Topological Defects and Phase Transitions In two dimensions

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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)

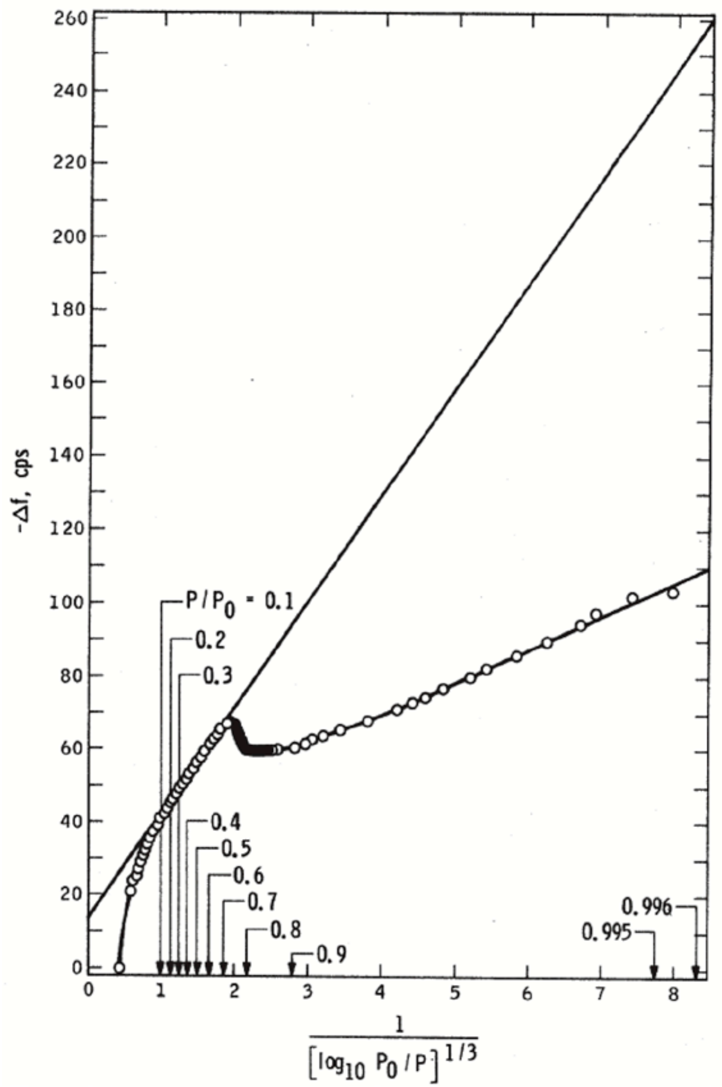
n=2: (superfluid He films): **maybe**

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)



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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:

$$\Delta E = \pi J \ln(L/a), \qquad H/kT=(J/4kT)\Sigma(s_i-s_j)^2=(K(T)/2)\Sigma(\theta_i-\theta_j)^2$$

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

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!

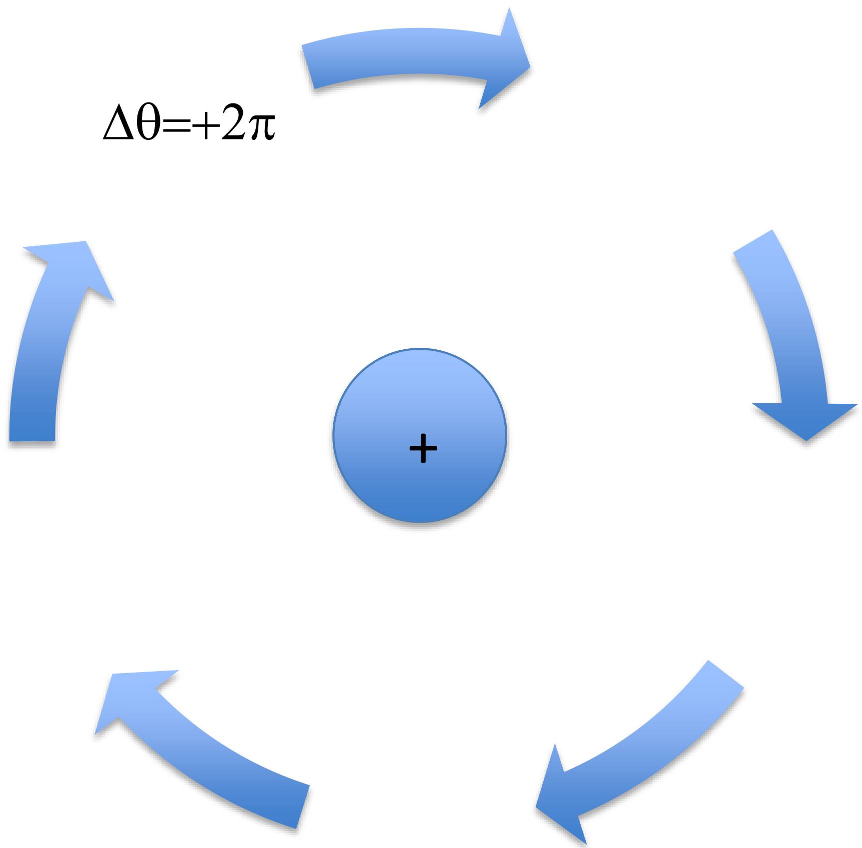
The Heisenberg model has $n = 3$ components, $\mathbf{s} = (\cos\theta, \sin\theta\cos\phi, \sin\theta\cos\phi)$ and there is one topological invariant $N = 0, \pm 1, \pm 2, \cdots$ where

