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30 June - 22 August 1997
MINIWORKSHOP ON
QUANTUM MONTE CARLO SIMULATIONS OF LIQUIDS AND SOLIDS
30 JUNE - 11 JULY 1997
and
CONFERENCE ON
QUANTUM SOLIDS AND POLARIZED SYSTEMS
3 - 5 JULY 1997

"Quantum Solids and Polarised Systems"

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These are preliminary lecture notes, intended only for distribution to participants.

Quantum Solids and Polarised Systems
ICTP, Trieste, July 1997

Recent experiments on helium films adsorbed on graphite

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1. **Heat capacity of ^{3}He - ^{4}He mixture films**
   2D and layered Fermi fluids

2. **Superfluidity of atomically layered ^{4}He films**
   Observation of sub-monolayer superfluidity

3. **NMR and heat capacity of 2D ^{3}He solid**
   Frustrated 2D magnets and multiple spin exchange

Research in collaboration with Marcio Siquiera, Martin Dann, Bob Ray, Jan Nyéki and Brian Cowan

Supported by the Engineering and Physical Sciences Research Council (United Kingdom)

2D FERMI LIQUIDS

$$g(\varepsilon) = \text{const.} = \frac{A}{\pi\hbar^2} m^*$$

$$T_F = \frac{\pi\hbar^2}{k_B m^*} \cdot n_3 = \frac{0.505}{(m^*/m)} \cdot n_3 \quad \text{K nm}^{-2}$$

heat capacity $\quad c = \gamma T \quad$ where $\gamma = \frac{\pi k_B^2 m^*}{3\hbar^2} \cdot A$

$$= 8.99 \cdot 10^{-2}\, A\, \frac{m^*}{m} \quad \frac{\text{nJ}}{\text{K}^2}$$

SYSTEMS

1. ^{3}He on bare graphite — 1st or 2nd layer fluid

$$m^* = m\left(1 + \tfrac{1}{2}F_1^s\right)$$

as $n_3 \to 0$ $\quad m^* \to m$; $\quad \frac{m^*}{m} \sim 6$ at $5.5\ \text{nm}^{-2}$

(cf bulk liquid at $p = 0$ $\quad \frac{m^*}{m} = 2.80$, 1 bulk "liquid layer" $\equiv 6.5\ \text{nm}^{-2}$ $\Rightarrow$ low dimensionality $\to$ bigger interactions

ideal gas value $\to$ $\frac{\chi}{\chi_0} = \frac{m^*/m}{1 + F_0^a}$ $\qquad F_0^a \to -0.76$

Greywall Phys. Rev. B41, 1842 (1990) ; Lusher, Saunders and Cowan Phys. Rev. Lett. 67, 2497 (1991) ; Morhard, Bäuerle, Bossy, Bunkov, Fisher and Godfrin, Phys. Rev. 53, 2658 (1996)

2. ^{3}He at the surface of ^{4}He (Andreev Sov. Phys. JETP 23, 939 (1966))

$$m^* = m_H\left(1 + \tfrac{1}{2}F_1^s\right)$$

(cf in bulk solutions $m_H/m = 2.24$)

↖ hydrodynamic mass

$\frac{m_H}{m} = 1.45 \pm 0.1$ at surface of bulk $\quad$ Edwards & Saam. Prog Low Temp Phys VII A (1978)

HEAT CAPACITY ANOMALY IN TWO DIMENSIONAL FLUID ^{3}He

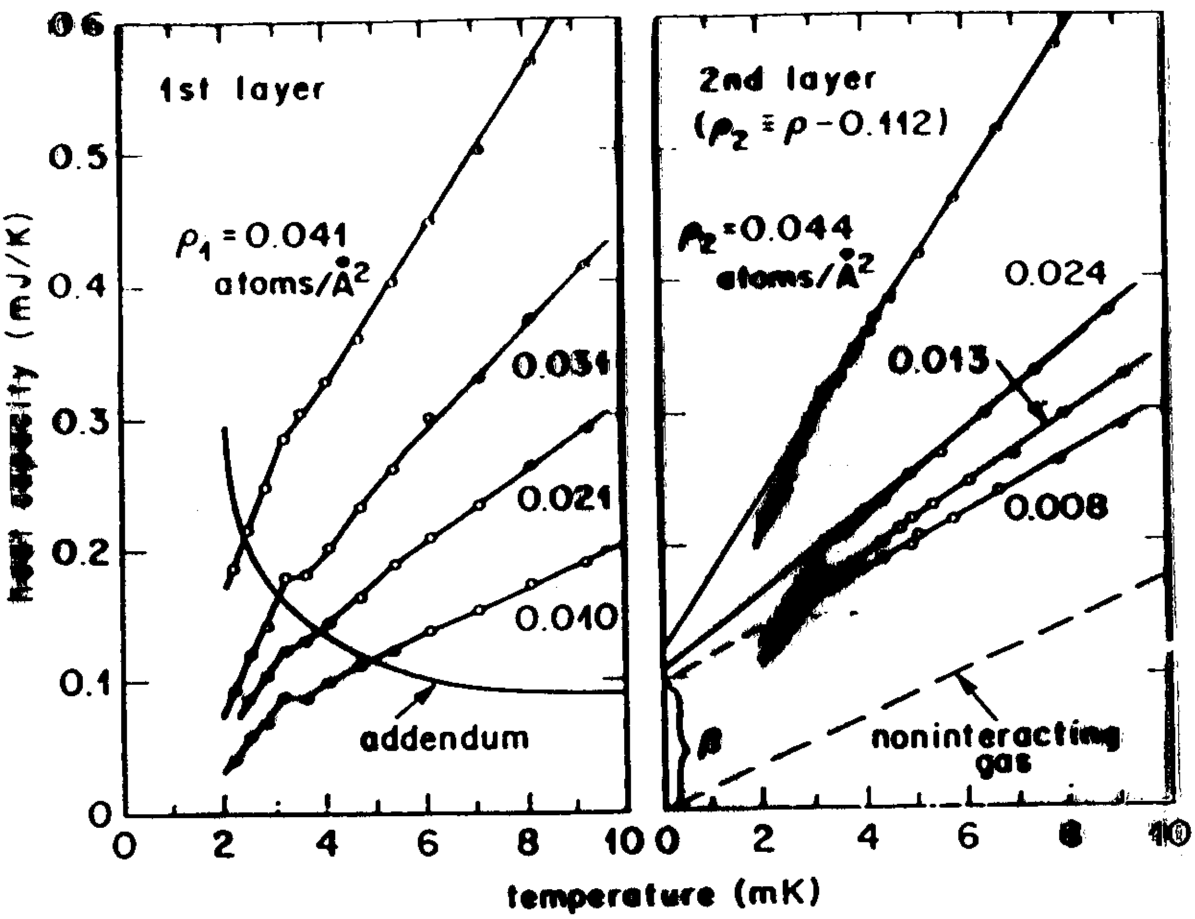


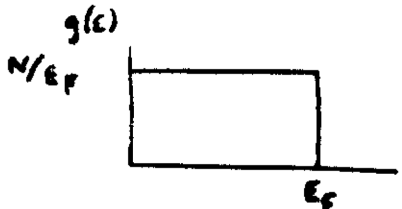
FIG. 2. First- and second-layer fluid heat capacities in the vicinity of a sharp feature at 3.2 mK. Also indicated are the addendum and the heat capacity of an ideal degenerate 2D Fermi gas.

