Expansion of Landau theory with Magnetic Susceptibility and Heat Capacity

Xuran Qi

School of physics, University of Utah, UT, USA

u1271727@umail.utah.edu

Abstract. Landau theory employs free energy to depict the work potential of molecules and utilizes order parameters to signify the degree of molecular organization. By applying a Taylor expansion of the free energy with respect to the order parameter in the vicinity of a phase transition, the theory elucidates how molecular arrangements can influence the system's energy. The universality of Landau theory stems from the order parameter within the framework of free energy expansion. The application of critical exponents exemplifies the universality of Landau theory, showcasing the properties of materials that share the same dimensionality and similar correlation lengths. This article aims to derive formulas and discuss practical applications of Landau theory, such as analyzing the heat capacity and magnetic susceptibility of materials across a range of temperatures.

Keywords: Landau theory, Phase transitions, critical point, critical temperature, free energy expansion, critical exponents.

1. Introduction

The significance of Landau theory in the study of phase transitions cannot be overstated, as it provides a fundamental framework for understanding these phenomena. Phase transitions, such as condensation, involve a substance changing from one state to another under certain conditions. For example, water is liquid at temperatures above zero degrees Celsius under standard atmospheric pressure, but it becomes solid when the temperature drops below zero. These different states—liquid and solid—are distinct phases of water, and the change between them is known as a phase transition. Landau's theory introduces the concept of an order parameter, which characterizes the properties of each phase and aids in comprehending the transition process. Imagine a cube-shaped building with a robust structural framework that is evenly distributed and supports the entire structure. If an earthquake occurs with relatively low energy, it may not be enough to destroy the building's bearing structures. However, if the earthquake carries a significant amount of energy, it could lead to the collapse of the building by damaging these critical supports. In this analogy, the intact building represents an ordered state, where the bearing structures all support the building in a unified direction. The destruction of these structures signifies a move to a disordered state, where the supporters no longer act in concert. Although this is a simplified example, it serves to illustrate the basic concepts. Various factors can influence the order parameter, with temperature being a primary one. Landau's theory also introduces critical exponents, which are universal results derived from calculations and can be used to predict material properties. These exponents are particularly useful when searching for materials with specific characteristics, such

as high resistance at high temperatures. The universality of critical exponents across materials in the same dimensional space is crucial for predicting their properties. While different dimensions may yield different critical exponents, each set of calculated exponents within a dimension is universal, making the study of Landau's theory invaluable for understanding and predicting material behavior.

2. Landau Theory and the Applications

Landau theory provides methodology to understand how different states of matter transform into one another, which is crucial in condensed matter physics and materials science. Transitions can be described as either first-order or second order. First-order phase transitions are characterized by a discontinuous change in density and latent heat. For example, the melting of a solid metal into a liquid is a first-order transition. Second-order transformations are characterized by a continuous change of an order parameter. For example, a change from ferromagnetic to paramagnetic states at the Curie temperature is a second-order transition.

2.1. Function of order parameter

Order parameters are crucial variables in Landau theory, used to describe the state of a system, particularly during phase transitions. They help distinguish between ordered and disordered states by indicating changes in symmetry and energy states. Above the critical temperature, the system is in a disordered state, characterized by an order parameter value of zero. In this high-temperature phase, the system exhibits high symmetry. The increased thermal energy provides enough agitation to allow electrons or other entities to populate higher energy states freely, which disrupts any preference for specific energy levels, leading to a disordered arrangement. The reduced thermal energy during this state means that electrons tend to occupy lower energy states, which stabilizes the ordered phase and contributes to the distinct characteristics of this lower-symmetry phase. Different levels of order are related to different states, and the state of order refers to the degrees of freedom of the system's components, such as atoms, molecules, spins, etc. From the properties of these components, we can predict the arrangement or behavior of the entire system.

2.2. Deduction of free energy expansion

Landau theory the free energy can be expressed as a Taylor-expansion of the order parameter close to the phase transition point, where order parameter is close to zero. Thus, we can write the expression as:

$$F(\emptyset) = A\emptyset + B\emptyset^2 + C\emptyset^3 + D\emptyset^4 + \cdots. \tag{1}$$

$F(\emptyset)$, Free energy expansion with order parameters. A,B,C, and D are temperature related values. Order parameter approaches a small value indicating that the expansion is nearing the critical point. A small order parameter means that higher-order terms have less impact than lower-power terms, allowing for a 'good' approximation with just a few terms. In the equation, it's necessary to eliminate all odd terms due to symmetrical considerations and stability requirements. This requirement is linked to stability, as the system prefers a state of lower energy, implying that the free energy should have a minimum value in the equilibrium state.

