Statistical Physics (PHY831): Part 3 - Interacting systems

Phillip M. Duxbury, Fall 2012

Part 3: (H, PB) Interacting systems, phase transitions and critical phenomena (11 lectures) Interacting spin systems, Ising model. Interacting classical gas, cluster expansion, van der Waals equation of state, Virial Expansion, phase equilibrium, chemical equilibrium. Interacting quantum gases in atom traps. BCS theory of Superconductivity, Landau and Ginzburg Landau theory. Topological excitations and topological phase transitions.

I. INTRODUCTION

There are many methods for interacting systems, which may be broadly classified as follows: (i) Decoupling schemes based on expansions in the fluctuations (e.g. mean field theory), equation of motion methods, integral equations etc.; (ii) Perturbation theory. High temperature expansions, low temperature expansions, expansions away from solvable models, diagrammatic methods; (iii) Computational approaches, MC, MD, Transfer matrix; (iv) Coarse grained models, field theory, Landau-Ginzburg and Landau-Ginzburg-Wilson theory. Each method has its strengths and weaknesses. We first analyse three problems using the mean field/decoupling scheme approach.

Interactions bring the possibility of new states of matter and phase transitions between different states. Understanding and describing new states of matter and phase transitions and is challenging and continues to be at the forefront of physics. Understanding of different states of matter and phase transitions centers around the order parameter and order parameter fluctuations. Landau theory is a built on the concept of a characteristic order parameter used to describe a phase and phase transitions within this theory occur by spontaneous symmetry breaking. Landau theory is a mean field theory and can be extended to include fluctuations. If the leading order term in the order parameter fluctuations is added to Landau theory, then we have the Ginzburg Landau theory. Sometimes this is also called Ginzburg-Landau-Wilson theory as Wilson used a similar formulation to develop his approach to calculating critical exponents. Landau theory is a long wavelength theory. A different and more specific approach is to start with a microscopic model. A mean field theory of microscopic models can be developed by using a perturbation theory in the fluctuations and if only the leading order term in the fluctuations is taken, then we have the mean field model. In the long wavelength limit, mean field theories reduce to Landau theory.

If there is no phase transition in a system, then the phase is the same at all temperatures which is quite uninteresting. Interactions provide the source of most phase transitions and can lead to very complex phase diagrams, even for simple systems such as ice (see Fig. 1). Phase transitions can be continuous or discontinuous. We define the correlation length through the pair correlation function. For an Ising spin system the pair correlation function is,

$$C_{ij} =< (S_i- < S_i >)(S_j- < S_j >) >=< S_iS_j > -m_im_j. \tag{1}$$

The asymptotic behavior of C_{ij} near a continuous phase transition is found to be of the form,

$$C_{ij} \to C(r) \sim \frac{1}{r^{d-2+\eta}} e^{-r/\xi} \tag{2}$$

$\xi \approx |T - T_c|^{-\nu}$ is the correlation length. Discontinous or first order transitions do not have a diverging correlation length and the correlations are then confined to finite clusters. When the correlation length diverges, fluctuations on all length scales occur, so that special techniques such as the renormalization group are required to integrate over all of them. Fundamental concepts and methods developed for phase transitions with a diverging correlation length have contributed to developments throughout physics, including fractals, self-organized criticality, power law networks, percolation phenomena and many others. We begin our discussion of phase transitions with the mean field theory for the Ferromagnetic Ising model. This theory does a suprisingly good job of indentifying different phases and the topology of the phase diagram. However the critical behavior that it predicts is often not correct in low dimensions. The theory of phase transitions and critical phenomena has several important concepts that we have looked at before but it is worth stating again:

- There is a lower critical dimension, d_{lc}, for every system below which a true phase transition cannot occur at finite temperature. For the short range Ising model we found that there was no phase transition in one dimension and for this system $d_{lc} = 1 + \delta$, while for the non-relativistic ideal Bose gas we found Bose condensation does not occur in two dimensions but it does in three dimensions and $d_{lc} = 2 + \delta$. Here δ is a small number and we allow the possibility of studying phase transitions on objects with non-integer dimensions, such as fractals.
- There is an upper critical dimension, d_{uc}, above which Landau theory or mean field theory gives the correct critical exponents. We will calculate this dimension later using Ginzburg-Landau theory.

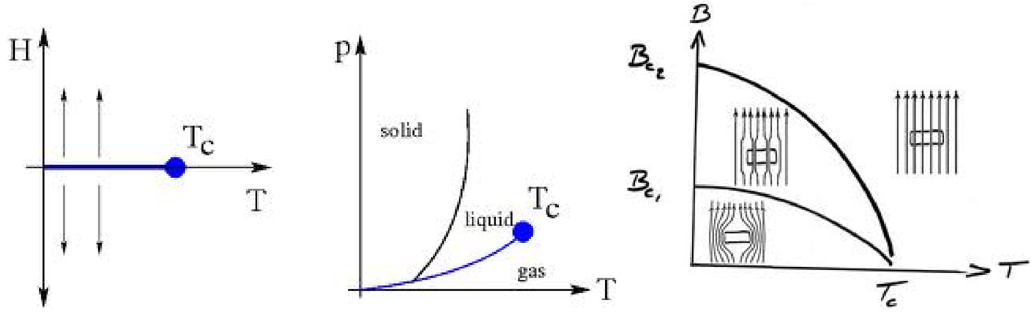

FIG. 1. Ising (left), water (middle) and type II superconductor (right) phase diagrams. Behaviors near the critical point (T_c) obey the laws of universality.

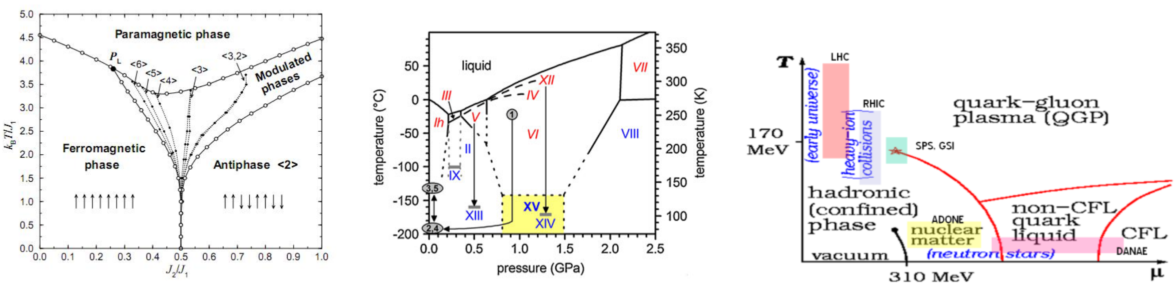

FIG. 2. Examples of more complex phase diagrams produced by competing interactions: A frustrated magnet (left), ice structures (middle), hot dense nuclear matter (right), from ALICE group at CERN-LHC. The group at Bielefeld argue the critical point at temperature around 170 MeV in right figure is in the 3-d Ising universality class.

- Between the lower and upper critical dimensions, the critical exponents change as a function of dimension.
- The behavior near continuous phase transitions is controlled by long wavelength physics, so critical exponents only depend on general features of the problem. The universality hypothesis states that the critical exponents at second order phase transitions only depend on: (i) The dimension, (ii) The symmetry of the order parameter, (iii) The range of the interaction. There are violations of this hypothesis but it is almost always true.
- Recently a new type of phase transition has been studied, where the phase transition cannot be described by a local order parameter. An example of these "topological" phase transitions is the quantum hall state of the two dimensional electron gas in a magnetic field. We shall discuss this issue and extend Ginzburg-Landau theory to consider this problem.

In most phase transitions whether they are continuous (second order) or discontinuous (first order) a change in symmetry occurs on crossing a phase boundary. This applies to problems such as, structural phase transitions, magnetic transitions, superfluid and superconducting phase transitions, Bose condensation, the liquid-gas transition, ferroelectric transitions, metal-insulator transitions etc. Phase diagrams for simple Ising, gas-liquid-solid, and superconducting systems are presented in Figure 1.

II. MEAN FIELD THEORY OF THE ISING MODELS

We start with the Ising model that has played an important role in the theory of phase transitions as it is relatively simple and illustrates many of the basic principles.

A. General spin half mean field theory

The Hamiltonian we consider is,

$$H = -\frac{1}{2}\sum_{ij} J_{ij} S_i S_j - \sum_i h_i S_i \tag{3}$$

and the mean field approximation makes an expansion in the fluctuations,

$$S_iS_j = [m_i + (S_i - m_i)][m_j + (S_j - m_j)] \tag{4}$$

so that

$$S_iS_j = m_im_j + m_i(S_j - m_j) + m_j(S_i - m_i) + (S_j - m_j)(S_i - m_i) \tag{5}$$

where we defined $m_i =< S_i >$ to be the local magnetization. The mean field approximation drops the term $(S_j - m_j)(S_i - m_i)$ which is quadratic in the fluctuations, so that,

$$S_iS_j \approx m_iS_j + m_jS_i - m_im_j \tag{6}$$

The mean field Hamiltonian is then,

$$H_{MF} = -\frac{1}{2}\sum_{ij} J_{ij}(m_iS_j + m_jS_i - m_im_j) - \sum_i h_iS_i \tag{7}$$

The canonical partition function for the spin half model ($S_i = \pm 1$) is then,

$$Z_{MF} = 2^N e^{-\frac{1}{2}\beta\sum_{ij} J_{ij}m_im_j} \prod_{i=1}^{N}(Cosh(\beta\sum_j J_{ij}m_j + \beta h_i)). \tag{8}$$

This is the general mean field theory for Ising spin 1/2 systems. For other spin possibilities (e.g. $S_i = 0, \pm 1$), the Hamiltonian is the same, but the spin sum changes so the partition function is different. The mean field equations are found by taking the average $< S_i >= m_i$,

$$m_i =< S_i >= \frac{1}{Z}\sum_{S_j=\pm 1} S_ie^{-\beta H_{MF}} = Tanh(\beta(\sum_{ij} J_{ij}m_j + h_i)) = \frac{1}{\beta}\frac{\partial(lnZ_{MF})}{\partial h_i} \tag{9}$$

Alternatively we can consider the free energy derived from Z_{MF} to be an energy landscape with the free energy that is observed being a minimum on this landscape. We therefore write,

$$ln(Z) = -\beta F_{MF} = Nln2 - \frac{1}{2}\beta\sum_{ij} J_{ij}m_im_j + \sum_{i=1}^{N} ln(Cosh[\beta(\sum_j J_{ij}m_j + h_i)]) \tag{10}$$

and minimize with respect to m_i (assuming $J_{ii} = 0$)

$$\frac{\delta(-\beta F_{MF})}{\delta m_i} = 0 = -\beta\sum_j J_{ij}m_j + \sum_i \beta J_{ij}Tanh[\beta(\sum_j J_{ij}m_j + h_i)] \tag{11}$$

which is satisfied provided the mean field equation is true. The mean field theory above may then be considered to be a variational theory as we have chosen an approximate free energy and we have minimized this free energy with respect to the magnetizations m_i. Then according to the variational principle, $F_{exact} \leq F_{MFT}$, so the mean field free energy always lies above the true free energy of the problem.

The Hamiltonian and its mean field theory formulated above encompasses a wide range of problems that have been intensively studied, including ferromagnets, frustrated magnets, random field magnets and spin glasses. Here we only consider the case of a ferromagnet.

B. Mean field theory for spin half ferromagnet

Now we explore the predictions of mean field theory for the case of an Ising ferromagnet. In that case the $m_i = m$ is the same everywhere, so the mean field equation reduces to,

$$H_{MF} = -\sum_{<i>} S_i(Jzm + h) + J\frac{z}{2}Nm^2 \tag{12}$$

where $\sum_j J_{ij} \to Jz$ is also assumed to be the same everywhere, and z is the co-ordination number of the lattice. This is true for ferromagnets on translationally invariant lattices. In cases where that is not the case the local mangetization m_i varies throughout the lattice and a numerical solution to the N non-linear MF equations is required. The partition function for a ferromagnet is,

$$Z_{MF} = e^{-\frac{1}{2}\beta JzNm^2}[2Cosh(\beta Jzm + \beta h)]^N \tag{13}$$

and the mean field Helmholtz free energy is,

$$F_{MF} = N[\frac{1}{2}Jzm^2 - k_BTln(2) - k_BTln(Cosh(\beta Jzm + \beta h))] \tag{14}$$

and the mean field equation are,

$$m = Tanh(\beta Jzm + \beta h) \tag{15}$$

Notice that this is the same form as the infinite range model that we solved exactly in Part II (we solved the zero field case only).

Now we extract the critical exponents, defined by,

$$m \approx t^{\beta}; \quad \chi \approx t^{-\gamma}; \quad C_v \approx t^{-\alpha}; \quad m(T_c) \approx h^{1/\delta} \tag{16}$$

and $t = |T - T_c|$. To find these critical exponents, we only need to consider small values of m and h so we will use the expansions,

$$Tanh(y) = y - \frac{1}{3}y^3 + O(y^5); \qquad ln(Cosh(y)) = \frac{1}{2}y^2 - \frac{1}{12}y^4 + O(y^6). \tag{17}$$

so that,

$$-f_R = \frac{-\beta F_{MF}}{N} + ln(2) = -\frac{1}{2}Jzm^2 + ln(Cosh(\beta Jzm+\beta h))] \approx -\frac{1}{2}\beta Jzm^2 + \frac{1}{2}(\beta(Jzm+h))^2 - \frac{1}{12}(\beta(Jzm+h))^4 + O(m^6) \tag{18}$$

and,

$$m = \beta Jzm + \beta h - \frac{1}{3}(\beta Jzm + \beta h)^3 + ... \tag{19}$$

First, consider the case $h = 0$, where the magnetization approaches zero continuously as $T \to T_c$ from below, so we find,

$$m \approx \beta Jzm - \frac{1}{3}(\beta Jzm)^3 + O(m^5) \tag{20}$$

with solutions,

$$m = 0, \quad m = \pm\left(3\frac{(\beta Jz - 1)}{(\beta Jz)^3}\right)^{1/2} \approx (T_c - T)^{\beta} \tag{21}$$

where $k_BT_c = Jz$, and $\beta_e = 1/2$ is the mean field order parameter critical exponent for the ferromagnetic Ising model. The behavior as a function of field at the critical point is found by including the field in the leading order term only.

$$m = \beta Jzm + \beta h - \frac{1}{3}(\beta Jzm)^3; \quad \text{so at } \mathrm{T_c} \quad m = \frac{(3\beta h)^{1/3}}{\beta Jz} \approx h^{1/3} \tag{22}$$

so the exponent δ for the mean field Ising model is 1/3. To find the behavior of the zero field susceptibility in the limit $h \to 0$, we include the h in the leading order term in the expansion of the mean field equation, so that,

$$m = \beta Jzm + \beta h - \frac{1}{3}(\beta Jzm)^3 \tag{23}$$

A derivative with respect to h yields,

$$\chi = \beta Jz\chi + \beta - (\beta Jz)^3 m^2 \chi \quad \text{where} \quad \chi = \frac{\partial m}{\partial h} \tag{24}$$

Solving for χ and using $\beta Jz = T_c/T$ gives,

$$\chi = \frac{\beta}{1-\frac{T_c}{T}+m^2(\frac{T_c}{T})^3} \approx |T-T_c|^{-\gamma} \tag{25}$$

which demonstrates that the mean field susceptibility exponent is $\gamma = 1$. To find the specific heat exponent, we expand the free energy and find C_V from it. From (), we find,

$$C_V = \frac{\partial U}{\partial T} = -T\frac{\partial^2 F}{\partial T^2} \approx |T-T_c|^{-\alpha} \tag{26}$$

where $\alpha = 0$. Calculation of the pair correlation function is more technical and is provided below for completeness. The results are that within mean field theory the exponents for the Ising model are $\nu = 1/2$ and $\eta = 0$.

