Leftrightarrow x = 1$$

T_* - Boyle temperature in vdW approximation,
$T^* = T_B^{vdW} = a_{vdW}/b$ and:

$$n_* = T_* \frac{B_2'(T_*)}{B_3(T_*)}$$

Mapping between binodals of the lattice gas and the fluid

Ising model (lattice gas) binodal maps onto the binodal of the fluid

$$\boxed{n(t) = n_* \frac{x(t)}{1 + a\,t}\,, \;\; T(t) = T_* \,\frac{a\,t}{1 + a\,t}}$$

Mapping between binodals of the lattice gas and the fluid

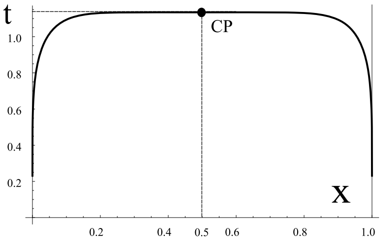

Figure : Binodal of 2D Ising model (Onsager exact solution).

$$x(t) = 1/2 \pm f(t)^{1/8}\,, \quad f(t) = 1 - \frac{1}{\sinh^4(\,2J/t\,)}$$

Mapping between binodals of the lattice gas and the fluid

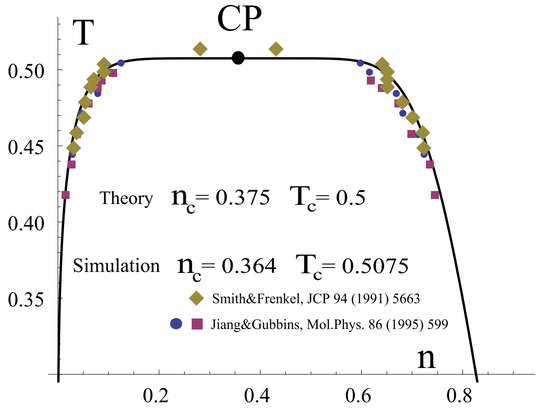

Figure : Binodal of 2D Lennard-Jones fluid $a = 1/3$, $T_* = 2.03 \approx T_B^{(vdW)} = 2$ and $n_* = 0.971$ ($n_*^{(theor)} = 0.91$) and the simulations data (Smith& Frenkel).

Mapping between binodals of the lattice gas and the fluid

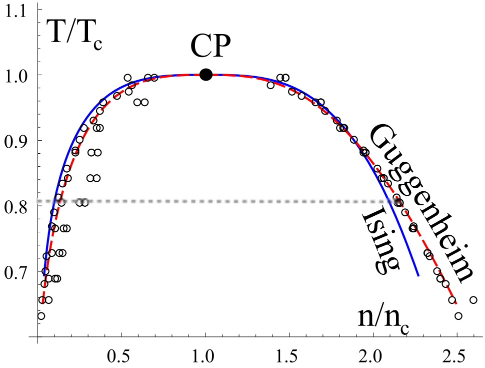

Figure : Binodal of 3D L-J fluid (blue) obtained via mapping (with $a = 1/2$) of the binodal of 3D Ising model (numerical data). Red line is the Guggenheim cubic law.

Scaling nature of z

Scaling symmetry

Different liquids differs by T_c and n_c because of different scales for energy interaction and the molecular sizes. The lattice gas hamiltonian obeys the scaling symmetry:

$$t_c \to \lambda^2\, t_c\,,\;\; x_c \to \lambda^{-1}\, x_c$$

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$$\frac{d\ln\left(\frac{T_c}{T_*}\right)}{d\ln\left(\frac{n_c}{n_*}\right)} = -\frac{1}{a}$$

Consistency condition

The attractive part of the potential in d dimensions has the form $\Phi_{attr}(r) \sim r^{-(d+\varepsilon)}$, $\varepsilon > 0$. The energy of interaction is:

$$E_{int} = \frac{1}{2}\sum_{i,j}\Phi_{attr}(|r_i - r_j|) = \frac{V}{2}\int \Phi_{attr}(r_{12})\, n(r_1)\, n(r_2)\, dr_{12}$$

$$n_c \sim \frac{1}{r_c^d}\,, \quad T_c \sim \Phi(r_c) \sim \frac{1}{n_c^{1+\varepsilon/d}}$$

naive scaling:

