J. Halpin-Healy, Troisième Cycle de la Physique en Suisse Romande, 22 October 1992

INTERFACIAL CRITICAL PHENOMENA

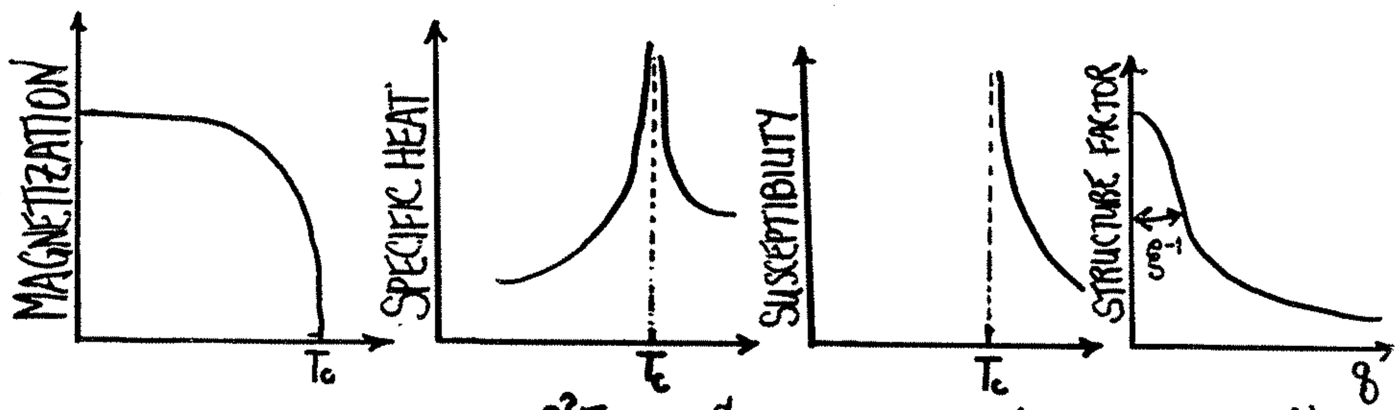
1. QUICK RECAP
   PHASE TRANSITIONS & RG → BULK SYSTEMS
2. 2d CRITICAL WETTING
3. EXPERIMENTAL REALIZATIONS – COMPLETE WETTING
   i) Ar/Au(111) ~ NEAR LIQUID-GAS CRITICAL PT
   ii) SURFACE PREMELTING – NEON MULTILAYERS
   iii) EDGE MELTING
4. COMMENSURATE - INCOMMENSURATE TRANSITION → Br_2 INTERCALATED GRAPHITE

BRISK TUTORIAL - PHASE TRANSITIONS & RENORMALIZATION GROUP

$\nearrow$ BULK CRITICAL PHENOMENA (KADANOFF, FISHER, WILSON, ...)

TESTING GROUNDS: ISING MODEL (MAGNETISM, LIQUID-GAS, BINARY FLUID MIXTURES)

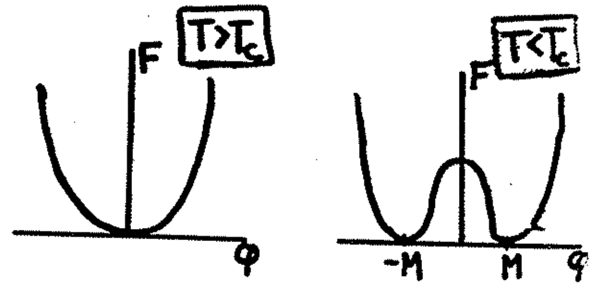
EXPTS: $0, \infty$ AT T_{CURIE}



$M \sim t^{\beta}$ $\quad C = \frac{\partial^2 F}{\partial T^2} \sim t^{-\alpha}$ $\quad \chi \sim t^{-\gamma}$ $\quad \xi \sim t^{-\nu}$

MEAN FIELD THEORY (LANDAU)

$$F = -\tfrac{1}{2} t \varphi^2 + \tfrac{g}{4!} \varphi^4$$



MINIMIZE FREE ENERGY $\left(\frac{\delta F}{\delta \varphi} \Big|_{\varphi = M} = 0 \right)$

$\Rightarrow$

$M \sim \sqrt{t}$

$F \sim t^2$

$-\varphi h$ $\quad \chi \sim 1/t$

$\frac{1}{2}(\nabla\varphi)^2$ $\quad \xi \sim t^{-1/2}$

$$\underset{(DISC.)}{\alpha = 0}, \beta = \tfrac{1}{2}, \gamma = 1, \nu = \tfrac{1}{2}$$

MFT EXPONENTS

1d - TRANSFER MATRIX APPROACH

PERMITS EXACT CALCULATION OF PARTITION FUNCTION

$$Z = \sum_{\text{CONFIGS}} \exp\left\{ J \sum_i \sigma_i \sigma_{i+1} + \underbrace{H}_{\text{EXTERNAL FIELD}} \sum_i \sigma_i \right\}$$

LINEAR CHAIN -

$$Z = \sum_{\sigma_i = \pm 1} \prod_i e^{J\sigma_i\sigma_{i+1} + H\sigma_i} = \sum_{\sigma_i = \pm 1} \langle \sigma_1 | T | \sigma_2 \rangle \langle \sigma_2 | T | \sigma_3 \rangle \langle \sigma_3 | \cdots$$