1. *Pair correlation function - mean field calculation (Optional)*

To find the behavior of the pair correlation function within mean field theory, note that,

$$< S_i S_j >= \frac{\partial m_i}{\partial h_j} = \frac{1}{\beta^2}\frac{\partial^2(ln(Z))}{\partial h_i h_j}. \tag{27}$$

A derivative of Eq. () yields,

$$\beta\sum_l J_{il}\frac{\partial m_l}{\partial h_j} + \beta\delta_{ij} = \frac{1}{1+m_i^2}\frac{\partial m_i}{\partial h_j} \tag{28}$$

so that,

$$\beta\sum_l J_{il}C_{lj} + \beta\delta_{ij} = \frac{1}{1+m_i^2}C_{ij} \tag{29}$$

We define,

$$C(\vec{k}) = \sum_j C_{ij}e^{i\vec{k}\cdot\vec{r}_{ij}}; \qquad J(\vec{k}) = \sum_j J_{ij}e^{i\vec{k}\cdot\vec{r}_{ij}} \tag{30}$$

so that,

$$\sum_j e^{i\vec{k}\cdot\vec{r}_{ij}}\sum_l J_{il}C_{lj} + \beta\sum_i e^{i\vec{k}\cdot\vec{r}_{ij}}\delta_{ij} = \frac{1}{1+m_i^2}\sum_i e^{i\vec{k}\cdot\vec{r}_{ij}}C_{ij} \tag{31}$$

Noting that for translationally invariant systems $\vec{r}_{ij} = \vec{r}_{il} + \vec{r}_{lj}$, we find,

$$\beta C(\vec{k})J(\vec{k}) + \beta = \frac{1}{1+m_i^2}C(\vec{k}); \qquad \text{or} \qquad C(\vec{k}) = \frac{1-m^2}{1-(1-m^2)\beta J(\vec{k})} \tag{32}$$

For nearest neighbor ferromagnetic interactions in a hypercubic lattice, we have,

$$J(\vec{k}) = \sum_{\alpha=1}^{d} 2Jcos(k_\alpha a) \approx J(2d - k^2a^2) \tag{33}$$

where the last expression on the RHS is correct in the long wavelength (small k) limit. The correlation function is then,

$$C(r) \approx \int d^dk C(\vec{k})e^{-i\vec{k}\cdot\vec{r}} \approx \int d^dk \frac{e^{-i\vec{k}\cdot\vec{r}}}{1/(1-m^2) - \beta J(2d-k^2a^2)} \tag{34}$$

we write this as

$$C(r) \approx \int d^dk \frac{e^{-i\vec{k}\cdot\vec{r}}}{1/(1-m^2) - \beta J(2d-k^2a^2)} = \int d^dk \frac{e^{-i\vec{k}\cdot\vec{r}}}{k^2+1/\xi^2} \tag{35}$$

where

$$\xi^2 = \frac{1-m^2}{1-2d\beta J(1-m^2)} \approx \frac{1}{|T-T_c|^{2\nu}}; \quad \text{with} \quad \nu = 1/2 \tag{36}$$

To show that this is the correlation length, we need to carry out the integral (), which is assisted by using the identity,

$$\frac{1}{x} = \int_0^\infty due^{-ux}du \tag{37}$$

so that,

$$C(r) \approx \int d^d k \frac{e^{-i\vec{k}\cdot\vec{r}}}{k^2+1/\xi^2} = \int_0^\infty du \int d^d k e^{-u(k^2+1/\xi^2)+i\vec{k}\cdot\vec{r}}. \tag{38}$$

The k integrals are Gaussian and can now be carried out to find,

$$C(r) \approx \int_0^\infty due^{-u/\xi^2}(\frac{\pi}{u})^{d/2}e^{-r^2/4u} \tag{39}$$

In the limit $r >> \xi$, we can use the saddle point method to find $C(r >> \xi) \approx e^{-r/\xi}$. In the small r limit, we find $C(r) \approx r^{2-d}$. These two limiting values are combined into the approximate form,

$$C(r) \approx \frac{e^{-r/\xi}}{r^{d-2}} \tag{40}$$

which is exact in three dimensions.

III. CRITICAL EXPONENTS, LANDAU THEORY AND SCALING

A. Critical exponents, Landau and Ginzburg-Landau theory

It is useful to summarize MFT exponents for the the Ising model are to compare them with the exponents that are found in two and three dimensions: The critical exponents found by more accurate methods, and confirmed in many experiments are,

$$\alpha = 0; \quad \beta_e = 1/8; \quad \gamma = 7/4; \quad \delta = 15; \quad \nu = 1; \quad \eta = 1/4; \quad 2-\text{D Ising} \tag{41}$$

$$\alpha = 0.110; \quad \beta_e = .327; \quad \gamma = 1.237; \quad \delta = 4.789; \quad \nu = 0.630; \quad \eta = 0.036 \quad 3-\text{D Ising} \tag{42}$$

$$\alpha = 0; \quad \beta_e = 1/2; \quad \gamma = 1; \quad \delta = 3; \quad \nu = 1/2; \quad \eta = 0; \quad \text{Ising MFT} \tag{43}$$

Clearly there is a dependence of the critical behavior on the spatial dimension that is not captured in the mean field theory. We know that in one dimension there is no finite temperature phase transition in the Ising model, as seen in the exact solution. We therefore introduce the concept of the "lower critical dimension", d_l. In dimensions $d < d_l$ there is no phase transition at finite temperature. For dimensions $d > d_l$ there is a phase transition at finite temperature. As we shall see later there is also an upper critical dimension d_u. In dimensions $d > d_u$ mean field critical exponents are correct. The dimension dependence in the critical exponents only occurs in the regime $d_l < d < d_u$. Nevertheless, mean field theory provides a surprisingly good method for predicting stable phases in many problems in three dimensions. It fails as it does not treat fluctuations correctly, and the modern theory of phase transitions addresses this issue in much more detail.

The field theory approach to treating fluctuations starts with the expansion of the free energy near the critical point leading to the free energy,

$$F_L \approx f_R \approx a(T-T_c)m^2 + bm^4 - hm \tag{44}$$

as found from the mean field expansion above. This expansion and its generalizations form the foundation of Landau theory. To add fluctuations, the leading order correction (added by Ginzburg) is, $|\nabla m|^2$, which takes into account local variations in the magnetization. We then have the G-L free energy for the Ising model,

$$F_{GL} = \int d^d r[a(T-T_c)m^2 + bm^4 - hm + c|\nabla m|^2] \tag{45}$$

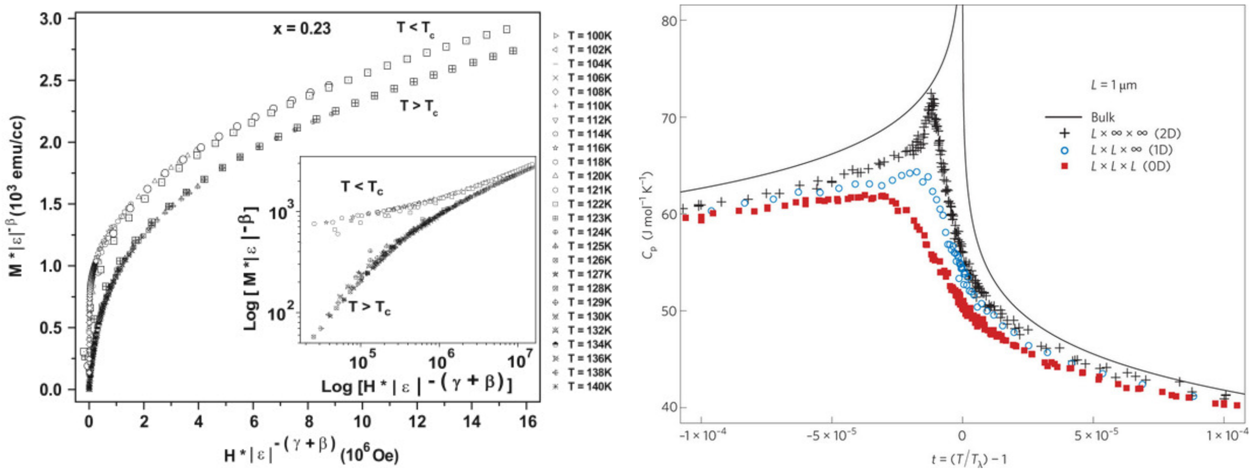

FIG. 3. Left: Scaling plot for the magnetization of a rare earth manganite. Here $\epsilon = |T - T_c|$. Right: Dependence of Helium 4 heat capacity on dimension of the sample.

where a, b, c are positive constants. This is considered to be a coarse-grained model and the behavior of the system is found by integration over all possible fluctuations in $m(\vec{r})$, which leads to the functional integral,

$$Z_{GL} = \int Dm(\vec{r})\; e^{-\beta F_{GL}} \tag{46}$$

which is now a classical field theory.

In the case where there is a vector spin like the one we studied for a paramagnet with a continuous degree of freedom, the GL free energy to describe the critical behavior looks very similar,

$$F_{GL} = \int d^d r[a(T-T_c)\vec{m}^2 + b\vec{m}^4 - \vec{h}\cdot\vec{m} + c|\nabla\vec{m}|^2] \tag{47}$$

The mean field critical exponents are the same, but the lower critical dimension is now $2+\epsilon$ instead of $1+\epsilon$ which applies the Ising case. A new feature is that the lowest free energy symmtery broken states are degenerate so spontaneous symmetry breaking (SSB) chooses one state from among a continuum of possible states. Superfluids, superconductors, Heisenberg magnets etc have vector order parameters where this occurs. In the case of superfluids and superconductors the ground state breaks symmetry under phase, so that one specific phase is chosen. In the case of vector order parameters topological excitions such as rotons and vortices become important, as well as domain walls and wavelike excitions.

B. Scaling theory

Though finding exact critical exponents is difficult, scaling theory provides exact relations between critical exponents providing methods to check behaviors calculated in different ways. First we go through the scaling theory of magnetic phase transitions. We then extend the analysis to consider scaling under changes in length.

1. *Scaling theory of Ising phase transitions*

The objective of the analysis is to find relations between the critical exponents $\alpha, \beta, \delta, \gamma, \eta, \nu$ that control behavior near the Ising critical point. We use the definitions,

$$\beta H = K\sum_{ij} S_i S_j + h\sum_i S_i; \qquad M \sim \frac{\partial F}{\partial h}; \qquad \chi \sim \frac{\partial M}{\partial h} \tag{48}$$

We also define the correlation function,

$$C(r) =< S(0)S(r) > - < S(0) >< S(r) >; \qquad \text{and} \qquad \chi \sim \int dV C(r) \tag{49}$$

Now we assume that the correlation length is the key quantity in the scaling theory so that the scaling behavior is of the form,

$$F(T,h) = t^{2-\alpha}F_s(h\xi^y); \qquad M(T,h) = t^{\beta}M_s(h\xi^y); \qquad \chi(T,h) = t^{-\gamma}\chi_s(h\xi^y); \quad C(r) = r^{-p}C_s(r/\xi, h\xi^y) \tag{50}$$

where $t = |T - T_c|$, and $y > 0$. We also define $\xi^y = t^{-\Delta}$, so that $\nu y = \Delta$, where Δ is the gap exponent. We also have $p = d - 2 + \eta$, and $\xi = t^{-\nu}$. The scaling functions have the property that as their argument $x = h\xi^y = h/t^{\Delta}$ goes to zero, the scaling functions must approach a constant. Moreover the scaling assumption states that for $h < \xi^{-y}$ the scaling functions are constant. Moreover, as $x \to \infty$, the scaling functions go to zero. First consider the behavior of the magnetization when we are at the critical point, so that,

$$M(t=0, h \neq 0) \sim t^{\beta}M_s(x \to \infty) \sim h^{1/\delta}; \quad \text{so that} \quad M_s(x) \sim x^k \tag{51}$$

where,

$$t^{\beta}x^k = t^{\beta}(\frac{h}{t^{\Delta}})^k = h^{1/\delta}; \quad \text{so that} \quad k = 1/\delta; \quad \text{and} \quad \Delta = \beta\delta \tag{52}$$

Now consider the relation between the magnetization and the susceptibility,

$$M \sim \int_0^{t^{\Delta}} \chi dh \sim t^{-\gamma}t^{\Delta} \sim t^{\beta}; \qquad \text{so that} \quad \beta = \Delta - \gamma \tag{53}$$

In a similar manner,

$$F \sim \int_0^{t^{\Delta}} M dh \sim t^{\beta}t^{\Delta} \sim t^{2-\alpha}; \qquad \text{so that} \quad \beta + \Delta = 2 - \alpha \tag{54}$$

Finally, consider the scaling of the correlation function in the case where $h\xi^y$ is zero, so that C_s is a constant for $r < \xi$ and zero otherwise. We then have,

$$\chi \sim \int d^3 r C(r) \sim \int_a^{\xi} dr r^{d-1} r^{-p} C_s(r/\xi, h\xi^y) \sim \xi^{d-(d-2+\eta)} \sim t^{-\gamma}; \quad \text{so that} \quad \gamma = \nu(2-\eta) \tag{55}$$

These exponent relations are usually written in the form,

$$\Delta = \beta + \gamma; \quad \gamma = \nu(2-\eta) \ \ (Fisher); \quad \alpha + 2\beta + \gamma = 2 \quad (Rushbrooke); \quad \gamma = \beta(\delta - 1) \quad (Widom) \tag{56}$$

Since we have added the "gap" exponent Δ, there are seven exponents in the problem. We have four exponent relations so that only three exponents are independent. Josephson introduced another relation, called the hyperscaling relation. He introduced the hypothesis that the singular part of the free energy scales as $1/\xi^d$. This implies that,

$$f_{sing} \approx \xi^{-d} \approx t^{2-\alpha}; \quad \text{so that} \quad d\nu = 2 - \alpha \ \ (Josephson,\ or\ hyperscaling\ relation) \tag{57}$$

The hyperscaling relation is considered the most likely of the scaling relations to fail and for example is known to fail in some heterogeneous models such as the Spin glass model.

These exponent relations extend to the liquid gas phase transition and to many other problems that have more complex order parameters, such as superconductivity and $O(n)$ magnets. If there are more parameters in the problem that must be tuned to find the critical point, then it may be necessary to extend the model to a system with three independent exponents.

