KT: Two dimensional melting

- In two dimension, no long range order
- What is the order parameter?
- Zero shear modulus, fluid
- Dislocation unbinding. Dislocations are topological defects. One has to remove a whole line of atoms to get back to the perfect solid and cannot get back to the perfect solid by continuous deformation of the system.
- Kosterlitz Thouless transition, part of their Nobel prize

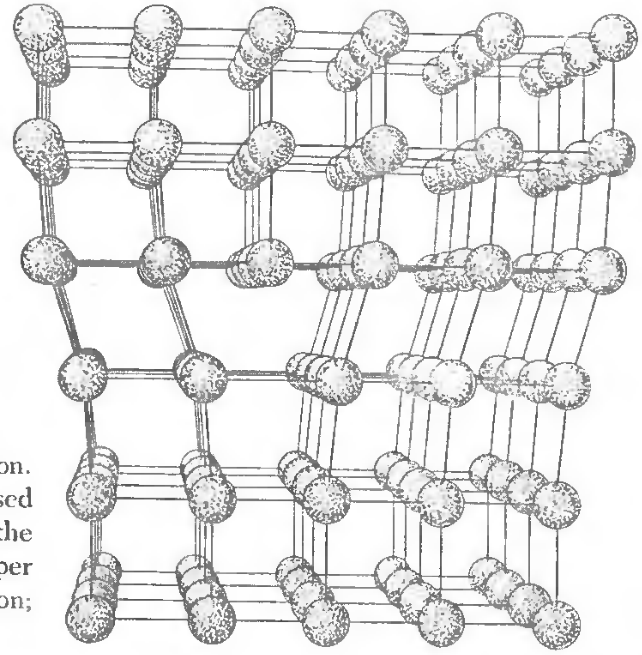


Figure 4 Structure of an edge dislocation. The deformation may be thought of as caused by inserting an extra plane of atoms on the upper half of the y axis. Atoms in the upper half-crystal are compressed by the insertion; those in the lower half are extended.

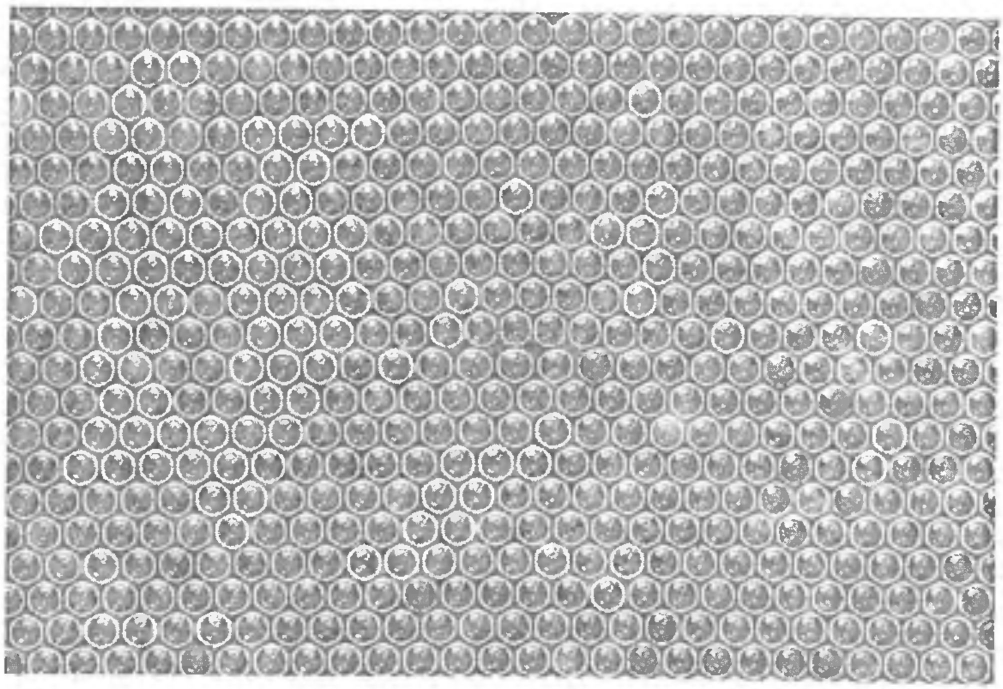


Figure 5 A dislocation in a two-dimensional bubble raft. The dislocation is most easily seen by turning the page by 30° in its plane and sighting at a low angle. (W. M. Lomer, after Bragg and Nye.)