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

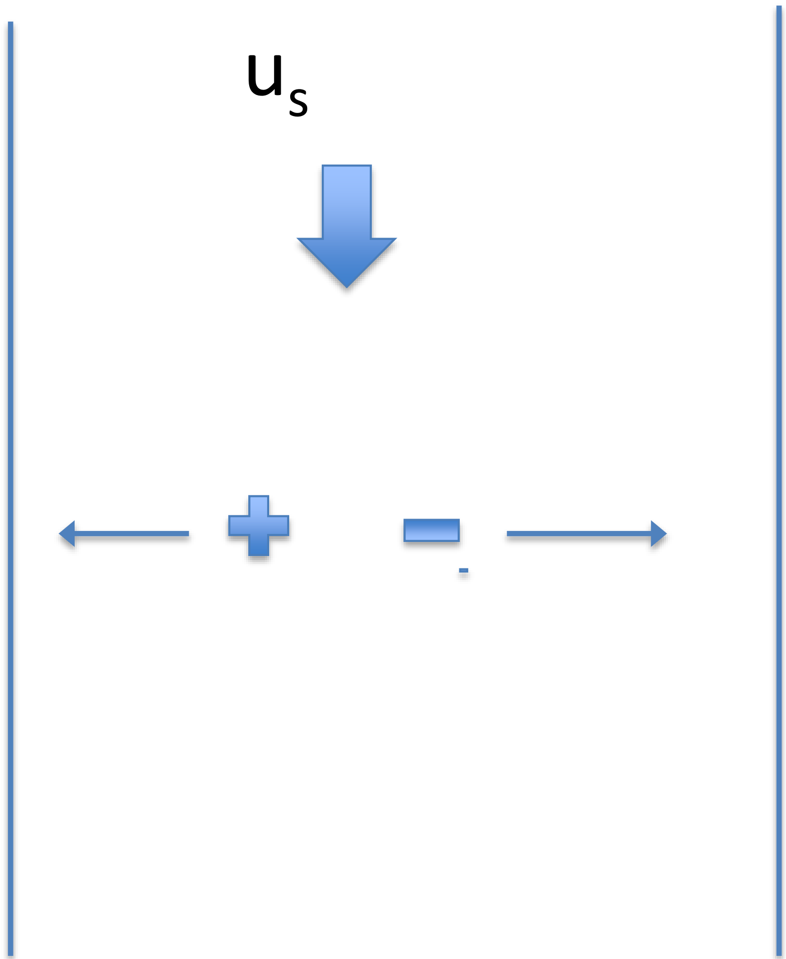
If we regard the direction of the magnetization in space as giving a mapping of the space on to the surface of a unit sphere, the invariant N measures the number of times space encloses the unit sphere. This invariant is of no consequence in statistical mechanics because the energy barrier separating 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

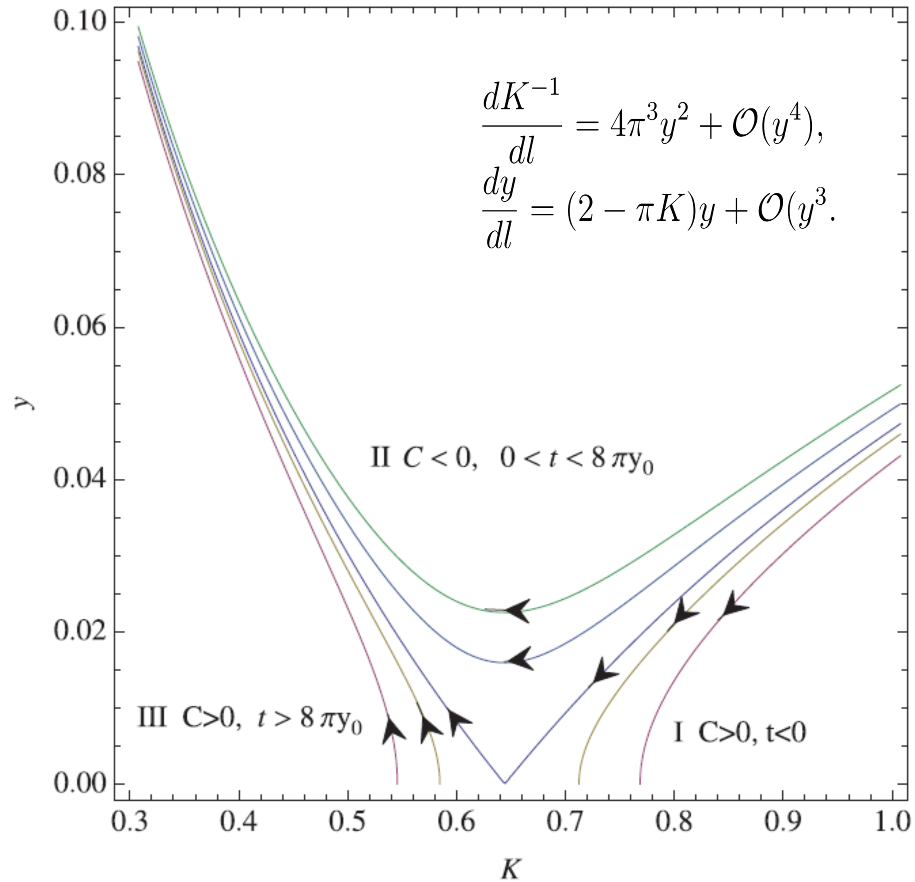
Vortex with n=+1. n=-1 vortex, fluid flow is in opposite direction.