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naive scaling:

$$n_c \to n_c(0)\, e^{-\lambda}\,, \quad T_c \to T_c(0)\, e^{(1+\varepsilon/d)\lambda}\,.$$

Consistency condition

naive scaling:

$$-\frac{1}{a} = \frac{d\ln\left(\frac{T_c}{T_*}\right)}{d\ln\left(\frac{n_c}{n_*}\right)} = -\left(1+\frac{\varepsilon}{d}\right) \quad \Rightarrow \quad a = \frac{1}{1+\frac{\varepsilon}{d}}\,.$$

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For LJ-systems with $\Phi_{attr} \propto r^{-6}$ in d dimensions $z = \frac{d}{6}$:

$$\boxed{d = 2:\ a = 1/3\,, \quad d = 3:\ a = 1/2}$$

CP in d-dimensions

$$\frac{T_c}{T_*} = \frac{1}{2+\frac{\varepsilon}{d}}\,, \quad \frac{n_c}{n_*} = \frac{1+\frac{\varepsilon}{d}}{2\left(2+\frac{\varepsilon}{d}\right)}\,.$$

$$T_* = \frac{4d}{6-d}\,, \quad a_{vdW} = 2^{d-1}\,\frac{4d}{6-d}\,, \quad b = 2^{d-1}\,,$$

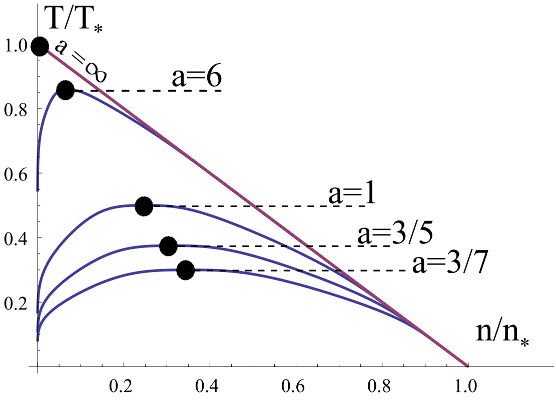
hard core volume is normalized so that $n_* = 1$.

Comparison with the simulations

LJ “6-12“ fluid	2D	3D	4D	5D
T_c	0.5	1.33	3.2	9.1
$T_c^{(num)}$	0.515	1.312	3.404	8.8 (?)
n_c	0.375	0.33	0.3	0.27
$n_c^{(num)}$	0.355	0.316	0.34	-