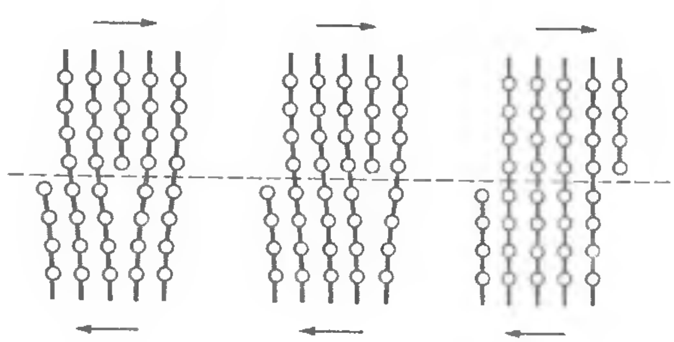


Figure 6 Motion of a dislocation under a shear tending to move the upper surface of the specimen to the right. (D. Hull.)

Other systems with the same physics

- For thin Helium films, there cannot be long range order in the coherence of the system due to large thermal fluctuation in low dimension, the same reason as the lack of positional order in 2D solids.
- However there can be a superfluid transition.
- Dissipation of fluid flow can be caused by vorticies. If there are no free vorticies, then the system is a superfluid.
- The superfluid transition is associated with unbound vorticies.

What is a renormaliation group (RG) transformation?

- The statistical averages such as the calculation of the partition function involves summing over all possible configurations for the variables of interest.
- We do a partial sum over configurations of a certain length scale in the (grand) partition function, usually with some approximations.
- We then redefine parameters so that the result of the partial sum involves an energy of the same functional form as the original energy.
- The relationship between the new and original parameters is called a RG transformation.

KT RG

- We consider a collection of dislocations so the energy of two dislocations is (for a pair of opposute charge, $\mathrm{q} = -\mathrm{q}'$)

$H_0 = 2q'q \quad \ln\left(\frac{r}{r_0}\right) + 2\mu',$ for r>r_0 fthe size of a dislocation.

- Assume low density with , $y_0 = e^{-\beta\mu\prime}$ small, $\beta = 1/kT$
- Do RG transformation by integrating out in the grand partition function configurations with the pairs of opposite charges that are close by with r_0<r<r_0+dr. The length scale of the problem, r_0, is increased but the free energy is of the same form .
- We have renormalized pairs with renormalized r_0, y_0 and a renormalized coupling $\mathrm{K} = \beta q^2$, $\beta = \frac{1}{kT}$.

RG eqn

- $dK^{-1} = (b-1)\pi y_0^2$
- $dy_0^2 = y_0^2\ (b^{-2K+4}-1)$
- Let b=1+dl,
- $dK^{-1}/dl = \pi y_0^2$
- $dy_0\ /\mathrm{dl} = y_0\ (2-K)$
- At K=2, y=0, the parameters do not change. This is called a fixed point of the transformation.

Fixed point analysis for general systems

- $\frac{dK^{-1}}{d\ln l} = f\left(K^{-1}\right)$. At a fixed point K_c^{-1}, f=0.
- Let $\epsilon = K_c\ \left(K^{-1} - K_c^{-1}\right), \epsilon$ is just (T−$T_c)/T_c$, then
- $\frac{d\epsilon}{d\ln l} = \ g(\epsilon)$, g(0)=0
- Close to the fixed point
- $\frac{dln\ \epsilon}{d\ln l} = y,\ \ y = g'(0).\ \epsilon = \epsilon_0 l^y$,
- We also have, for the free energy,
- $F(\epsilon\ l^y) = l^d F(\epsilon\ )$ for spatial dimension d. This is the scaling hypothesis.