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:

$$\frac{\hbar^2 \rho_s^R(T)}{m^2 k_B T} = K^R(K_0, y_0) = K^R(K(\infty), y(\infty) = K(\infty) = \frac{2}{\pi} + b\sqrt{|t|}, \quad t<0$$

$$\frac{\rho_s^R(T_c^-)}{T_c} = \frac{2m^2 k_B}{\pi \hbar^2} = 3.491 \times 10^{-8} \mathrm{gm\ cm}^{-2}\ \mathrm{K}^{-1}.$$

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)

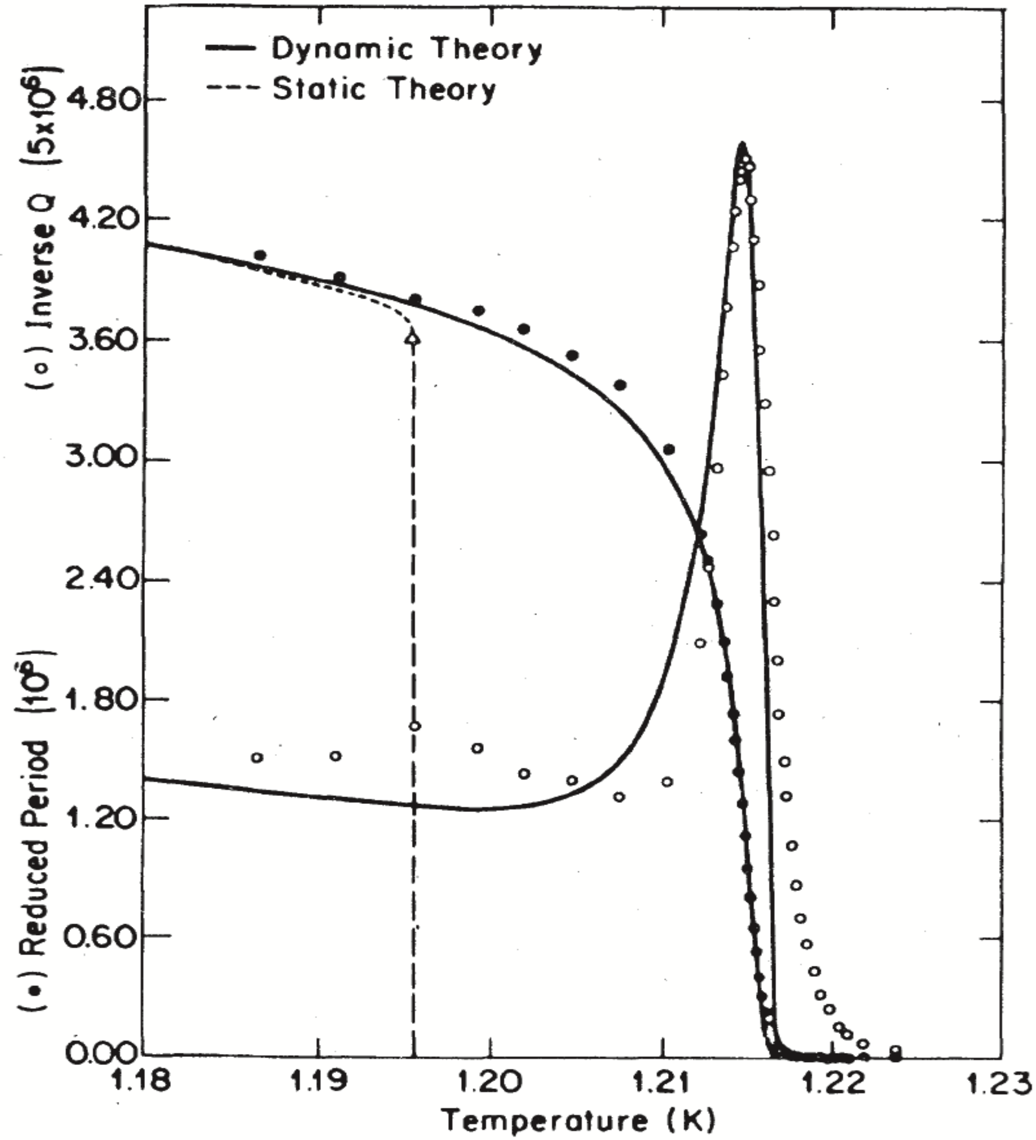
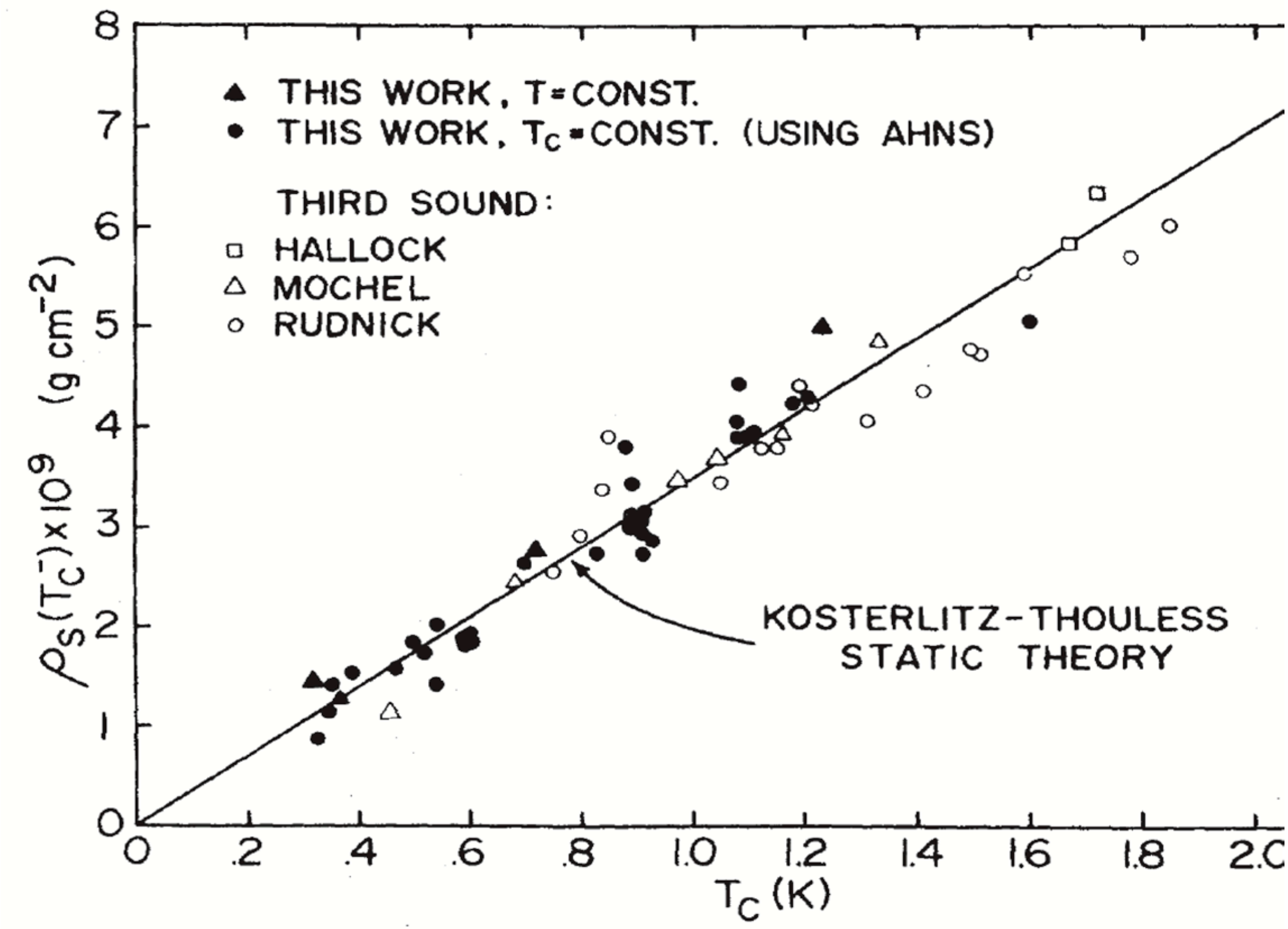