2. Generalized scaling relations, finite size scaling and fractals

In the renormalization group theory and in the analysis of results of simulations and experiments, it is interesting to consider the change in properties under rescaling by a length b. In this more general case we postulate that,

$$M(t,h) = b^{-\beta/\nu}M_s(hb^{D_h}, tb^{D_t}); \qquad \chi(t,h) = b^{\gamma/\nu}\chi_s((hb^{D_h}, tb^{D_t}); \quad C(r) = b^{-p}C_s(r/b, hb^{D_h}, tb^{D_t})) \tag{58}$$

This reduces to the scaling behavior of Eq. (50) if we use $b = \xi = t^{-\nu}$. However now we are able to study the bahavior as a function of the system size, the finite size scaling behavior. At the critical point where $h = t = 0$, we

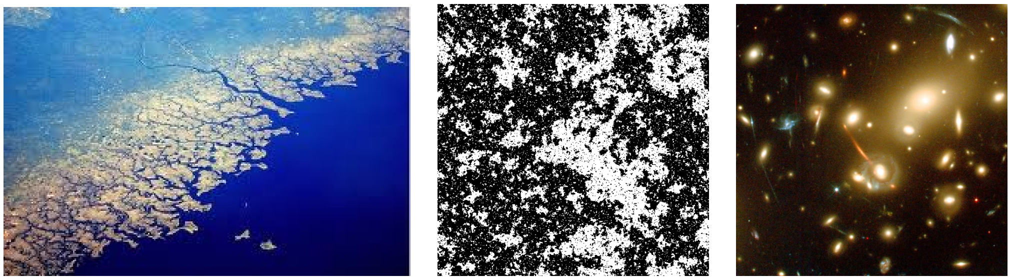

FIG. 4. Left: Fractal coastline. Middle: Fractal Ising clusters at the critical point of a two dimensional system. Right: There is some evidence that the mass distribution in the universe has fractal properties over some length scales.

find that $M \sim L^{-\beta/\nu}$, which is the finite size scaling behavior of the magnetization at the critical point. Comparing this formulation with the formulation above, we find that,

$$D_t = 1/\nu; \quad D_h = \Delta/\nu \tag{59}$$

The renormalization group method studies the change in parameters such and temperature and field under a change in length scales and hence finds the exponents D_t and D_h.

For length scales $r < \xi$, the fluctuations in the order parameter have a fractal geometry. If we have a connected cluster of spins the fractal dimension is found by finding the number of spins, $M(R)$ in the cluster at a distance less than $r < R$. For $R < \xi$, the largest cluster is fractal so that,

$$M(R) \sim R^{D_f} \tag{60}$$

The magnetization is then,

$$m \sim M(R)/R^d = R^{D_f - d} \sim R^{-\beta/\nu} \tag{61}$$

The fractal dimension of clusters for length scales $R < \xi$ are then related to the magnetization critical behavior using,

$$d - D_f = \frac{\beta}{\nu} \tag{62}$$

C. Lower critical dimension

The lower critical dimension is the dimension below which thermal fluctuations are always relevant. In english that means thermal fluctuations are strong at any temperature and they destroy long range order. For the fluctuations to destroy long range order of, for example, a ferromagnet, large scale fluctuations must have finite energy. We can find the typical energy of a long range fluctuation by considering a domain wall. First consider an Ising model where a domain wall consists of an interface between an up spin half-space and a down spin half-space. It is easy to calculate the enery of this interface (at zero temperature), and we write,

$$E_{interface} = 2JL^{d-1}; \quad \text{Ising domain wall, so} \quad d_{lc} = 1 \tag{63}$$

From this expression it is clear that for $d = 1$ the domain wall energy is finite so that thermal fluctuations destroy long range order at any finite temperature. However for any $d > 1$, the interface energy grows with the size of the domain wall, so the ordered state is stable for small but finite temperature. At high enough temperature order is destroyed because the surface tension goes to zero. This low critical dimension also applies to the liquid-gas phase transition.

Now consider a superconductor where the order parameter has a phase degree of freedom. This enables the domain wall energy to be reduced. In a system of size L, the domain wall width is L instead of 1 as occurs in the ising case. The simplest model to illustrate this behavior is a spin model where the spin can rotate with one angular degree of freedom. In that case,

$$H = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j = \sum_{ij} J_{ij} |S|^2 Cos(\theta_{ij}) \tag{64}$$

where θ_{ij} is the angle between the two spins. If we make a domain wall of width l in this model, the angle between adjacent spins is π/l, so the energy of the domain wall is,

$$E_{interface} = 2JL^{d-1}l(cos(\pi/l) - 1) \approx 2\pi^2 J\frac{L^{d-1}}{l} \to 2\pi^2 JL^{d-2}; \quad \text{so,} \quad d_{lc} = 2 \tag{65}$$

where the last expression is found by setting $l \to L$. This shows that two dimensional superconductors are unstable to domain formation. This is similar to what we found for the Bose gas, where there is no true Bose condensation in two dimensions, however the physical origin of the two effects is different. In the limit where the thickness of a sample is of order or less than the coherence length, we expect strong fluctuations in superconducting domains due to this effect.

D. Upper critical dimension - Lifshitz criterion

Below the lower critical dimension, no finite temperature phase transition occurs. Nevertheless there are sometimes interesting behaviors as $T \to 0$, especially in quantum systems where quantum critical points may occur at zero temperature.

As the spatial dimension increases, the fluctuations become less important due to the higher connectivity of the systems. The upper critical dimension is the the dimension above which fluctuations have no effect on the critical exponents. They may still change non-universal properties such as the critical temperature, however they do not alter the leading order critical exponents. This means that above the upper critical dimension mean field theory is correct.

Lifshitz considered the ratio, $\frac{C(\xi)}{m^2}$ which compares the fluctuations to the order parameter squared. If this ratio goes to zero as we approach the critical point, then fluctuations are irrelevant. Carrying this through we find that,

$$\frac{\xi^{-p}}{m^2} \approx t^{(d-2+\eta)\nu-2\beta} \tag{66}$$

To find the critical dimension, we use the mean field values $\beta = 1/2, \nu = 1/2$, to find that,

$$(d-2+\eta)\nu - 2\beta = 0 \quad \to \quad d_{uc} = 4 \tag{67}$$

The upper critical dimension is then four, and below that value the fluctuations modify the critical exponents. Note that the critical dimension for a tricritical point is different and there are other cases where $d = 4$ is not correct. However for superconductors, liquid-gas transitions and homogeneous magnets it is four.

From the discussion of upper and lower critical dimensions it is evident that we happen to live in the window of dimensions where fluctuations are relevant. In many ways three dimensions is the most interesting and complex dimension for critical phenomena, at least for the models we have discussed in this course.

The above exponent relations and critical dimensions are EXACT, which is surprising given the simplicity of the analysis. Finding the values of the two remaining unknown exponents for $d_l < d < d_u$ is much more challenging and lead to the development of many different tools and approaches, including the renormalization group, series expansions and high precision computational methods.

IV. MEAN FIELD THEORY OF CLASSICAL GASES - VAN DER WAALS EQUATION OF STATE

A. Phenomenology

The phase behavior of a monatomic particle systems consists, in the simplest case, of solid, liquid and gas phases. However even monatomic systems can have much more interesting behavior, as occurs in the case of Helium 4, where there is the additional possibility of a superfluid phase. The case of Helium 3 is still more interesting as this monatomic systems is a Fermionic system (2 protons, one neutron, two electrons), but it still undergoes a transition to superfluidity. The BCS theory has been extended to this case and predicts not only a singlet state, but also a triplet superfluid. This has been observed experimentally. There are also more than one solid phase. Molecular systems are even more complex with for example many different solid structures for ice, with 11 confirmed crystalline phases at the time of writing this. There are also the possibility of different fluid phases, with the case of liquid crystals being heavily studied due to a variety of applications in optics.

B. 3-D Van der Waals model, a mean field theory of gas-liquid phase transitions

We consider a monatomic interacting classical gas of particles that interact through central force pair potentials, so the Hamiltonian of the system is given by,

$$H = \sum_i \frac{p_i^2}{2m} + \sum_{i>j} u(|\vec{r}_i - \vec{r}_j|) \tag{68}$$

This interaction is quite good for many systems including,

$$V_{Yukawa} = -g\frac{e^{-\alpha r}}{r}; \quad V_{SC} = -\frac{Q}{4\pi\epsilon_0}\frac{e^{-k_0 r}}{r}; \quad V_{LJ} = 4\epsilon[(\frac{\sigma}{r})^{12} - (\frac{\sigma}{r})^6] \tag{69}$$

For the Yukawa potential, the parameter α is proportional to the mass of the particle mediating the interaction, for example the meson in nuclear physics. g is the coupling constant for the interaction and for the nuclear force is proportional to the meson-fermion interaction. For the screened Coulomb potential (SC), the screening parameter k_0 in an electron gas is $k_0 = [me^2 k_f/(\epsilon_0 \pi^2 \hbar^2)]^{1/2}$. The Lennard-Jones interaction is widely applicable and is used, with additional terms, in modeling many materials. For inert gases including Argon and Neon it is a good approximation to only use the LJ interaction. A further simplication that works well for these systems is to assume that the pair potential may be divided into a hard core replusion and an attactive part, for the LJ interaction we have,

$$u(r < \sigma) = \infty; \quad u(r > \sigma) = -4\epsilon(\frac{\sigma}{r})^6 \tag{70}$$

The Yukawa and screened Coulomb interactions are monotonic decreasing and must have a cutoff if they are used in classical calculations. In a quantum calculation the cutoff is the average radius of the ground state wavefunction.

Our objection is to develop a mean field approximation to any classical particle system described by central force pair potential where we can divide the pair potential into a short range repulsive part and a more diffuse long range attraction, as occurs in the cases discussed above. One objective is to find the isotherms and the co-existence curves of the van der Waals gas, as illustrated in Fig. 5.

The canonical partition function for a classical particle system is given by,

$$Z = \frac{1}{N! h^{3N}} \int d^3q_1 ... d^3q_N \int d^3p_1 .... d^3p_n e^{-\beta H}. \tag{71}$$

Recall that the partition function of the ideal classical gas is given by,

$$Z = \frac{V^N}{N! \lambda^N}; \quad where \quad \lambda = \frac{h}{\sqrt{2\pi m k_B T}} \tag{72}$$

For particle systems with central force pair interactions, the partition function is,

$$Z = \frac{1}{N! \lambda^{3N}} \int d^3r_1 ... d^3r_N e^{-\beta \sum_{i>j} u(|\vec{r}_i - \vec{r}_j|)}. \tag{73}$$

To account for the hard core repulsion and the attractive part of the interation, we make the replacement $V \to V - Nb$, where $b = 2\pi\sigma^3/3$, which takes into account the reduction in the volume available to the particles (it is 2π instead of 4π to remove overcounting of pairs). Here σ is twice the hard core radius of a particle. This is a mean field approximation as it treats the average effect of the hard core repulsions but not their fluctuations. The attractive contribution is also treated within mean field using the approximation,

$$\int d^3r_1 ... d^3r_N e^{-\beta \sum_{i>j} u(|\vec{r}_i - \vec{r}_j|)} \to I^N \tag{74}$$

where

$$I = Exp[-\beta \frac{N}{2V} \int_\sigma u(r) 4\pi r^2 dr] = Exp[\beta a \frac{N}{V}] \tag{75}$$

where $a = -\frac{1}{2}\int u(r) 4\pi r^2 dr$. The reduction of the integral I may be understood by making the replacement,

$$\sum_{i>j} u(|\vec{r}_i - \vec{r}_j|) \to \frac{1}{2} \int d^3r \int d^3r' u(|\vec{r} - \vec{r}'|) \rho(\vec{r}) \rho(\vec{r}') \to \frac{1}{2} < \rho >^2 V \int dr 4\pi r^2 u(r) \tag{76}$$

where $\rho(\vec{r}) = \sum_i \delta(\vec{r} - \vec{r}_i)$, and $< \rho >= N/V$. This procedure replaces the densities by their averages as is typical of mean field theory. An expansion to leading order in the fluctuations leads to the same result because the potential only depends on the difference of the position vectors. The canonical partition function is then,

$$Z = \frac{q^N}{N!\lambda^N}; \quad \text{where} \quad q = (V - Nb)e^{aN/(Vk_BT)} \tag{77}$$

and the Helmholtz free energy is given by,

$$F = -k_BTln(Z) = -k_BTln\left(\frac{(V-bN)^N}{N!\lambda^{3N}}\right) - a\frac{N^2}{V} \tag{78}$$

The thermodynamics may then be calculated following the same procedures as for the classical ideal gas, to find the van der Waals equation of state,

$$P = -\left(\frac{\partial F}{\partial V}\right)_{T,N} = \frac{Nk_BT}{V-Nb} - \frac{N^2a}{V^2} \tag{79}$$

The entropy is,

$$S = -\left(\frac{\partial F}{\partial T}\right)_{V,N} = k_Bln\left(\frac{(V-bN)^N}{N!\lambda^{3N}}\right) + \frac{3}{2}Nk_B \tag{80}$$

and the internal energy is,

$$U = F + TS = \frac{3}{2}Nk_BT - \frac{N^2a}{V} \tag{81}$$

To find the thermodynamic state, F, S and U above need to be suplemented by the Maxwell construction for $T < T_c$. They are correct above T_c where the Helmholtz energy remains convex.

C. Phase behavior and scaling near the critical point

It is convenient to work with the form,

$$P = \frac{k_BT}{v-b} - \frac{a}{v^2} \tag{82}$$

where $v = V/N$. The free energy may then be written in the reduced form,

$$f = \frac{F}{N} = f_0 - ln(v-b) - \frac{a}{v}; \quad \text{where} \quad f_0 = k_BT(ln(\lambda^3) - 1). \tag{83}$$

f_0 does not play a role in most of the discussion below. The Gibbs free energy or chemical potential are found using, $G = \mu N = F + PV$ to find,

$$\mu = \frac{G}{N} = f_0 - k_BTln(v-b) - \frac{a}{v} + Pv \tag{84}$$

The critical point is defined by,

$$\frac{\partial P}{\partial v}(T_c) = 0; \qquad \frac{\partial^2 P}{\partial v^2}(T_c) = 0 \tag{85}$$

which lead to the two equations,

$$\frac{-k_BT_c}{(v_c-b)^2} + \frac{2a}{v_c^3} = 0; \qquad \frac{2k_BT_c}{(v_c-b)^3} - \frac{6a}{v_c^4} = 0 \tag{86}$$

Solving gives,

$$v_c = 3b; \quad k_BT_c = \frac{8}{27}\frac{a}{b}; \qquad P_c = \frac{a}{27b^2} \tag{87}$$

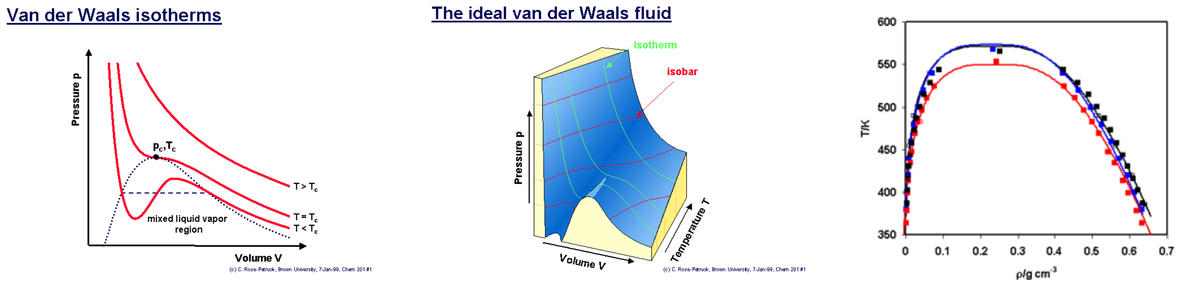

FIG. 5. Left: Van der Waals isotherms, showing the Maxwell construction. Middle: Three dimensional view. Right: Experimental and modeling (solid lines) results for the co-existence curves of three isomers of octane.