Magnetic systems

Atoms in magnets are charged particles with angular momenta **S** called spins that, in some units, are interger or half integer.

Their magnetic moments **M** = $g\mu_B$**S** where $g\mu_B$ is some constant.

In a magnetic field **B**, the energy is -**H.M** = -$g\mu_B H$**.S**.

Including heat change, we get the total energy change of a magnetic system is

dE=TdS+other terms-**H.**d**M**

One can define a quantity G=F+BM so that dF'=-SdT+MdH+other terms

Thus $\frac{\partial G}{\partial H} = M$

For processes under a constant magnetic field and at fixed temperature, G is minimized.

Critical exponents from the scaling hypothesis

- For the magnetic system, we have the dimensionless coupling kT/J and H=magnetic field /kT, the coupling close to Tc, $\epsilon = (\mathrm{T}-T_c)/T_c$
- $G(\epsilon \quad L^y, H\ L^x) = L^d G(\epsilon_, H)$
- This can be written as ($\lambda = L^d, a_\epsilon = \frac{y}{d}, a_H = x/d$)
- $G(\epsilon \quad \lambda^{a_\epsilon}, H\ \lambda^{a_H}) = \lambda G(\epsilon_, H)$
- This is called the static scaling hypothesis.
- From this, we can obtain different the critical exponents and the relationships between them.

- Derivation of critical exponents from the static scaling hypothesis.

Critical exponents

- $G(\epsilon \quad \lambda^{a_\epsilon}, H\,\lambda^{a_H}) = \lambda G(\epsilon_{,} H)$
- Differentiate both sides with respect to H
- $\lambda^{a_H} \partial G(\epsilon \quad \lambda^{a_\epsilon}, H\,\lambda^{a_H})/\partial(H\,\lambda^{a_H}) = \lambda \partial G(\epsilon_{,} H)/\partial H$

$$M(\epsilon_, 0) \quad \propto (-\epsilon)^{\beta}, \ \epsilon = (\mathrm{T}-T_c)/T_c$$

- $\lambda^{a_H} M(\epsilon_0 \lambda^{a_\epsilon}, H\ \lambda^{a_H}) = \lambda M(\epsilon_{0,}\ H)$
- Consider H=0
- $\lambda^{a_H - 1} M(\epsilon \quad \lambda^{a_\epsilon}, 0) = M(\epsilon_, 0)$
- Take λ =(-1/ϵ $\}^{1/a_\epsilon}$
- $M(\epsilon_, 0) = (-\epsilon)^{(1-a_H)/a_\epsilon} M(-1{,}0) \propto (-\epsilon)^{\beta}$
- $\beta = (1 - a_H)/a_\epsilon$

$$M(0, H) \quad \propto (H)^{1/\delta},$$

- $\lambda^{a_H} M(\epsilon \quad \lambda^{a_\epsilon}, H\, \lambda^{a_H}) = \lambda M(\epsilon, H)$
- Consider ϵ =0, H small
- $\lambda^{a_H - 1} M(0, H\, \lambda^{a_H}) = M(0, H)$
- Take λ =(H}$^{-1/a_H}$
- $M(0, H) \; = H^{(1-a_H)/a_H} M(0,1) \propto (H)^{\delta}$
- $\delta = a_H/(1 - a_H)$

$$\chi_T(\epsilon, 0) \qquad \propto (-\epsilon)^{-\gamma},$$

- $\lambda^{a_H} M(\epsilon \;\; \lambda^{a_\epsilon}, H\,\lambda^{a_H}) = \lambda M(\epsilon, H)$
- Magnetic susceptibility at constant T: $\chi_T = \partial M/\partial H$
- $\lambda^{2a_H} \chi_T(\epsilon \;\; \lambda^{a_\epsilon}, H\,\lambda^{a_H}) = \lambda \chi_T(\epsilon, H)$
- Take λ =(-1/ϵ $\}^{1/a_\epsilon}$, H=0
- $\chi_T(\epsilon, 0) = (-\epsilon)^{(1-2a_H)/a_\epsilon} \chi_T(-1,0) \propto (-\epsilon)^{-\gamma'}$
- $\gamma' = (2a_H - 1)/a_\epsilon$
- *Recall that* $\delta = a_H/(1-a_H)$, $\beta = (1-a_H)/a_\epsilon$
- $\gamma' = \beta(\delta - 1)$

