Topological Defects and Phase Transitions
In two dimensions

Nobel Symposium, Stockholm, 08/12/2016

John Michael Kosterlitz
Department of Physics
Brown University
Providence, RI, USA

Situation of 2D systems in 1970's

2D magnetic models:

$H/kT = K(1 - s(i).s(j))$ $s = (s_1 \ldots s_n)$, $|s| = 1$

Numerical simulations and high temperature series expansions indicated:

n=1: (Ising model): yes, transition (exact solution, L. Onsager, 1944)

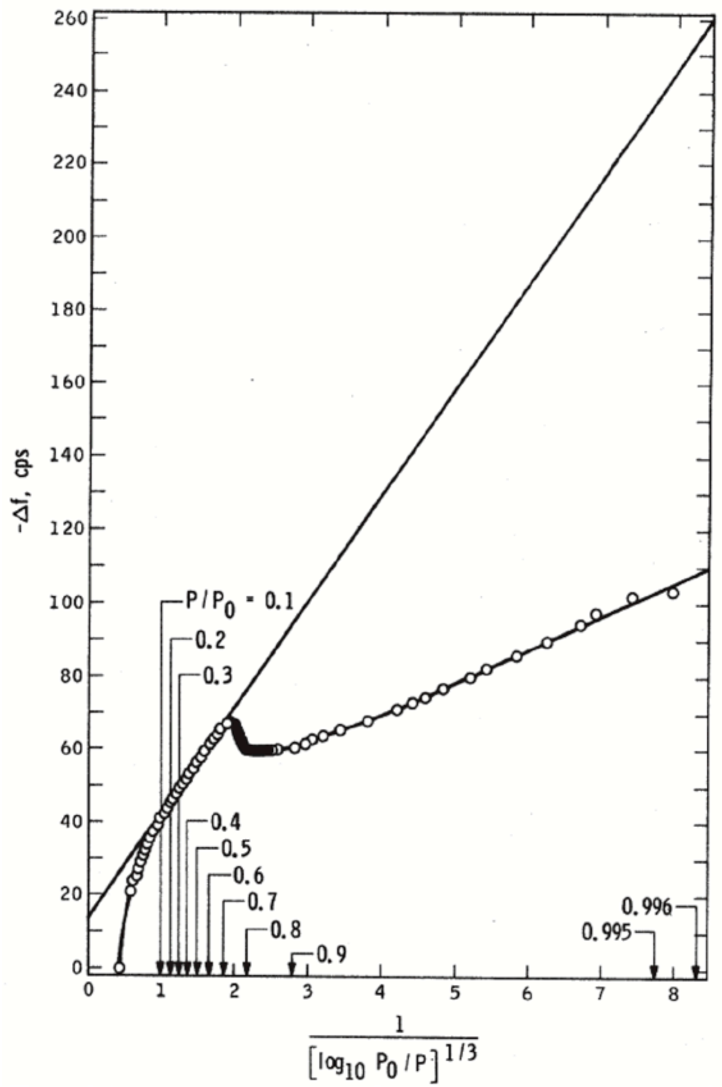
n=2: (superfluid He films): **maybe**

n>2 : probably not

n= infinity: NO phase transition (exact solution, H.E. Stanley, 1968)

This situation needed further study, especially for n=2 (Superfluid He^4 film, etc.)

Figure 1, M Chester, L C Yang and J B Stephens, Phys Rev Lett 29, 211 (1972)



1D Ising model: Topology defined by $s_i = \pm 1$ and spin configurations by positions of these domain walls or "topological defects".

Planar rotor model:

$$\mathrm{s}_i = |s|(\cos\theta_i, \sin\theta_i)$$

$$\Psi = s_x + is_y = |s|e^{i\theta_i} = |\Psi|e^{i\theta_i}.$$

Invariant under

$$\theta_i \to \theta_i + 2\pi n_i, \quad n_i = 0, \pm 1, \pm 2, \cdots$$

Topology is a torus $\Rightarrow$ global (topological) excitations are "vortices".

$$\oint_C d\theta = 2\pi n$$

Energy and entropy of isolated vortex in system of size L:

$$\Delta E = \pi J \ln(L/a),$$

$H/kT=(J/4kT)\Sigma(s_i-s_j)^2=(K(T)/2)\Sigma(\theta_i-\theta_j)^2$

$$\Delta S = k_B \ln(L^2/a^2).$$

Central quantity in statistical mechanics is the Free Energy, $F = E - TS$ because the probability of a configuration with free energy F is

$$P \propto \exp(-\beta F)$$

$$P(vortex) \to \left(\frac{L}{a}\right)^{-(\pi K-2)} = \begin{cases} 0, & \pi K > 2, \\ 1, & \pi K < 2 \end{cases}$$

When K(T) large, topological sector is stable and when K(T) small, have transitions between topological sectors!

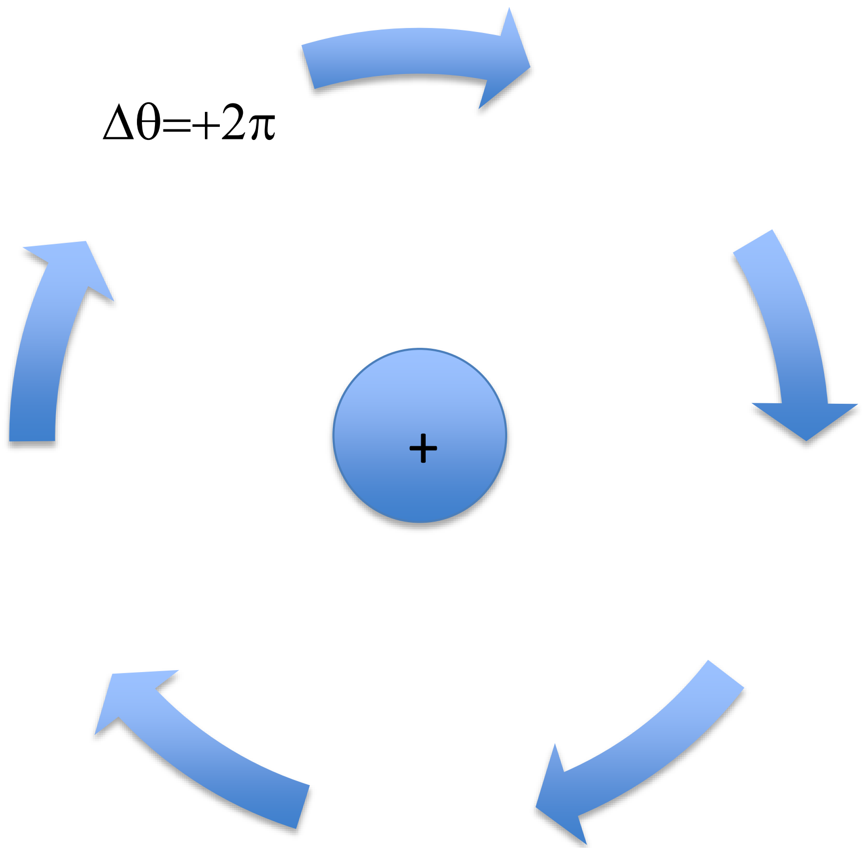
The Heisenberg model has $n = 3$ components, $\mathbf{s} = (\cos\theta, \sin\theta\cos\phi, \sin\theta\cos\phi)$ and there is one topological invariant $N = 0, \pm 1, \pm 2, \cdots$ where