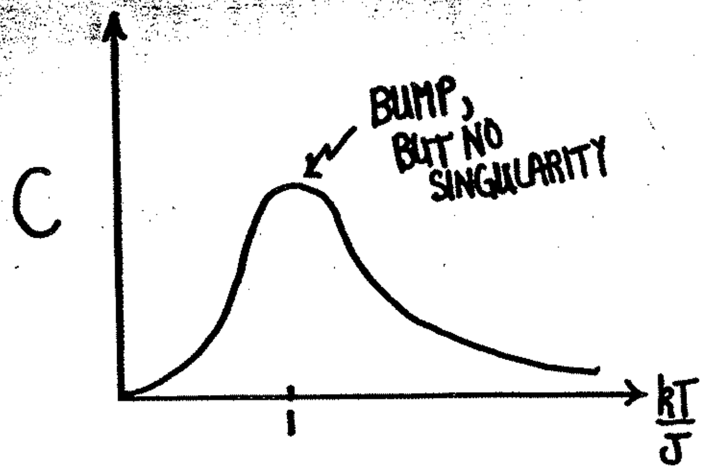
WRITTEN AS PRODUCT OF MATRICES WITH

$$\langle | T | \rangle = \begin{array}{c c} & \begin{array}{cc} + & - \end{array} \\ \begin{array}{c} + \\ - \end{array} & \begin{pmatrix} e^{J+H} & e^{-J} \\ e^{-J} & e^{J-H} \end{pmatrix} \end{array}$$

$\Rightarrow$

$$Z = \mathrm{Tr}\, T^N = \lambda_+^N + \lambda_-^N \qquad (N = \#\ \text{SPINS})$$

FREE ENERGY GIVEN BY LARGEST EIGENVALUE OF TRANSFER MATRIX $\rightarrow$ $F/N = -kT \log\left[\cosh H + \sqrt{\cosh^2 H - 2e^{-2J}\sinh 2J}\right]$



NO PHASE TRANSITION IN 1d

2d Ising Model

- RUDE AWAKENING $\Longrightarrow$ ONSAGER'S EXACT SOLUTION VIA TRANSFER MATRIX

ONSAGER (1944)
KAC + WARD (1952)
YANG (1952)
VDOVICHENKO (1964)

$$\underset{(\log)}{\alpha=0}, \ \beta=\frac{1}{8}, \ \gamma=\frac{7}{4}, \ \nu=1$$

- KRAMERS + WANNIER (1941) DUALITY (DOMAIN WALLS) $\quad \tanh J_c = \sqrt{2}-1$

- CLUSTER RSRG

3d Ising Model ~ ε-EXPANSION, FIELD THEORETIC METHODS

$$\alpha\approx 0.09, \ \beta\approx 0.33, \ \gamma\approx 1.25, \ \nu\approx 0.64$$

- INDEX RELATIONS

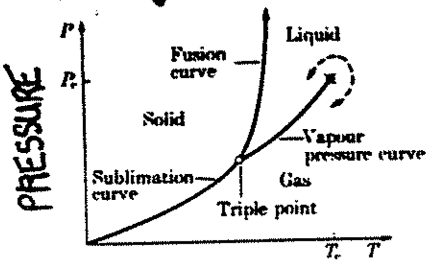
$$\alpha+2\beta+\gamma=2$$

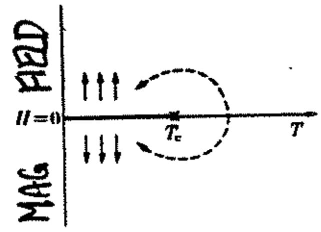
$$2-\alpha=\nu d \quad \text{(HYPERSCALING)} \Rightarrow d_{UCD}^{ISING}=4$$

MORAL ~ UNIVERSALITY
SCALING ~ ξ
EXPONENTS + IDENTITIES
IMPORTANCE OF FLUCTUATIONS
BREAKDOWN MFT

* RENORMALIZATION GROUP LANGUAGE OF "FIXED PTS" + "RG FLOWS"

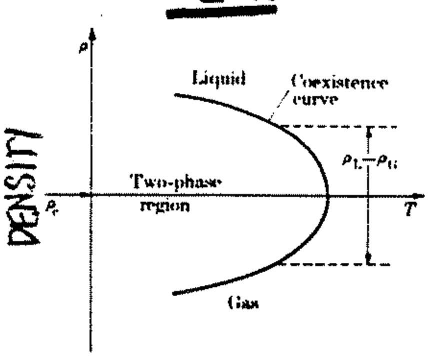
PHASE DIAGRAMS:

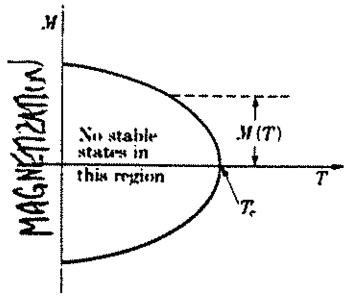




FLUID

MAGNET





VANISHING ORDER PARAMETER

CRITICAL PHENOMENA: BASIC RESULTS

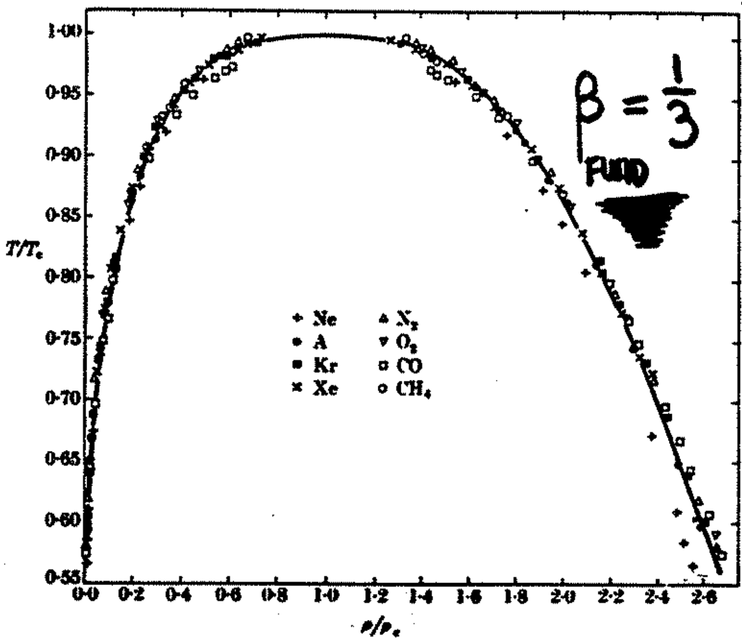


FIG. 1.8. Measurements on eight fluids of the coexistence curve (a reflection of the $P\rho T$ surface in the ρT plane analogous to Fig. 1.3). The solid curve corresponds to a fit to a cubic equation, i.e. to the choice $\beta = \frac{1}{3}$, where $\rho - \rho_c \sim (-\epsilon)^\beta$. From Guggenheim (1945).

FLUID COEXISTENCE CURVE

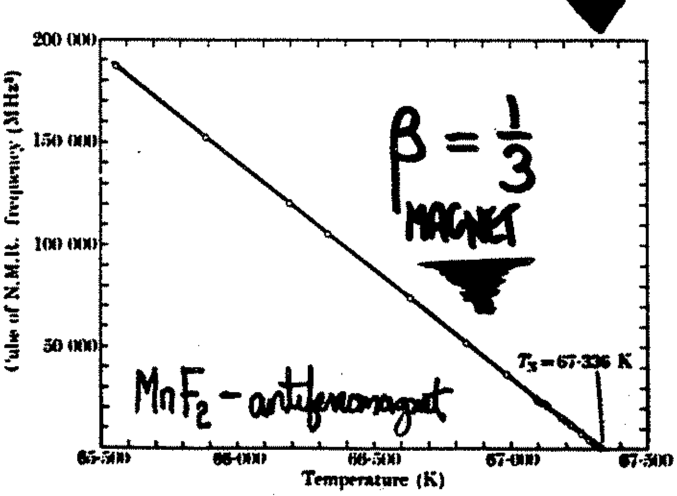


FIG. 1.9. Dependence upon temperature of the cube of the zero-field magnetization for MnF_2. Since MnF_2 is an antiferromagnet instead of a ferromagnet, the critical temperature is denoted by T_N rather than by T_c. After Heller and Benedek (1962).

MAGNETIZATION

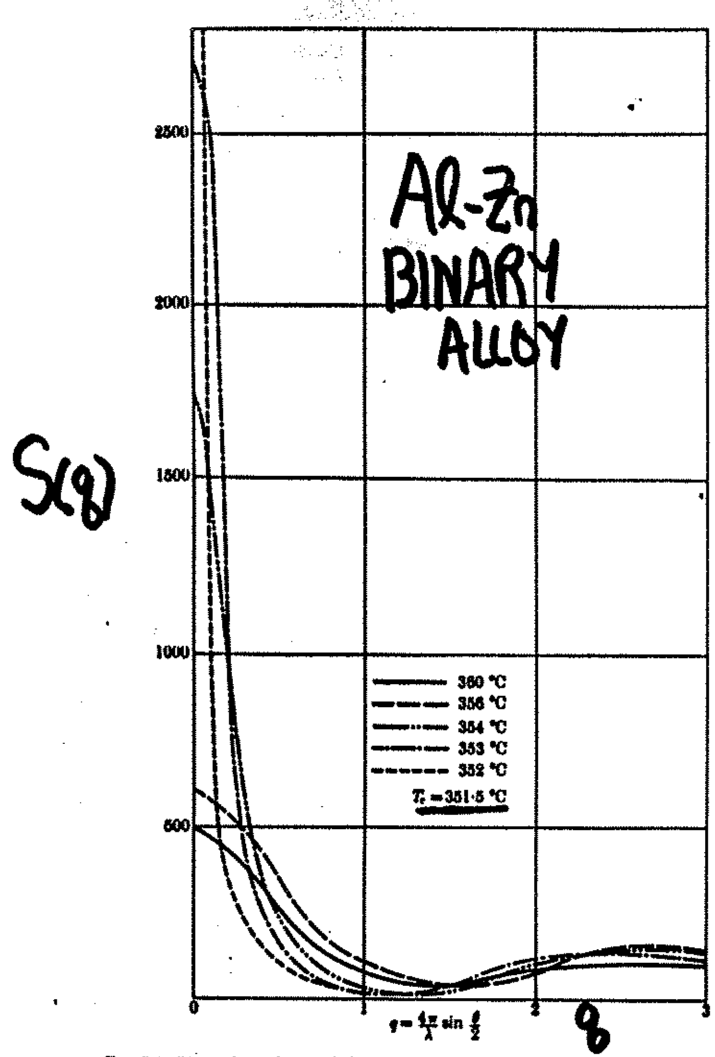


Fig. 7.4. The q dependence of the structure factor $S(q)$ for several temperatures just above the critical temperature $T_c = 351{\cdot}5$°C. After the work of Münster and Sagel (1958) on Al–Zn alloy. The 'lattice-gas' model of a simple fluid (cf. §1.1) also provides a useful model for a binary alloy.