$$c = \beta + \gamma T$$

believed to arise from heterogeneity

NUCLEAR MAGNETIC SUSCEPTIBILITY OF TWO DIMENSIONAL FLUID ^{3}He

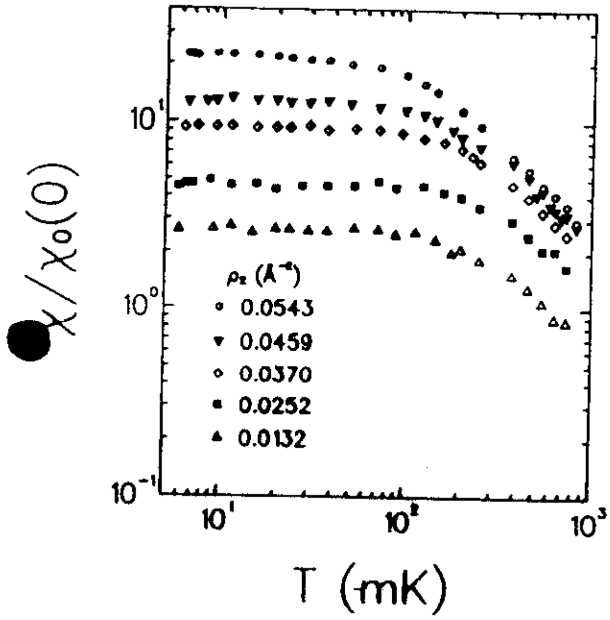
FERMI GAS



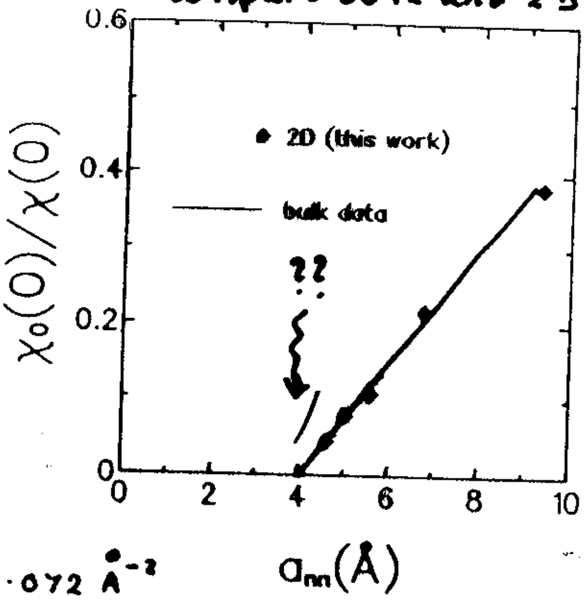
$$\chi = \mu^2 g(\epsilon_F) = \frac{N\mu^2}{k_B T_F} \qquad T_F = \frac{\pi \hbar^2}{k_B m} \cdot \frac{N}{A}$$

$\chi_0 = C/T_F$ independent of $\rho = N/A$

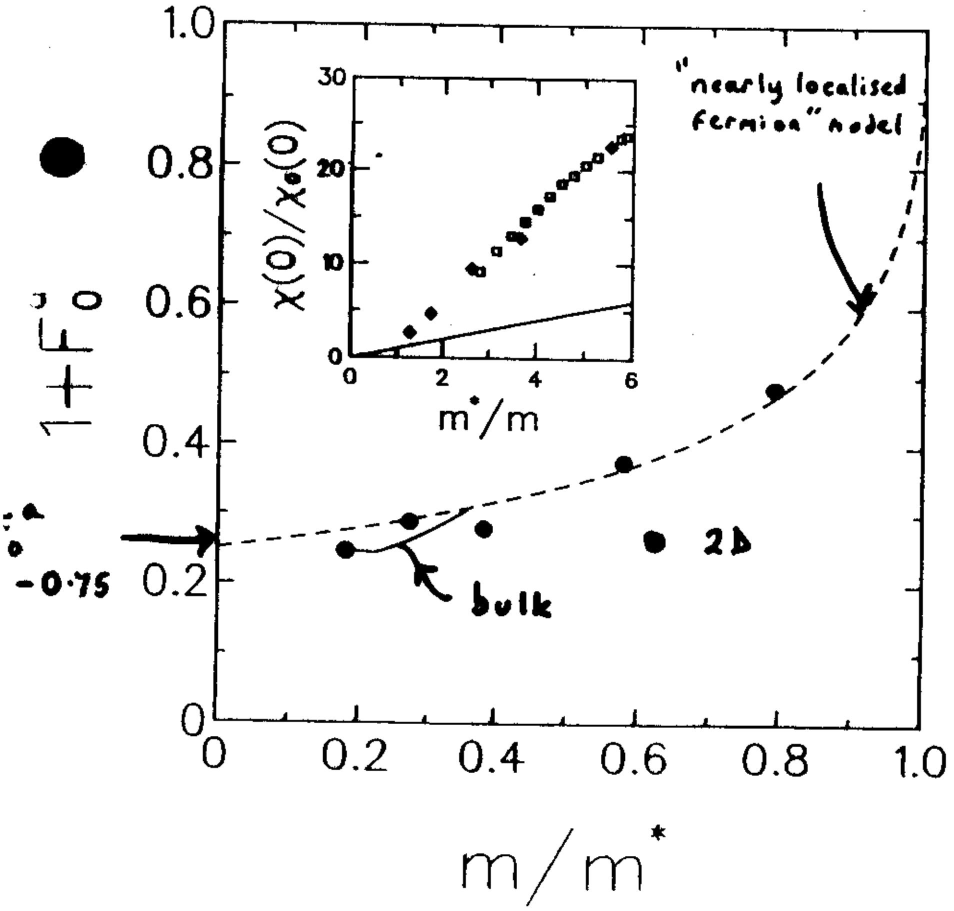
FERMI LIQUID $\quad \chi/\chi_0 = m^*/m \, (1 + F_0^a)^{-1}$ (INTERACTIONS)