$$N = \frac{1}{4\pi} \int d^2\mathbf{r} \sin\theta(\mathbf{r}) \left(\frac{\partial\theta(\mathbf{r})}{\partial x} \frac{\partial\phi(\mathbf{r})}{\partial y} - \frac{\partial\phi(\mathbf{r})}{\partial x} \frac{\partial\theta(\mathbf{r})}{\partial y} \right).$$

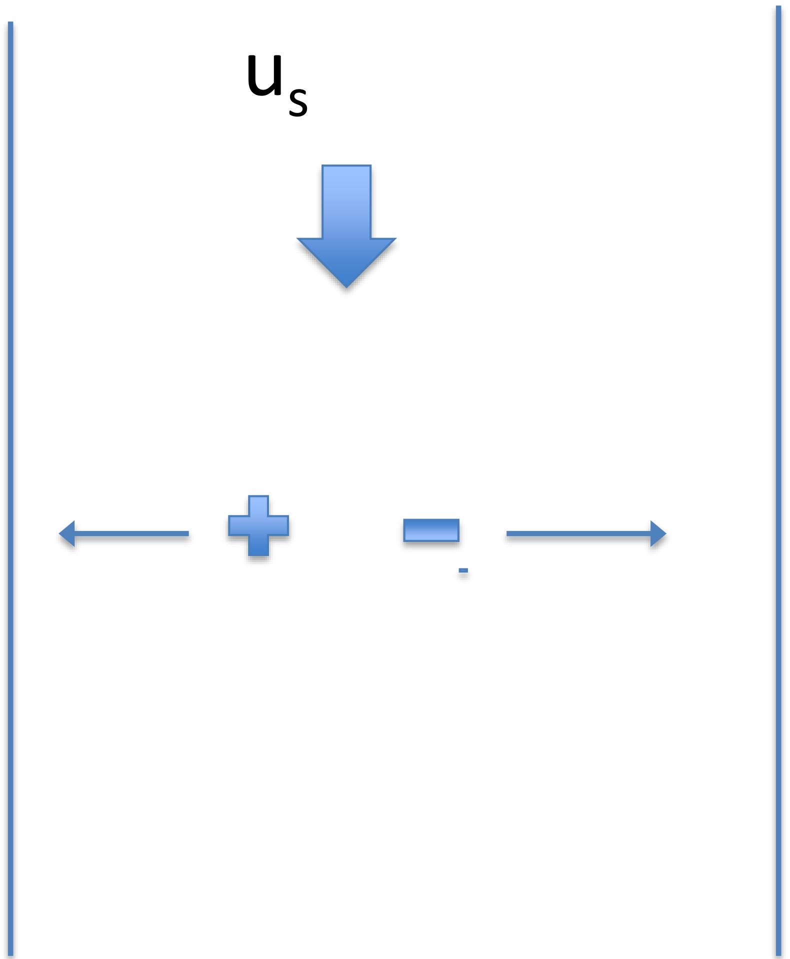
If we regard the direction of the magnetization in space as giving a mapping of the space on to the surface of a unit sphere, the invariant N measures the number of times space encloses the unit sphere. This invariant is of no consequence in statistical mechanics because the energy barrier separating configurations with different values of N is of order unity. Thus, there is no barrier between different topological sectors which implies that there is no ordered state for the $2D$ $n = 3$ Heisenberg magnet.

N.D. Mermin, H. Wagner, 1966

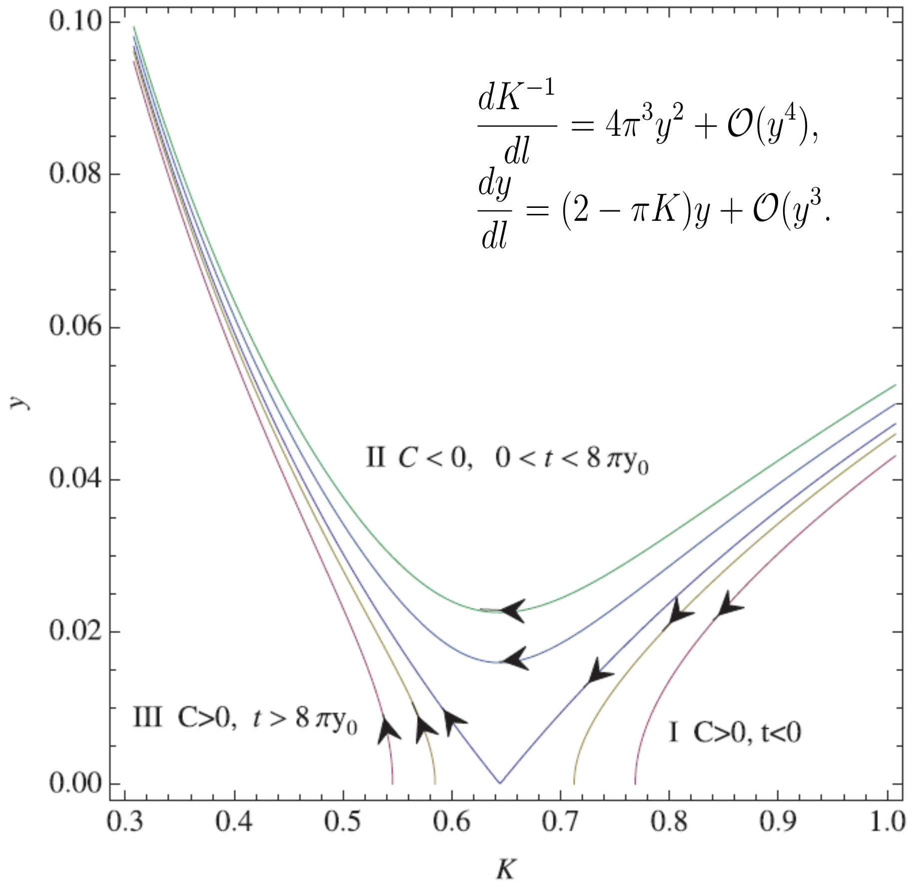
Vortex with n=+1. n=-1 vortex, fluid flow is in opposite direction.