Figure 3: DJ Bishop and JD Reppy, Phys Rev Lett 40, 1727 (1978).



Two possible orders in 2D crystal:

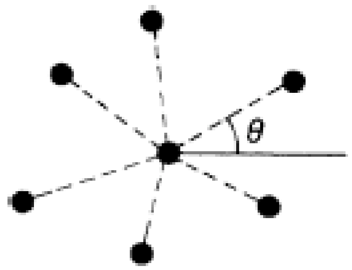
Translational order: Particle positions at **R=r+u(r)**

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

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

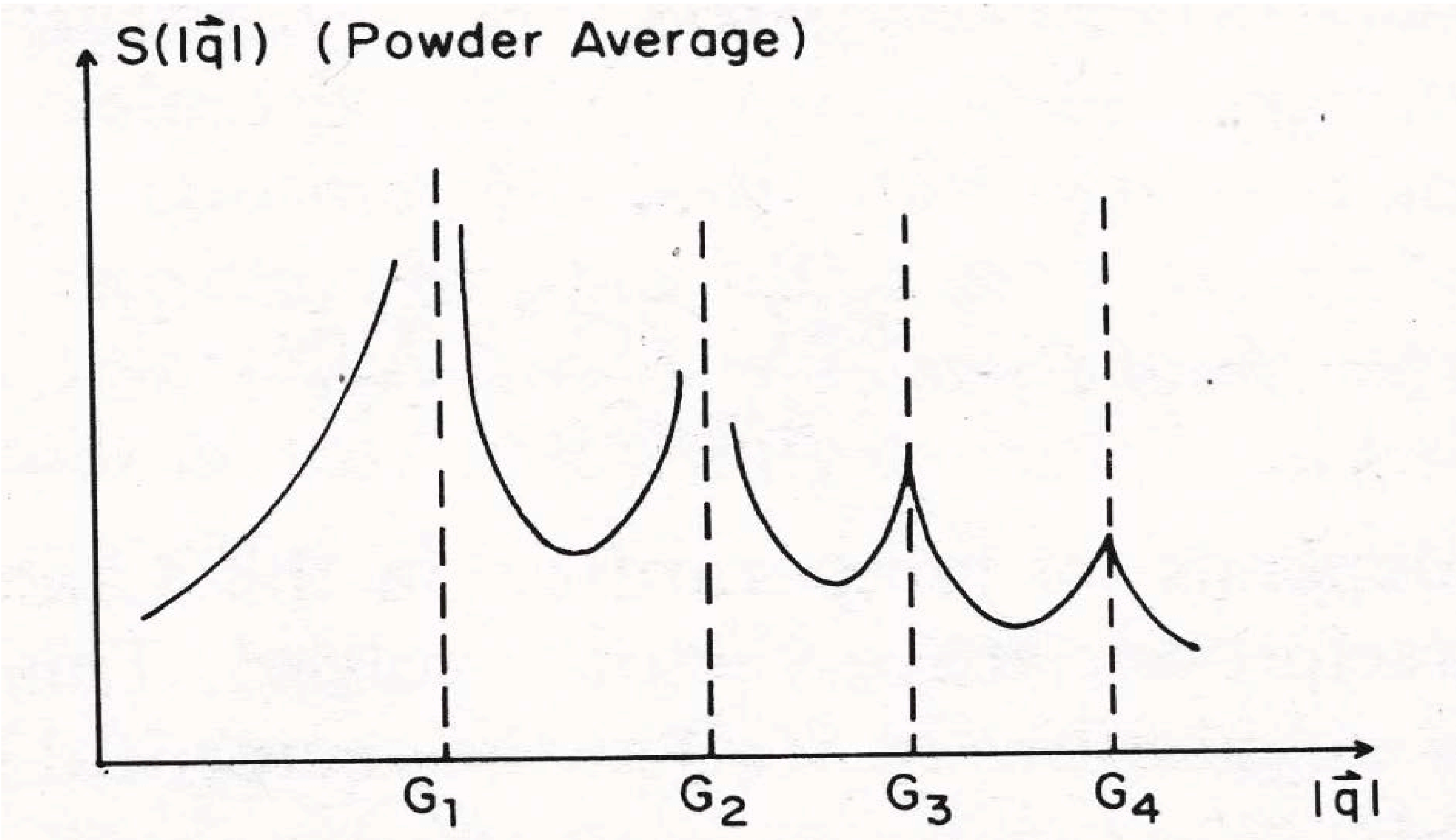
$$C_G(\mathbf{r}) = \langle \rho_{\mathbf{G}}(\mathbf{r})\rho_{\mathbf{G}}^*(0)\rangle \sim r^{-\eta_G(T)} \qquad \rho_{\mathbf{G}}(\mathbf{r}) = \exp\left(i\mathbf{G}\cdot(\mathbf{r}+\mathbf{u}(\mathbf{r}))\right)$$