$$M\left(\epsilon_{,}0\right) \qquad \propto (-\epsilon)^{\beta},\ \epsilon = (\mathrm{T}-T_c)/T_c$$

- Take $\lambda \quad =(1/|\epsilon \quad |)^{1}$
- $M\left(\epsilon_{,}H\right) \; = (|\epsilon|)^{(1-a_H)/a_\epsilon} M(\epsilon \quad /|\epsilon \quad |, H\ /|\epsilon \quad |^{a_{H/a_\epsilon}})$
- $\lambda^{a_H-1} M(\epsilon \quad \lambda^{a_\epsilon}, H\ \lambda^{a_H}) = M(\epsilon_{,}H)$
- $\beta = (1-a_H)/a_\epsilon, \delta = a_H/(1-a_H)$
- $M\left(\epsilon_{,}H\right) /(|\epsilon|)^{\beta} = M(\epsilon \quad /|\epsilon \quad |, H\ /|\epsilon \quad |^{\beta\delta})$

Define

$m = M\left(\epsilon_{,}H\right) /(|\epsilon|)^{\beta}$, h=$H\ /|\epsilon \quad |^{\beta\delta}$,$F_{\pm} = M(\pm 1, h)$,

$$m = F_{\pm}(\mathrm{h})$$

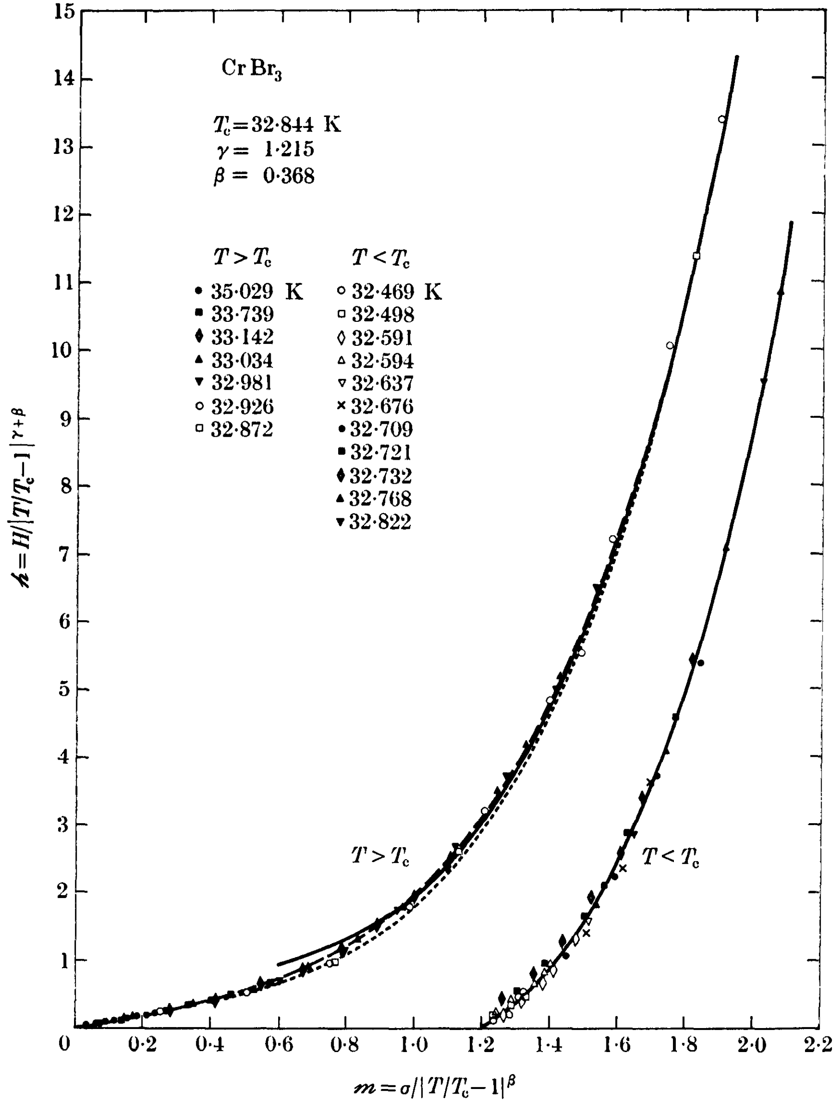