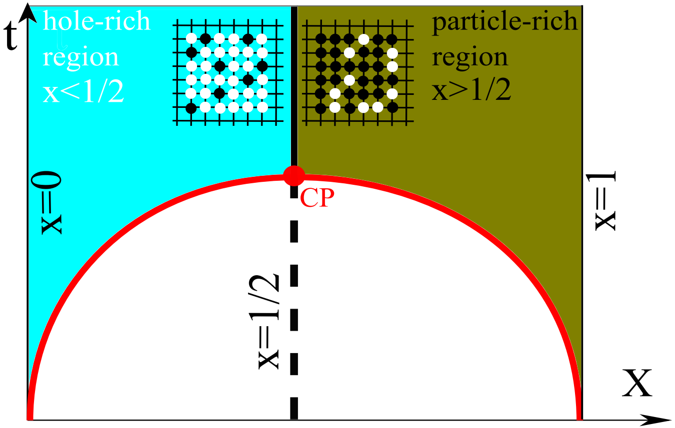
Binodal as function of a

Binodal as function of z

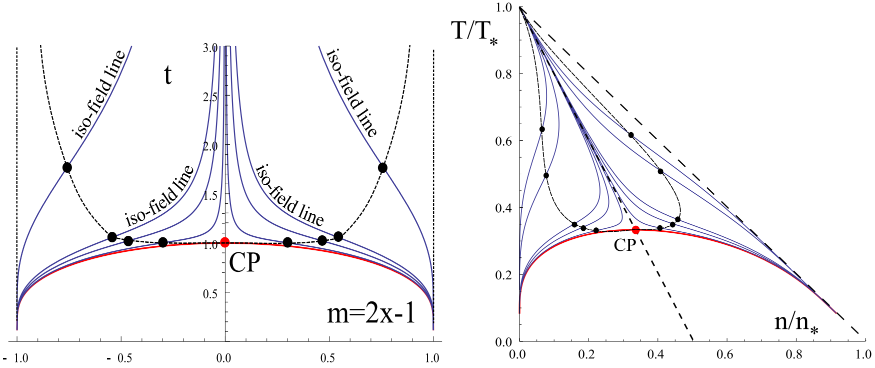


$a \to \infty$ Flory θ-point?

“particle-hole“ symmetry



Correspondence of thermodynamic states



$$n/n_* = \frac{x}{1 + a\,t}\,, \quad T/T_* = \frac{a\,t}{1 + a\,t}\,.$$

Connection between lattice and fluid

Proposition

Projective form of the lattice-fluid transformation is the consequence of the projective nature of the thermodynamic limit:

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Projective form of the lattice-fluid transformation is the consequence of the projective nature of the thermodynamic limit:

$$\text{FLUID} \quad \begin{pmatrix} \mathrm{U} \\ \mathrm{S} \\ \mathrm{V} \\ \mathrm{N} \end{pmatrix} = \hat{\mathrm{L}} \begin{pmatrix} \mathfrak{U} \\ \mathfrak{S} \\ \mathfrak{N} \\ \mathcal{N} \end{pmatrix} \quad \text{Ising Model}$$

Relation between bulk thermodynamic potentials

$$\mathrm{n}/\mathrm{n}_* = \frac{\mathrm{x}}{1 + \mathrm{a}\,\mathrm{t}}\,, \quad \mathrm{n} = \left.\frac{\partial\,\mathrm{J}}{\partial\,\mu}\right|_{\mathrm{T}}\,, \quad \mathrm{x} = \left.\frac{\partial\,\mathfrak{G}}{\partial\,\mathrm{h}}\right|_{\mathrm{t}}$$

we get relation between grand potentials:

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we get relation between grand potentials:

$$\mathrm{J}(\mu,\mathrm{T},\mathrm{V}) = \mathrm{P}(\mu,\mathrm{T}),\mathrm{V} = \mathfrak{G}\left(\,\mathrm{h}(\mu,\mathrm{T}),\mathrm{t}(\mathrm{T}),\mathcal{N}\,\right)$$

Relation between bulk thermodynamic potentials

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$$\mathrm{J}(\mu,\mathrm{T},\mathrm{V}) = \mathrm{P}(\mu,\mathrm{T})\,\mathrm{V} = \mathfrak{G}\,(\,\mathrm{h},\mathrm{t},\mathcal{N}\,) = \mathcal{N}\,\mathfrak{g}(\mathrm{h},\mathrm{t})$$

$$\mu - \mu_0(\mathrm{T}) = \frac{\mathrm{h}}{1+\mathrm{a\,t}}$$

$\mu_0(\mathrm{T})$ - chem. potential along coexistence curve

Relation between surface thermodynamic potentials (?)

The surface tension of 2D Ising model is determined by the next eigenvalue of the transfer matrix $\Lambda_1 < \Lambda_{\mathrm{max}}$:

$$\Sigma_{\mathrm{m}\times\mathrm{n}}^{(\mathrm{lat})} = \Lambda_{\mathrm{max}}^{\mathrm{m}} + \Lambda_1^{\mathrm{m}} + \ldots$$