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

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

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

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

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:

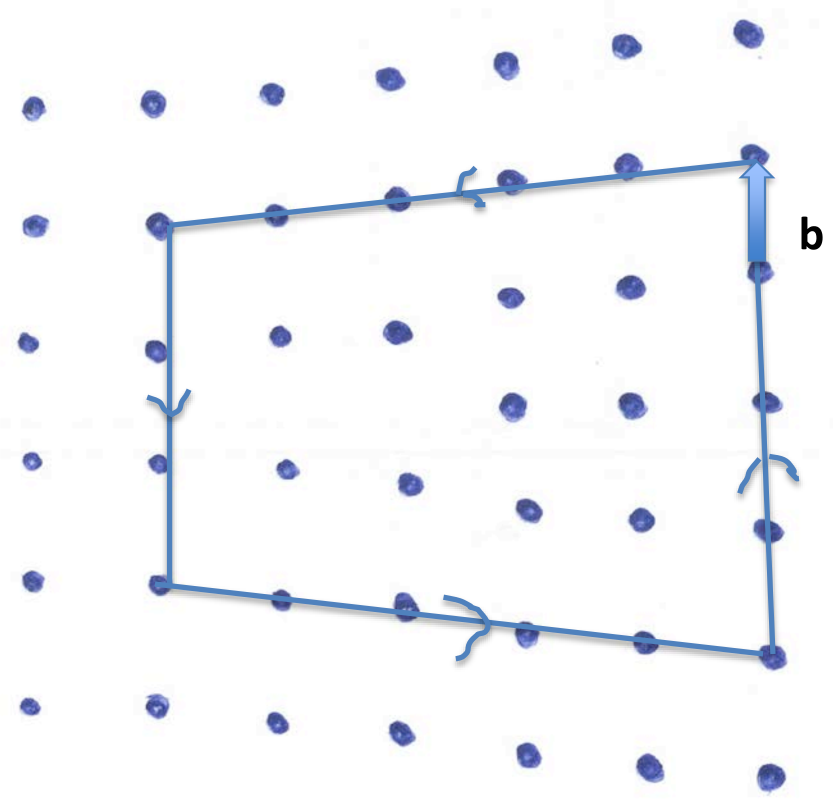
$$\oint d\vec{u} \;=\; \vec{b}(\vec{r}) = n(\vec{r})\vec{e}_1 + m(\vec{r})\vec{e}_2$$

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.