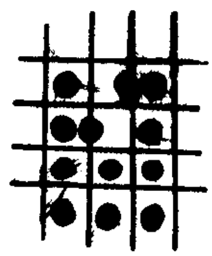


compare bulk and 2D



$?? \equiv 0.072$ Å^{-2}





lattice gas model

repulsive interaction

$I = U/U_c$

$m^*/m = (1 - I^2)^{-1}$

$F_0^a \sim -[1 - (1+I)^{-2}]$

note as $I \to 1$

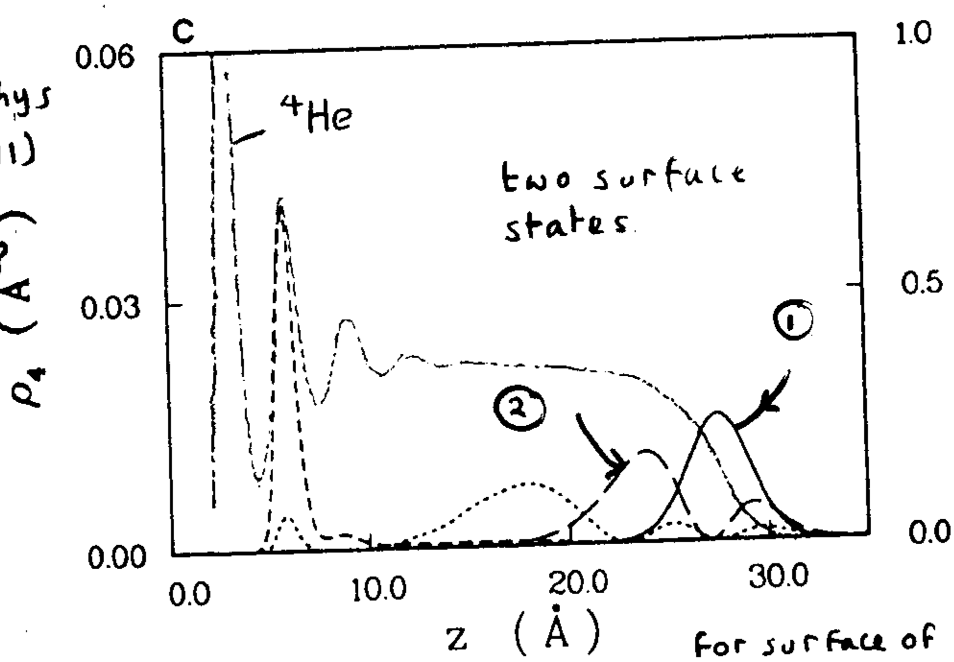
$m^*/m \to \infty$

$F_0^a \to -0.75$

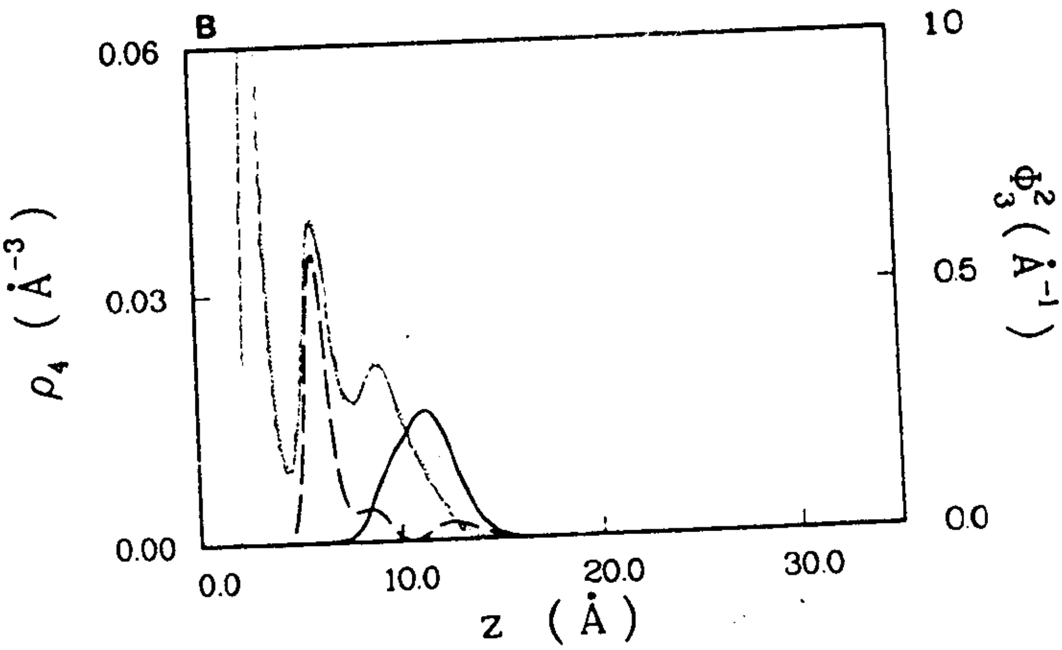
Structure of ^{4}He films

^{3}He surface states on ^{4}He films

these pictures from Pavloff e Treiner J. Low Temp Phys 83, 331 (1991)



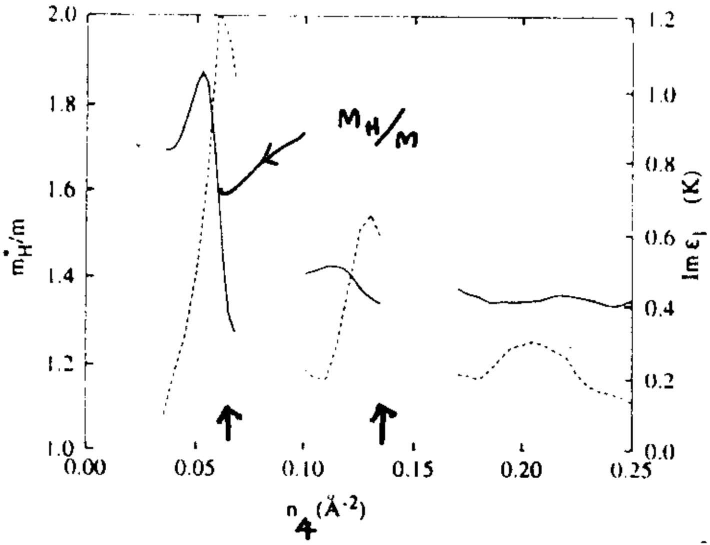
For surface of bulk liquid see Dalfovo e Stringari, Physica Scripta 38, 204 (1988)



calculations by Krotschech and co-workers since ~1985 see Clements, Krotscheck, Saarela Phys. Rev B55, 5959 (1997) and refs. therein

Predicted coverage dependence of hydrodynamic effective mass

Krotscheck, Clements, Saarela



gaps arise from layer by layer 2D condensation of ^4He film

↑ indicates where new layer begins to form

Energetics of surface states

Dynamics of ^{3}He Impurities in ^{4}He Films 181

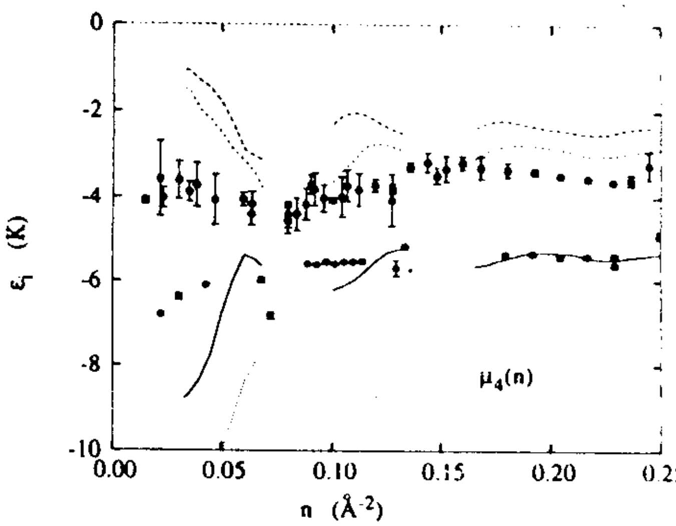
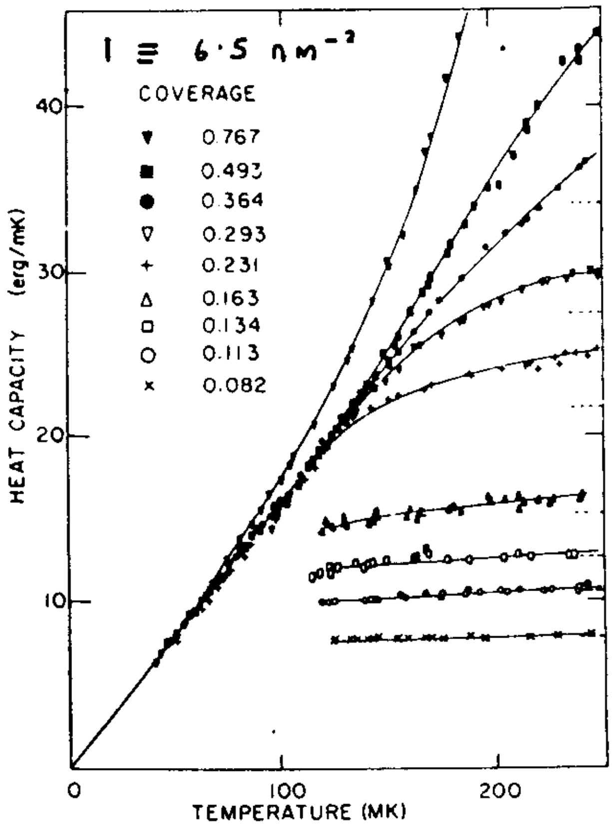


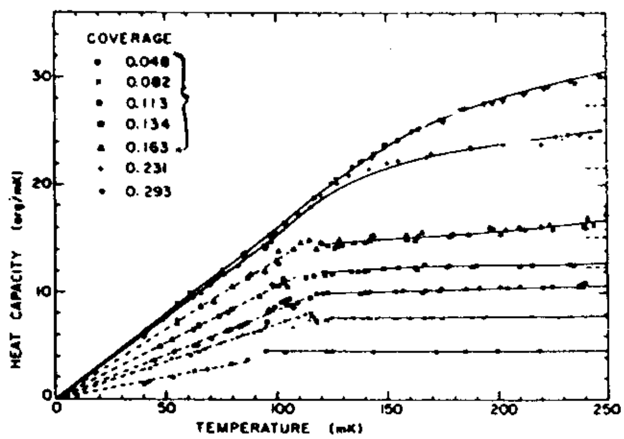
Fig. 1. Our theoretical results for the ground-state energy of ^{3}He impurities in ^{4}He films (solid line) and the first excited state (short-dashed line) are compared with the data of Ref. 5 for the ground state (solid circles) and the first excited state (open circles) with error bars. Also shown is the first excitation energy calculated within the static approximation (long-dashed line) and the chemical potential of the background (dotted line). The experimental data were shifted horizontally by 0.25 Å^{-2} to account for the first two solid layers.

Early heat capacity data

Gasparini and co-workers (State University of New York, Buffalo).
substrate; nuclepore filter paper



- anomalous results at low coverages $n_3 < 1.3$ nm^{-2}
  Puddling?