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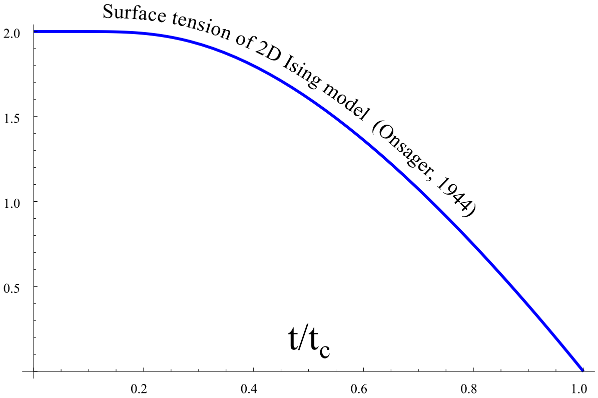
$$\Sigma^{(\mathrm{lat})}_{\mathrm{m}\times\mathrm{n}} = \Lambda^{\mathrm{m}}_{\max} + \Lambda^{\mathrm{m}}_{1} + \ldots$$

$$\mathrm{V\,T}\ln\Xi_{\mathrm{V}}(\mu,\mathrm{T}) = \mathrm{V\,P} + \sigma\,\mathrm{A} = \mathcal{N}\,\mathfrak{g} + \mathfrak{s}\,\mathcal{A} = \mathcal{N}\,\mathrm{t}\ln\Sigma_{\mathcal{N}}(\mathrm{h},\mathrm{t})$$

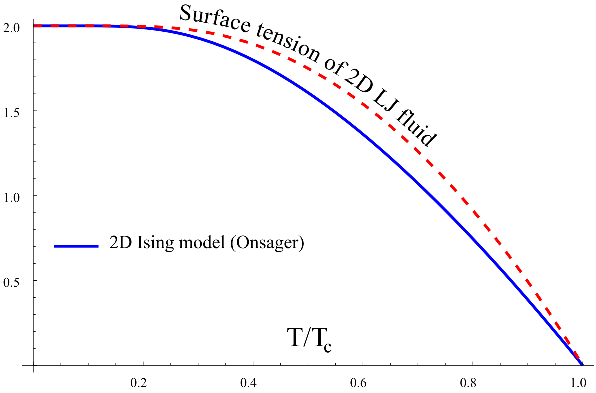
Surface tension of 2D Ising model

$$\mathfrak{s}(t) = 2 + t\,\ln\left(\tanh\frac{1}{t}\right) = 4\left(1 - t/t_c\right) + \ldots$$



Surface tension of 2D LJ fluid

$$\sigma_{\mathrm{LJ}}(\mathrm{T}) = \mathfrak{s}(\mathrm{t}(\mathrm{T})) = \frac{16}{3}\left(1 - \mathrm{T}/\mathrm{T_c}\right) + \dots\,,$$



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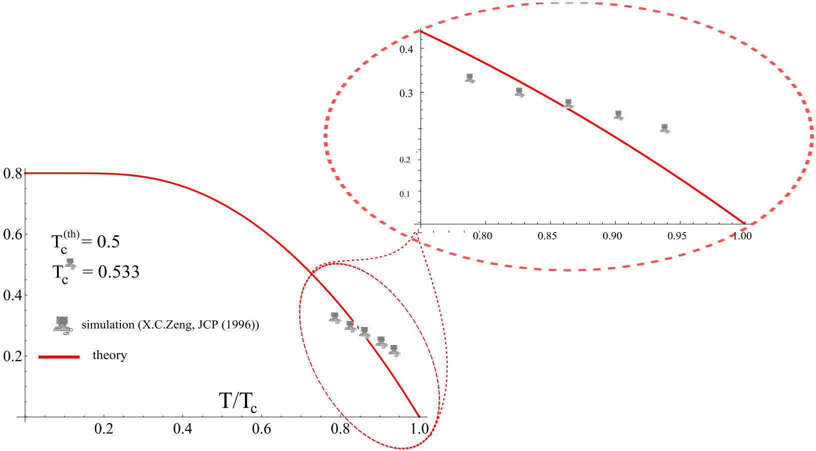