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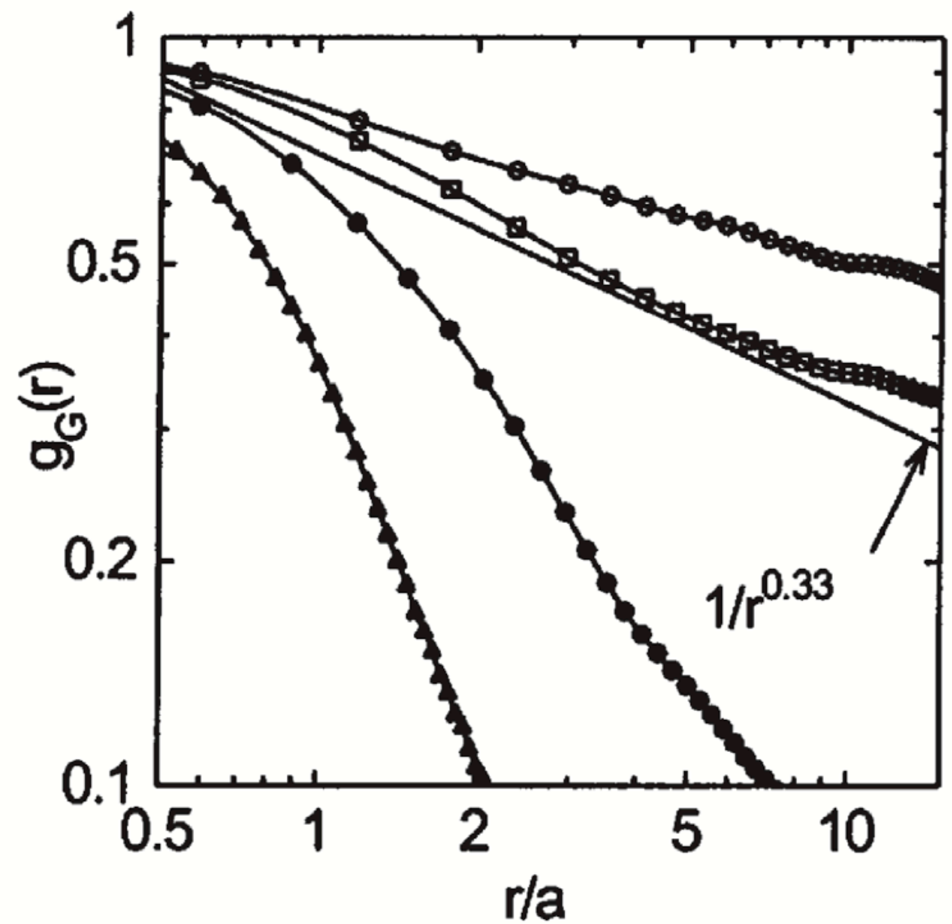


Orientational correlation function $g_6(r)=1/r^{\eta_6(T)}$. Reprinted with permission from K Zahn, R Lenke and G Maret, Phys Rev Lett 82, 2721 (1999)

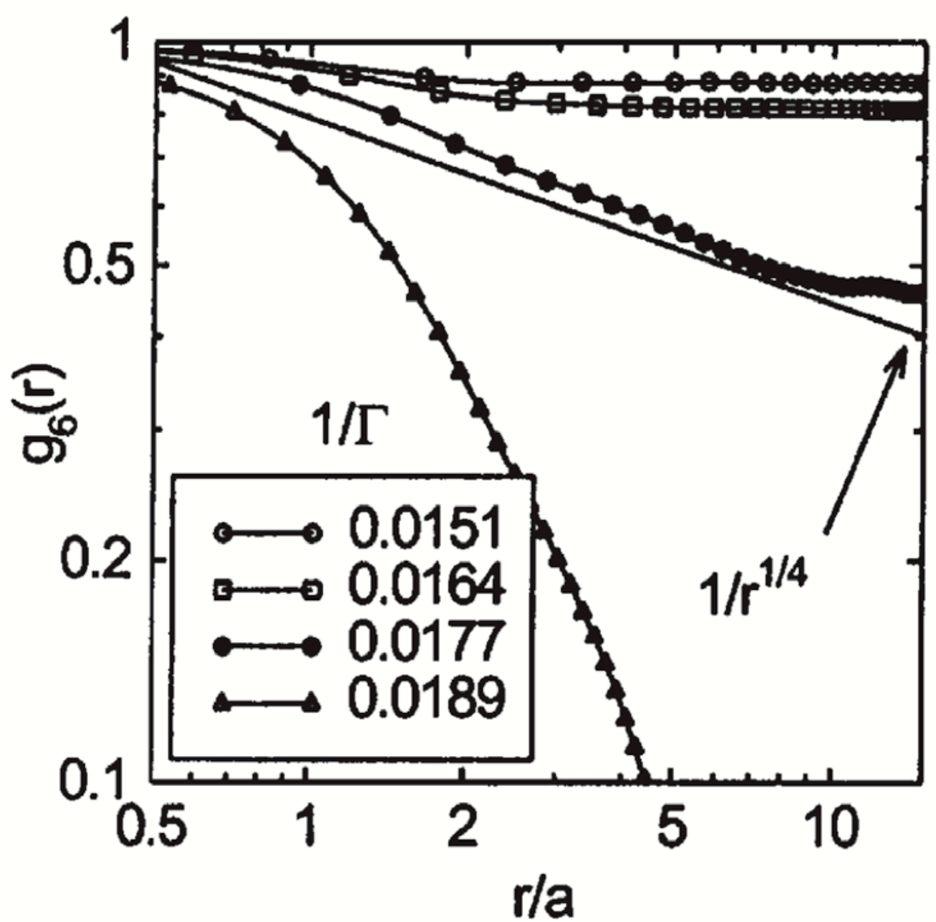
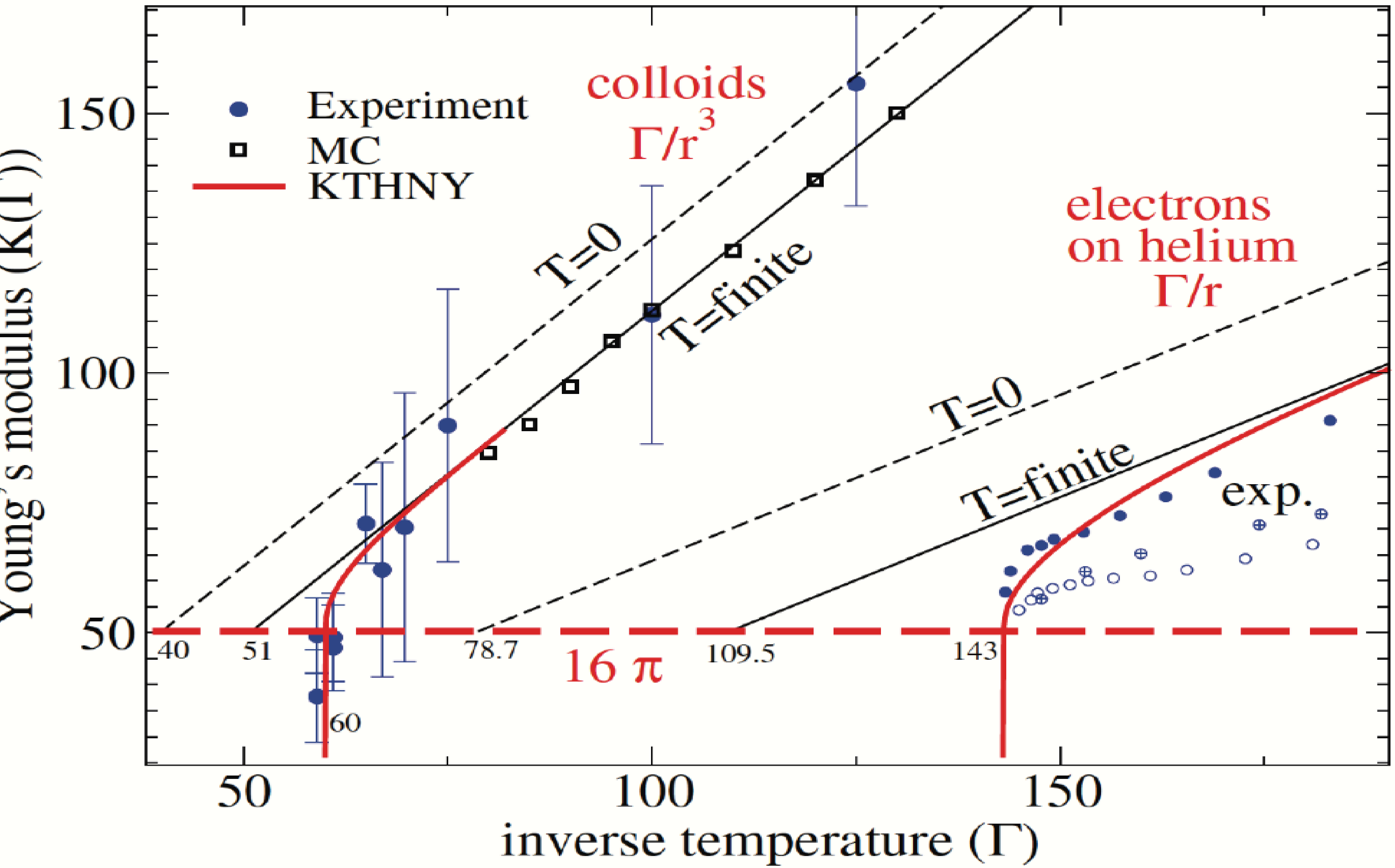