Uniform superfluid velocity u_s reduced by h/mL when vortex goes across system.



RG flows in the (K,y) plane. The transition temperature $T_c(y)$ is the straight line on the right ending at $K=2/\pi$.



Crucial predictions of our theory

Measured stiffness: $$K^R(K_0, y_0) = K^R(K(l), y(l)),$$

Correlation lengths:
$$\xi_-(T) \sim \exp\left(b|t|^{-\frac{1}{2}}\right), \ \ t < 0, \quad t \equiv \frac{T - T_c}{T_c}$$
$$\xi_+(T) \sim \exp\left(\frac{2\pi}{b} t^{-\frac{1}{2}}\right), \ \ t > 0,$$

Superfluid density:
$$\frac{\hbar^2 \rho_s^R(T)}{m^2 k_B T} = K^R(K_0, y_0) = K^R(K(\infty), y(\infty) = K(\infty) = \frac{2}{\pi} + b\sqrt{|t|}, \quad t<0$$
$$\frac{\rho_s^R(T_c^-)}{T_c} = \frac{2m^2 k_B}{\pi \hbar^2} = 3.491 \times 10^{-8} \mathrm{gm\ cm^{-2}\ K^{-1}}.$$

J M Kosterlitz. The critical properties of the two-dimensional xy model. *Journal of Physics C: Solid State Physics*, 7(6):1046, 1974.

J M Kosterlitz and D J Thouless. Long range order and metastability in two dimensional solids and superfluids.(Application of dislocation theory). *Journal of Physics C: Solid State Physics*, 5(11):L124, 1972.

J M Kosterlitz and D J Thouless. Ordering, metastability and phase transitions in two-dimensional systems. *Journal of Physics C: Solid State Physics*, 6(7):1181, 1973.

Figure 2: DJ Bishop and JD Reppy, Phys Rev Lett 40, 1727 (1978)

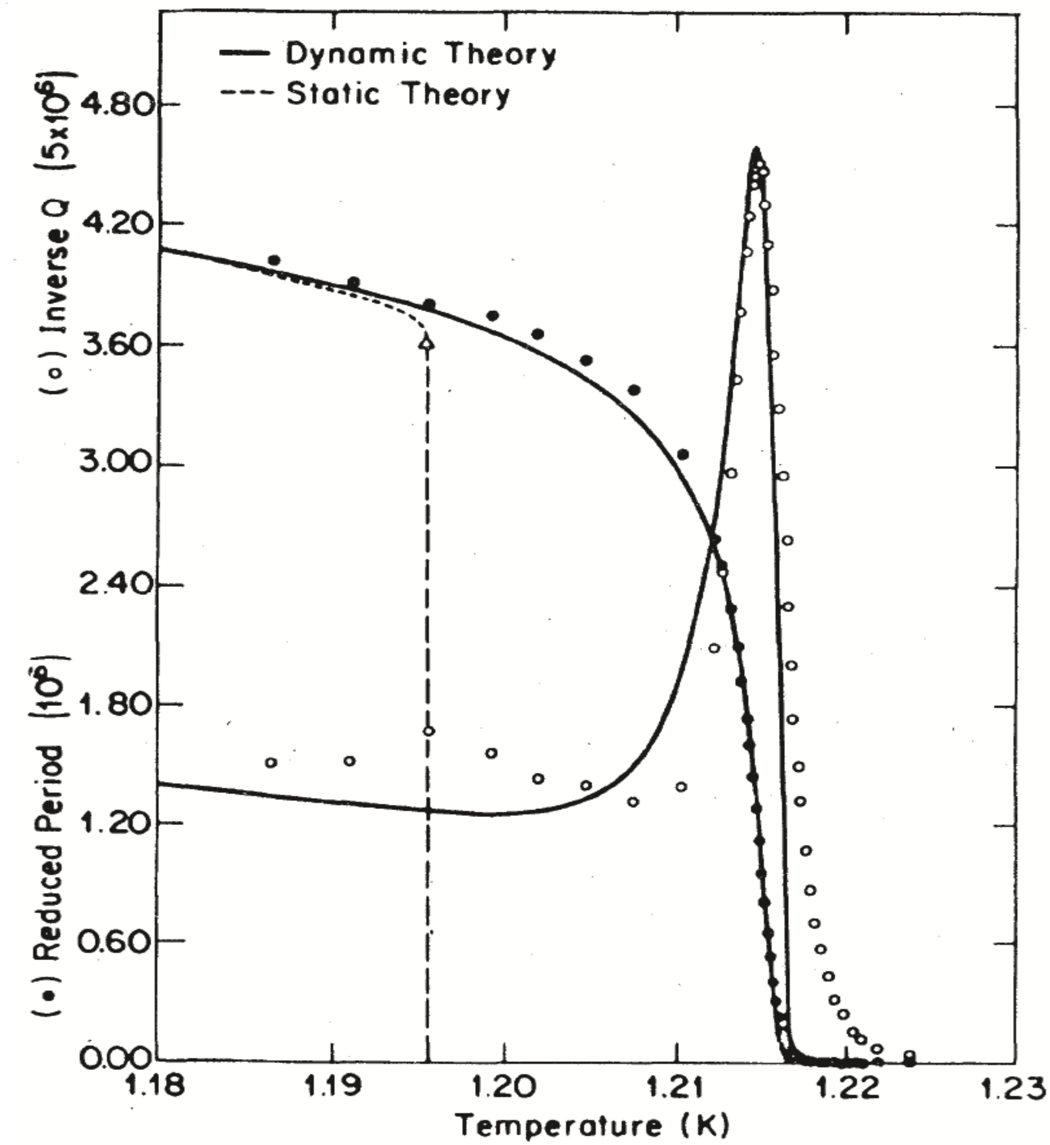
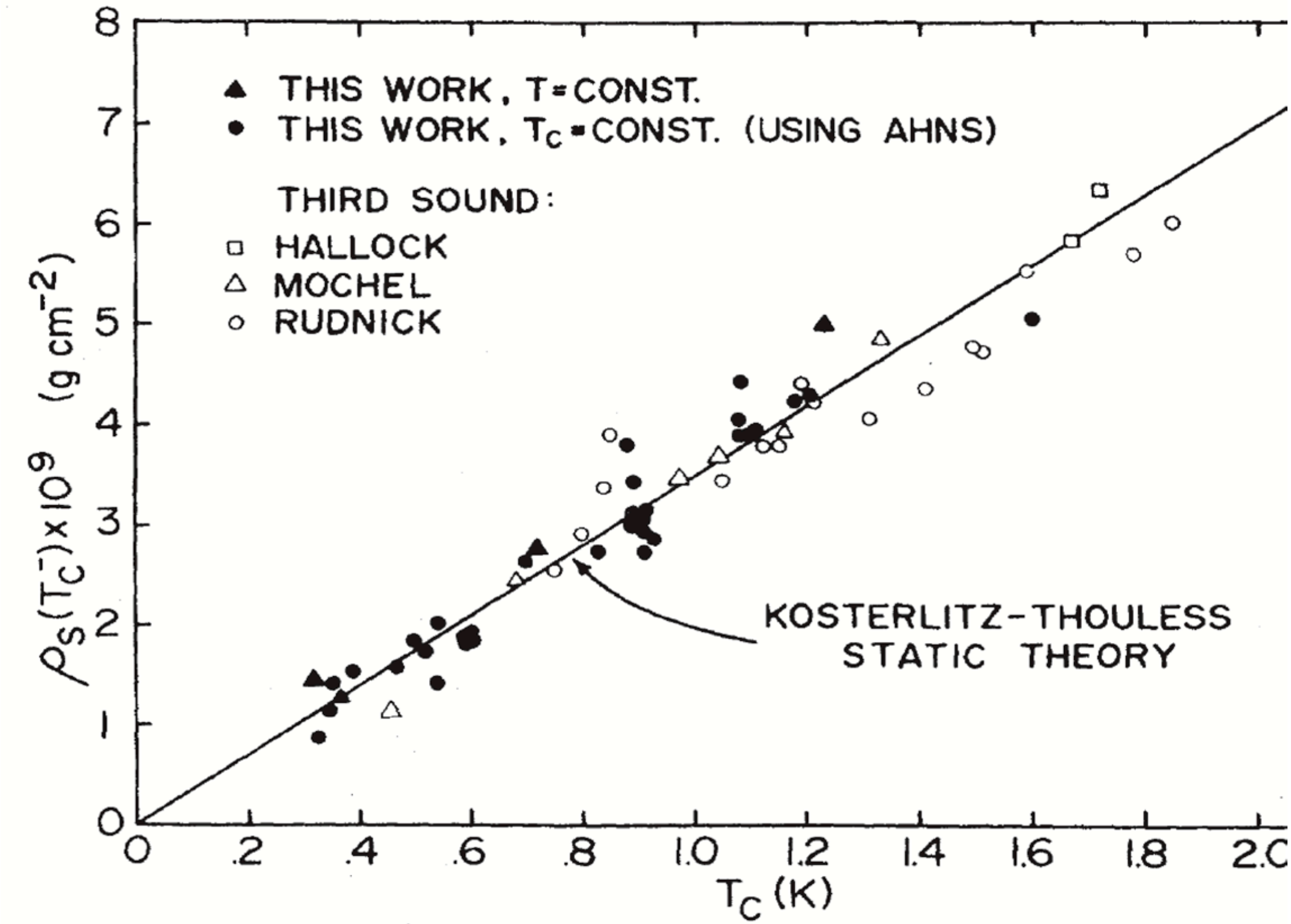