STRUCTURE FACTOR

$$S(q) \propto \frac{1}{q^2 + \xi^{-2}}$$

Ar LIQUID-GAS CRITICALITY

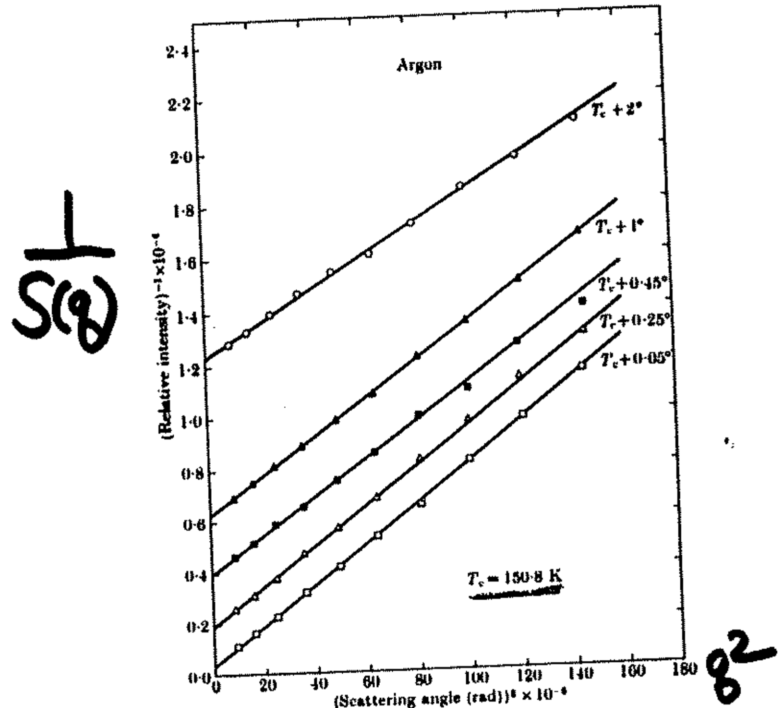


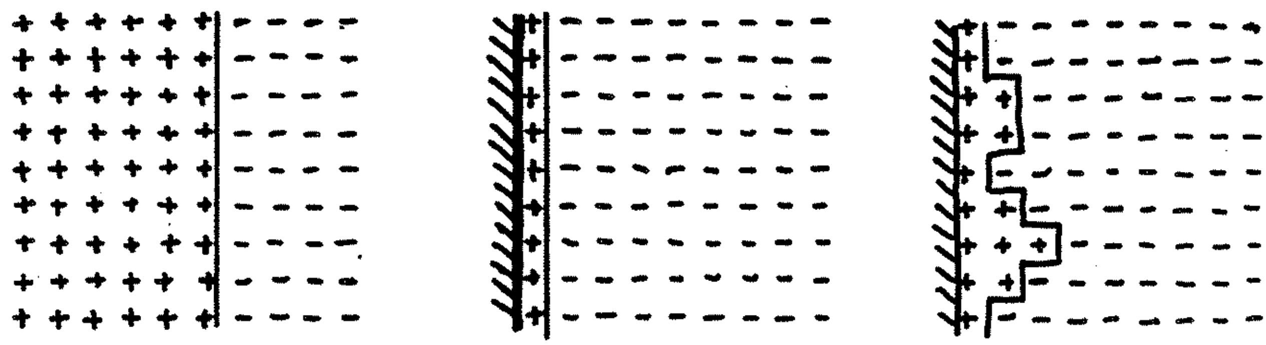
Fig. 7.6. Dependence on q^2 of the inverse scattering intensity for argon. Apparently the predictions of the Ornstein–Zernike theory are borne out by these measurements. Taken from Thomas and Schmidt (1963). Note that the slopes of the lines increase as $T \to T_c$, corresponding to an increase in the parameter R^2 defined in eqn (7.43).

DIVERGING CORRELATION LENGTH $\xi \xrightarrow[T]{T_c} \infty$

$\Downarrow$

VANISHING INTERCEPT!

2d CRITICAL WETTING – EXACT SOL'N SEMI-INFINITE ISING MODEL ~ D. ABRAHAM



T=0 INFINITE ISING MODEL (APERIODIC BC)

T=0   T>0

SEMI-INFINITE ISING MODEL

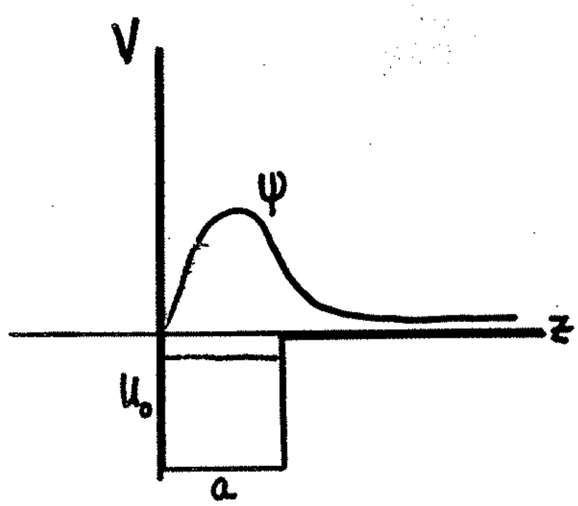
- CONTINUUM SOLID-ON-SOLID MODEL OF THERMALLY FLUCTUATING INTERFACE:

$$\mathcal{Z} = \underbrace{\int \mathcal{D}z}_{\text{CONFIGS INTERFACE}}\; e^{-\frac{1}{T}\int dx \left\{ \underbrace{\frac{1}{2}\gamma\left(\frac{dz}{dx}\right)^2}_{\text{"ELASTICITY"}} + \underbrace{V(z)}_{\text{LOCALIZING POTENTIAL}} \right\}}$$