Using these values we define scaled variables $v_s = v/v_c$, $P_s = P/P_c$ and $T_s = T/T_c$ which lead to the expressions,

$$P_s = \frac{8T_s}{3v_s - 1} - \frac{3}{v_s^2}; \quad f_s = \frac{8F}{3Nk_BT_c} = -\frac{3}{v_s} - \frac{8}{3}T_s ln(3v_s - 1) + s(T), \tag{88}$$

where $s(T)$ does not depend on P or v. We also have,

$$g_s = \frac{8G}{3Nk_BT_c} = -\frac{3}{v_s} - \frac{8}{3}T_s ln(3v_s - 1) + P_s v_s + s(T). \tag{89}$$

For temperatures below the critical isotherm, the van der Waals equation of state has a “wiggle” instead of a flat behavior in the co-existence region. This wiggle is not a thermodynamically stable state as if $\partial P/\partial V > 0$ at any value of v, the system can find a lower free energy state by segregating into two phases with different density, leading to co-existence of the two phases, gas and liquid. The two co-existing phases are at equilibrium with each other so they must have the same chemical potential $\mu_g = \mu_l$, and the same pressure $P_l = P_g$. The condition for the same pressure gives,

$$P_l = -\frac{\partial F}{\partial V}|_l = P_g = -\frac{\partial F}{\partial V}|_g. \tag{90}$$

The slopes of the free energy versus v graphs at the co-existing phases must then be the same. By connecting these points, a “tie” line is produced and this is the actual equilibirum free energy of the co-existing system, removing the unstable regime of the van der Waals free energy. This is the “Maxwell” construction. The Maxwell construction can also be drawn on the graph of pressure versus volume. On that graph we know that the pressure of the liquid and gas phases must be the same so we draw a line parallel to the horizontal axis (see Figure 5). The location of the horizontal line can be found by taking the values of v_l and v_g found from the Maxwell construction for the Helmholtz energy. Alternatively we can integrate the relation between $P = (\partial F/\partial V)$ to find,

$$F_g - F_l = -N\int_{v_l}^{v_g} P dv. \tag{91}$$

From the construction of the tie line on the free energy plot we also have,

$$F_g - F_l = -P_*(V_g - V_l), \tag{92}$$

where this uses the fact that the pressure P^* defines the slope of the tie line on the free energy graph. Combining these relations we find the Maxwell construction, which states that we should draw a flat line that has equal areas above and below the line defined by the pressure P^*, as stated by the Maxwell “equal area” condition

$$P^*(v_l - v_g) = \int_{v_g}^{v_l} P dv. \tag{93}$$

We are now ready to find the critcal behavior. To define them, recall that the response functions for a particle system are defined as follows;

$$C_V = \left(\frac{\partial U}{\partial T}\right)_{V,N}; \quad \kappa_T = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_{T,N}; \quad \alpha_P = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_{P,N}; \quad C_P = C_V + \frac{TV\alpha_P^2}{\kappa_T} \tag{94}$$

For any liquid-gas transition, the response functions κ_T, α_P, C_P diverge, while the response function C_V may diverge (e.g. for the Bose condensate is remains finite). We will look at the way in which these response functions behave near the critical point. The critical exponents for the liquid-gas phase transition are defined as follows;

$$C_V \approx t^{-\alpha}; \quad v_g - v_l \approx t^{\beta}; \quad \kappa_T \sim t^{-\gamma}; \quad |v - v_c| \approx |P - P_c|^{1/\delta} \tag{95}$$

Here $n = N/V = 1/v$. These expressions indicate that there is an analogy between magnetic behavior in the Ising model and the behavior near the critical point of liquid-gas systems. To be concrete, the analogies are $n_{liq} - n_{gas} \approx v_g - v_l \to 2m$, $P - P_c \to h$, $T - T_c \to T - T_c$.

The specific heat exponent is found using,

$$C_V = \frac{\partial U}{\partial T} = \frac{\partial}{\partial T}[\frac{3}{2}Nk_BT - \frac{Na^2}{V}] \approx |T - T_c|^{-\alpha} \quad T \geq T_c \tag{96}$$

where $\alpha = 0$. The isothermal compressibility is given by,

$$\kappa_T = -\left(V(\frac{\partial P}{\partial V})_T\right)^{-1}; \tag{97}$$

where

$$(\frac{\partial P}{\partial V})_T(V_c) == \frac{1}{Nb^2}\left[\frac{8a}{27b} - T\right] \approx |T - T_c| \quad T \geq T_c \tag{98}$$

comparing () and (), we find that $\gamma = 1$. Calculation of the order parameter behavior is more tedious. We first write,

$$\delta t = 1 - \frac{T}{T_c}; \quad \delta p = \frac{P}{P_c} - 1; \quad \delta v = \frac{V}{V_c} - 1 \tag{99}$$

In these variables, the equation of state is,

$$\delta p = \frac{8(1 - \delta t)}{2 + 3\delta v} - \frac{3}{(1 + \delta v)^2} - 1 \tag{100}$$

Expanding to third order in δv yields,

$$\delta p = -4\delta t + 6\delta t\delta v - 9\delta t(\delta v)^2 - \frac{3}{2}(\delta v)^3 \tag{101}$$

At T_c, $\delta t = 0$, so we find,

$$P - P_c \approx a(v - v_c)^3 \tag{102}$$

so that $\delta = 3$.

To find the order parameter behavior below T_c, we use the Maxwell construction, and we note that,

$$\delta p_l = \delta p_g; \quad \delta v_l = -\delta v_g \tag{103}$$

Writing Eq. (101) for both the gas and liquid, and using the above relations, leads to,

$$12t\delta v_g = 3(\delta v_g)^3; \quad \text{so that} \quad \delta v_g = 0, \delta v_g = \pm 2(\delta t)^{1/2} \tag{104}$$

The order parameter exponent is then $\beta_e = 1/2$. The order parameter in this problem is the density, so the correlation function that we use to characterize the critical fluctuations is the density-density correlation function,

$$C(\vec{r}) = \sum_{ij} \delta(|\vec{r}_i - \vec{r}_j| - r)[< n(\vec{r}_i)n(\vec{r}_j) > - < n(\vec{r}_i) >< n(\vec{r}_j) >] \tag{105}$$

and we expect that

$$C(r) \approx \frac{Exp[-r/\xi]}{r^{d-2+\eta}} \tag{106}$$

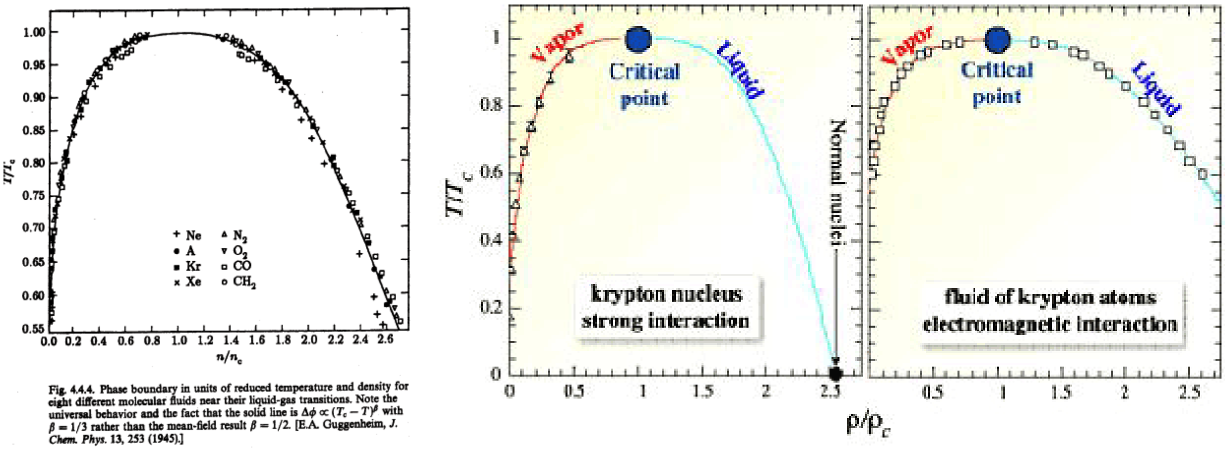

FIG. 6. Left: Co-existence curve data for various fluids, from 1945 (Guggenheim, J. Chem Phys) indicating the $\beta \approx 1/3$, instead of the mean field value (1/2). Recent simulations and experiments indicate that $\beta = 0.325 \pm 0.003$, which is consistent with the Ising universality class. Right: Co-existence curves for Krypton nucleus and Krypton fluid.

From the analysis above it is evident that the critical behavior of the van der Waals gas is essentially the same as that of the mean field theory of the Ferromagnetic Ising model. Moreover the mean field theory of the fluid-gas transitions maps to that of the Ising model by using the relation $h \to \delta p$. Using the universality theory and the scaling theory we can then infer that the liquid-gas transition is in the same universality class as the ferromagnetic Ising model. The upper critical dimension is then four, and the critical exponents in three dimensions are the same as the Ising model in three dimensions, so for example the exponent β describing the order parameter behavior, $\delta v = \delta t^\beta$ should be 0.327 (see Eq. (42)). This is predicted to be exact, so that the exponents for the liquid-gas transition are exactly the same as those of the Ising model, a result which helps a great deal in theoretical work.

It is remarkable that two systems that are so different exhibit the same critical behavior, indicating that "long-wavelength" properties are the most important in determining the behavior near critical points. The question then arises "what is important in determining the value of critical exponents". We already have a partial answer, the spatial dimension is important. A second related answer is that the range of the interactions is important, as we have seen that the infinite range Ising model behaves like a mean field problem and is independent of dimension, whereas a short range problem depends on dimension. A more complete answer to our question depends on more developments. But first we explore probably the most important interacting quantum model in physics, the BCS theory of superconductivity.

1. *When does co-existence occur - constraint is needed*

In the ferromagnetic Ising and liquid-gas systems, co-existence occurs when the system is not able to convert completely to a symmetry broken ground state and it is forced to take up a mixed or co-existence state where symmetry broken ground states co-exist. In the Ising system that we studied earlier, the order paramater fluctuations and boundary conditions made it possible to convert the whole system to either an all up phase or an all down phase. However in the case of a liquid gas system with fixed volume, the system instead is force to have co-existence. This is due to the boundary conditions so that when the volume of the system is fixed and the number of particles in the system is fixed, it is not possible for the system to convert to either all liquid or all gas phases so the system is forced into the co-existence state. Co-existence causes an energy cost as the interface between the gas and liquid phases is not favorable, just as the interface between up and down spins domains in the Ising system is not favorable. When the system can remove these interfaces and convert to a single symmetry broken phase, it will do so.

We can ask how to change the boundary conditions of the gas-liquid system so that the unfavorable interface is removed and co-existence does not occur. There are several ways to do this. We can allow exchange of particles with a reservoir so that the system can adjust the average density to that of either the gas or the liquid phases and in that way remove the interface. Similarly if we fix the pressure instead of the volume, the volume can adjust to find the equilibrium value and in that way choose either a phase that is all gas or all liquid.

In the Ising system where we consider varying the temperature at fixed volume and zero field, we found that the equilibrium state is either the up magnetized or down magnetized state, so that co-existence does not occur. So then we can ask how to modify or contrain the Ising system so that co-existence does occur. One way to do this is to fix the number of up spins in the system so that when the system is cooled, it phase segregates into domains of up and down spins. This is the binary alloy model and is used to model order disorder transitions in materials such and CuAu.

It is also important to note that even in cases where the equilibrium state is a single symmetry broken phase, we often observe a state where there are domains of each of the lowest energy phases. For example in crystals we usually have polycrystalline samples and in magnets we have domains of different spin orientations. This occurs in systems with both discrete and continuous symmetry and the stability of the domain structures depends on the dynamics in the system. If we start at high temperature where there are many different domain orientations and quench into a temperature regime where symmetry breaking is expected, we usually see growth of domains so the low temperature phase is a phase of domain coarsening which gets slower as the domains get larger. In both experiment and theory it can be difficult to avoid domain structures and strategies to achieve uniform single phase systems has to be developed for each system. In the case of materials growth of single crystals is an art form, while in magnets we have the nice capability of applying a magnetic field to orient the sample in one spin direction. In ferroelectrics we can apply an electric field to do this. In the liquid gas system super-cooling or superheating are due to similar effects and can be a problem. They can be overcome by providing nucleation centers, as occurs for example in cloud seeding to produce rain, or by dropping an ice crystal into supercooled water.

V. PERTURBATION THEORY AND SERIES EXPANSIONS

Decoupling strategies like mean field theory, or related approaches like decoupling of integral equation hierarchies or equations of motion, may be applied to any system and are widely used. An alternative approach that can produce similar results and in some ways is more appealing is to use a systematic pertubation theory approach. This approach can always be applied at high enough temperature as we know the limiting behavior about which to carry out the perturbation. If we know the ground state we can also carry out a systematic low temperature expansion.

Two general and basic elements of thermodynamic perturbation theory are as follows: (i) *The linked cluster theorem*: Expansions in statistical physics are most naturally carried out in terms of the partition function, however the quantities of interest are the free energies, entropy and averages such as the order parameters and response functions. Many of the terms in the expansion of the partition function are not extensive, so that when we take a logarithm or carry out averages we end up with many terms that are not extensive. These terms must cancel out in the end so one approach is to ignore them on physical grounds. However it is satisfying, this ad hoc procedure is justified by rigorous work demonstrating that for most systems of interest the non-extensive terms cancel in an expansion to arbitrary order. The proof is quite technical and we shall carry it through for the classical interacting gas. (ii) *Diagrammatic expansions and resummation*: It is usually best to classify terms in perturbation theory using graphs or diagrams. This is true for the Ising model, classical gases, in field theory and in most other problems. Diagrams are just a book keeping tool. For each problem there are rules for constructing them, counting them and evaluating them. The diagrams and rules are also different for different quantities even for the same problem, though they are often quite similar. Once we have a diagrammatic expansion it is possible to classify different classes of diagrams and to resum within a class. Once the diagrams within a class are resummed, the resulting theoretical expressions may reproduce the results of a particular decoupling scheme, so we can talk about “mean field”diagrams etc.

We shall illustrate these issues using two problems, the Ferromagnetic Ising model and the classical lattice gas.

A. Perturbation theory for the spin half Ferromagnetic Ising model

We consider the square lattice Ising model with nearest neighbor interactions, so that,

$$H = -J\sum_{<ij>} S_i S_j; \qquad \text{where} \qquad S_i = \pm 1, \quad J > 0 \tag{107}$$

The partition function is then,

$$Z = \sum_{S_i=\pm 1}\prod_{<ij>} e^{KS_iS_j} = (Cosh(K))^{zN/2}\sum_{S_i=\pm 1}\prod_{<ij>}(1+tS_iS_j) \tag{108}$$

When we take the sum of the spin values $S_i = \pm 1$, the only terms that survive in the expansion of the product are terms where the spin operators S_i are raised to an even power. We can represent this graphically, by placing a bond for each spin pair S_iS_j. Terms with n spin pairs are then represented by n edges in the square lattice. All possible placement of edges appear in the product, but only those cases where the spins appear as even powers are finite. The first "graph" or "diagram" that is finite is a square () that appears with weight t^4, with one factor of t for each edge. The number of ways of placing this diagram on a square lattice is N where N is the number of sites in the lattice. The next finite term is a rectangle with 6 sites with six edges, so it is of order t^6, and it has degeneracy $2N$. The next term is of eighth order with eight edges. This case is more interesting as there are four connected diagrams that must be considered, in addition to the disconnected diagrams. The degeneracy for the connected diagrams is $9N$, while the disconnected diagrams have degeneracy $N(N-9/2)$. For the 2-D Ising model this procedure can be carried to infinite order leading to the exact solution (see LL). To order t^8, the partition function is,

$$-\beta F = ln(Z) = \frac{zN}{2} ln(Cosh(K)) + Nln(2) + ln[1 + Nt^4 + 2Nt^6 + N(N + \frac{9}{2})t^8 + 0(t^{10})] \tag{109}$$

Expanding the logarithm and dropping terms that are not extensive (using the linked cluster theorem), gives,

$$-\beta F = \frac{zN}{2} ln(Cosh(K)) + Nln(2) + N[t^4 + 2t^6 + \frac{9}{2}t^8 + ...] \tag{110}$$

Note that the higher order terms in the expansion of the logarithm are not needed (linked cluster theorem) as they lead to non-extensive terms. This clearly simplifies the analysis a great deal. Note also that the expansion of the logarithm is clearly divergent, so that only the linked cluster theorem makes the expansion valid. Similar expansions may be carried out for different properties, for any lattice or graph structure, and for Ising model with spins different than $S_i = \pm 1$. For each case the appropriate diagrams have to be designed.