Figure 3: DJ Bishop and JD Reppy, Phys Rev Lett 40, 1727 (1978).



Two possible orders in 2D crystal:

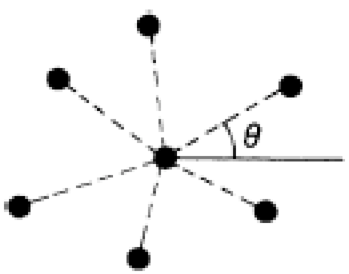
Translational order: Particle positions at **R=r+u(r)**

r=n$\mathbf{e}_1$+m$\mathbf{e}_2$ define ideal periodic lattice.

u(**r**) is displacement from ideal lattice position.

Order Parameters: $$\rho_{\mathbf{G}}(\mathbf{r}) = \exp\left(i\mathbf{G}\cdot(\mathbf{r}+\mathbf{u}(\mathbf{r}))\right)$$

Orientational order: Triangular lattice has 6 crystal axes $\pi/3$ apart.



Orientational order parameter: $$\psi(\mathbf{r}) = \exp\left(6i\theta(\mathbf{r})\right)$$

Harmonic crystal in 2D described by elastic free energy

$$\frac{H}{kT} = \frac{1}{2}\int d^2r(2\mu u_{ij}^2 + \lambda u_{kk}^2) \qquad u_{ij}(\vec{r}) = \frac{1}{2}\left(\frac{\partial u_i(\vec{r})}{\partial r_j} + \frac{\partial u_j(\vec{r})}{\partial r_i}\right)$$