Figure 2 (J Zanghellini et al 2005 J. Phys: Condens. Matter 17 S3579)



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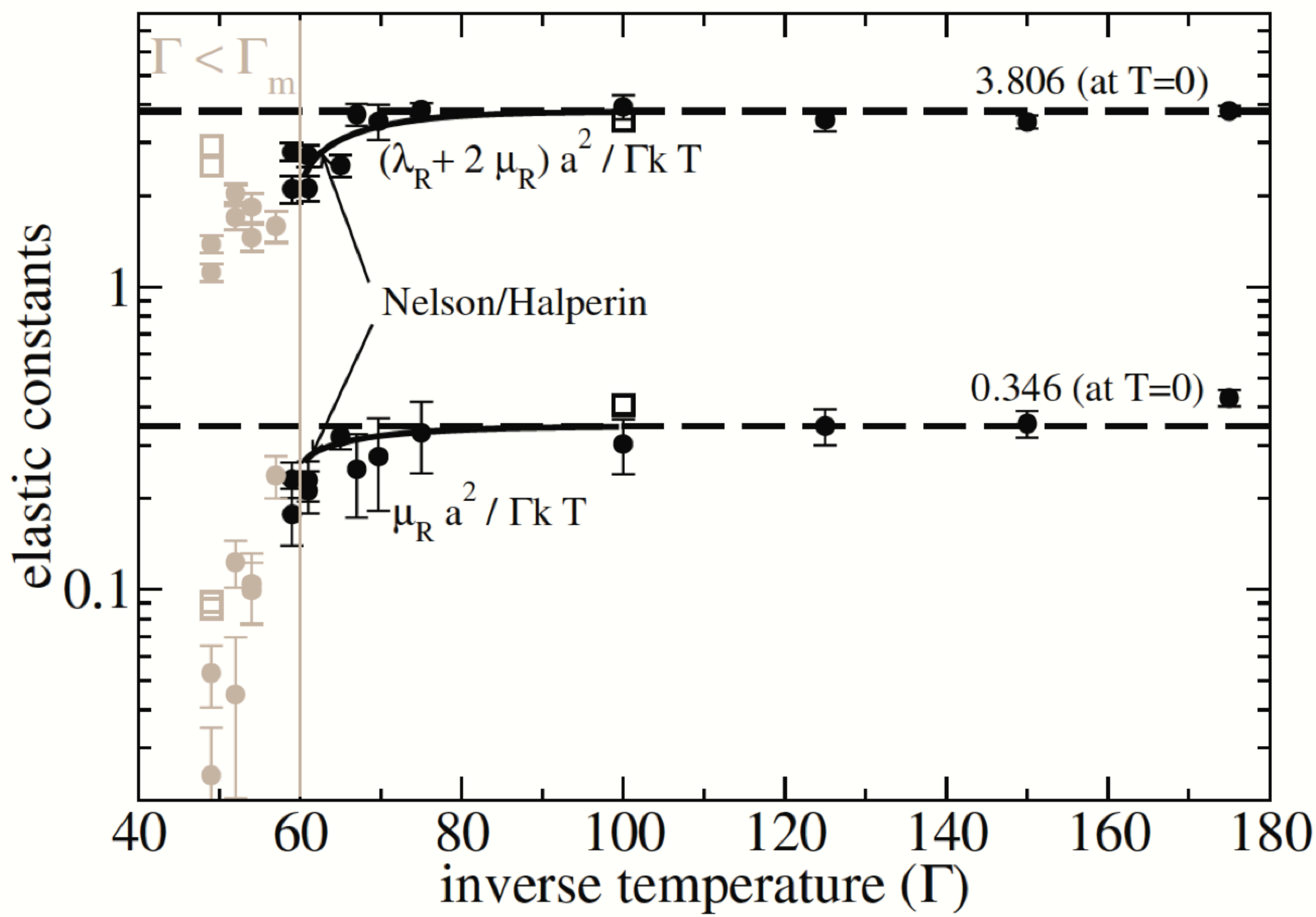