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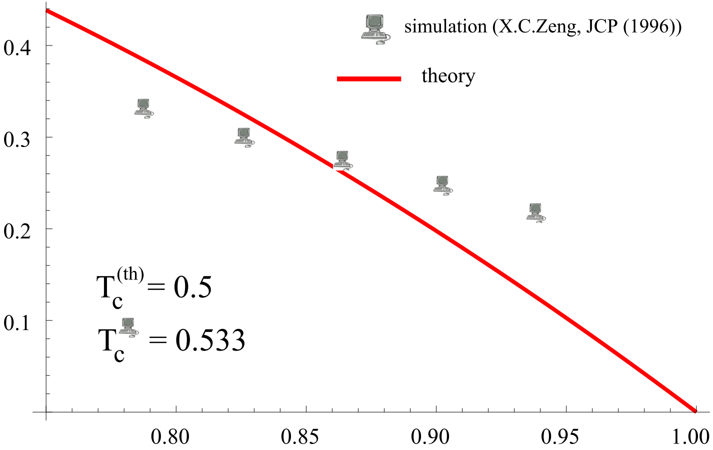

Surface tension of lattice model

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General Equation for the Surface Tension of the Lattice Gas

GEORGE W. WOODBURY, JR.*
Department of Chemistry, University of Montana, Missoula, Montana 59801

(Received 30 December 1968)

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General Equation for the Surface Tension of the Lattice Gas

GEORGE W. WOODBURY, JR.*
Department of Chemistry, University of Montana, Missoula, Montana 59801

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Local representation of the surface tension

$$\sigma = \mathrm{t}\left(\langle\,\eta\,\rangle_{\mathrm{gas}} - \langle\,\eta\,\rangle_{\mathrm{liq}}\right)$$

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$$\sigma = \frac{\mathrm{t}}{2\,\mathrm{a}}\,(\,\mathrm{x_{liq}} - \mathrm{x_{gas}}\,)\,\ln\,\frac{\mathrm{x_{liq}}}{\mathrm{x_{gas}}}$$

a - lattice spacing

Surface tension of lattice model

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$$\sigma = \mathrm{t}\,\left(\langle\, \eta \,\rangle_{\mathrm{gas}} - \langle\, \eta \,\rangle_{\mathrm{liq}} \right)$$

Modified form:

$$\sigma = \frac{\mathrm{t}}{2\,\xi^{1-\eta}}\,(\,\mathrm{x}_{\mathrm{liq}} - \mathrm{x}_{\mathrm{gas}}\,)\,\ln\frac{\mathrm{x}_{\mathrm{liq}}}{\mathrm{x}_{\mathrm{gas}}}$$

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$\xi(\mathrm{t})$ - effective thickness of the interface

Test: 2D Ising model

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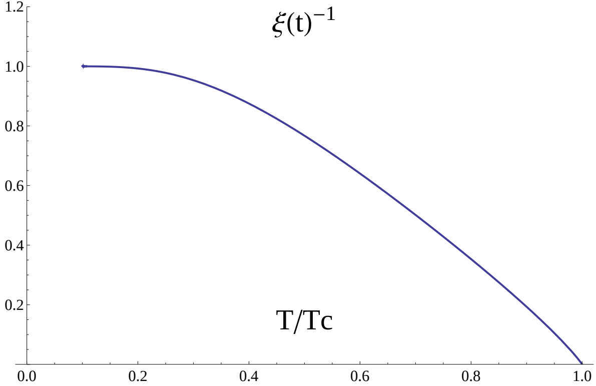

Figure : Effective interfacial thickness, $\eta = 1/4$, $\nu = 1$.

Surface tension of 3D fluid

$$\sigma = \frac{\mathrm{t}}{2\,\xi^{1-\eta}}\,\left(\,\mathrm{x_{liq}} - \mathrm{x_{gas}}\,\right)\,\ln\,\frac{\mathrm{x_{liq}}}{\mathrm{x_{gas}}}$$

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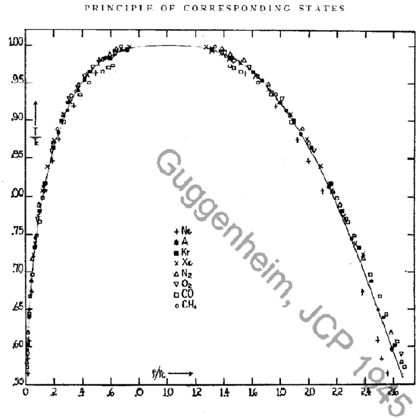
$\xi = (1/\mathrm{t} - 1)^{-\nu}$, $\eta \approx 0.03$ - Fisher's critical exponent, ν taken as fitting parameter