Now consider the low temperature series expansion about the ferromagnetic state. In this case, we consider a perturbation about the ground state. The ground state has all spins in one direction, so we choose all up spins. The first excited state has one down spin, so it differs in energy from the ground state by $8J$. The number of ways of choosing to flip one spin in the system is N. The next contribution is from flipping two spins. These two spins can be neighbors (connected) or non-neighbors (disconnected). The connected case has energy $12J$ with respect to the ground state, and they have degeneracy $2N$. The disconnected two spin flip diagrams have energy $16J$ with respect to the ground state and have degeneracy $N(N-5/2)$. There are two connected third order diagrams that also have energy $16J$ with respect to the ground state, and they have degeneracy $4N$ and $2N$. There is also a connected four flip cluster with energy $16J$ with respect to the ground state. It has degeneracy N. The disconnected diagrams with three flipped spins are of higher order. The low temperature series expansion is then

$$Z = \sum_{S_i=\pm 1} \prod_{<ij>} e^{KS_iS_j} = e^{KzN/2}[1 + Ns^4 + 2Ns^6 + N(N + \frac{9}{2})s^8 + O(s^{10})] \tag{111}$$

so the Helmholtz free energy is given by,

$$-\beta F = N[\frac{1}{2}Kz + s^4 + 2s^6 + \frac{9}{2}s^8 + ...] \tag{112}$$

where again we invoked the linked cluster theorem to omit any non-extensive diagrams. Comparing Eq. () and (), we see that term by term they look the same. This equivalent turns out to be true to all orders, and is called duality. It corresponds to mapping the high temperature phase to the low temperature phase of the Ising system. This kind of mapping has been used extensively in other contexts. The Ising model on a square lattice is "self-dual" which leads to the idea that there is a special point at which the high and low temperature phases look the same, except for irrelevant prefactors in Z. These prefactors are irrelevant as the behavior near the critical point is determined by high order terms in the series expansions. Based on this observation, for this self dual model, we can find the critical point from the relation,

$$e^{-2K_c} = tanh(K_c); \quad so; \quad x = \frac{1-x}{1+x} \tag{113}$$

where $x = Exp(-2K_c)$. Solving we find $x = \frac{1}{2}(\sqrt{2}-1)$, so that,

$$K_c = \frac{J}{k_B T_c} = -\frac{1}{2} ln[(\sqrt{2}-1)] \approx 0.441, \tag{114}$$

which is the exact critical point of the square lattice Ising ferromagnet.

Series expansions have been carried out to high order from many spin systems. Critical behavior can be deduced by various extrapolation procedures, such as Pade approximates. Prior to the RG and advanced MC high order series expansions were the most accurate approach for finding critical exponents.

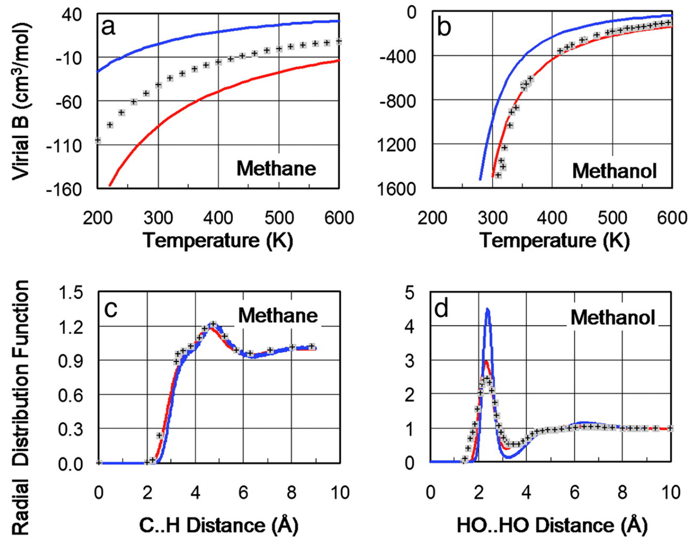

FIG. 7. Second virial coefficient and pair distribution function. Comparison between theory and experiment for methane and methanol

B. High temperature expansions for particle systems - the virial expansion

The virial expansion leads to a systematic series of corrections to the ideal gas law, in the form,

$$\frac{Pv}{k_BT} = \sum_{l=1}^{\infty} a_l(T)(\frac{\lambda^3}{v})^{l-1} \tag{115}$$

where $v = V/N$ and the thermal wavelength $\lambda = h/\sqrt{2\pi m k_B T}$, and $a_l(T)$ is the l^{th} virial coefficient. $a_1(T) = 1$, so the first non-trivial terms is the second virial coefficient. The expansion variable λ^3/v is small at high temperature and low density.

Derivation of the virial expansion is best carried out using the Grand Canonical Ensemble, where we will see that the pressure may be expanded as a power series in the fugacity, so that,

$$\frac{P}{k_BT} = \frac{1}{\lambda^3}\sum_{l=1}^{\infty} b_l z^l; \qquad N = z\frac{\partial(ln(\Xi))}{\partial z} = \frac{V}{\lambda^3}\sum_{l=1} l b_l z^l \tag{116}$$

where we used the relations $PV = k_BTln(\Xi)$, $N = z\partial(ln(\Xi))/\partial z$, and $b_1 = 1$ to recover the ideal gas law at high enough temperatures. If we find the coefficients b_l in the fugacity expansion then the virial coefficients, $a_l(T)$ may be found by noting that,

$$\frac{Pv}{k_BT} = \frac{\sum_{l=1}^{\infty} b_l z^l}{\sum_{l=1}^{\infty} l b_l z^l} = \sum_{l=1}^{\infty} a_l(T)(\frac{\lambda^3}{v})^{l-1} \tag{117}$$

and using the fugacity equation for N/V in Eq. (158), we write

$$\sum_{l=1}^{\infty} b_l z^l = [\sum_{l=1}^{\infty} a_l(T)(\sum_{k=1} k b_k z^k)^{l-1}][\sum_{l=1}^{\infty} l b_l z^l]. \tag{118}$$

Expanding and keeping terms to order z^3 gives,

$$b_1 z + b_2 z^2 + b_3 z^3 = [a_1 + a_2(b_1 z + 2b_2 z^2 + 3b_3 z^3) + a_3(b_1 z + 2b_2 z^2 + 3b_3 z^3)^2 + ...](b_1 z + 2b_2 z^2 + 3b_3 z^3) \tag{119}$$

Equating the coefficients of z^n in this expression leads to relations between a_l and b_l, for example,

$$a_1(T) = 1; \qquad a_2(T) = -b_2(T); \qquad a_3(T) = 4b_2^2 - 2b_3 \quad etc \tag{120}$$

where $b_1 = 1$.

Now we want to find the coefficiencts b_l. For the ideal Bose and Fermi gases we already know that,

$$b_l = \frac{(-1)^{l+1}}{l^{5/2}}; \quad (Fermi) \qquad b_l = \frac{1}{l^{5/2}}; \quad (Bose) \tag{121}$$

Moreover, a general expression for b_l is found from the relation between the grand canonical partition function and the canonical partition function,

$$\Xi = \sum_{N=0} z^N Z_N; \qquad \textbf{so that} \quad \frac{PV}{k_B T} = ln(1 + zZ_1 + z^2 Z_2 + z^3 Z_3 + ...) = \frac{V}{\lambda^3} \sum b_l z^l \tag{122}$$

Expanding the logarithm and comparing coefficients, we can find a relation between b_l and the canonical partition functions Z_l. For example,

$$b_1 = \frac{\lambda^3}{V} Z_1; \quad b_2 = \frac{\lambda^3}{V}(Z_2 - \frac{1}{2} Z_1^2); \quad b_3 = \frac{\lambda^3}{V}(Z_1^3 - Z_1 Z_2 + \frac{1}{3} Z_3) \tag{123}$$

Though this is useful, the canonical partition function (Z_l) grows rapidly with l, so we have to subtract large quantities to find small residuals. In this case, it is better to try to find a smaller quantity to use for the perturbation theory. We shall do this for a classical particle system with pair interactions $u(\vec{r}_{ij})$, with partition function,

$$Z_N = \frac{1}{\lambda^{3N} N!} I_N; \qquad \text{where} \qquad I_N = \int \prod_i d^3 r_i e^{-\beta \sum_{i<j} u(\vec{r}_{ij})} \tag{124}$$

We define the quantity $f_{ij} = Exp[-\beta u(\vec{r}_{ij})] - 1$ that is small at high temperatures. We therefore write,

$$I_N = \int \prod_i d^3 r_i \prod_{i<j} (1 + f_{ij}) = \int \prod_i d^3 r_i [1 + \sum_{i<j} f_{ij} + \sum_{i<j, k<l} f_{ij} f_{kl} + ...] \tag{125}$$

Graphically, I_N consists of all graphs with N circles and n lines joining the circles, with at most one line between each pair of circles. The integrals corresponding to these graphs can be broken up into separate pieces. The first reduction considers connected clusters. A connected cluster is as it sounds, the circles are connected by edges. We define,

$$b_l = \frac{1}{l! \lambda^{3l-3} V}(sum\ over\ all\ l - connected - cluster\ integrals) \tag{126}$$

so that $b_1 = \frac{1}{V} \int d^3 r = 1$; and,

$$b_2 = \frac{1}{2! \lambda^3 V} \int d^3 r_1 d^3 r_2 f_{12} = \frac{1}{2\lambda^3} \int dr_{12} f_{12} \tag{127}$$

The third order term is more complex. However in general we note that the set of N particle graphs are composed of all clusters with the restriction,

$$\sum_{l=1}^{N} l m_l = N \tag{128}$$

where l is the size of a connected cluster and m_l is the number of times that cluster size appears. The contribution of each graph has a degeneracy factor due to the number of ways of arranging the clusters, each of which has degeneracy m_l. We then have to assign lines within these clusters. We may then write,

$$I_N = \sum_{m_l} T_1 T_2 = \sum_{m_l} \frac{N!}{\prod_l m_l!} \prod_l \frac{(l! \lambda^{3(l-1)} V b_l)^{m_l}}{(l!)^{m_l}} = \sum_{m_l} \frac{N!}{\prod_l m_l!} \prod_l (\lambda^{3(l-1)} V b_l)^{m_l} \tag{129}$$

where the sums over m_l must satisfy the constraint (170). The canonical partition function is then

$$Z_N = \sum_{m_l} \prod_{l=1}^{N} \frac{1}{m_l!} \left(\frac{V b_l}{\lambda^3}\right)^{m_l} \tag{130}$$

This sum is hard to do as the configurations $\{m_l\}$ are constrained by Eq. (170). The grand partition function that is given by,

$$\Xi = \sum_{N=0}^{\infty} z^N Z_N = \sum_{m_l} z^{\sum_l l m_l} \prod_{l=1}^{\infty} \frac{1}{m_l!}\left(\frac{V b_l}{\lambda^3}\right)^{m_l} = \sum_{m_l} \prod_{l=1}^{\infty} \frac{1}{m_l!}\left(\frac{V b_l z^l}{\lambda^3}\right)^{m_l} \tag{131}$$

where now the sums $_l$ can be carried out without the constraint. which simplifies to,

$$\Xi = \prod_{l=1} Exp[\frac{V}{\lambda^3} z^l b_l]; \quad \text{so} \quad \frac{PV}{k_B T} = ln(\Xi) = \frac{V}{\lambda^3} \sum_{l=1}^{\infty} b_l z^l \tag{132}$$

Which proves that the cluster integrals appear in the virial expansion, and that the terms in the expansion are extensive.

VI. MICROSCOPIC THEORY OF SUPERCONDUCTIVITY - BCS THEORY

A. Introduction and history

The theory of superconductivity is spectacular with ramifications throughout all areas of physics and in many aspects of technology. This brief historical review will give some of the highlights.

The adventure starts with the successful liquifaction of Helium by the group of Kamerlingh Onnes in 1911. This enabled the group to study properties at lower temperatures and quickly lead to the observation that the resistance of mercury seems to go to zero abruptly at $4.18K$. In addition the group noticed that the viscosity of Helium 4 appears to go to zero at around $2.17K$ at STP. The group thus discovered both superconductivity and superfluidity, and the focus of the interest around the world on these new quantum phenomena. It took many years for the theorists to catch up, and though the theory of Bose-Einstein condensation was developed in 1924 by Einstein it was quickly noted that it is not an accurate model for either superfluidity in Helium 4 or for superconductivity in Hg. The nobel prize was awarded to Onnes in 1913.

The next big discovery was by Meissner and Oshenfeld in 1933, who characterized the property of perfect diamagnetism in the superconducting phase of materials such as Hg. Perfect diamagnetism occurs when screening currents are set up inside the superconducting so that an applied magnetic field is prevented from penetrating the superconductor. Though all materials have a diamagnetic response (due to Lenz's law), superconductors have the special property of perfect diamagnetism at low fields. This discovery was never awarded a nobel prize which is considered an oversight by the community.

In the period $1935 - 1941$ the London brothers (Fritz and Heinz) developed a theory to describe the way in which flux penetrates into superconductors. Screening currents flow in superconductors in order to set up a magnetization to oppose a magnetic field and these screening currents exist over a length scale at the surface. This length is called the London penetration depth, usually denoted by λ, and the applied magnetic field also penetrates over this depth. The London equation to describe the magnetic field penetration into a superconductor is,

$$\nabla^2 B = \frac{B}{\lambda^2} \tag{133}$$

where B is the magnetic field vector.

Theorists where still struggling to understand how superconductivity arises and a big step forward was the suggestion in 1950 by Fröhlich that an attraction between electrons near the Fermi surface can be generated by phonons or lattice distortions. Motivated by this suggestion, Reynolds also in 1950 measured the superconducting transition temperature T_c of Hg as a function of isotope substitution, for isotopes in the range $A = 198 - 203$. He found that T_c decreased as $T_c = a + \frac{b}{\sqrt{A}}$. The fact that the critical temperature depends on the mass of the isotope with a square root dependence suggests that the critical temperature is related to the lattice vibrations as suggested by Frölich.