FIG. 11.4. Scaled magnetic field h is plotted against scaled magnetization m for the insulating ferromagnet $CrBr_3$, using data from seven supercritical ($T > T_c$) and from eleven subcritical ($T < T_c$) isotherms. Here $\sigma \equiv M/M_0$. After Ho and Litster (1969).

Note that the determination of the values of two of the exponents is not sufficient to check the validity of the scaling predictions; we need at least three exponents. Of course, if we assume the validity of the scaling hypothesis, (11.30), then determination of two exponents

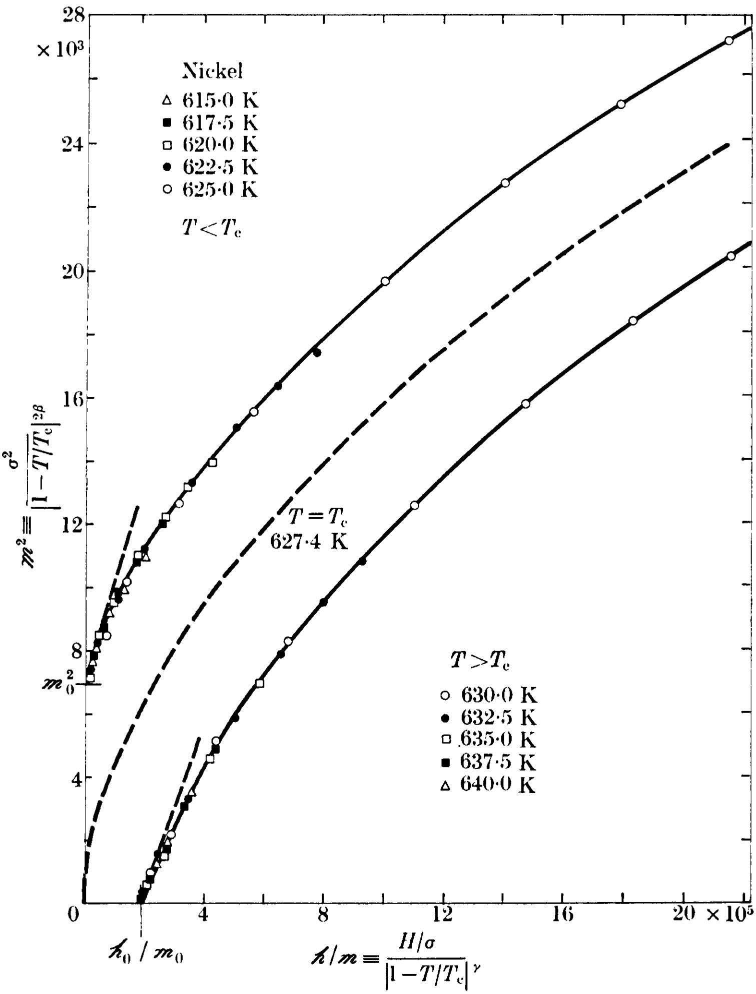


FIG. 11.5. A plot of m^2 against h/m, where m is the scaled magnetization and h is the scaled magnetic field. The data are from measurements on the metallic ferromagnet nickel. Here $\sigma \equiv M/M_0$. After Kouvel and Comly (1968).