$\gamma \propto n_3$

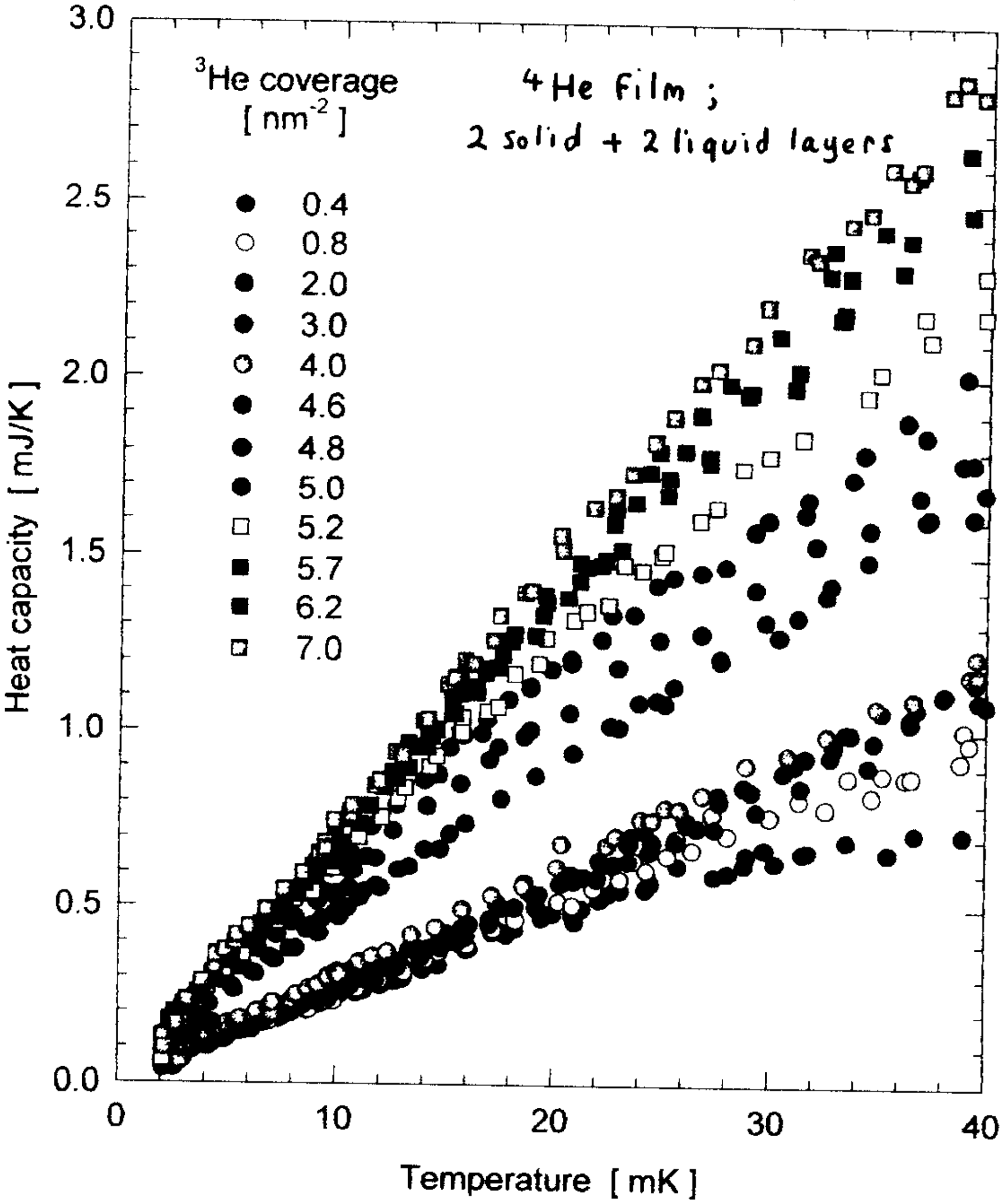
FIG. 1. Heat capacity of ^{3}He at various coverages on a 10-Å ^{4}He film. The solid lines represent a fit of the data under the assumption that the ^{3}He is homogeneously spread out over the surface of the film. The dashed lines are drawn to guide the eye.

^3He - ^4He mixture films on graphite

(Dann, Nyéki, Cowan, Saunders - submitted to J. Low Temp. Phys. (QFS 97)

Fit data to $c = \gamma T + B T^3$ ~~β~~

note; (i) no β term (ii) for $n_3 < 4\,nm^{-2}$ no strong n_3 dependence so no 'puddling'



$$\gamma = 8.99 \cdot 10^{-2} \times 182 \times \frac{m^*}{m} \quad (mJ\,K^{-2})$$

total surface area $A = 182\ m^2$

EFFECTIVE MASS

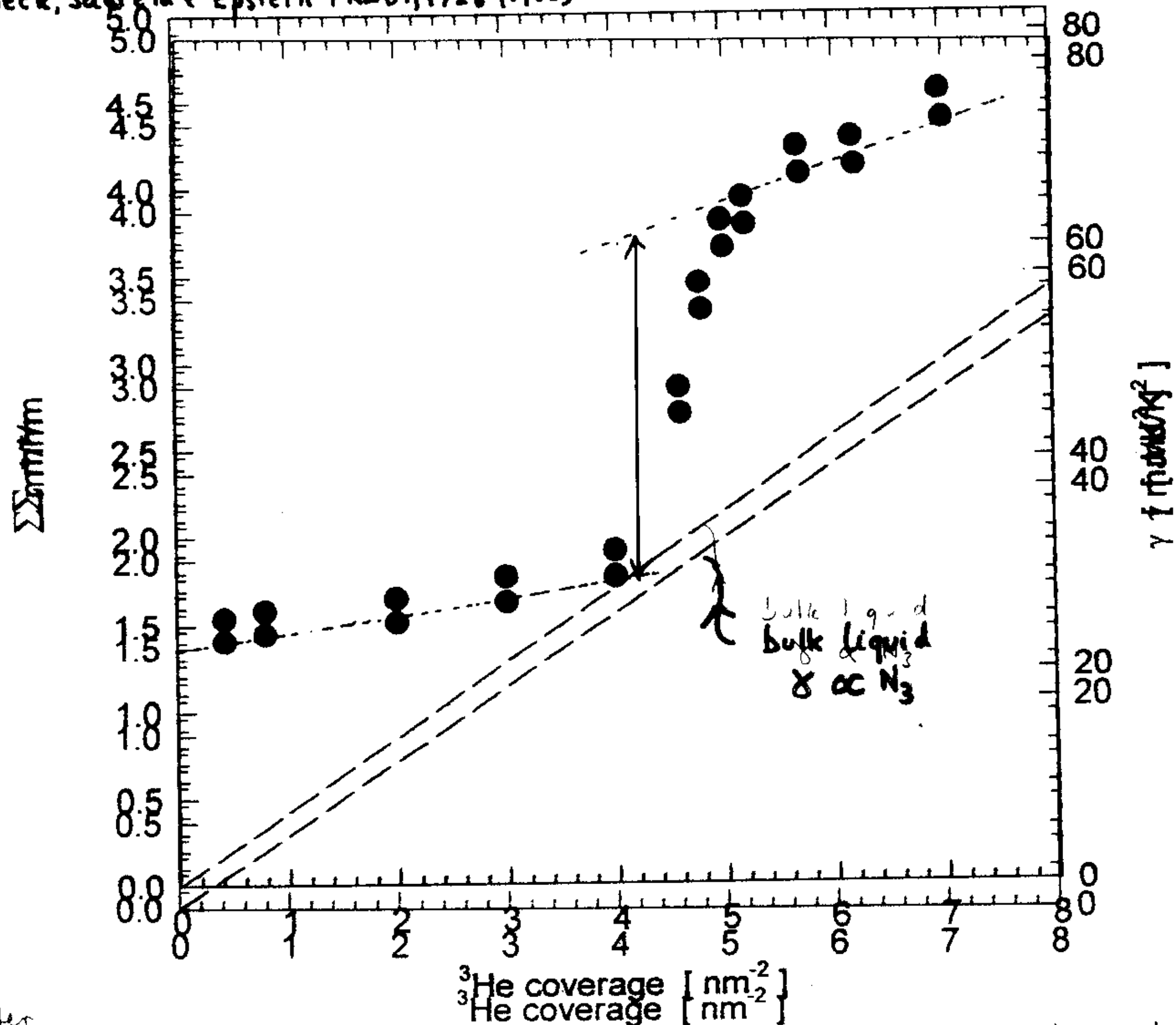
- before step $n_3 < 4\ nm^{-2}$

  2D Fermi liquid $m^* = m_H\left(1 + \frac{1}{2}F_1^s\right)$

  $\Rightarrow \frac{m_H}{m} = 1.48$ $F_1^s = 0.40 \pm 0.04$ at $n_3 = 3.2\ nm^{-2}$