Surface tension of 3D fluid

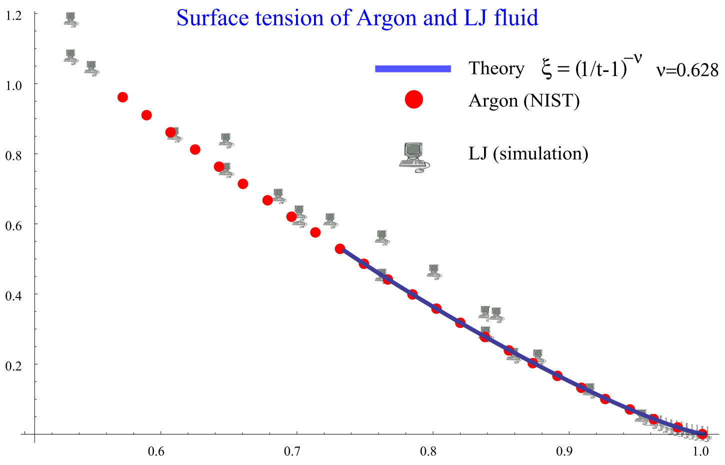
$$x_{\text{liq,gas}}(T) = \frac{1}{2\,(1+a)}\,\frac{\rho_{\text{liq,gas}}}{1-\frac{T}{T_c}\,\frac{a}{1+a}}\,,\qquad t(T) = \frac{t_c}{1+a}\,\frac{T/T_c}{1-\frac{T}{T_c}\,\frac{z}{1+a}}$$



$$\frac{\rho_l}{\rho_c} = 1 + \frac{3}{4}\left(1-\frac{T}{T_c}\right) + \frac{7}{4}\left(1-\frac{T}{T_c}\right)^{\frac{1}{3}}$$

$$\frac{\rho_g}{\rho_c} = 1 + \frac{3}{4}\left(1-\frac{T}{T_c}\right) - \frac{7}{4}\left(1-\frac{T}{T_c}\right)^{\frac{1}{3}}$$

Surface tension of 3D fluid



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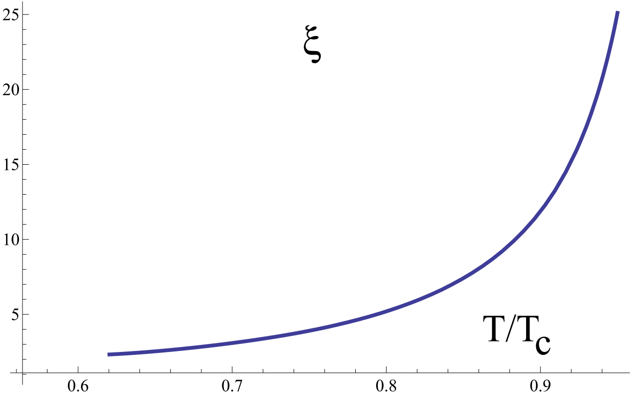

Figure : Temperature dependence of the effective interfacial thickness

Surface tension of 3D fluid

Microscopic form (Kirkwood-Buff):

$$\sigma_\infty = \frac{1}{4}\int dz_1 \int d\vec{r}\, r\, u'(r)\,(1-3\cos^2\theta)\, n_2(z_1, z_2, r)\,,$$

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Fluctuational (mesoscopic) form (Triezenberg-Zwanzig, 1972):

$$\sigma_{\infty} = T \iint dz_1\, dz_2\, \frac{d\, n(z_1)}{d\, z_1}\, K_2(z_1, z_2)\, \frac{d\, n(z_2)}{d\, z_2}$$

$$K_2(z_1, z_2) = \frac{1}{4} \int d^{d-1}\boldsymbol{\rho}\; \rho^2\, C_2\,(\, z_1, z_2; \rho\,)$$