STATISTICAL MECHANICAL PARTITION FUNCTION

WHERE

$$V(z) = \begin{cases} \infty & z<0 \\ -u_0 & 0<z<a \\ 0 & z>a \end{cases}$$



FEINMAN PATH INTEGRAL QM PARTICLE IN ASYMMETRIC SQUARE WELL

(THERMAL FLUCTUATIONS) $T \leftrightarrow \hbar$ (QM FLUCTUATIONS)

T SUFFICIENTLY LARGE $\Rightarrow$ INTERFACE WILL BE LIBERATED

$$\psi \sim \begin{cases} \sin kz & 0<z<a \\ e^{-\kappa z} & z>a \end{cases}$$

SCHRODINGER EQ

$\Downarrow$

$$E = -\frac{\hbar^2\kappa^2}{2m} = -\frac{\hbar^2 k^2}{2m} - U_0$$

CONTINUITY OF ψ'/ψ AT $z=a$

$\Downarrow$

$$k \cot ka = -\kappa$$

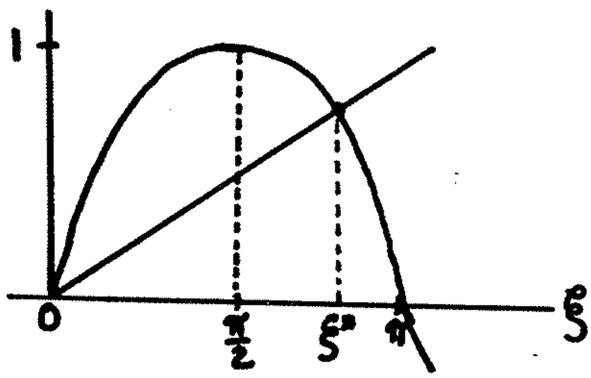
GROUND-STATE ENERGY DETERMINED BY ROOT OF

$$\sin \xi = \eta \xi$$

WHERE

$$\xi = ka$$

$$\eta = \frac{\hbar}{a\sqrt{2mU_0}}$$



QM PARTICLE ESCAPES WELL $\Rightarrow$ $\hbar_c = \frac{2a}{\pi}\sqrt{2mU_0}$

CAN SHOW

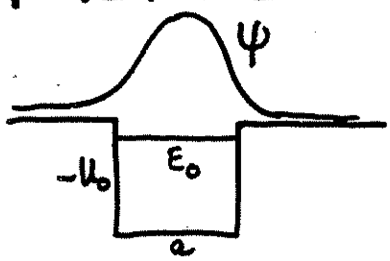
$$E_{\text{GROUND STATE}} \propto -(\hbar_c - \hbar)^2$$

$$\langle z \rangle \propto (\hbar_c - \hbar)^{-1}$$

$\Rightarrow$ INTERFACIAL FREE ENERGY VANISHES <u>QUADRATICALLY</u> $\alpha = 0$

" MEAN POSITION DIVERGES <u>LINEARLY</u> $\beta = 1$

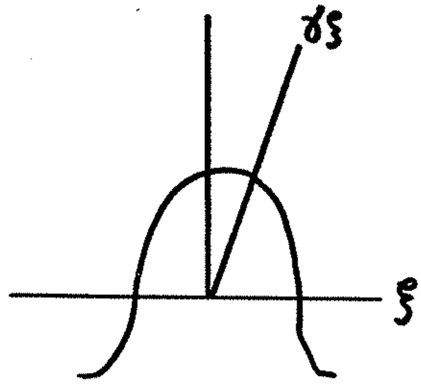
SYMMETRIC SQUARE WELL



matching condition

$\Downarrow$

$$\cos\xi = \gamma\xi$$



$\Rightarrow$

ALWAYS A BOUND-STATE

NO ENTROPY LOSS $\rightleftarrows$ NO DEPINNING TRANSITION

SPECIAL CASE: $U_0 = \infty$

$$E_{GS} = \frac{\pi^2\hbar^2}{2ma^2} \propto \frac{1}{a^2}$$

FREE ENERGY COST OF CONSTRAINING INTERFACIAL WANDERING

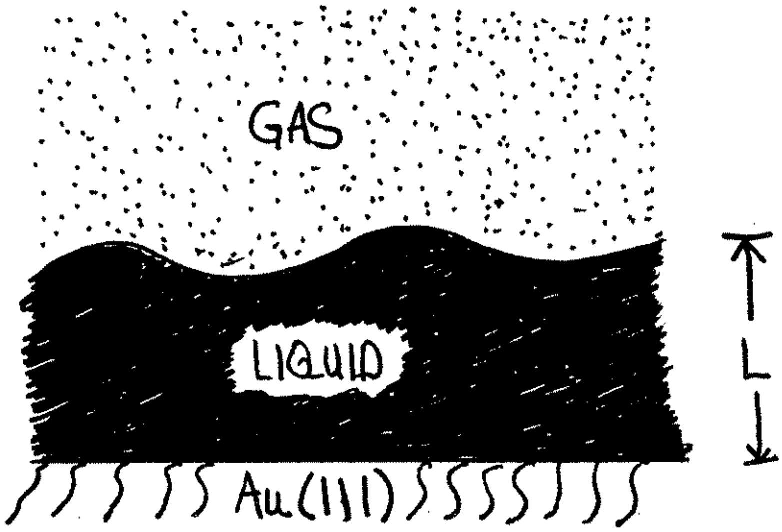
(polymer physics de Gennes)