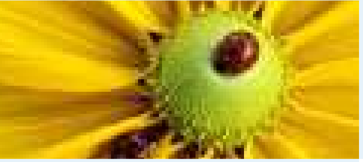
suffices to fix the values of all the remaining exponents. For example, the reader can easily verify from Table 11.1 that for $CrBr_3$ the data of (11.64) together with the scaling assumption imply that

$$\left.\begin{aligned} \alpha &\simeq 0{\cdot}05, \\ \Delta &\simeq 1{\cdot}6, \\ \varphi &\simeq 0{\cdot}03, \\ \psi &\simeq 0{\cdot}60. \end{aligned}\right\} \tag{11.66}$$

Correlations

- We can also apply scaling considerations to correlation functions such as the correlation function

$$\Gamma_{ij} \equiv \langle \sigma_i \sigma_j \rangle - \langle \sigma_i \rangle \langle \sigma_j \rangle.$$



Correlations

- We can also apply scaling considerations to correlation functions such as the covariance
$$\Gamma_{ij} \equiv \langle \sigma_i \sigma_j \rangle - \langle \sigma_i \rangle \langle \sigma_j \rangle.$$
- If the system has translational and rotational symmetry,[2] we can write this as a function of the relative displacement of spins i and j:
$$\Gamma_{ij} = \Gamma(\vec{r}_{ij}) \approx \Gamma(r_{ij}), \qquad \vec{r}_{ij} \equiv \vec{r}_i - \vec{r}_j.$$

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- The spin-spin correlation function $\Gamma(\vec{r})$ is analogous to the total correlation function $h(\vec{r}) \equiv g(\vec{r}) - 1$ that we studied in fluids.
- The Ornstein–Zernike theory we used there is also applicable here, leading to the same result (in 3D)

$$\Gamma(r) \sim \frac{1}{r} \exp(-r/\xi) \qquad (r \gg \xi),$$

where $\xi(t, h)$ is called the correlation length.

[2] For spins on a lattice, these are discrete symmetries, but we approximate them as continuous.

- In d dimensions, this relationship generalizes to

$$\Gamma(r) \sim \frac{1}{r^{(d-1)/2}} \exp(-r/\xi) \qquad (r \gg \xi).$$

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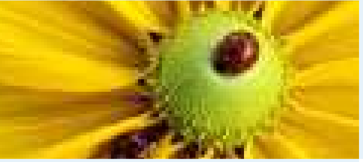
- In our study of fluids, we showed that ξ could be written as

$$\xi = R(nk_\mathrm{B}TK_T)^{1/2} = R\left(\frac{nk_\mathrm{B}T}{B_T}\right)^{1/2} \qquad (R = \text{constant}),$$

  where K_T is the isothermal compressibility.



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where K_T is the isothermal compressibility.
- Assuming that the bulk modulus $B_T = 1/K_T$ vanishes linearly with T at the critical point, we get

$$\xi(t,0) \sim |t|^{-1/2}.$$

- The “classical” (i.e., mean field) value of ν is therefore $\nu = 1/2$.

- Is there any way to use scaling arguments to find the exponent ν?

Scaling of ξ

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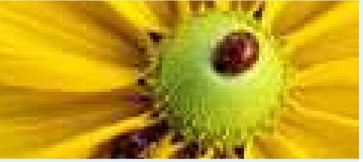
- Note first that ξ has units of length.
- If we increase the units of length by a factor λ, we would expect ξ to have the value ξ/λ in the new system of units.



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we obtain

$$\xi(t, 0) = |t|^{-1/y}\xi(\operatorname{sgn} t, 0).$$

- We can therefore identify $\nu = 1/y$, where y can be obtained from our previous relation

$$\alpha = \frac{2y - d}{y}.$$

Correlation exponent ν

- We see that the correlation exponent ν is related to the heat capacity exponent α by
$$\nu = \frac{2-\alpha}{d},$$
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  which is known as the Josephson scaling law.
- Unlike the Rushbrooke and Widom scaling laws, the Josephson relation depends explicitly on the spatial dimension d.
- For this reason, it is sometimes called a hyperscaling relation.