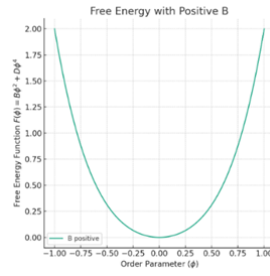$$F(\emptyset) = B\emptyset^2 + D\emptyset^4. \tag{2}$$

Figure 1. (We use free energy to label y and order parameter in x label and the coefficient B is always positive.)

Order parameter equal to zero when temperature equals to critical temperature. When B is equal to zero it means the free energy has a single minimum at an order parameter equal to zero, indicating a stable phase without spontaneous symmetry breaking.
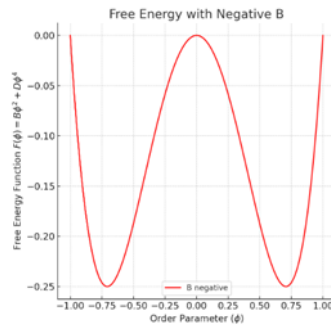

Figure 2. (We use free energy to label y and order parameter in x label and the coefficient B is always negative.)

Order parameter equal to zero when temperature equals to critical temperature. This graph shows two minima, indicative of two equivalent stable states at non-zero values of the order parameter. This represents a situation of spontaneous symmetry breaking, typical for temperatures below the critical temperature, where the system can spontaneously choose one of two ordered phases. First derivative of first four term in free energy expansion. In equilibrium, for a system to be stable, the first derivative of the free energy with respect to the order parameter should be zero.

$$\frac{dF}{d\phi} = F'(\phi) = 2B\phi + 4D\phi^3 = \phi(2B + 4D\phi^2) = 0. \tag{3}$$

Second derivative of first four term in free energy expansion. This curvature is directly related to the stability of the equilibrium state.

$$\frac{d^2F}{d\phi^2} = F''(\phi) = 2B + 12D\phi^2. \tag{4}$$

The second derivative gives different meanings for each condition. ($\frac{d^2F}{d\phi^2} < 0$), Indicates an unstable equilibrium. ($\frac{d^2F}{d\phi^2} = 0$), At this point, the system is marginally stable, and the response to perturbations can lead to qualitative changes in the system's behavior. ($\frac{d^2F}{d\phi^2} > 0$), Indicates a stable equilibrium. Then we can consider how B works in the free energy expansion. Could we make a connection between B and temperature? We can make a linear correlation between the change in temperature and the change in our constant B from positive to negative.

$$B \sim \blacksquare \frac{(T - T_c)}{T_c} + \blacksquare \ or \ B(T) \sim T - T_c. \tag{5}$$

Then we can rewrite the expression:

$$F(\emptyset) = F_0 + \frac{1}{2}a(T)\emptyset^2 + \frac{1}{4}b(T)\emptyset^4 + \cdots. \tag{6}$$

The coefficient number is used to cancel the extra value from derivative. Then we can determine the Order Parameter Exponent (β). The order parameter behaves as $\emptyset \sim (T - T_c)^\beta$ below T_c. To find the Order Parameter Exponent we need to Minimization of Free Energy, which is take the first derivative. Finally, we get $\emptyset \sim (T - T_c)^{1/2}$ and this exponent (1/2) is the critical component. Critical components have the property of Universality. This property gives us a way to predict behavior of material close to critical points. The critical exponent correlates to correlation length and disruption. In Landau theory, the heat capacity of a material near a phase transition can be analyzed by considering the expansion of the free energy in terms of order parameters. The heat capacity at constant volume is defined as the temperature derivative of the internal energy, and, equivalently, it can be expressed as the negative second temperature derivative of the free energy assuming constant volume:

$$C_v = \frac{dU}{dT}\bigg|_v = -T\frac{d^2F}{dT^2}\bigg|_v. \tag{7}$$

C_v is heat capacity at constant volume. $\frac{dU}{dT}$ is temperature derivative of the internal energy. $\frac{d^2F}{dT^2}$ is the second temperature derivative of free energy. As temperature approaches the critical temperature, the free energy becomes highly sensitive to changes in temperature due to the critical fluctuations of the order parameter. Near the critical temperature, the order parameter changes significantly, typically going from nonzero in the ordered phase to zero in the disordered phase. This significant change in the order parameter results in an anomaly in the heat capacity, which may exhibit a peak or discontinuity at the critical temperature.