Surface tension of 3D fluid

$$\frac{1}{\mathrm{T}}\left(\frac{\partial\,\mathrm{p}}{\partial\,\mathrm{n}}\right)_{\mathrm{T}} = 1 - \mathrm{n}\int \mathrm{C}_2(\mathrm{n};\mathrm{r}_{12})\,\mathrm{d}\mathrm{r}_{12}\,,$$

$$\left(\frac{\partial\,\mathrm{p}}{\partial\,\mathrm{n}}\right)_{\mathrm{T}} \propto |\tau|^{\gamma} \quad \mathrm{T}\to\mathrm{T}_c\,.$$

$$\mathrm{C}_2(\mathrm{n};\mathrm{r}_{12}) \propto |\tau|^{2-\alpha+\gamma} \propto \frac{1}{\xi^{\mathrm{d}+2-\eta}}$$

$$\mathrm{K}_2 = \frac{1}{4}\int \mathrm{d}^{\mathrm{d}-1}\boldsymbol{\rho}\;\rho^2\,\mathrm{C}_2\left(\mathrm{z}_1,\mathrm{z}_2;\rho\right) \propto \frac{\xi^{\mathrm{d}+1}}{\xi^{\mathrm{d}+2-\eta}} \propto \frac{1}{\xi^{1-\eta}}\,.$$

Surface tension of 3D fluid

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$$d\,\nu = 2 - \alpha\,, \quad 2 - \alpha = \beta + \gamma\,, \quad \gamma = \nu\,(2 - \eta)\,, \quad \sigma \propto |\tau|^{(d-1)\nu}$$

$$\sigma_\infty \sim \frac{\left(n_{liq} - n_{gas}\right)^2}{\xi^{1-\eta}} \propto |\tau|^{2\beta+\nu(1-\eta)} = |\tau|^{(d-1)\nu}$$

Tolman length

Definition

$$\Delta p = \frac{2\,\sigma_\infty}{R}\left(1 - \frac{\delta_T}{R} + \ldots\right) \;\Rightarrow\; \sigma = \sigma_\infty\left(1 - 2\,\frac{\delta_T}{R} + \ldots\right)$$

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Microscopic form δ_T (Bokhuis&Bedeaux, 1992)

$$\delta_T = -\frac{1}{8\,\sigma_\infty}\int dz_1 \int d\vec{r}_{12}\, u'(r)\, r\,(1-3\cos^2\theta)\,(z_1+z_2)\,n_2(z_1,z_2,r)\,.$$

Tolman length

Question

Does the fluctuational (mesoscopic) form similar to Trietzenberg-Zwanzig for σ_∞ exist for δ_{T}?

Tolman length

Square-gradient approx (Fisher&Wortis, PRB (1984))

$$\delta_{\mathrm{T}} = \frac{\int\limits_{-\infty}^{+\infty} \mathrm{z}\,\mathrm{n}'(\mathrm{z})\,\mathrm{dz}}{\int\limits_{-\infty}^{+\infty} \mathrm{n}'(\mathrm{z})\,\mathrm{dz}} - \frac{\int\limits_{-\infty}^{+\infty} \mathrm{z}\,\mathrm{n}'^{2}(\mathrm{z})\,\mathrm{dz}}{\int\limits_{-\infty}^{+\infty} \mathrm{n}'^{2}(\mathrm{z})\,\mathrm{dz}}$$

$\mathrm{n}(\mathrm{z})$ is the equilibrium density profile.

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Anisimov's expression, PRL (2007)

$$\delta_{\mathrm{T}} \simeq \frac{\mathrm{n_d} - 1}{\mathrm{n_{liq}} - \mathrm{n_{gas}}}\,\xi$$

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Symmetry

If there is “particle-hole“ symmetry (Ising model) then $\delta_{\mathrm{T}} \equiv 0$.