Correlation exponent η

- Another critical exponent η is defined by writing the correlation function in the form[3]

$$\Gamma(r) = \frac{f(r/\xi)}{r^{d-2+\eta}},$$

where the function $f(x)$ varies asymptotically as $\exp(-x)$ times some power of x in the limit $x \longrightarrow \infty$.
- This is another type of scaling hypothesis, since $\Gamma(r)$ is assumed not to depend on any length parameter other than ξ.

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  where the function $f(x)$ varies asymptotically as $\exp(-x)$ times some power of x in the limit $x \to \infty$.
- This is another type of scaling hypothesis, since $\Gamma(r)$ is assumed not to depend on any length parameter other than ξ.
- To find a scaling relation for the exponent η, we start by establishing the following connection between the correlation function $\Gamma_{ij} = \Gamma(r_{ij})$ and the susceptibility $\chi = \partial m/\partial h$:

$$\chi = \frac{1}{N k_{\mathrm{B}} T} \sum_{i,j} \Gamma_{ij}.$$

[3] In the mean-field approximation, $\eta = 0$.

Susceptibility

- To do this, let us return to the original definition of the free energy:

$$\tilde{A}(t,h) = -k_{\mathrm{B}} T \log Z_C\,,$$

$$Z_C = \sum_{\sigma} \exp\left(\beta \sum_{i<j} J_{ij}\sigma_i\sigma_j + \beta h \sum_i \sigma_i \right).$$

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- By differentiating with respect to h, we find

$$\frac{\partial}{\partial h} \log Z_C = \beta \sum_i \langle \sigma_i \rangle = \beta N m,$$

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where $m \equiv (1/N) \sum_i \langle \sigma_i \rangle$ is the order parameter.

- A second derivative then yields

$$\frac{\partial^2}{\partial h^2} \log Z_C = \beta^2 \sum_{i,j} (\langle \sigma_i \sigma_j \rangle - \langle \sigma_i \rangle \langle \sigma_j \rangle)$$
$$= \beta^2 \sum_{i,j} \Gamma_{ij} .$$

Fluctuation-dissipation theorem

- Comparing these two expressions, we obtain the desired relationship between susceptibility and correlations:

$$\chi = \frac{\partial m}{\partial h} = \frac{1}{\beta N} \frac{\partial^2}{\partial h^2} \log Z_C = \frac{\beta}{N} \sum_{i,j} \Gamma_{ij}.$$

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- If the system is translationally invariant, the sum on i does not depend on the value of j, hence

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- This result can be expressed as a d-dimensional volume integral:

$$\begin{aligned} \chi &\approx \frac{\beta}{v_0} \int \Gamma(\vec{r})\, \mathrm{d}^d r \\ &\propto \frac{\beta}{v_0} \int \Gamma(r) r^{d-1}\, \mathrm{d}r, \end{aligned}$$

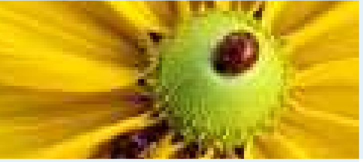
where v_0 is the volume occupied by each spin in the lattice.

Temperature dependence

- At this point, we can write the correlation function as

$$\Gamma(r) = r^{-(d-2+\eta)} f(r/\xi),$$

where $f(x) \sim \exp(-x)$ as $x \to \infty$.



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  where $f(x) \sim \exp(-x)$ as $x \to \infty$.
- The susceptibility is thus of the form

$$\begin{aligned} \chi &\propto \int_0^\infty r^{-(d-2+\eta)} f(r/\xi) r^{d-1}\, \mathrm{d}r \\ &= \xi^{-(d-2+\eta)} \xi^d \int_0^\infty x^{-(d-2+\eta)} f(x) x^{d-1}\, \mathrm{d}x, \end{aligned}$$

  or

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or

$$\chi \propto \xi^{2-\eta}.$$

- If we now set $h = 0$, we can use the relations

$$\chi(t,0) \propto |t|^{-\gamma}, \qquad \xi(t,0) \propto |t|^{-\nu},$$

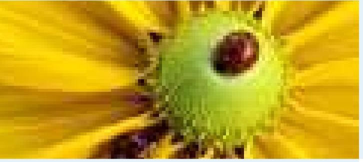
to write

$$\chi(t,0) \propto |t|^{-\gamma} \propto |t|^{-\nu(2-\eta)}.$$

- Upon matching the exponents, we see that

$$\gamma = \nu(2 - \eta),$$

which is known as the Fisher scaling law.