2.3. Magnetic Susceptibility

Magnetic susceptibility is a critical parameter that quantifies the response of a magnetic system to an applied magnetic field. For a magnetic system near a phase transition, the Landau free energy expansion in terms of the magnetization(M), which serves as the order parameter.

$$F(T, M) = F_0 + aM + \frac{1}{2}b(T)M^2 + \frac{1}{3}c(T)M^3 + \frac{1}{4}b(T)M^4 + \cdots - MH. \tag{8}$$

F is free energy. F_0 is the free energy in the absence of magnetization. T is temperature. M is net magnetization. H is applied magnetic field. MH is energy from external field.

To find the critical component of $F(T, M)$, we also need to minimize the free energy. First let's define $a = a(T) = a_0(T - T_c) < 0$. Make a temperature dependent.

$$\frac{dF}{dM} = aM + bM^3 - H = 0. \tag{9}$$

The magnetic susceptibility is defined as the derivative of magnetization with respect to the applied magnetic field at constant temperature:

$$x = \frac{dM}{dH} \tag{10}$$

For small fields and near critical temperatures, M also small, allowing us to approximate the equilibrium condition for magnetization by neglecting higher-order terms:

$$M = H/a. \tag{11}$$

Equation (11) gives the expression the susceptibility:

$$x = \frac{1}{a} = 1/a(T - T_c). \tag{12}$$

Which gives critical exponent equal to -1.

3. Results

3.1. Heat Capacity

In "Heat Capacity of Iron: A Review" by J.B. Austen, which is the cornerstone of metallurgical engineering and materials science. Austen meticulously documents how different alloying elements impact iron's heat capacity, providing a comprehensive dataset that distinguishes between the alpha (α) and gamma (γ) phases of iron, which are two of the several allotropes of iron that exist at different temperature ranges and pressures. Austen's work captures the thermal transitions between these phases, revealing how the intrinsic property of heat capacity responds as iron progresses through these structural and magnetic transformations. By focusing on the heat capacity of α-iron from 100°C to 906°C, Austen steps into a critical domain of temperature where the material exhibits significant changes in its physical properties.
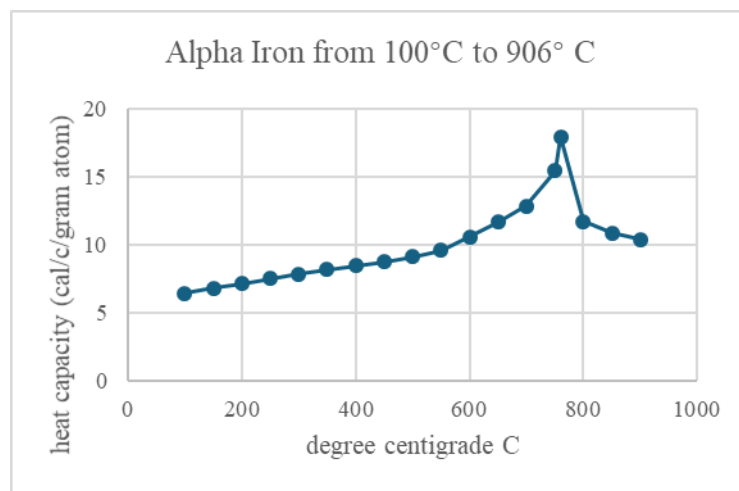

Figure 3. (This graph measures the heat capacity changes with different degree centigrade and there is an unexpected peak appear on the graph, which comes from A Review" by J.B. Austen. [3])

The heat capacity appears relatively stable at lower temperatures with a gradual increase as the temperature rises. This is typical for solids, as the heat capacity increases with temperature due to the increased vibrational energy of the atoms. There is a sharp peak observed in the graph. This could correspond to a phase transition. According to Landau's Theory, such a peak might be associated with a second-order phase transition, where the heat capacity shows critical behavior as the order parameter changes continuously. If this peak indeed corresponds to the Curie point, the graph provides experimental evidence that supports Landau's Theory. The theory predicts that the heat capacity will diverge at the critical temperature for a second-order phase transition.