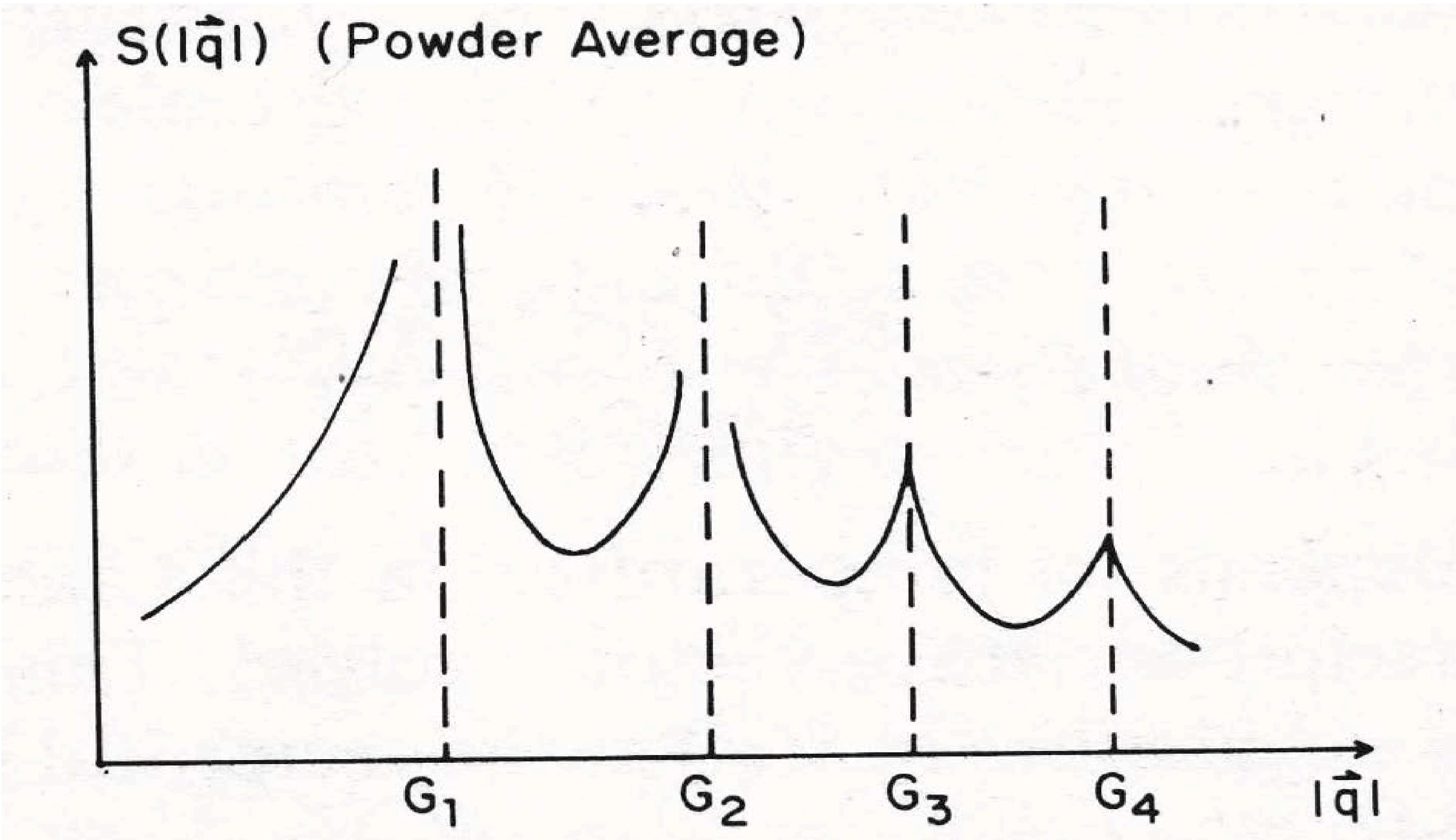
$$C_G(\mathbf{r}) = \langle \rho_{\mathbf{G}}(\mathbf{r})\rho_{\mathbf{G}}^*(0)\rangle \sim r^{-\eta_G(T)} \qquad \rho_{\mathbf{G}}(\mathbf{r}) = \exp\left(i\mathbf{G}\cdot(\mathbf{r}+\mathbf{u}(\mathbf{r}))\right)$$

$$\eta_G(T) = \frac{k_B T G^2(3\mu+\lambda)}{4\pi\mu(2\mu+\lambda)}$$

Structure function:

$$S(\mathbf{q}) = \langle \rho(\mathbf{q})\rho(-\mathbf{q})\rangle = \sum_{\mathbf{r}} e^{i\mathbf{q}\cdot\mathbf{r}}\langle \exp\left[i\mathbf{q}\cdot(\mathbf{u}(\mathbf{r})-\mathbf{u}(\mathbf{0}))\right]\rangle \sim |\mathbf{q}-\mathbf{G}|^{-2+\eta_G(T)}$$

Figure 2.19: D.R. Nelson ``Defects and Geometry in Condensed Matter Physics”
(Cambridge University Press) 2002



Bond Angle (or crystal axes) Order in Harmonic Crystal

$$\psi(\mathbf{r}) = \exp\left(6i\theta(\mathbf{r})\right) \qquad \theta(\mathbf{r}) = \frac{1}{2}\left(\frac{\partial u_y(\mathbf{r})}{\partial x} - \frac{\partial u_x(\mathbf{r})}{\partial y}\right)$$

$$\langle \psi(\mathbf{r})\psi^*(0)\rangle = constant$$

Gaussian theory says: (i) algebraic decay of translational order (Mermin-Wagner theorem)
(ii) long range orientational order
(iii) elastic moduli finite

Need to identify excitations which will lead to isotropic liquid – dislocations & disclinations

Dislocation:

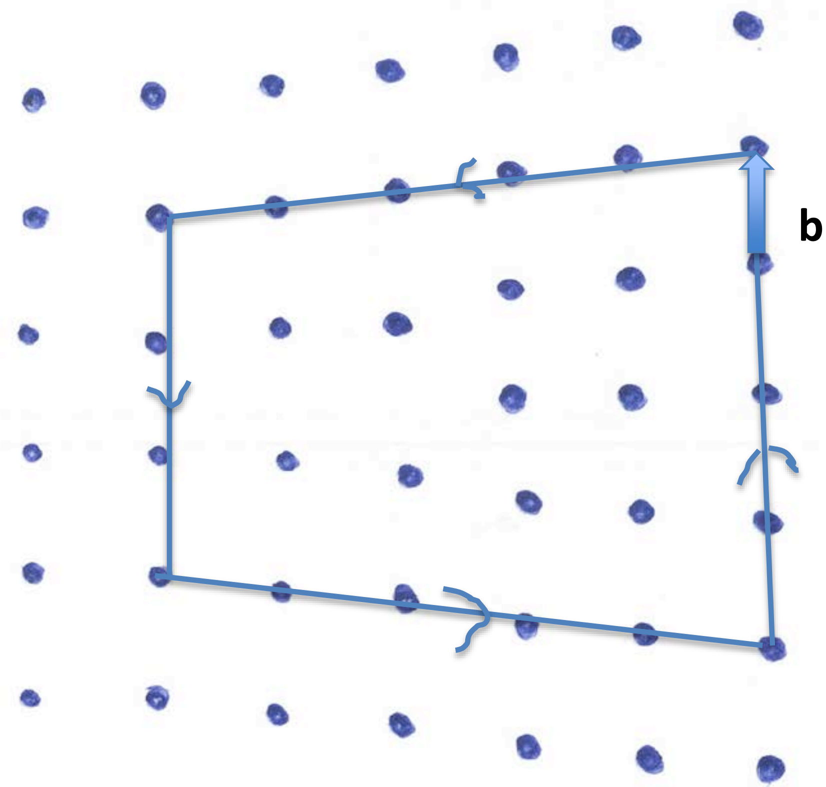
$$\oint d\vec{u} = \vec{b}(\vec{r}) = n(\vec{r})\vec{e}_1 + m(\vec{r})\vec{e}_2$$