Scaling laws

- Upon matching the exponents, we see that

$$\gamma = \nu(2-\eta),$$

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- Putting everything together, we have now derived the four scaling laws

$$\begin{aligned} \alpha + 2\beta + \gamma &= 2 && \text{(Rushbrooke)} \\ \gamma &= \beta(\delta - 1) && \text{(Widom)} \\ \gamma &= \nu(2-\eta) && \text{(Fisher)} \\ \nu d &= 2 - \alpha && \text{(Josephson).} \end{aligned}$$

- These laws show that only two of the six critical exponents α, β, γ, δ, ν, η are independent variables.

Test cases

- We can test these scaling laws using the exact critical exponents for the 2D Ising model:[4]

$$\alpha = 0, \quad \beta = 1/8, \quad \gamma = 7/4, \quad \delta \stackrel{?}{=} 15, \quad \nu = 1, \quad \eta = 1/4.$$

- All of the scaling laws are indeed satisfied, which provides support (but not proof) for the hypotheses used to derive them.

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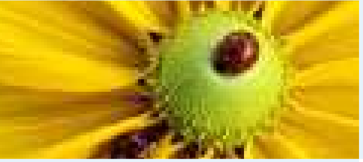
- We can test these scaling laws using the exact critical exponents for the 2D Ising model:[4]

$$\alpha = 0, \quad \beta = 1/8, \quad \gamma = 7/4, \quad \delta \stackrel{?}{=} 15, \quad \nu = 1, \quad \eta = 1/4.$$

- All of the scaling laws are indeed satisfied, which provides support (but not proof) for the hypotheses used to derive them.
- The corresponding critical exponents for the mean-field theory are

$$\alpha = 0, \quad \beta = 1/2, \quad \gamma = 1, \quad \delta = 3, \quad \nu = 1/2, \quad \eta = 0.$$

- These values satisfy all of the scaling laws except the Josephson (hyperscaling) relation,[5] which depends explicitly on the dimension d.



Test cases

- We can test these scaling laws using the exact critical exponents for the 2D Ising model:[4]

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- These values satisfy all of the scaling laws except the Josephson (hyperscaling) relation,[5] which depends explicitly on the dimension d.
- The scaling laws are also in good agreement with numerical calculations (e.g., for the 3D Ising and Heisenberg models) and experimental data, where available.

[4] Here the value $\delta = 15$ is taken from the Widom relation, since it has not yet been derived exactly in the 2D Ising model.

[5] The Josephson relation is satisfied in the special case $d = 4$, but not in general. It fails in the Landau theory because the Landau theory contains another length parameter in addition to ξ, thus violating the given hyperscaling hypothesis.

The idea of functions on different length scale is related to what is called “machine learning”

Machine Learning is very simple conceptually

- Machine learning = interpolation and extrapolation by fitting data with some functions and determining the parameters of the function.
- Possible functions:
  - polynomials
  - Fourier series
  - Neural network
- Learning= determining the parameters
- Deep learning=More parameters

Success depends on a good choice of functions

- Kolmogorov and Arnold
- It is possible to represent a function of several variables as a sum of functions of single variables.
- They show how to construct such functions by looking at sums of classes of functions representing different scale of magnitude.
- Kolmogorov is an expert on turbulence. In turbulence, one also has eddies (fluid flow) of different scales.
- No one has looked if ideas in critical phenomena can be of any use here.

Real life problem?

- Real life variables are logical variables
- There is no a priori mapping to real variables.
- A first step maybe is to find a metric.