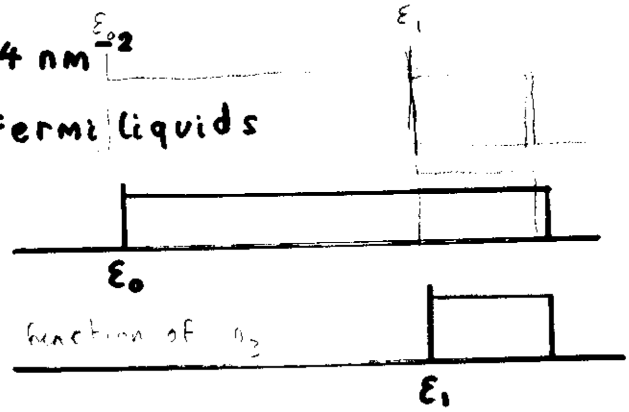
  ($\Rightarrow F_0^a \sim -0.4$ using magnetization data)

in reasonable agreement with Krotscheck, Saarela e Epstein PRL 61, 1728 (1988)



- after step $n_3 > 4\ nm^{-2}$

  two 'layered' 2D Fermi liquids



but $\varepsilon_1 - \varepsilon_0$ is a function of n_3

height of step $\Rightarrow \frac{M_H}{M} \sim 1.9$ in 1st excited state.

Magnetization measurements

Hallock and co-workers (University of Massachusetts)

Higley, Sprague and Hallock Phys. Rev. Lett 63, 2570 (1989)

observed magnetization step.

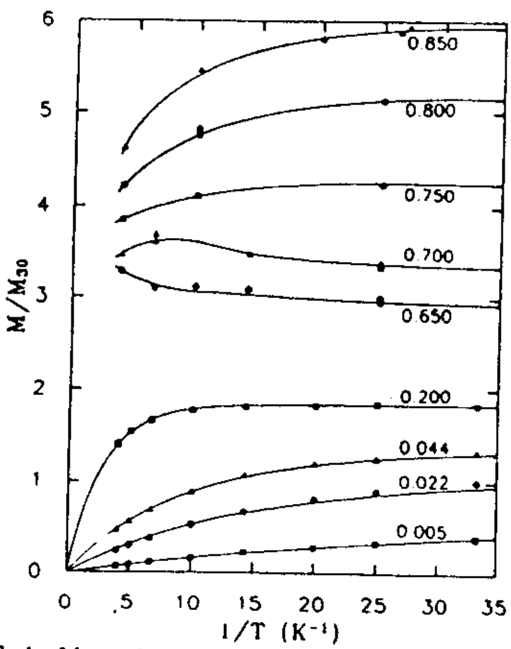


FIG. 1. Magnetization of the sample vs $1/T$ at fixed ^{4}He coverage 44 μmol/m^2 for the ^{3}He coverages shown at the right. The positive dM/dT at $d_3 = 0.65$ layer precedes the step in magnetization seen in Fig. 2. The curves for $d_3 \leq 0.2$ layer are 2D Fermi-gas fits, and the curves for $d_3 \geq 0.65$ layer are a guide to the eye.

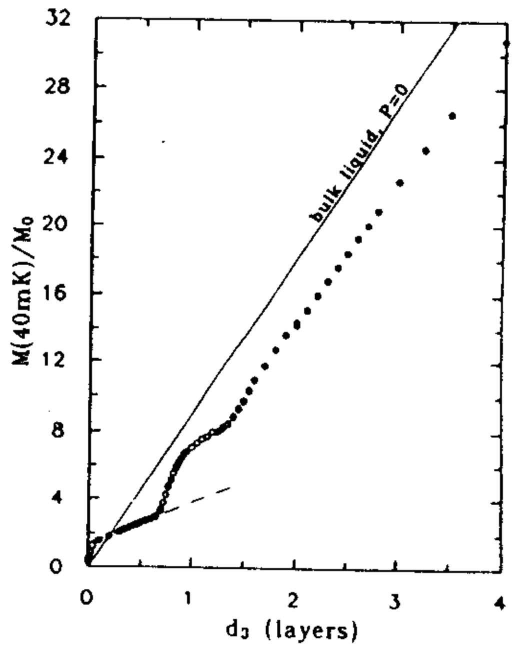


FIG. 2. Magnetization at $T = 40$ mK vs d_3, showing steps in magnetization at $d_3 \approx 0.8$ and 1.5 layers, and an increase in magnetization with the same slope as for bulk liquid above $d_3 = 2$ layers. The dashed line extrapolates low-coverage data to obtain the hydrodynamic mass $m_h = 1.38 m_3$.

bulk-like behavior is observed for rather than films

state of a thicker film

^{3}He

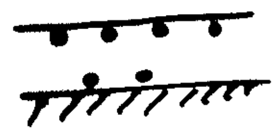
^{4}He

see review by Hallock in Prog.Low Temp.Phys. XIV (1985)

SOME FUTURE PROSPECTS

for ^3He – ^4He liquid "mixture films" on graphite

- In this system a ^4He film with an integral number of layers can be prepared with good precision
- to observe the predicted structure of M_H vs n_4 (2D phase separation) (M_H gives information about where ^3He sits in film)
- is there a substrate state ?

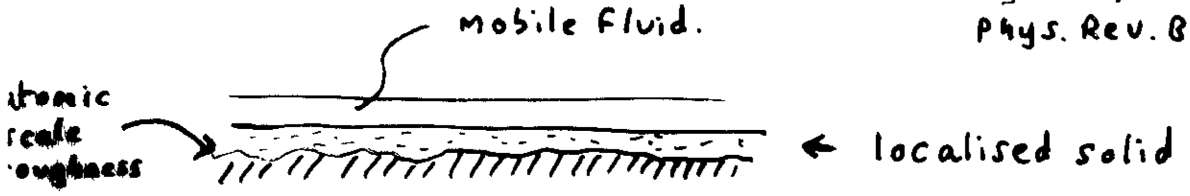


- quasiparticle interactions with $n_4 = 2$ (solid) layers and $n_4 = 3$ layers (2 solid + 1 sfl)
- measurements of χ and C → F_0^a & F_1^s on same system
- phase transitions – dimerization & superfluidity.

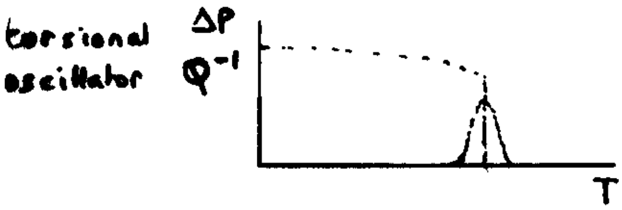
SUPERFLUIDITY OF THIN ^4He FILMS

1. Amorphous substrate

Bishop & Reppy PRL 40, 1727 (1980), Phys. Rev B22, 5171 (80)
Agnolet, McQueeney & Reppy Phys. Rev. B39, 8934 (1989)



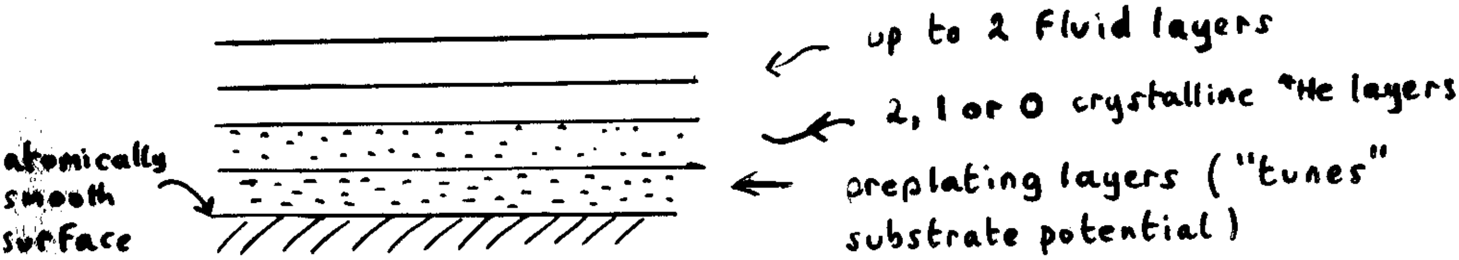
superfluidity observed for $n > n_d$ ← inert layer



universal Kosterlitz - Thouless relation

$$\frac{\rho_s(T_c)}{T_c} = \frac{2m^2 k_B}{\pi\hbar^2} = 5.254\ \mathrm{nm^{-2}K^{-1}}$$

2. Atomically flat substrate ⟶ atomically layered film



⬇

2 ^4He solid layers ⟵ no preplating.