Also in 1950 the Russian theoretical community was developing a field theory approach to phase transitions (Landau-Ginzburg theory) and this culminated with the Ginzburg-Landau theory to describe superconductors or charged superfluids in a magnetic field. Within this theory the Gibbs free energy, which is taken to be the difference between the superconducting and normal state free energies, is given by,

$$g_{GL} = \int dV \; [\frac{1}{2m}|(-i\hbar\nabla - qA)\psi(\vec{r}))|^2 + a(T)|\psi(\vec{r})|^2 + \frac{b(T)}{2}|\psi(\vec{r})|^4 + \frac{B^2}{2\mu_0} + \frac{\mu_0 H^2}{2} - B\cdot H]. \tag{134}$$

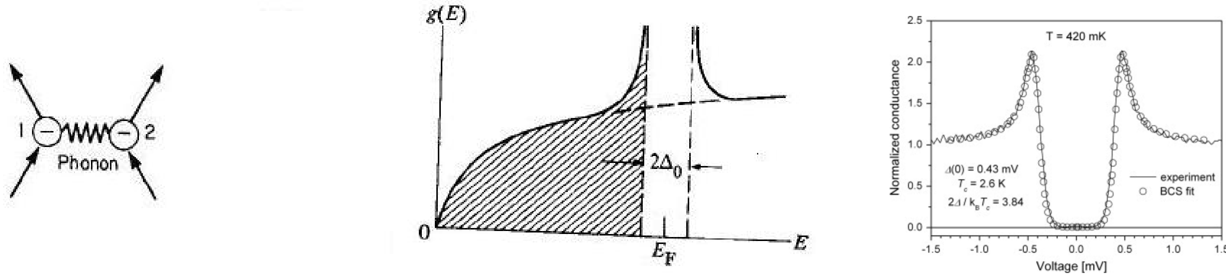

FIG. 8. Schematic of phonon mediated pairing (left); BCS prediction for the quasiparticle density of states (middle); and results of tunneling measurements of the quasiparticle density of states, compared to BSC for SrPd at low T (right).

This free energy is the basis of most analysis of the electromagnetic properties of superconductors and contains the London theory as a special case. Within this theory there are two lengths, the electromagnetic or London length λ and the healing length ξ. We shall return to these lengths later. Despite the important observation that phonons may lead to an attraction between electrons at the Fermi surface, theorists still had a basic problem. The phonon mediated attraction between electrons is weak and it is well known that for there to be a bound state between to quantum particles in three dimensions, the interaction strength has to be above a finite threshold. In 1956, Cooper resolved this threshold by calculating the pairing between two electrons in the Fermi sea. He found the surprising result that in the presence of the Fermi sea a bound state exists for arbitrarily weak attractive potential. This can be understood by noting that the Fermi sea imposes a constraint so that the electrons participating in pairing are moving on the surface of the Fermi sea, a two dimensional object. This is important because if we solve the quantum problem of two particles with an attractive interaction in two dimensions there is a bound state for arbitrarily weak interaction.

The Cooper calculation indicates that the Fermi sea is unstable to arbitrarily weak pair interactions so that a gap at the Fermi surface may open up by this mechanism. Fermi surface instabilities in Fermi liquids may be of many types (Peierls, charge density waves, superconductivity etc) and so superconductivity only occurs in some cases. Bardeen Cooper and Schrieffer (BCS) worked together to solve the problem of a Fermi sea in the presence of a weak attractive potential. Their theory does not depend on phonons as it proposes an attractive potential of magnitude V extending over a range of energies $\hbar\omega_c$ near the Fermi surface. It is thus used in a wide range of contexts ranging from neutron states to atomic nuclei to the Higg's mechanism as well as superfluids and superconductors. They received the nobel prize in 1972. Some of the key results of their analysis are the prediction for the superconducting gap Δ at zero temperate and as a function of the temperature, along with the relation between T_c, V and $\hbar\omega_c$,

$$\Delta(T=0) = 2\hbar\omega_c e^{-1/(N(E_F)V)}; \quad k_B T_c = \hbar\omega_c e^{-1/(N(E_F)V)}; \quad \Delta(T) \approx 3.06(T_c - T)^{1/2} \tag{135}$$

Superconductivity in pure metals is found to agree very well with this theory.

Also in 1957, using Ginzburg-Landau theory, Abrikosov predicted that there are two types of superconductor, type I and type II that have different electromagnetic properties. Type I superconductors make a direct transition from the Messner state to the normal phase, while type II superconductors have an additional "mixed phase" where quantized vortices penetrate the superconductor. The mixed phase is much more stable to applied magnetic fields so that superconductivity persists to very high magnetic fields in strongly type II superconductors. High T_c materials are strongly type II.

Soon after development of the BCS and GL theories for superconductivity they were extended to in many fields of physics including: superfluidity (Landau-Pitaevskii); to nuclear theory to explain odd-even effects in nuclear stability (Bohr-Mottelson - see review by Zelevinsky in 2003), awarded the 1975 nobel prize; in 1963 Anderson suggested that a mechanism like that in the GL theory of superconductivity could generate mass in non-abelian Yang-Mills field theory. Peter Higgs independently discovered this mechanism and put it in a relativistic context. Now that the Higgs particle has been discovered it is likely that the nobel prize will be awarded for the Higgs Boson, but who gets it is still a question. In 1965 Tony Leggett developed general theories for pairing in Fermi liquids. He shared the nobel with Abrikosov in 2003.

The most recent major discoveries have been experimental. In 1970 Osheroff, Richardson and Lee discovered superfluidity in Helium 3 (Nobel prize 1996). The phase diagram that includes both singlet and triplet phases is well described by BCS theory. In 1986 Bednorz and Muller discovered high temperature superconductivity in oxides (Nobel prize was very fast - 1987). This was a shock as there had been a very extensive experimental and theoretical program directed at increasing the T_c of materials, with the conclusion that the upper limit was around $30K$. Bednorz and Muller discovered superconductivity above 30K in relatively dirty, poorly conducting, tenary alloys. Soon after

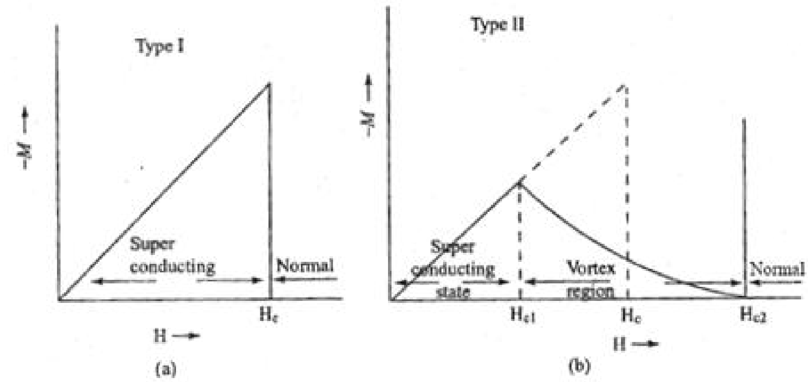

FIG. 9. Magnetization of type I (left) and type II superconductors (right). In the mixed phase vortices pentrate the superconductor but the superconductivity remains.

superconductors with T_c up to $126K$ were developed. The theorists are still trying to understand the mechanism and so far there is no predictive theory to say what the T_c of a new material will be. A third remarkable experimental result is the observation of Bose-Einstein condensation in trapped gases, by Cornell and Wieman in 1995 (Nobel with Ketterle in 2001). Below we go through the fundamentals of the two approaches to superfluidity and superconductivity, namely BCS theory and GL theory. We look at BCS theory first and prior to that there is some introductory material on second quantization for those unfamiliar with it.

B. Second quantization

First quantization is the transition from the classical momentum to the quantum momentum, i.e. $p \to -i\hbar\nabla$. A many body Hamiltonian is written in terms of these operators, and we solve for a many body wavefunction that has a specific number of particles. In second quantization we allow the possibility of any number of particles, as we did in the ideal Fermi and Bose gases. Moreover we work in the "number representation" rather than working with the many body wavefunctions. Before going to the many particle case it may be useful to remember the use of raising an lowering operators in the Harmonic oscillator.

1. *Second quantization of a harmonic oscillator*

Creation and annihilation operators are the same as raising and lowering operators, and for a harmonic oscillator they are defined by,

$$a = \alpha(x + i\frac{p}{m\omega}); a^\dagger = \alpha(x - i\frac{p}{m\omega}); \qquad \alpha = (\frac{m\omega}{2\hbar})^{1/2} \tag{136}$$

and

$$[a, a^\dagger] = 1; \quad [a, a] = [a^\dagger, a^\dagger] = 0; \tag{137}$$

and

$$\hat{n} = a^\dagger a; \quad \hat{n}|n >= n|n >; \qquad H = (\hat{n} + \frac{1}{2})\hbar\omega \tag{138}$$

with

$$a^\dagger|n >= (n+1)^{1/2}|n+1 >; \qquad a|n >= (n)^{1/2}|n-1 > . \tag{139}$$

2. *Second quantization of many-body Boson systems*

This formulation can be extended to treat a many body system composed of many harmonic oscillators that interact. In that case, if there are N harmonic oscillators, and the number representation of a state gives the number of bosons in each state, that is $|n_1, n_2....n_M>$ for a system with M single particle energy levels. The creation and annihilation operators obey the relations,

$$[a_i, a_j^\dagger] = \delta_{ij}; \quad [a_i, a_j] = 0; \quad [a_i^\dagger, a_j^\dagger] = 0 \tag{140}$$

and,

$$\hat{n}_i = a_i^\dagger a_i; \quad \hat{n}_i|n_1...n_i + 1...n_M >= n_i|n_1...n_i + 1...n_M >; \tag{141}$$

and

$$a_i^\dagger|n_1...n_i...n_m >= (n_i + 1)^{1/2}|n_1...n_i + 1...n_M >; \tag{142}$$

$$a_i|n_1...n_i...n_M >= (n_i)^{1/2}|n_1...n_i - 1...n_M > \tag{143}$$

These operators act in the state space of many body wavefunctions constructed from single particle states, for example for a set of Harmonic oscillators, we need to construct a correctly symmetrized N harmonic oscillator wavefunction basis set. A state of this type is written in second quantized form as,

$$|n_1....n_i...n_M >= (a_M^\dagger)^{n_M}..(a_i^\dagger)^{n_i}...(a_1^\dagger)^{n_1}|0 > \tag{144}$$

In field theory, the interactions are often written in real space where they are called field operators. Creation and annihilation then occurs at a point in space. Nevertheless Boson second quantized field operators obey the similar commutation relations,

$$[\psi(x), \psi^\dagger(x')] = \delta(x - x'); \quad [\psi(x), \psi(x')] = [\psi(x)^\dagger, \psi^\dagger(x')] = 0; \quad \hat{n}(x) = \psi(x)^\dagger\psi(x) \tag{145}$$

3. Second quantization of many-body Fermion systems

In the case of Fermions, there are two differences: (i) each state can only have one or zero particles, (ii) the commutators change to anticommutators, so that,

$$\{a_i, a_j^\dagger\} = \delta_{ij}; \quad \{a_i, a_j\} = 0; \quad \{a_i^\dagger, a_j^\dagger\} = 0 \tag{146}$$

and,

$$\hat{n}_i = a_i^\dagger a_i; \quad \hat{n}_i|n_1...n_i + 1...n_M >= n_i|n_1...n_i + 1...n_M >; \tag{147}$$

and

$$a_i^\dagger|n_1...n_i...n_m >= (-1)^{S_k}\delta(n_i)|n_1...n_i + 1...n_M >; \tag{148}$$

and

$$a_i|n_1...n_i...n_M >= (-1)^{S_k}\delta(n_i - 1)|n_1...n_i - 1...n_M > \tag{149}$$

where $S_k = \sum_{j=1}^{i-1} n_j$. These operators act in the state space of many body wavefunctions constructed from single particle states. In the case of Fermions, the correct wave functions are Slater determinants, which have the form,

$$\Psi(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_1(\mathbf{x}_1) & \psi_2(\mathbf{x}_1) & \cdots & \psi_N(\mathbf{x}_1) \\ \psi_1(\mathbf{x}_2) & \psi_2(\mathbf{x}_2) & \cdots & \psi_N(\mathbf{x}_2) \\ \vdots & \vdots & & \vdots \\ \psi_1(\mathbf{x}_N) & \psi_2(\mathbf{x}_N) & \cdots & \psi_N(\mathbf{x}_N) \end{vmatrix}. \tag{150}$$

A state of this type is written in second quantized form as,

$$|n_1....n_i...n_M >= (a_M^\dagger)^{n_M}..(a_i^\dagger)^{n_i}...(a_1^\dagger)^{n_1}|0 > \tag{151}$$

In field theory, the interactions are often written in real space where they are called field operators. Creation and annihilation then occurs at a point in space. Nevertheless Boson second quantized field operators obey the similar commutation relations,

$$\{\psi(x), \psi^\dagger(x')\} = \delta(x - x'); \quad \{\psi(x), \psi(x')\} = \{\psi(x)^\dagger, \psi^\dagger(x')\} = 0; \quad \hat{n}(x) = \psi(x)^\dagger\psi(x) \tag{152}$$

4. Hamiltonians in second quantized form, both Bosons and Fermions

To work with these operators, we need to write the quantum Hamilonians that we are interested in second quantized form. This is relatively straightforward, as we can write a single particle wavefunction as,

$$\psi(\vec{r}) = \sum_k \psi_k(\vec{r}) a_k^\dagger |0> \tag{153}$$

so the second quantized form for the kinetic energy may be written as,

$$\hat{O} = \sum_{k_1,k_2} a_{k_1} O_{k_1,k_2} a_{k_2}^\dagger, \quad O_{k_1,k_2} = \int d^3r \psi_{k_1}^*(\vec{r}) O(\vec{r}) \psi_{k_2}(\vec{r}) \tag{154}$$

and for a pair potential we have,

$$\hat{V} = \sum_{k_1,k_2,k_3,k_4} a_{k_1}^\dagger a_{k_2}^\dagger V_{k_1,k_2,k_3,k_4} a_{k_3} a_{k_3}, \quad V_{k_1,k_2,k_3,k_4} = \int d^3r d^3r' \psi_{k_1}^*(\vec{r}) \psi_{k_2}^*(\vec{r}') V(\vec{r},\vec{r}') \psi_{k_3}(\vec{r}) \psi_{k_4}(\vec{r}') \tag{155}$$

Note that the order of the operators must be with the destruction operators to the right so the vacuum state has zero energy. This form of the Hamiltonian applies to both Fermions and Bosons, as the commutation (Bosons) and anticommutation (Fermion) relations account for the symmetry of the particles.

C. BCS theory

The original BCS paper of 1957 solved a momentum space Hamiltonian using a variational approach. Below we solve this momentum space Hamiltonian using a mean field approach introduced by Bogoliubov and developed in real space by de Gennes. BCS theory using the real space approach is more convenient for analysis of interfaces and tunnelling. It is solved using methods similar to those described here.