TZ-like form for the Tolman length

We start with B&B expression:

$$\delta_{\mathrm{T}} = -\frac{1}{8\,\sigma_\infty} \int \mathrm{dz}_1 \int \mathrm{d}\vec{\mathrm{r}}_{12}\,(\mathrm{z}_1+\mathrm{z}_2)\,\mathrm{u}'(\mathrm{r})\,\mathrm{r}\,(1-3\cos^2\theta)\,\mathrm{n}_2(\mathrm{z}_1,\mathrm{z}_2,\mathrm{r})$$

TZ-like form for the Tolman length

proceed with:

$$\delta_{\mathrm{T}} = -\frac{1}{8\,\sigma_\infty} \int \mathrm{d}z_1 \int \mathrm{d}\vec{r}_{12}\,(2z_1 + z_{12})\,u'(r)\,r\,(1 - 3\cos^2\theta)\,n_2(z_1, z_2, r) =$$

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$$-\frac{1}{4\,\sigma_{\infty}}\int \mathrm{dz}_1\,\mathrm{dz}_2\,\mathrm{z}_1\,\mathrm{n}'(\mathrm{z}_1)\,\mathrm{K}_2(1,2)\,\mathrm{n}'(\mathrm{z}_2)$$

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$$-\frac{1}{4\,\sigma_\infty}\int \mathrm{d}z_1\,\mathrm{d}z_2\,z_1\,n'(z_1)\,K_2(1,2)\,n'(z_2)$$

$$-\frac{1}{4\,\sigma_\infty}\int \mathrm{d}Z\,\mathrm{d}\vec{r}\,z\left(x\frac{\partial\,u}{\partial\,x} - z\frac{\partial\,u}{\partial\,z}\right)\,n_2\left(\vec{R}, \vec{R} + \vec{r}\right)$$

Square Gradient approximation = local approximation for $K_2(1,2)$, so the first term goes to:

$$-\frac{1}{4\,\sigma_\infty}\int dz_1\, dz_2\, z_1\, n'(z_1)\, K_2(1,2)\, n'(z_2) \Rightarrow -\frac{\int\limits_{-\infty}^{+\infty} z\, n'^2(z)\, dz}{\int\limits_{-\infty}^{+\infty} n'^2(z)\, dz}$$

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the second:

$$-\frac{1}{4\,\sigma_\infty}\int dZ\,d\vec{r}\,z\left(x\frac{\partial u}{\partial x}-z\frac{\partial u}{\partial z}\right)n_2\left(\vec{R},\vec{R}+\vec{r}\right) \Rightarrow \frac{\int\limits_{-\infty}^{+\infty} z\,n'(z)\,dz}{\int\limits_{-\infty}^{+\infty} n'(z)\,dz}+\ldots?$$

Spinodal

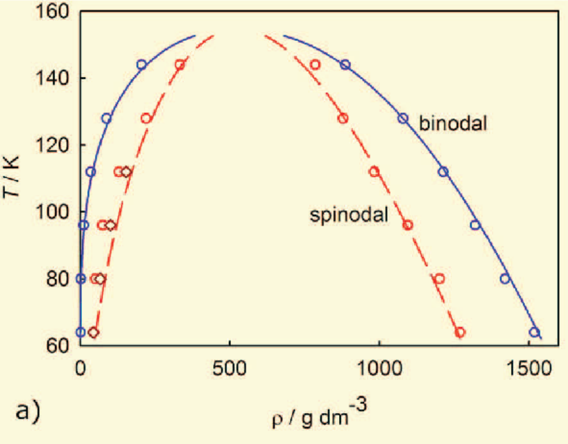

Figure : Binodal and spinodal for LJ fluid (Imre et al., JCP (2008))

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Corollary of the Global Isomorphism

The law of rectilinear diameter holds also for the spinodal

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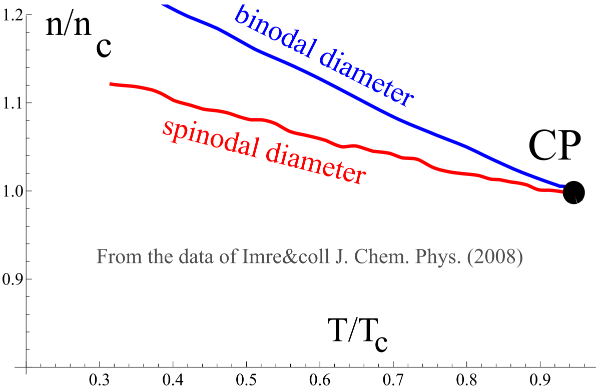

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- Is it possible to connect the transport coefficients of the fluid and the lattice gas?

The END

Thank you for attention!