3.2. Magnetic Susceptibility

The article "Temperature Dependence of the Magnetic Susceptibility for Triangular-Lattice Antiferromagnets with spatially anisotropic exchange constants" which written by "Weihong Zheng" and "Rajiv R. P. Singh." And their team gives a good example to illustrate the property of critical exponent.
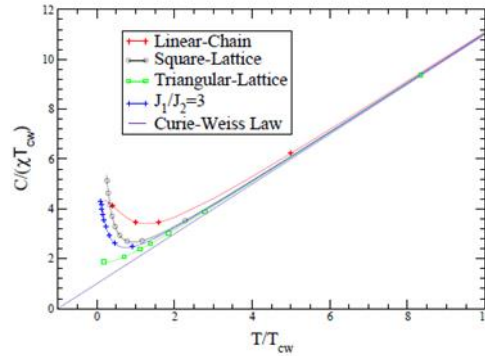
Figure 4. (The Curie-Weiss Law is represented by a straight line, which is the expected behavior for a paramagnetic material in the high-temperature limit, according to the Curie-Weiss law. Different symbols represent different lattice models (linear-chain, square-lattice, triangular-lattice, and an anisotropic model with $\frac{J_1}{J_2} = 3$ [2])

J_1 and J_2 are parameters that characterize the interactions between adjacent particles or spins in a lattice. C define as Curie constant and in their model expression in $C = Ag^2$. χ define as uniform magnetic susceptibility per mole of a substance in the context of Para magnetism. When it expresses by Curie-Weiss law $\chi = \frac{C}{T + T_{cw}}$. T_{cw} define as The Curie-Weiss temperature and express with $c = J_2 + \frac{J_1}{2}$. The uniformity of the critical exponent is assessed by how closely the data points for each lattice model approach the line representing the Curie-Weiss law as T approaches T_{cw}. If the lattice models follow the Curie-Weiss behavior closely, they exhibit a critical exponent consistent with the mean-field prediction. If they deviate, it suggests different critical exponents and possibly different universality classes for the phase transitions. For a paramagnetic to ferromagnetic transition, we would expect the susceptibility to diverge as T approaches T_{cw}. On the graph, this would be represented by the plotted points for each lattice system rising sharply and following the line as T/T_{cw} approaches 1, indicating that T is getting close to T_{cw}. In this graph, if all the data collapse to the same line near the critical region, it would imply that they share the same critical exponent. But when deviations happen as T they approach T_{cw}, indicating different magnetic ordering.

4. Conclusion and Outlook

Table 1. Critical exponents for percolation phase transition in dimensions

dimension	α	β	γ	δ	ν	η
1D	1	0	1	∞	1	1
2D	-2/3	5/36	43/18	91/5	4/3	5/24
3D	-0.625	0.418	1.793	5.29	0.876	0.46

[a]α This exponent characterizes how the specific heat of a system varies near its critical point.
[b]β This exponent describes how the order parameter, such as magnetization in a ferromagnetic material, changes as the system passes through the critical temperature from above.
[c]γ This exponent illustrates how the susceptibility or response function of the system behaves in the presence of an external field as the critical temperature is approached.
[d]δ This exponent demonstrates the relationship between the order parameter and the external field at the critical temperature.
[e]ν This exponent is associated with the correlation length, indicating how correlated regions of the system grow as the critical point is approached.
[f]η These exponents measure the decay of correlations at the critical point, describing the anomalous dimension or behavior of the correlation function at large distances.

Landau's theory of phase transitions is fundamentally about symmetry breaking [1]. The concept of symmetry refers to the invariance of the system's free energy under certain transformations. In a high-symmetry phase, temperature dropping below a critical value and a system may undergo a phase transition to a low-symmetry phase. For example, in Figure.2 we defined when temperature is lower than critical temperature and it will drop to one of the two minimum. When it is dropped, it means it is broken the symmetry and selected one of the lower energy states. In Table 1, we observe that varying dimensions can lead to markedly different outcomes for each parameter. However, it's important to note that not all materials possess similar operators. Within the same dimension, certain materials, such as cuprate superconductors, exhibit vastly different correlation lengths and spatial distances compared to classical materials. The correlation length measures how far apart two parts of a system can be while still maintaining some degree of correlation. Spatial distance, another factor that can influence critical exponents, refers to the physical length separating two points in space. In cuprate superconductors, the correlation length tends to be short due to the intense electronic correlations present, which result in the pairing of electrons into Cooper pairs over very brief distances. The role of spatial distance is crucial in determining the propagation of correlated states. Consequently, we can deduce that a critical exponent related to a physical property is based on the order parameter and could represent the spin of an electron in magnetic susceptibility. Altering the spatial distance between two electrons and the extent of their correlation undeniably modifies the resulting critical exponent.

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