The BCS pairing Hamiltonian is a simplified model in which only pairs with zero center of mass momentum are included in the analysis. In the original BCS theory a singlet state was also assumed, so that,

$$H_{pair} - \mu N = \sum_{\vec{k}\sigma} (\epsilon_{\vec{k}\sigma} - \mu)\ a_{\vec{k}\sigma}^\dagger a_{\vec{k}\sigma} + \sum_{\vec{k}\vec{l}} V_{\vec{k}\vec{l}}\ a_{\vec{k}\uparrow}^\dagger a_{-\vec{k},\downarrow}^\dagger a_{-\vec{l}\downarrow} a_{\vec{l}\uparrow}, \tag{156}$$

where $N = \sum_{\vec{k}\sigma} n_{\vec{k}\sigma}$ is the number of electrons in the Fermi sea. The creation and destruction operators in this Hamiltonian obey the Fermion anticommutator relations,

$$\{a_{\vec{k},\sigma}, a_{\vec{k}',\sigma'}^\dagger\} = \delta_{\vec{k},\vec{k}'}\delta_{\sigma,\sigma'}, \quad \{a_{\vec{k},\sigma}, a_{\vec{k}',\sigma'}\} = 0, \quad \{a_{\vec{k},\sigma}^\dagger, a_{\vec{k}',\sigma'}^\dagger\} = 0, \tag{157}$$

while the number operator $n_{\vec{k},\sigma} = a_{\vec{k},\sigma}^\dagger a_{\vec{k},\sigma}$. The 1957 Bardeen, Cooper, Schreiffer (BCS) solution to this "pairing" Hamilonian introduces the averages,

$$b_{\vec{k}} =< a_{-\vec{k}\downarrow} a_{\vec{k}\uparrow} >, \quad \text{and} \quad b_{\vec{k}}^* =< a_{\vec{k}\uparrow}^\dagger a_{-\vec{k}\downarrow}^\dagger > . \tag{158}$$

where $b_{\vec{k}}^*$ is the average number of pairs in the system at wavevector $\vec{k}$. We carry out an expansion in the fluctuations,

$$a_{-\vec{l}\downarrow} a_{\vec{l}\uparrow} = b_l + (a_{-\vec{l}\downarrow} a_{\vec{l}\uparrow} - b_l); \qquad a_{\vec{k}\uparrow}^\dagger a_{-\vec{k}\downarrow}^\dagger = b_k^* + (a_{\vec{k}\uparrow}^\dagger a_{-\vec{k}\downarrow}^\dagger - b_k^*) \tag{159}$$

The mean field Hamiltonian keeps only the leading order term in the fluctuations so that,

$$H_{MF} - \mu N = \sum_{\vec{k}\sigma} (\epsilon_{\vec{k}\sigma} - \mu)\ a_{\vec{k}\sigma}^\dagger a_{\vec{k}\sigma} + \sum_{\vec{k}\vec{l}} V_{\vec{k}\vec{l}}\ (a_{\vec{k}\uparrow}^\dagger a_{-\vec{k},\downarrow}^\dagger b_{\vec{l}} + b_{\vec{k}}^* a_{-\vec{l}\downarrow} a_{\vec{l}\uparrow} - b_{\vec{k}}^* b_{\vec{l}}) \tag{160}$$

This is the Hamiltonian that leads to the BSC solution. Suprisingly it gives excellent results that agree with the experiments except very close to the phase transition. In constrast mean field theory for the Ising model and liquid-gas transition is quite poor in quantitative terms, for example predicting a critical point that is off by over 30% in most

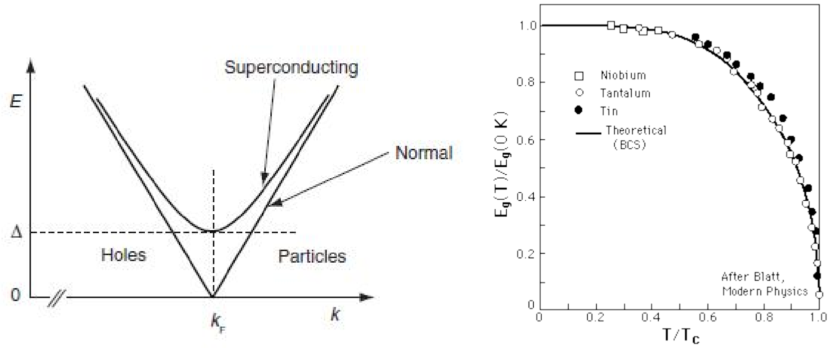

FIG. 10. Left: The opening of a gap in the excitation spectrum of the Fermi gas. Right: Comparison of BCS gap as a function of temperature with experiment.

cases. The reason that the BCS mean field theory works so well for low temperature superconductors is explained by a deeper discussion of the fluctuations. We shall return to this issue later in a more general context.

The mean field Hamiltonian can be solved using an interesting transformation called the Bogoliubov-Valatin transformation. This transformation can be tuned so that the new Hamiltonian is like that of a Free Fermion system. First we define the quantity (which will turn out to be the superconducting gap),

$$\Delta_{\vec{k}} = -\sum_{\vec{l}} V_{\vec{k}\vec{l}}\, b_{\vec{l}} \tag{161}$$

which reduces (160) to,

$$H_{MF} - \mu N = \sum_{\vec{k}\sigma} (\epsilon_{\vec{k}\sigma} - \mu)\; a^{\dagger}_{\vec{k}\sigma} a_{\vec{k}\sigma} - \sum_{\vec{k}} (\Delta_{\vec{k}} a^{\dagger}_{\vec{k}\uparrow} a^{\dagger}_{-\vec{k},\downarrow} + \Delta^*_{\vec{k}} a_{-\vec{k}\downarrow} a_{\vec{k}\uparrow} - b^*_{\vec{k}} \Delta_{\vec{k}}) \tag{162}$$

The key trick to transforming (162) to Free Fermion form is to use the following transformation (where up spin is considered to be positive ($i.e.\ \sigma = +,\ for,\ spin = \uparrow$),

$$a_{\vec{k}\sigma} = u_{\vec{k}} \gamma_{\vec{k}\sigma} + \sigma v^*_{\vec{k}} \gamma^{\dagger}_{-\vec{k}-\sigma}, \tag{163}$$

where $u_{\vec{k}} = u_{-\vec{k}},\ v_{\vec{k}} = v_{-\vec{k}}$. For example, we have

$$a_{\vec{k}\uparrow} = u_{\vec{k}} \gamma_{\vec{k}\uparrow} + v^*_{\vec{k}} \gamma^{\dagger}_{-\vec{k}\downarrow}; \quad a^{\dagger}_{\vec{k}\downarrow} = u^*_{\vec{k}} \gamma^{\dagger}_{\vec{k}\downarrow} - v_{\vec{k}} \gamma_{-\vec{k}\uparrow}$$

and

$$a^{\dagger}_{\vec{k}\uparrow} = u^*_{\vec{k}} \gamma^{\dagger}_{\vec{k}\uparrow} + v_{\vec{k}} \gamma_{-\vec{k}\downarrow}; \quad a_{\vec{k}\downarrow} = u_{\vec{k}} \gamma_{\vec{k}\downarrow} - v^*_{\vec{k}} \gamma^{\dagger}_{-\vec{k}\uparrow}$$

The inverse transformation is,

$$\gamma_{\vec{k}\sigma} = u^*_{\vec{k}} a_{\vec{k}\sigma} - \sigma v_{\vec{k}} a^{\dagger}_{-\vec{k}-\sigma} \tag{164}$$

Using the Bogoliubov-Valatin transformation, it is possible to show that u_k, v_k may be chosen so that the mean field Hamiltonian is diagonal in the quasiparticle operators $\gamma_{\vec{k},\sigma}$.

To ensure that the new operators (e.g. $\gamma_{\vec{k}\uparrow}$) obey the Fermi anticommutation relations, we must have,

$$|u_{\vec{k}}|^2 + |v_{\vec{k}}|^2 = 1 \tag{165}$$

The Hamiltonian in the new operators is,

$$H_{MF} - \mu N = \sum_{\vec{k}} (\epsilon_{\vec{k}} - \mu - E_{\vec{k}} + \Delta_{\vec{k}} b^*_{\vec{k}}) + \sum_{\vec{k}} E_{\vec{k}} (\gamma^{\dagger}_{\vec{k}\uparrow} \gamma_{\vec{k}\uparrow} + \gamma^{\dagger}_{\vec{k}\downarrow} \gamma_{\vec{k}\downarrow}), \tag{166}$$

provided we impose the condition,

$$2(\epsilon_{\vec{k}} - \mu)u_{\vec{k}}v_{\vec{k}} + \Delta_{\vec{k}}v_{\vec{k}}^2 - \Delta_{\vec{k}}^* u_{\vec{k}}^2 = 0, \tag{167}$$

and we define $E_{\vec{k}}$ to be,

$$E_{\vec{k}} = (\epsilon_{\vec{k}} - \mu)(|u_{\vec{k}}|^2 - |v_{\vec{k}}|^2) + \Delta_{\vec{k}}u_{\vec{k}}^* v_{\vec{k}} + \Delta_{\vec{k}}^* v_{\vec{k}}^* u_{\vec{k}}. \tag{168}$$

Equations (165)-(168) along with the definition of $\Delta_{\vec{k}}$ (Eq. (161)) are the BCS solution. Now we have to extract the physics and to give physical meaning to the quantities $E_{\vec{k}}$, $\Delta_{\vec{k}}$, $b_{\vec{k}}$, $u_{\vec{k}}$ and $v_{\vec{k}}$. Without loss of generality, we can choose one of $u_{\vec{k}}$ or $v_{\vec{k}}$ to be real. We choose $u_{\vec{k}}$ to be real. Using Eq. (165) in (167), we have,

$$2(\epsilon_{\vec{k}} - \mu)(1 - |v_{\vec{k}}|^2)^{1/2}v_{\vec{k}} + \Delta_{\vec{k}}v_{\vec{k}}^2 - \Delta_{\vec{k}}^*(1 - |v_{\vec{k}}|^2) = 0, \tag{169}$$

This is simplified if we write $v_{\vec{k}}$ as,

$$v_{\vec{k}} = \frac{g_{\vec{k}}}{(1 + |g_{\vec{k}}|^2)^{1/2}} \tag{170}$$

and hence,

$$|u_{\vec{k}}|^2 = 1 - |v_{\vec{k}}|^2 = \frac{1}{1 + |g_{\vec{k}}|^2}. \tag{171}$$

so that Eq. (167) reduces to,

$$2(\epsilon_{\vec{k}} - \mu)g_{\vec{k}} + \Delta_{\vec{k}}g_{\vec{k}}^2 - \Delta_{\vec{k}}^* = 0. \tag{172}$$

with solution,

$$g_{\vec{k}} = \frac{-2(\epsilon_{\vec{k}} - \mu) \pm (4(\epsilon_{\vec{k}} - \mu)^2 + 4|\Delta_{\vec{k}}|^2)^{1/2}}{2\Delta_{\vec{k}}}.$$

For positive energy excitations, we take the positive root so that,

$$g_{\vec{k}} = \frac{E_{\vec{k}} - (\epsilon_{\vec{k}} - \mu)}{\Delta_{\vec{k}}} \tag{173}$$

where we defined,

$$E_{\vec{k}} = [(\epsilon_{\vec{k}} - \mu)^2 + |\Delta_{\vec{k}}|^2]^{1/2} \tag{174}$$

From this definition, and the definition of $g_{\vec{k}}$, we have,

$$|g_{\vec{k}}|^2 = \frac{E_{\vec{k}} - (\epsilon_{\vec{k}} - \mu)}{E_{\vec{k}} + (\epsilon_{\vec{k}} - \mu)}$$

and,

$$|v_{\vec{k}}|^2 = \frac{g_{\vec{k}}}{(1 + |g_{\vec{k}}|^2)^{1/2}} \frac{g_{\vec{k}}^*}{(1 + |g_{\vec{k}}|^2)^{1/2}} = \frac{(E_{\vec{k}} - (\epsilon_{\vec{k}} - \mu))^2}{|\Delta_{\vec{k}}|^2} \frac{|\Delta_{\vec{k}}|^2}{|\Delta_{\vec{k}}|^2 + (E_{\vec{k}} - (\epsilon_{\vec{k}} - \mu))^2}. \tag{175}$$

Using (170) we also find,

$$|v_{\vec{k}}|^2 = \frac{E_{\vec{k}} - (\epsilon_{\vec{k}} - \mu)}{2E_{\vec{k}}}$$

and from Eq. (170) and the normalisation condition (165), we have,

$$|u_{\vec{k}}|^2 = \frac{1}{(1 + |g_{\vec{k}}|^2)} = \frac{E_{\vec{k}} + (\epsilon_{\vec{k}} - \mu)}{2E_{\vec{k}}}. \tag{176}$$

Combining (174) and (175) it follows that,

$$u^*_{\vec{k}} v_{\vec{k}} = \frac{g_{\vec{k}}}{1+|g_{\vec{k}}|^2} = g_{\vec{k}} |u_{\vec{k}}|^2 = \frac{\Delta^*_{\vec{k}}}{2E_{\vec{k}}} \tag{177}$$

Using these relations it is possible to show that Eqs. (168) and (174) are the same.

The gap at zero temperature

To proceed further, we need to evaluate the quantity $b_{\vec{k}}$ which measures the number of superconducting pairs in the condensate. Using the transformation (163), we have,

$$b_{\vec{k}} =< a_{-\vec{k}\downarrow} a_{\vec{k}\uparrow} >=< (u_{\vec{k}} \gamma_{-\vec{k}\downarrow} - v^*_{\vec{k}} \gamma^\dagger_{\vec{k}\uparrow})(u_{\vec{k}} \gamma_{\vec{k}\uparrow} + v^*_{\vec{k}} \gamma^\dagger_{-\vec{k}\downarrow}) > \tag{178}$$

The expectation value $< Operator >$ is taken over the ground state of the interacting Hamiltonian. The ground state has no quasiparticle excitations so that $< \gamma^\dagger_{\vec{k}\sigma} \gamma_{\vec{k}\sigma} >= 0$. From (178), we find that,

$$b_{\vec{k}} = u_{\vec{k}} v^*_{\vec{k}} \tag{179}$$

Combining Eqs. (161), (177) and (178), we find the famous "gap equation"

$$\Delta_{\vec{k}} = -\sum_{\vec{l}} V_{\vec{k}\vec{l}} \frac{\Delta_{\vec{l}}}{2E_{\vec{l}}} \tag{180}$$

with the quasiparticle excitations having the energy spectrum,

$$E_{\vec{k}} = ((\epsilon_{\vec{k}} - \mu)^2 + |\Delta_{\vec{k}}|^2)^{1/2} \tag{181}$$

In the special case of an angle independent gap $\Delta_{\vec{k}} = \Delta$, and assuming a constant pairing potential $-V$ in a band near the Fermi surface of width $\hbar\omega_c$, Eq. (180) reduces to,

$$1 = \frac{N(\epsilon_F)V}{2} \int_{\epsilon_F - \hbar\omega_c}^{\epsilon_F + \hbar\omega_c} \frac{d\epsilon}{((\epsilon - \epsilon_F)^2 + |\Delta|^2)^{1/2}} = N(\epsilon_F)V \int_0^{\hbar\omega_c/\Delta} \frac{dx}{(1+x^2)^{1/2}} = N(\epsilon_F)V \ Sinh^{-1}(\frac{\hbar\omega_c}{\Delta}) \tag{182}$$

From (182), we take the weak coupling limit $\hbar\omega_c/\Delta >> 1$ to find the BCS gap *at zero temperature*,

$$\Delta = 2\hbar\omega_c Exp[\frac{-1}{N(\epsilon_F)V}] \tag{183}$$

Note that, following convention, $N(\epsilon_F)$ is the density of states *for one electron spin*, whereas the density of states quoted in most other applications is a factor of two larger. In the weak coupling limit $N(\epsilon_F)V << 1$, this expression is of the same form as the gap found in the Cooper problem, except for a factor of two in the exponential. The ground state energy is given by,

$$f_s(T=0) - f_n(T=0) = \sum_{\vec{k}} (\epsilon_{\vec{k}} - \mu - E_{\vec{k}} + \Delta_{\vec{k}} b^*_{\vec{k}}) = -\frac{1}{2} N(\epsilon_F)\Delta^2 \tag{184}$$

This is also called the condensation energy. As we shall show later using Landau theory, the difference in free energy between the normal and superconducting states $f_n(H=0) - f_s(H=0) = \frac{1}{2}\mu_0 H_c^2$. Combining these two equations we get an extimate of the critical field of type one superconductors in terms of the gap,

$$H_c^2 = N(\epsilon_F)\Delta^2/\mu_0 \tag{185}$$

The *density of states* for the excitations is very important as it is measured in tunnelling. The density of states is found from,

$$D(E)dE = N(\epsilon)d\epsilon \approx N(\epsilon_F)d\epsilon \tag{186}$$

Since,

$$dE = \frac{2(\epsilon - \mu)d\epsilon}{2((\epsilon - \mu)^2 + \Delta^2))^{1/2}}, \tag{187}$$

we have,

$$D(E) = \frac{N(\epsilon_F)((\epsilon-\mu)^2+\Delta^2))^{1/2}}{\epsilon-\mu} = \frac{N(\epsilon_F)E}{(E^2-\Delta^2)^{1/2}} \tag{188}$$

This density of state applies for $E > |\Delta|$, while the density of states is zero otherwise.