FORCE ON WALLS - QM PARTICLE IN A BOX

$$-\frac{\partial E_{GS}}{\partial a} = \frac{\pi^2\hbar^2}{2ma^3}$$

3d COMPLETE WETTING I – NEAR LIQUID-GAS CRITICALITY

KRIM, DASH & SUZANNE PRL 52, 640 (1984)

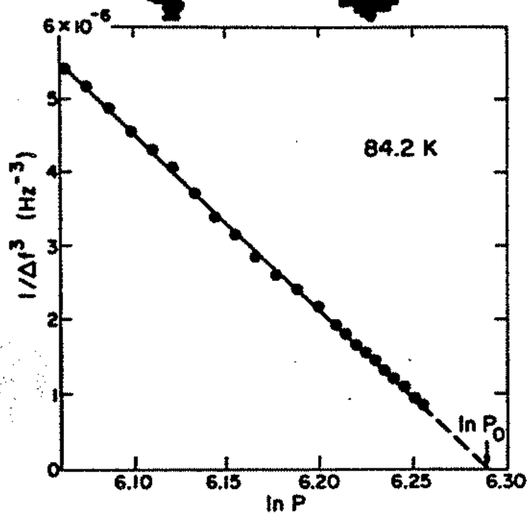


$$V_{BINDING}(L) = \Delta\mu L + \frac{const}{L^2} \longrightarrow L \sim (\Delta\mu)^{-1/3}$$

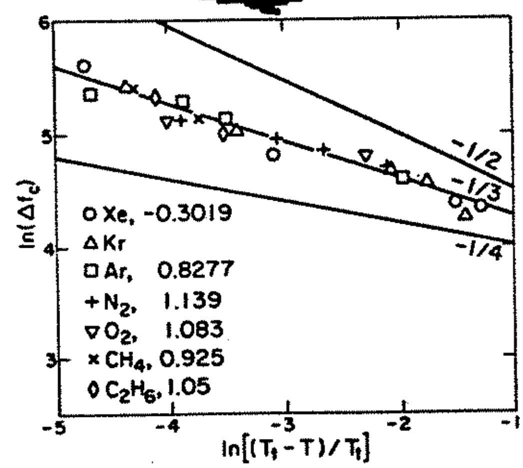
ATTRACTIVE PIECE

REPULSIVE PIECE

ARGON ADSORPTION

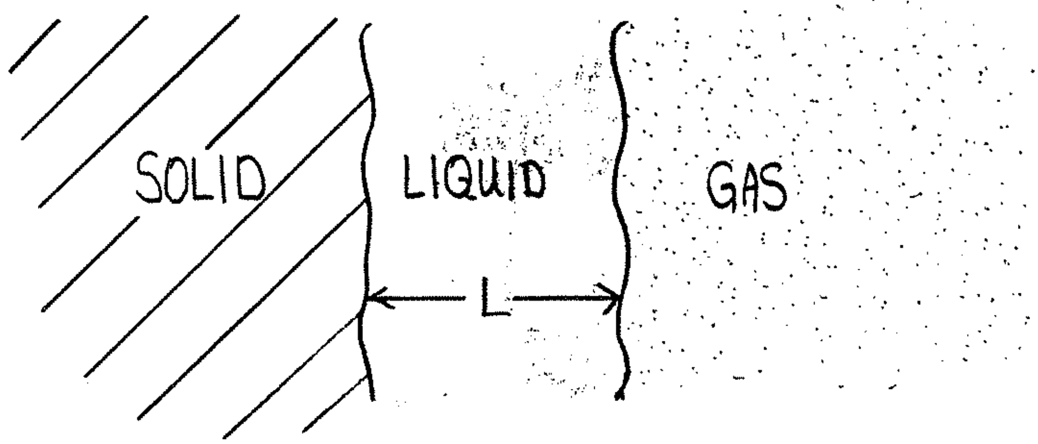


UNIVERSALITY



* 3d COMPLETE WETTING II - "SURFACE MELTING"

ZHU + DASH, PRL 60, 432 (1988)



NEON MULTILAYERS:

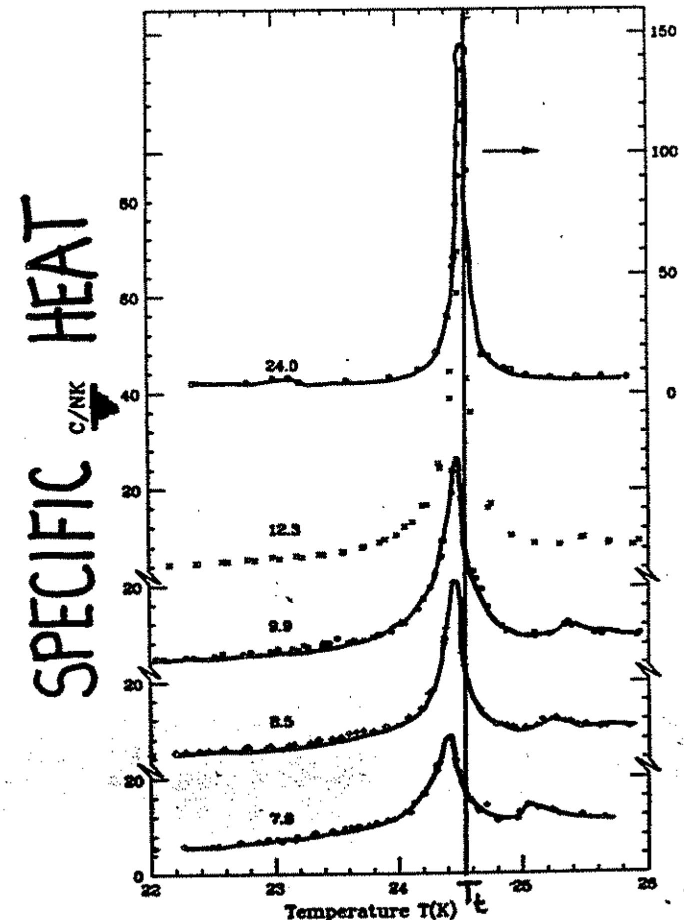


FIG. 1. Heat capacity of Ne films, showing melting anomalies near the triple point. The numbers are the film thicknesses in layers at 24.54 K. The rises, beginning well below the peaks, are due to surface melting. The small cusps at temperatures above the main peaks are caused by melting of substrate-field–compressed single layers next to the substrate.

$$L \sim (\Delta\mu)^{-1/3} \sim (T_t - T)^{-1/3}$$

$$\Downarrow$$

$$\text{PEAK SHIFT} \sim L^{-3}$$

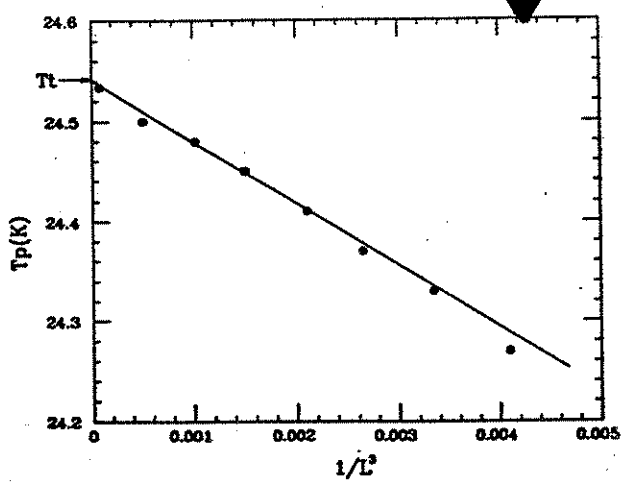


FIG. 2. Peak temperatures, showing the trend to higher temperature with increasing thickness. Proportionality to L^{-3} corresponds to surface melting controlled by long-range dispersion forces. The intercept is identified with the bulk triple-point temperature 24.541 K.

"EDGE MELTING" — 2d COMPLETE WETTING

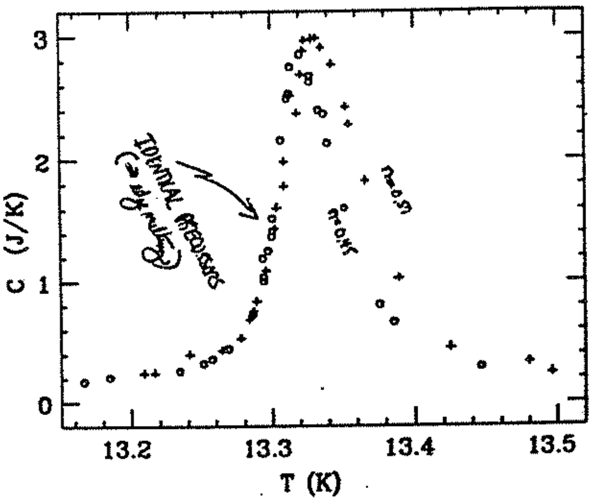
ZHU, PENGRA + DASH — PRB 37, 5586 (1988)

REPULSIVE PIECE $\sim L^{d+1-\sigma} \sim L^{-3}$ 2d LJ particles

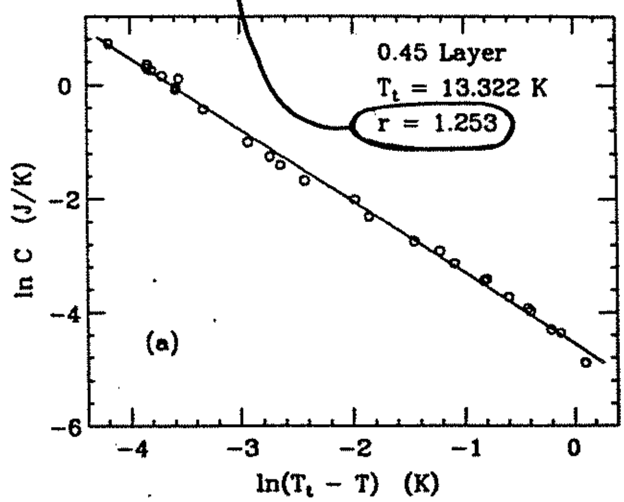
$$\Rightarrow L \sim (T_t - T)^{-1/4}$$

$\Rightarrow$ SPECIFIC HEAT PRECURSOR $\quad C \sim (T_t - T)^{-5/4}$

NEON MONOLAYERS ON GRAPHITE:



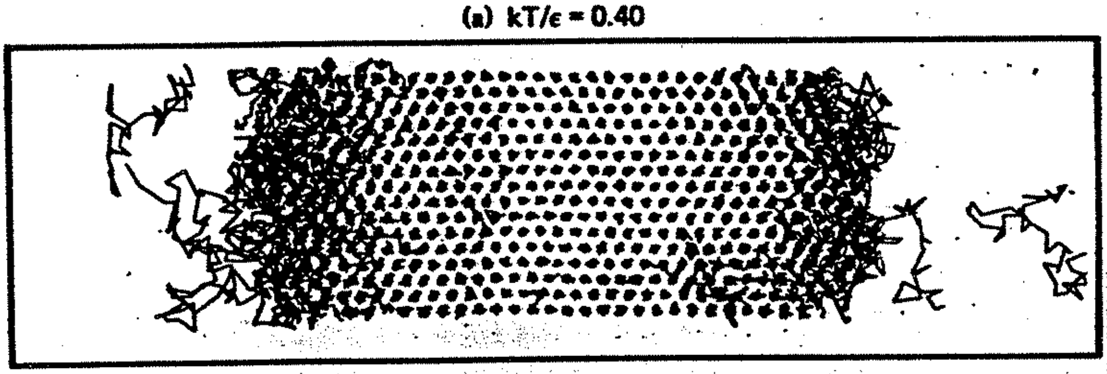
SPECIFIC HEAT EXPONENT:



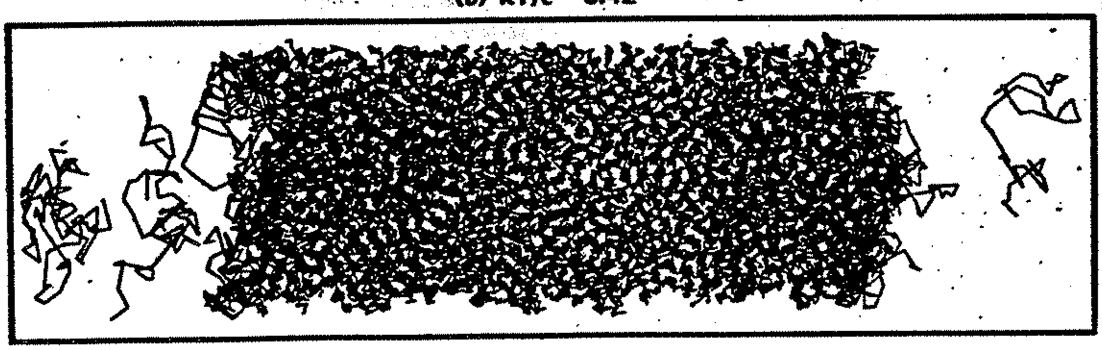
COMPUTER SIMULATIONS

HALPIN-HEALY + ABRAHAM (IBM)

(a) $kT/\epsilon = 0.40$



(b) $kT/\epsilon = 0.42$

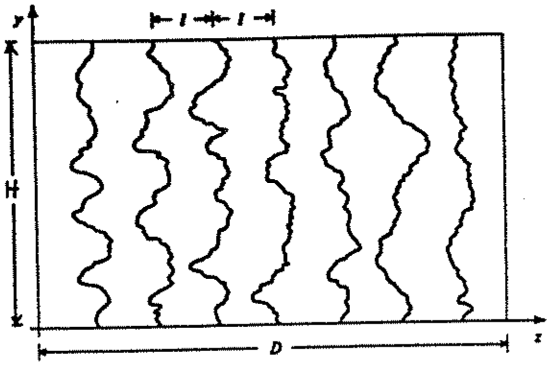


COMMENSURATE - INCOMMENSURATE TRANSITION

POKROVSKY + TALAPOV
PRL 42, 65 (1979)
SOV. PHYS. JETP 51, 134 (1980)

THEORY:

STRIPED IC
2d PHASE



$N = \frac{D}{l}$ = # WALLS

H = WALL LENGTH

free energy/length of one wall

"FREE ENERGY" $\rightarrow F = NH\boxed{\Sigma_0} + NH\,W(l)$ ← STERIC repulsion between walls

$-\Sigma' t$, where $t = [T - T_c(\mu)]$ measures the distance from the transition

$\Downarrow$

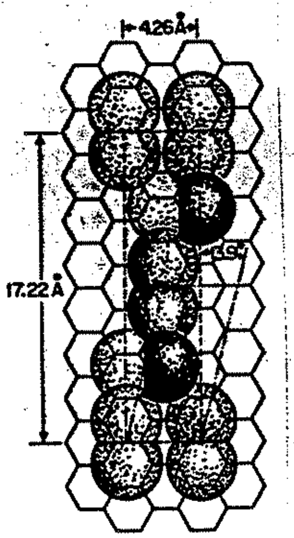
"FREE ENERGY DENSITY" $\rightarrow f = \frac{F}{HD} = -\Sigma' \frac{t}{l} + \frac{\text{cnst}}{l^3}$

DIVERGENT WALL SPACING

$\bar{l} \sim t^{-1/2}$

EXPERIMENT:

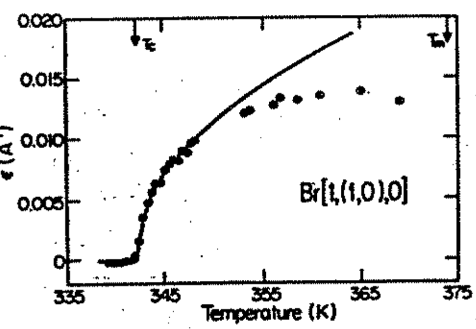
Br_2 - INTERCALATED GRAPHITE



KORTAN, BIRGENEAU, EROL, DRESSELHAUS
PRL 49, 1427 (1982)

⇒ ASSOCIATED WAVEVECTOR:

"INCOMMENSURABILITY" $\varepsilon \sim t^{1/2}$



$\beta_{EXPT} = 0.50 \pm 0.02$