Disclination

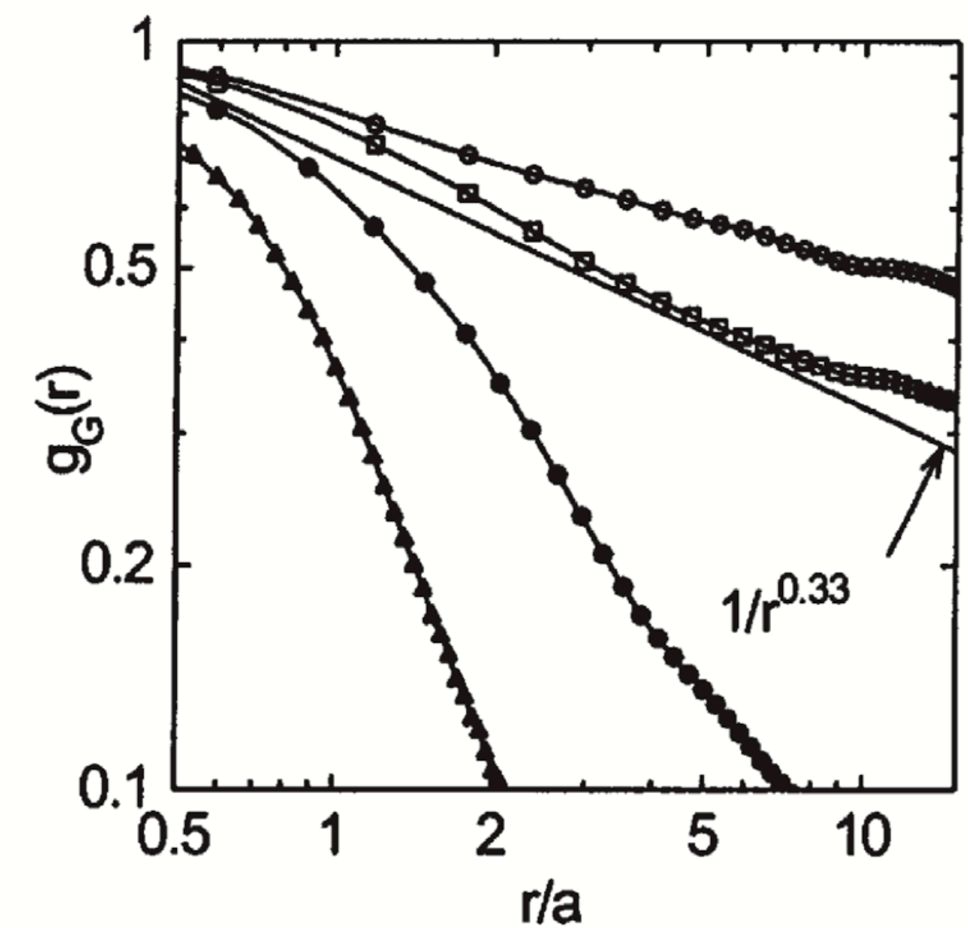
$$\oint d\theta = \frac{2\pi}{6}n \qquad n = 0, \pm 1, \pm 2, \cdots$$

$$\vec{e}_1 = (1, 0)$$
$$\vec{e}_2 = (-1/2, \sqrt{3}/2)$$
$$\vec{e}_3 = (-1/2, -\sqrt{3}/2)$$

Dislocation in square lattice. Burger's vector b amount 3x5 contour fails to close.



Reprinted with permission from Figure 1: K Zahn, R Lenke and G Maret, Phys Rev Lett 82, 2721 (1999). A plot of the correlation function $g_G(r)=r^{-\eta}$



Orientational correlation function $g_6(r)=1/r^{\eta_6(T)}$. Reprinted with permission from K Zahn, R Lenke and G Maret, Phys Rev Lett 82, 2721 (1999)