The excitation or quasiparticle spectrum is also important. Recall that for a free Fermi system near the Fermi energy, we have,

$$\epsilon_k - \epsilon_F = \frac{\hbar^2 k^2}{2m} \approx \frac{\hbar^2 k_F}{m}(k-k_F) \tag{189}$$

which is found by using $k = k_F + (k - k_F)$ and expanding to leading order in $k - k_F$. In a superconductor the quasiparticle spectrum is,

$$E_k = ((\epsilon_k-\epsilon_F)^2+\Delta^2)^{1/2} \approx ((\frac{\hbar^2 k_F}{m}(k-k_F))^2+\Delta^2)^{1/2} \tag{190}$$

Assigned problems and sample quiz problems

Sample Quiz Problems

Quiz Problem 1. Draw the phase diagram of the Ising Ferromagnet in an applied magnetic field. Indicate the critical point. Plot the magnetization as a function of the applied field for three temperatures $T < T_c$, $T = T_c$, $T > T_c$.

Quiz Problem 2. Plot the behavior of the magnetization of the Ising ferromagnet as a function of the temperature, for three applied field cases: $h < 0$, $h = 0$, $h > 0$. Indicate the critical point.

Quiz Problem 3. Write down the definition of the critical exponents α, β_e, γ, δ, η and ν. What values do these exponents take within mean field theory.

Quiz Problem 4. Write down the mean field equation for the Ising ferromagnet in an applied field, on a lattice with co-ordination number z and exchange constant J. From this equation find the critical exponent δ for the Ising ferromagnet within mean field theory.

Quiz Problem 5. Write down the scaling hypothesis for the magnetization, susceptibility, free energy and correlation function. From these relations, find the Fisher, Widom and Rushbrooke critical exponent relations. Also write down the hyperscaling relation.

Quiz Problem 6. Find the domain wall energy for the Ising ($O(1)$ model) and for the $O(2)$ model. From these expressions find the lower critical dimension for these two problems.

Quiz Problem 7. Write down the van der Waals equation of state. Draw the P, v phase diagram of the van der Waals gas and indicate the critical point.

Quiz Problem 8. Make plots of the van der Waals equation of state isotherms, for $T > T_c$, $T < T_c$ and for $T = T_c$. For the case $T < T_c$ explain why the non-convex part of the curve cannot occur at equilibrium and the Maxwell construction to obtain a physical P, v isotherm.

Quiz Problem 9. Write down the Landau free energy for the Ising and fluid-gas phase transitions. Explain the correspondences between the quantities in the magnetic and classical gas problems.

Quiz Problem 10. Derive the Helmholtz free energy of the van der Waals gas and explain the physical meaning of the parameters a and b. Using your free energy explain the Maxwell construction.

Quiz Problem 11. Write down the Gibb's free energy of the van der Waals gas. What is the equilibrium co-existence condition in terms of the Gibb's free energy.

Quiz Problem 12. Explain the meaning of the upper critical dimension and lower critical dimension in the theory of critical phenomena.

Quiz Problem 13. State the universality hypothesis in the theory of critical phenomena and using it explain why the liquid gas phase transition is in the same universality class as the Ising mdoel.

Quiz Problem 14. Explain the importance of the "linked-cluster" theorems in perturbation theory of many particle systems.

Quiz Problem 15. Draw the high temperature series expansion diagrams to order t^8 (where $t = tanh(\beta J)$) for the square lattice, nearest neighbor, spin half Ising ferromagnet partition function. What is the degeneracy of each of these diagrams? Write down the expansion for the Helmholtz free energy and give a physical reason why only the terms of order N are kept.

Quiz Problem 16. Draw the low temperature series expansion diagrams to order s^8 (where $s = Exp[-2\beta J)$ for the square lattice, nearest neighbor, spin half Ising ferromagnet partition function. What is the degeneracy of each of these diagrams? Write down the expansion for the Helmholtz free energy and give a physical reason why only the terms of order N are kept.

Quiz Problem 17. Write down the mathematical form of the virial expansion for many particle systems and explain why it is important. What physical properties can be extracted from the second virial coefficient?

Quiz Problem 18. Explain the meaning of second quantization. Discuss the way that it can be used in position space and in the basis of single particle wavefunctions. Write down the commutation relations for Bose and Fermi second quantized creation and annihilation operators.

Quiz Problem 19. Write down the Hamiltonian for BCS theory, and the decoupling scheme used to reduce it to a solvable form. Explain the physical reasoning for the decoupling scheme that is chosen.

Quiz Problem 20. Consider the inverse Bogoliubov-Valatin transformation,

$$\gamma_{\vec{k}\sigma} = u^*_{\vec{k}} a_{\vec{k}\sigma} - \sigma v_{\vec{k}} a^\dagger_{-\vec{k}-\sigma}. \tag{191}$$

Show that if the operators $a, a^\dagger$ obey standard fermion anti-commutator relations, then the operators $\gamma, \gamma^\dagger$ also obey these relations, provided,

$$|u_k|^2 + |v_k|^2 = 1 \tag{192}$$

Quiz Problem 21. Given that the energy of quasiparticle excitations from the BCS ground state have the spectrum,

$$E = [(\epsilon - \epsilon_F)^2 + \Delta^2]^{1/2}, \tag{193}$$

where Δ is the superconducting gap and E_F is the Fermi energy, show that the quasiparticle density of states if given by,

$$D(E) = \frac{N(\epsilon_F)E}{(E^2 - \Delta^2)^{1/2}} \tag{194}$$

Quiz Problem 22. Describe the physical meaning of the superconducting gap, and the way in which BCS theory describes it.

Quiz Problem 23. (omit) BCS theory works very well even quite near the superconducting transition, despite the fact that it is a mean field theory. Use the Ginzburg criterion to rationalize this result. (we will do this after midterm III)

Quiz Problem 24. Given the general solutions to the BCS mean field theory

$$\Delta_{\vec{k}} = -\sum_{\vec{l}} V_{\vec{k}\vec{l}} \frac{\Delta_{\vec{l}}}{2E_{\vec{l}}}, \qquad E_{\vec{k}} = ((\epsilon_{\vec{k}} - \mu)^2 + |\Delta_{\vec{k}}|^2)^{1/2} \tag{195}$$

Describe the assumptions that are made in deducing that,

$$1 = \frac{N(\epsilon_F)V}{2} \int_{\epsilon_F - \hbar\omega_c}^{\epsilon_F + \hbar\omega_c} \frac{d\epsilon}{((\epsilon - \epsilon_F)^2 + |\Delta|^2)^{1/2}} =$$

$$N(\epsilon_F)V \int_0^{\hbar\omega_c/\Delta} \frac{dx}{(1+x^2)^{1/2}} = N(\epsilon_F)V \; Sinh^{-1}(\frac{\hbar\omega_c}{\Delta}) \tag{196}$$

and hence,

$$\Delta = 2\hbar\omega_c Exp[\frac{-1}{N(\epsilon_F)V}] \tag{197}$$

Assigned problems

Assigned Problem 1. From Eq. (18) of the notes, derive the Landau form Eq. (44). Explain the approximations that are made. Plot F_L as a function if m for $T > T_c$ and $T < T_c$ for $h = 0$ and for $h \neq 0$. Explain the concept of spontaneous symmetry breaking (SSB) using your graphs.

Assigned Problem 2. Consider the Ising ferromagnet in zero field, in the case where the spin can take three values $S_i = 0, \pm 1$. a) Find equations for the mean field free energy and magnetization. b) Find the critical temperature and the behavior near the critical point. Are the critical exponents $(\beta, \gamma, \alpha, \delta)$ the same as for the case $S = \pm 1$? Is the critical point at higher or lower temperature than the spin ± 1 case? c) Is the free energy for the the spin $0, \pm 1$ case higher or lower than the free energy of the ± 1 case? Why? d) Carry out an expansion of the free energy to fourth order in the magnetization. Does this free energy have the Landau form expected for an Ising ferromagnet?

Assigned Problem 3. By using $b = \xi$ show that Eqs. (58) reduces to Eqs. (50).

Assigned Problem 4. Consider the Landau free energy,

$$F = a(T - T_c)m^2 + bm^4 + cm^6 \tag{198}$$

where $c(T) > 0$ as required for stability. Sketch the possible behaviors for $a(T), b(T)$ positive and negative, and show that the system undergoes a first order transition at some value T_c. Find the value of $a(T_c)$ and the discontinuity in m at the transition.

Assigned Problem 5. Consider a Landau theory with a cubic term,

$$F = a(T - T_c)m^2 + bm^3 + cm^4. \tag{199}$$

Analyse the behavior of this model, particularly the nature of the different phases and phase transition(s) that occur.

Assigned Problem 6.
A spin half Ising model with four spin interactions on a square lattice has Hamiltonian,

$$H = -\sum_{ijkl \; in \; square} J S_i S_j S_k S_l \tag{200}$$

where the sum is over the smallest squares on an infinite square lattice, the interaction is ferromagnetic $J > 0$ and $S_i = \pm 1$. Each elementary square is counted only once in the sum.

Using a leading order expansion in the fluctuations (i.e. write $S_i = m_i + (S_i - m_i)$ and expand to leading order in the fluctuations), find the mean field Hamiltonian for this problem (Here $m_i =< S_i >$ is the magnetization at site i).

Using the mean field Hamiltonian and assuming a homogeneous state where $m_i = m$, find an expression for the mean field Helmholtz free energy, and the mean field equation for this problem.

Taking $J = 1$, sketch the behavior of the solutions to the mean field equation as a function of temperature. Does the non-trivial solution move continuously toward the $m = 0$ solution as the temperature increases? Is the behavior of the order parameter at the critical temperature discontinuous or continuous? Do you expect the correlation length to diverge at the critical point in this problem?

Assigned Problem 7. The Dieterici equation of state for a gas is,

$$P = \frac{k_B T}{v - b} e^{-a/(k_B T v)} \tag{201}$$

where $v = V/N$. Find the critical point and the values of the exponents β, δ, γ for this model.

Assigned Problem 8. Consider a phase co-existence curve in a $P - T$ phase diagram, separating two phases "A" and "B". Consider two points on the phase coexistence curve at P, T and $P + \Delta P, T + \Delta T$. Since the chemical potential of the phases A and B are the same at any given point on the co-existence curve, we have,

$$\Delta g_A = g_A(P + \Delta P, T + \Delta T) - g_A(P, T) = g_B(P + \Delta P, T + \Delta T) - g_B(P, T) = \Delta g_B \tag{202}$$

From this relation, prove the Clausius-Clapeyron relation,

$$\frac{\partial P}{\partial T} = \frac{L}{T(V_B - V_A)} \tag{203}$$

where L is the latent heat. Find the form of this relation for the van der Waals equation of state. What is the dependence of the latent heat as $T \to T_c$. Is this exponent related to any of the other exponents in the problem?

Assigned Problem 9. Recent work on black hole thermodynamics has suggested that a black hole with charge Q obeys the equation of state,

$$P = \frac{T}{v} - \frac{1}{2\pi v^2} + \frac{2Q^2}{\pi v^4} \tag{204}$$

where the physical pressure and temperature are given by,

$$Press = \frac{\hbar c}{l_P^2}; \quad Temp = \frac{\hbar c}{k_B} T; \quad v = 2 l_P^2 r_+ \tag{205}$$

where $l_P = \hbar G_N / c^3$ is the Planck length and r_+ is the black hole event horizon. Find the critical point of this equation of state and find the critical exponents δ and β.

Assigned Problem 10. Consider a ferromagnetic nearest neighbor, spin 1/2, square lattice Ising model where the interactions along the x-axis, J_x, are different than those along the y-axis, J_y. Extend the low and high temperature expansions to this case. Does duality still hold? From your expansions, find the internal energy and the specific heat.

Assigned Problem 11. Find and compare the second virial coefficient for four cases: (i) the classical hard sphere gas; (ii) Non-interacting Fermions; (iii) Non-interacting Bosons; (iv) The van der Waals gas.

Assigned Problem 12. The BCS pairing Hamiltonian is a simplified model in which only pairs with zero center of mass momentum are included in the analysis. We also assume that the fermion pairing that leads to superconductivity occurs in the singlet channel. The BCS Hamiltonian is then,

$$H_{pair} - \mu N = \sum_{\vec{k}\sigma} (\epsilon_{\vec{k}\sigma} - \mu) \; a^\dagger_{\vec{k}\sigma} a_{\vec{k}\sigma} + \sum_{\vec{k}\vec{l}} V_{\vec{k}\vec{l}} \; a^\dagger_{\vec{k}\uparrow} a^\dagger_{-\vec{k},\downarrow} a_{-\vec{l}\downarrow} a_{\vec{l}\uparrow}, \tag{206}$$

where $N = \sum_{\vec{k}\sigma} n_{\vec{k}\sigma}$ is the number of electrons in the Fermi sea. By making an expansion in the fluctuations and defining,

$$b_{\vec{k}} =< a_{-\vec{k}\downarrow} a_{\vec{k}\uparrow} >, \quad \text{and} \quad b^*_{\vec{k}} =< a^\dagger_{\vec{k}\uparrow} a^\dagger_{-\vec{k}\downarrow} > . \tag{207}$$

where $b^*_{\vec{k}}$ is the average number of pairs in the system at wavevector $\vec{k}$, show that the mean field BCS Hamiltonian is given by,

$$H_{MF} - \mu N = \sum_{\vec{k}\sigma}(\epsilon_{\vec{k}\sigma} - \mu)\ a^\dagger_{\vec{k}\sigma} a_{\vec{k}\sigma} + \sum_{\vec{k}\vec{l}} V_{\vec{k}\vec{l}}\ (a^\dagger_{\vec{k}\uparrow} a^\dagger_{-\vec{k},\downarrow} b_{\vec{l}} + b^*_{\vec{k}} a_{-\vec{l}\downarrow} a_{\vec{l}\uparrow} - b^*_{\vec{k}} b_{\vec{l}}) \tag{208}$$

This is the Hamiltonian that we will solve to find the thermodynamic behavior of superconductors, using an atomistic model.

Assigned Problem 13. Using the Bogoliubov-Valatin transformation (Eq. 163), show that the mean field BCS Hamiltonian (Eq. (162)) reduces to Eq. (166), provided Equations (167) and (168) are true.

Assigned Problem 14. If we define,

$$v_{\vec{k}} = \frac{g_{\vec{k}}}{(1 + |g_{\vec{k}}|^2)^{1/2}} \tag{209}$$

show that Eq. (167) reduces to (173).

Assigned Problem 15. Show that $E_{\vec{k}}$ as defined in Eq. (174) is in agreement with Eq. (168).

Assigned Problem 16. Prove the relations Eq. (175-177).