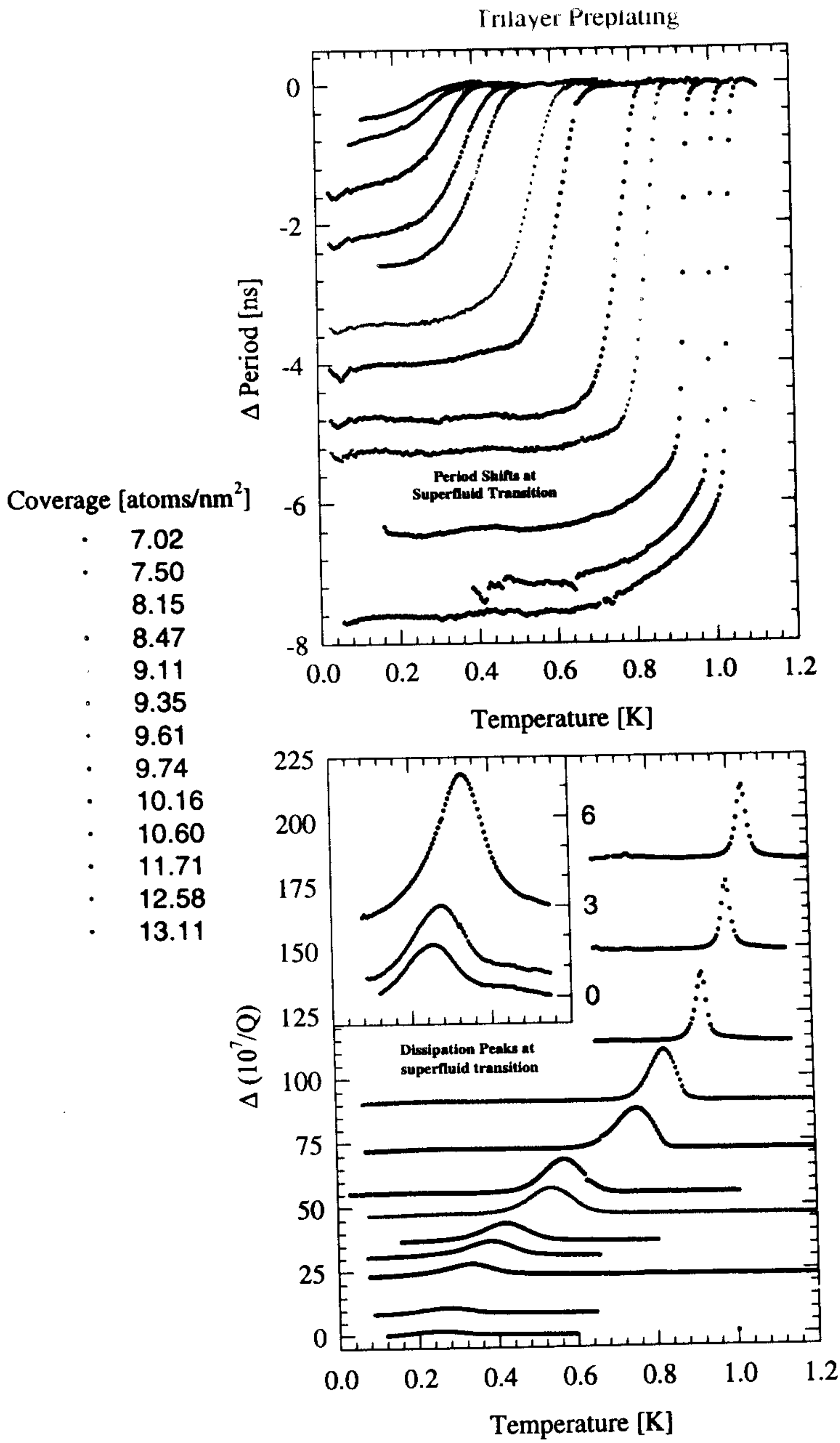
1 ^4He solid layer ⟸ 2 layers HD / 3 layers HD

no ^4He solid layer ⟵ 2 layers Ne + 5 layers HD

⇓

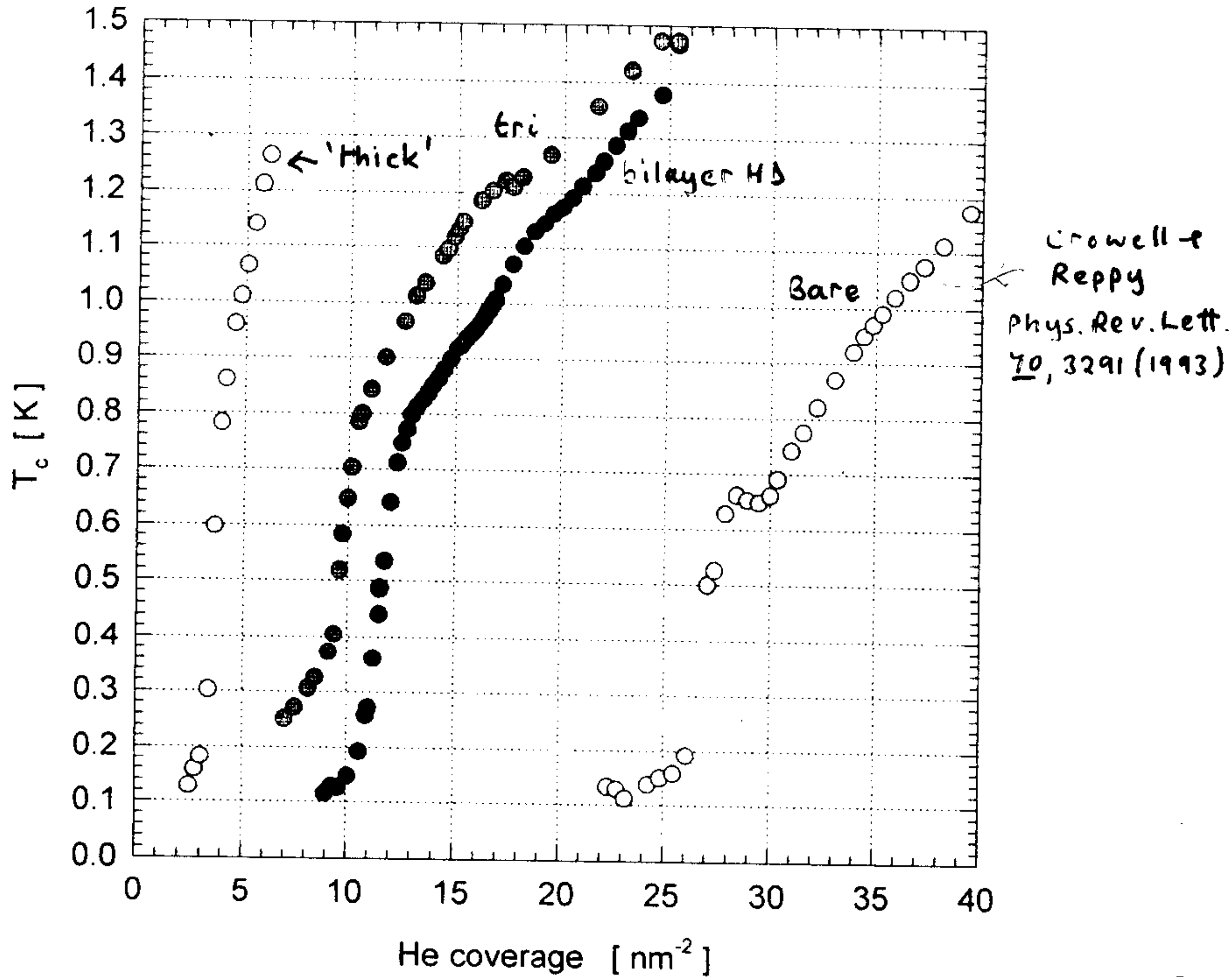
SUBMONOLAYER SUPERFLUIDITY !