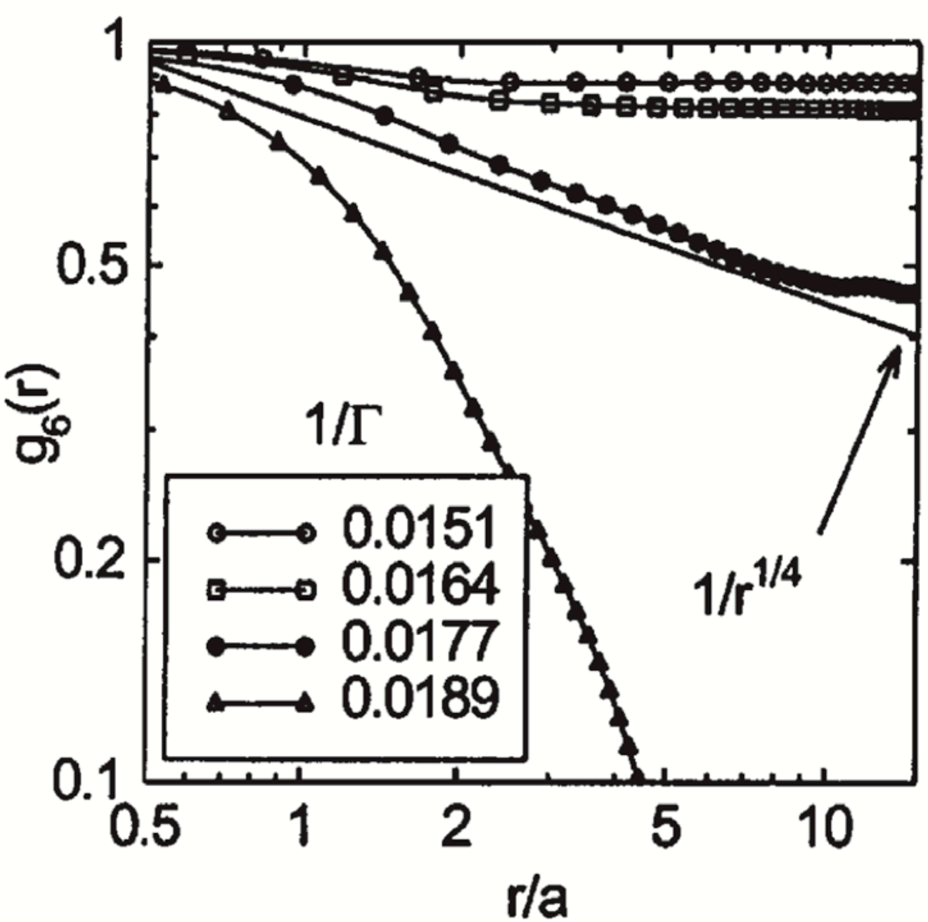
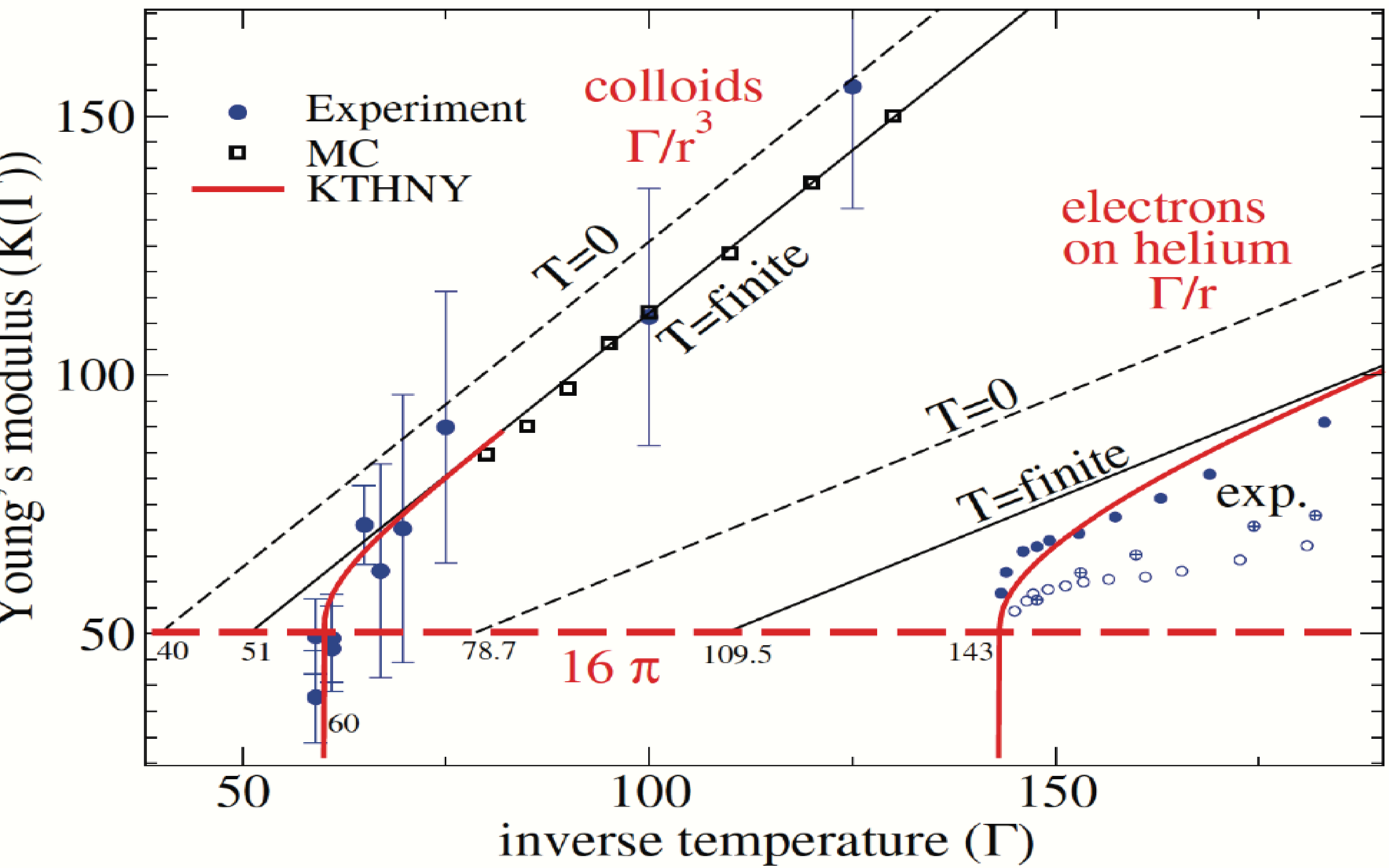


Figure 2 (J Zanghellini et al 2005 J. Phys: Condens. Matter 17 S3579)



Reprinted figure with permission from HH von Gruenberg, P Keim and G Maret, Phys Rev Lett 93,255703 (2004). Copyright 2004 by the American Physical Society.