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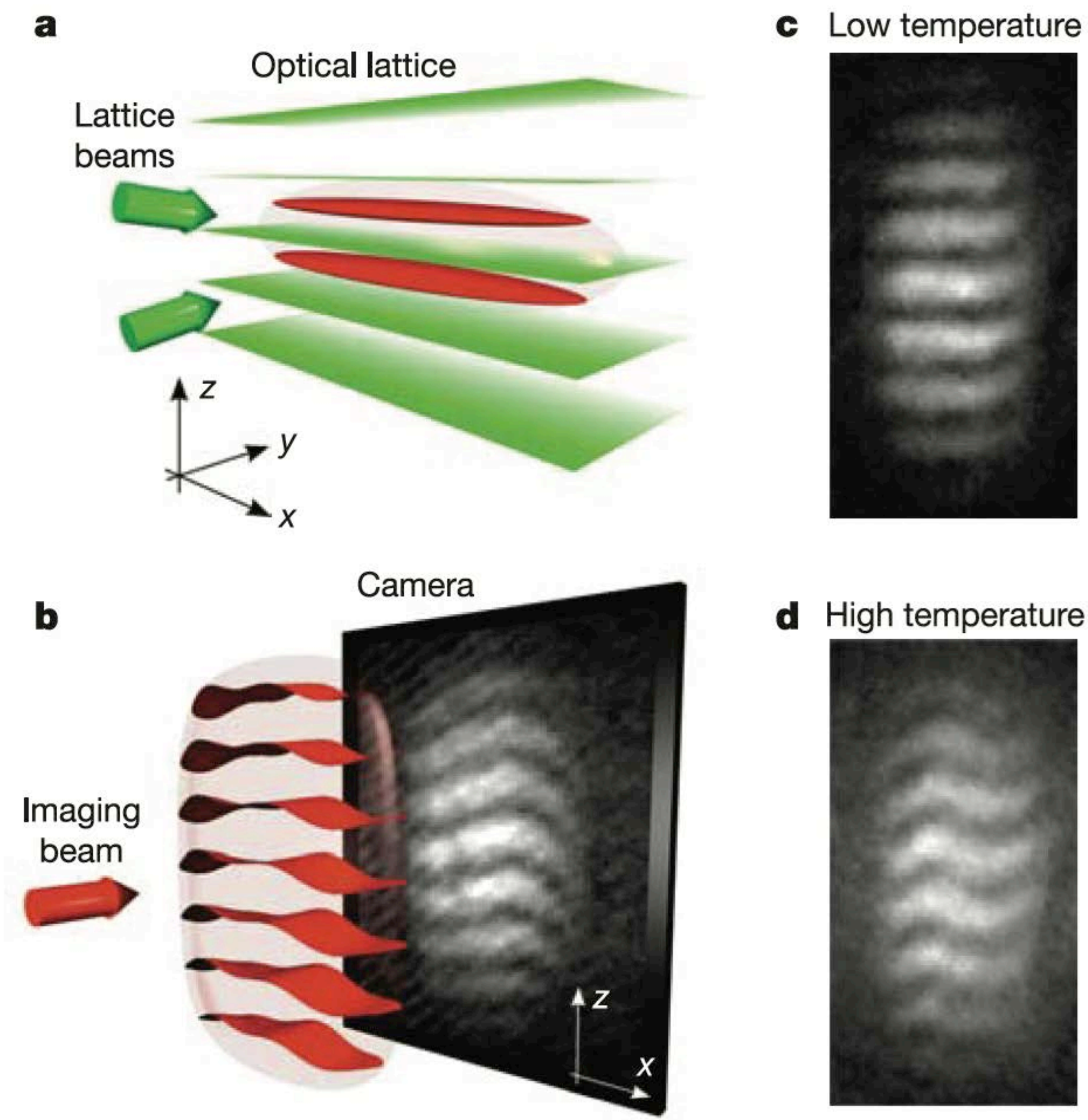

Conclusion Remarks

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