- PIMC calculations of ^4He on H_2 — Wagner & Ceperley J. Low Temp. Phys. 94, 185 (1994)
- 3rd sound studies by Mochel & co-workers


Trilayer Preplating
Δ Period [ns]
Period Shifts at Superfluid Transition
Temperature [K]
Coverage [atoms/nm²]
7.02
7.50
8.15
8.47
9.11
9.35
9.61
9.74
10.16
10.60
11.71
12.58
13.11
Δ (10⁷/Q)
Dissipation Peaks at superfluid transition
6
3
0
Temperature [K]

Temperature of Dissipation Peak as a Function of Coverage

for various preplatings



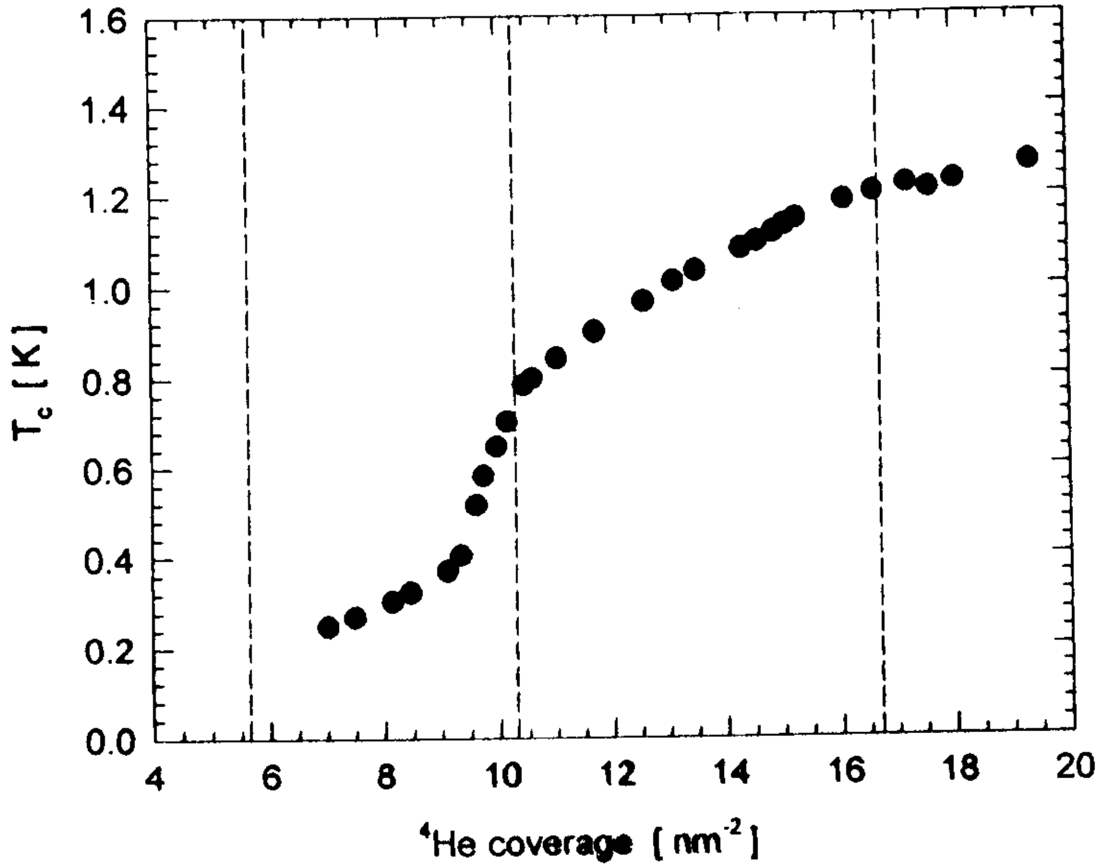
35.6 ?

Bare grafoil - no preplating [1]. First two He layers are solid.
3rd layer completion at 28 nm-2
4th layer completion at 35.6 nm-2

Grafoil preplated by HD trilayer. Total HD density 27.54 nm^{-2}
Isothermal compressibilty of He film has minima at
5.65 nm^{-2}, 10.3 nm^{-2}, 16.7 nm^{-2} and 24.0 nm^{-2}, respectively

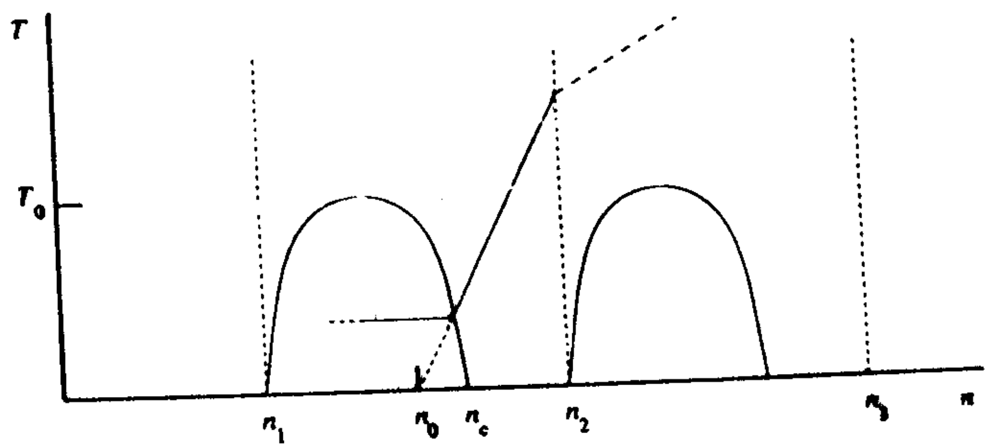
Grafoil preplated by HD bilayer. Total HD coverage 19.16 nm^{-2}
Compressibility minima at
7.3 nm^{-2}, 12.5 nm^{-2}, 18.7 nm^{-2}, 25.2 nm^{-2}

Temperature of the dissipation peak



CLEMENTS, KROTSCHECK, LAUTER, PRL 70 (1993) 1287 – theory

EBEY, VILCHES, private communication, heat capacity measurements on H_2 plated graphite



Cheng, Cole, Saam, Treiner; PRB 46 (1992) p. 13 967

KT relation $$T_c = \frac{n_s(T_c)\pi\hbar^2}{2mk_B} \approx 0.82\,\frac{n_s(0)\pi\hbar^2}{2mk_B}$$

TWO DISTINCT REGIMES

I single fluid layer

structure 2D gas liquid coexistence region (puddles) $n < n_c$

↓

uniform fluid $n > n_c$

- coverage dependence of T_c and ΔP suggest that superfluidity is suppressed in the uniform film. This suppression is coverage dependent.*

possible mechanism ? (Saarela, Clements, Krotscheck, Kusmartsev J. Low Temp. Phys 93, 971 (1993) find that for $n < 3.7\ nm^{-2}$ vortex-antivortex pairs are spontaneously created)