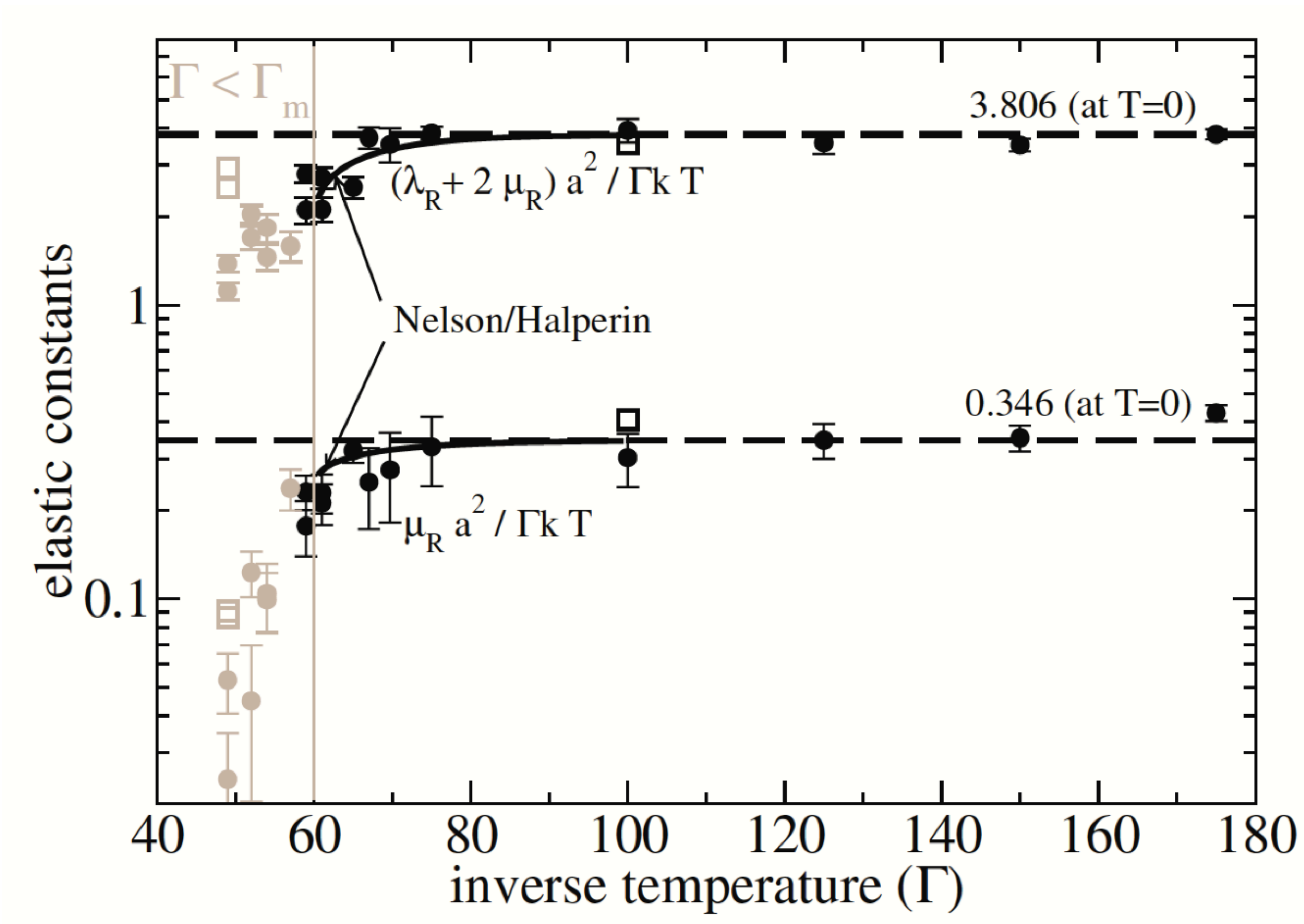
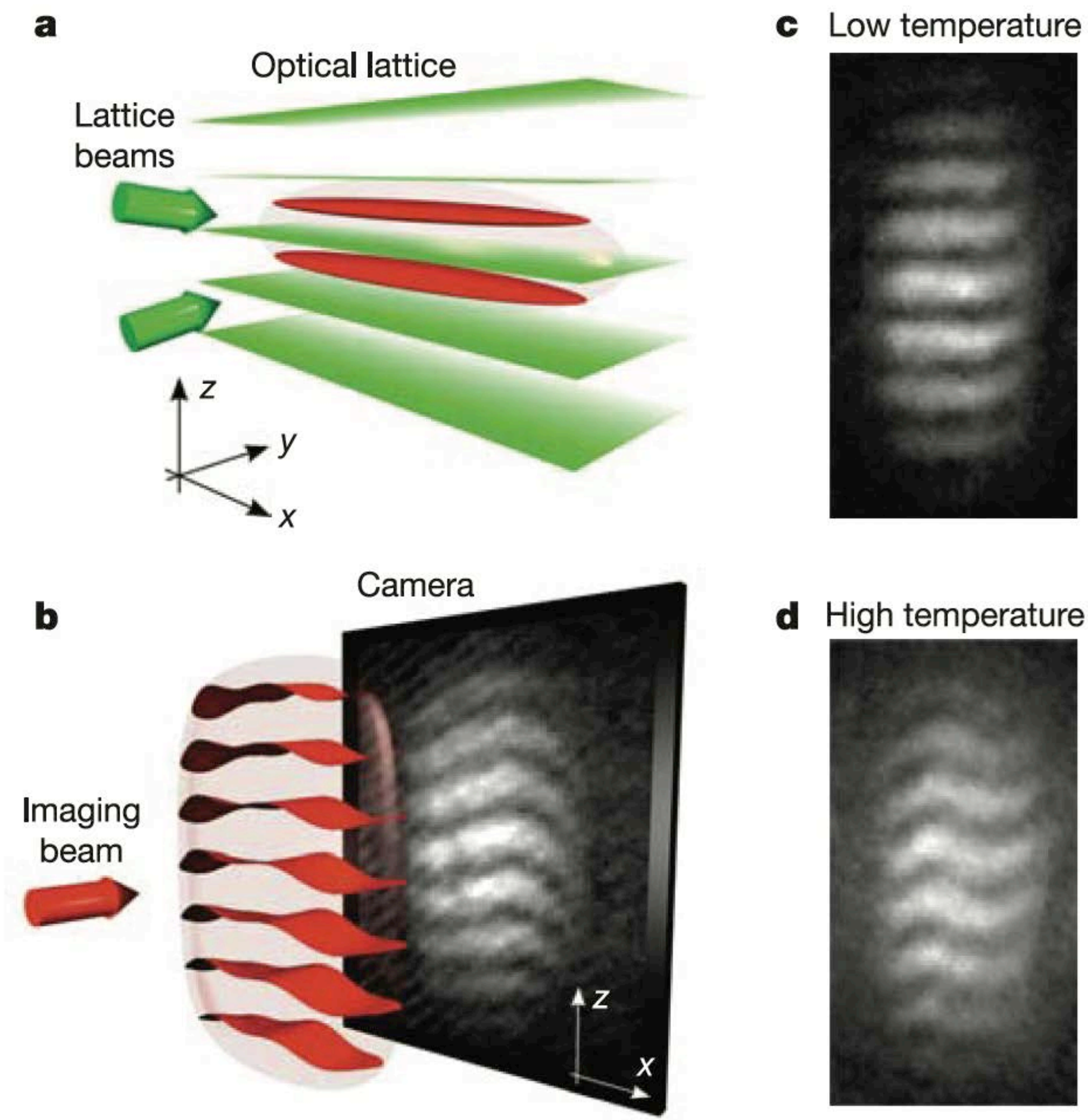


Figure 1 reprinted with permission from Z Hadzibabic, P Kruger, M Cheneau, B Battelier and J Dalibard, Nature 441, 1118 (2006). Copyright 2006 Nature Publishing Group



Conclusion Remarks

I would like to thank David Thouless for introducing me to this beautiful problem, and David Nelson for collaboration and discussions, and John Reppy for many useful discussions, and the Nobel Committee for the recognition.

I wish to thank my wife Berit for an incredible life journey taking us from Birmingham to Providence; finally, but not least, my children Cairn, Jonanthan, Elizabeth for putting up with me.