* i.e. ∃ inert layer in a uniform fluid film

II two fluid layers

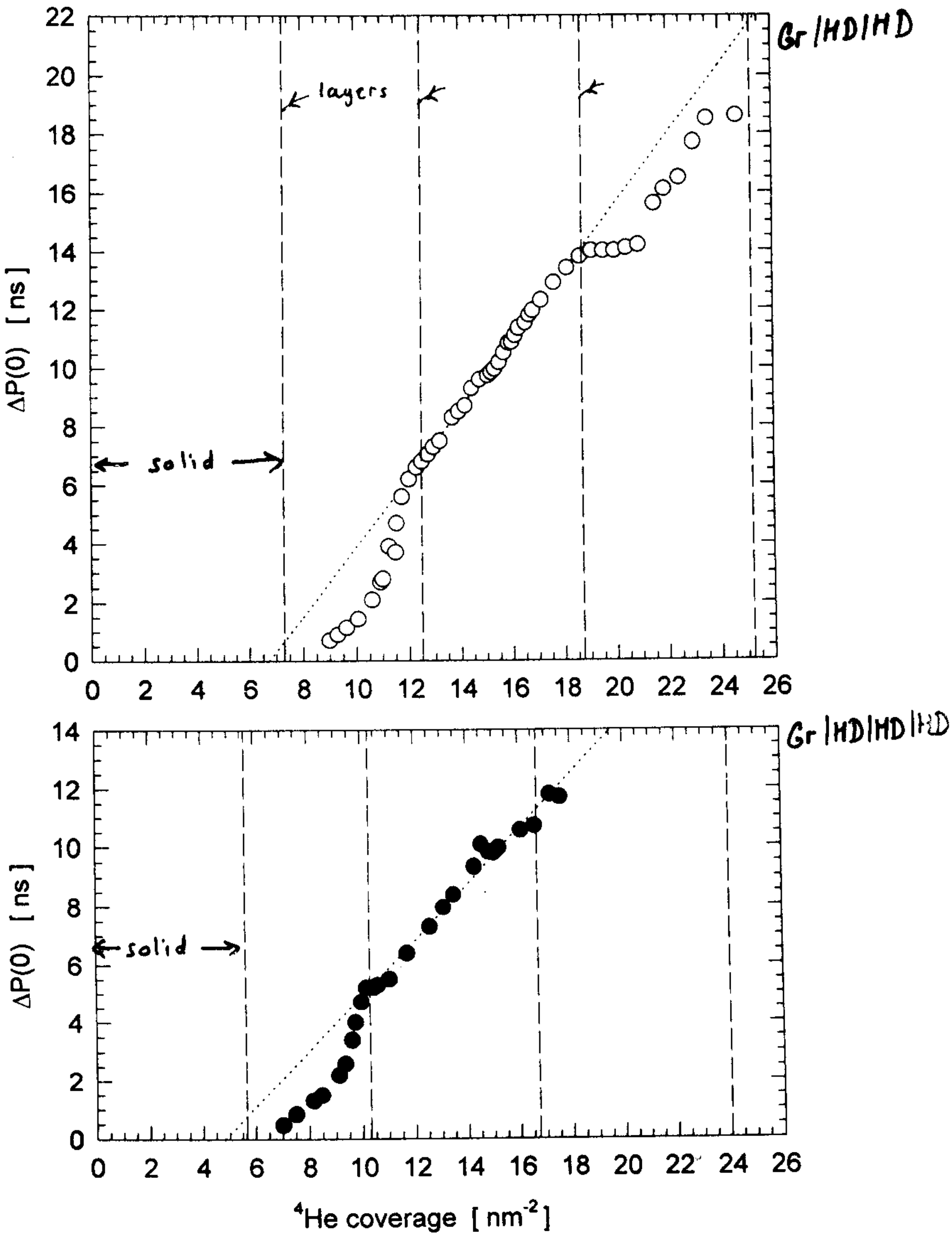
- all of the two fluid layers participates in superfluidity (see period shift data) (i.e. "dead" or "inert" layer is just solid layer)

- T_c depends much more weakly on n than K-T relation ($T_c = 0.156\ n \quad K\,nm^{-2}$) (similar to mylar data)

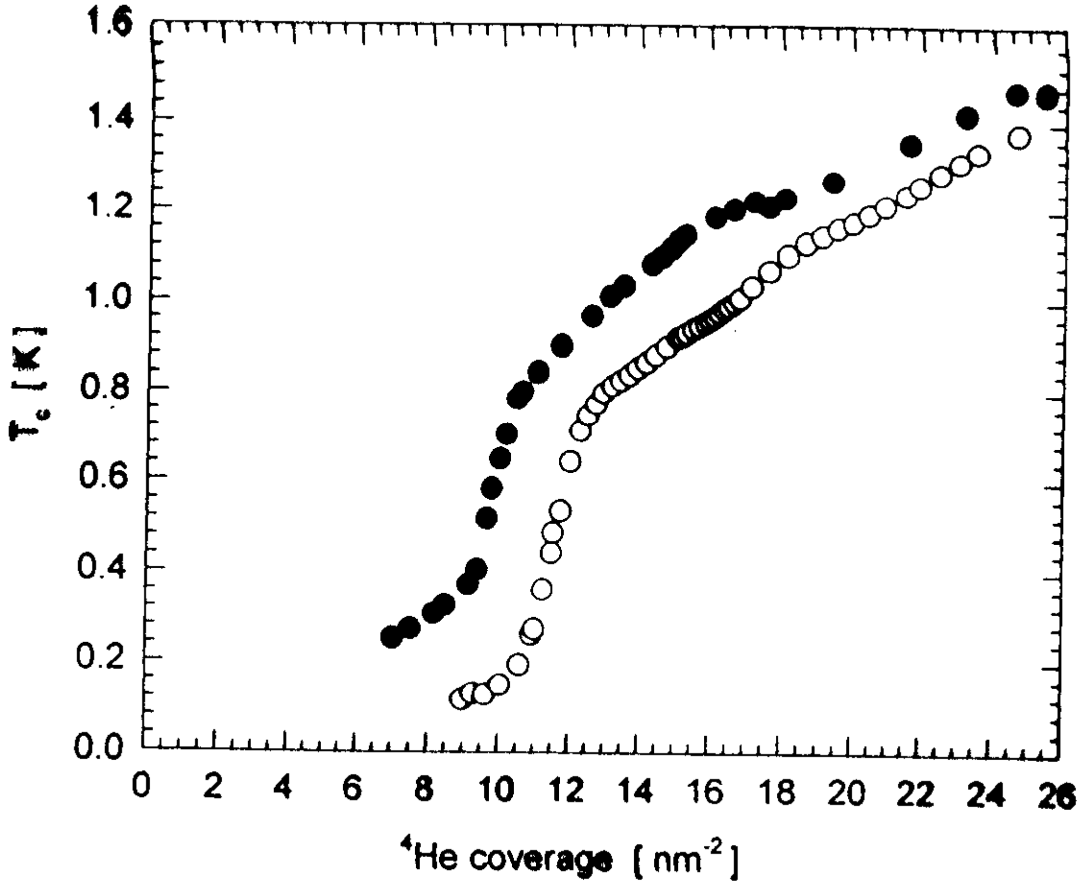
⇒ K-T theory does not apply to bi-layer

dynamics of vortices in a superfluid bi-layer ?

Low temperature period shift



Temperature of the dissipation peak



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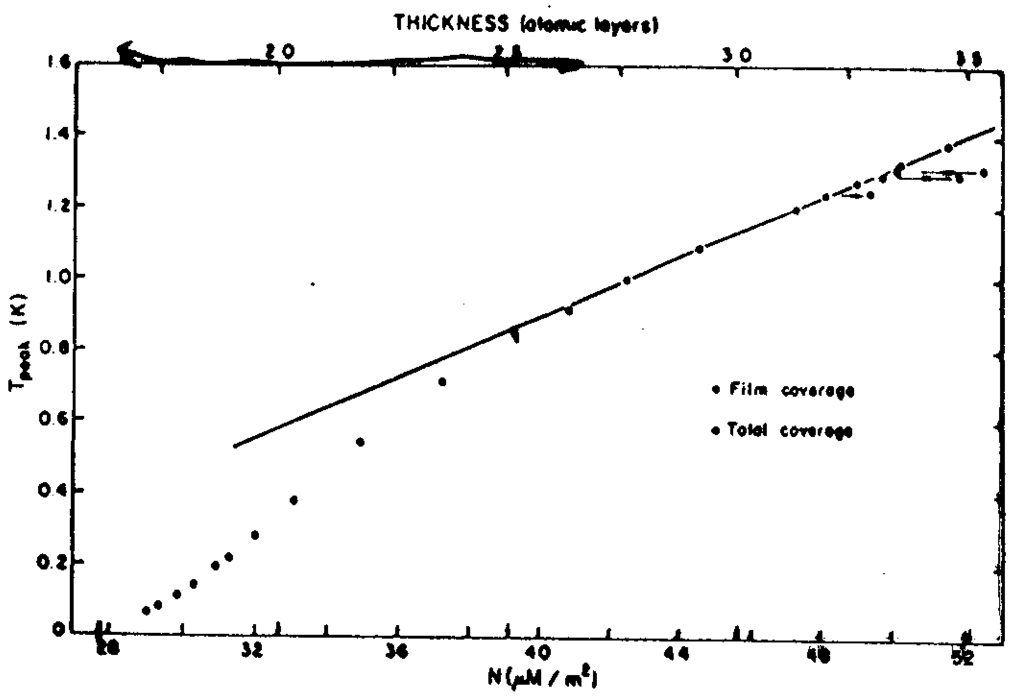

FIG. 14. Variation of T_{peak} with film coverage. The line is drawn to emphasize the coverage dependence of the lower covera data. The higher coverages have been corrected for depletion by the gas. The nominal thickness in atomic layers is shown.