Critical Phenomena of Mott transition

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Abstract

Due to interaction between electrons, half-filled band materials can be insulators at finite temperature. The metal-insulator transition in such system is known as Mott transition. The order parameter for Mott transition is believed in the Ising universality class which has been verified both theoretically and experimentally. However, recent experiments find that Mott transitions in 2D system may belong to other universality class. In this essay, we discuss the Mott transition in Ising universality class and the possibility of it being in different universality classes.

1. Introduction

It is surprising that simple physical laws can describe critical phenomena no matter whether the system is classical or quantum. Even though the microscopic details of the underlying systems may be completely different, they can have similar scaling property near critical point . Such scaling laws were found in magnetic transitions, liquid-gas transitions, and so forth [1]. With similar phase diagram proposed for Mott transition (also known as metal-insulator transition) [2], it is natural to ask whether Mott transition has the same scaling property.

The Mott transition is phase transition between Mott insulator and metal. From band theory, materials with half-filled band should be metallic, but if interactions between electrons are taken into account, they may become insulators called Mott insulators [3]. Some typical Mott insulators are Cr-doped V_2O_3 [4] and layered organic charge-transfer salts κ-(BEDT-TTF)$_2$X with X representing monovalent anions [5][6][7]. The transition is usually triggered by changing the ratio between the local Coulomb repulsion and kinetic energy of the relevant electrons and the ratio can be controlled by changing temperature, applying pressure or changing lattice spacing [5]. As shown in Fig.1, The typical temperature-pressure phase diagram consists a first order transition line separating the two phases: insulator and metal, and a critical point at the end of this first order transition line [5].

Mott transition is usually described by half-filled Hubbard model [2]:

$$H = t \sum_{\langle i,j\rangle,\sigma} C^{\dagger}_{i,\sigma} C_{j,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow} \tag{1}$$

where t is nearest-neighbor hopping coefficient, U is repulsion between electrons on the same site and $n_{i,\sigma} = C^{\dagger}_{i,\sigma} C_{i,\sigma}$ is the number operator of site i and spin σ.

Theoretical studies on half-filled Hubbard model are done by methods such as renormalization-group [8][9], dynamical mean field theory (DMFT) [10][11][12] and cluster DMFT [13]. Early theoretical work suggested that the transition lies in the Ising universality class. Castellani et al derived a new effective Hamiltonian from half-filled Hubbard Hamiltonian and found out that it is a generalization of Blume-Emery-Griffith Hamiltonian for He^3-He^4 mixtures [2]. By comparing with previous works, they gave a clear physical interpretation of the phase diagram and indicated that the critical behavior of Mott transition is in Ising universality class. Using DMFT, Kotliar

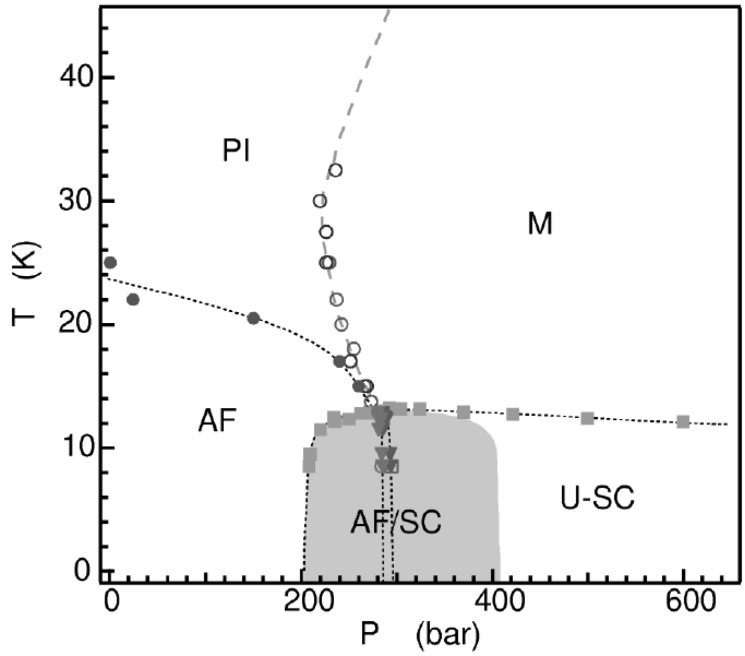

Figure 1: A typical phase diagram of Mott transition retrieved from Ref. [5]. The Mott transition line is represented by open circles. The low pressure phase is paramagnetic insulator (PI) and the high pressure phase is metal (M). The first order transition line ends at a critical point at (P_c, T_c)≈(220 bar, 32.5 K).

reached the similar conclusion [10].

In 2003, Limelette *et al.* reported the critical exponents of Cr-doped V_2O_3 which is consistent with the prediction by previous theories, indicating the system is in the Ising universality class [4]. It seems perfect that theoretical predictions are verified by experiment results. However, the later discovery of unconventional critical behavior in quasi-2D organic charge-transfer salts put this seemingly settled issue into debate [6]. Possible explanations include existence of quantum critical points [14] and wrong interpretation of experimental results [15]. In 2010, Bartosch *et al.* pointed out that the definition of critical exponent is problematic in the vicinity of critical point [15]. They suggested that the seemingly controversial results of experiment and theory are in fact consistent if the experimental results are fitted with a correct scaling law. By developing new scaling functions in the vicinity of critical end point, they successfully fitted previously reported experimental results within 2D Ising universality class.

This essay presents and analyzes the main result of the work done by Bartosch *et al* [15]. and discusses the universality class of that Mott transition may belong. The second part presents the main procedure and results in the paper. The third part evaluates the reliability of their work and the forth part compares several experiment results and discusses whether Mott transition is in Ising universality class or not. The last part gives a summary of the whole essay.

2. Main Results of the Paper

Begin with the singular part of Gibbs free energy for 2D Ising universality class, the authors first proved that Gruneisen ratio diverges at critical point, and then derived a new scaling function for expansivity.

The singular part of Gibbs free energy f can be written as

$$f_s(t,h) = \frac{t^2}{8\pi}\ln t^2 + |h|^{d/y_h}\Phi(t/|h|^{y_t/y_h}) \tag{2}$$

where $t = (T - T_c)/T_c$, $h = (p - p_c)/p_c$ and Φ is the scaling function.

The thermal expansivity is defined as

$$\alpha_p = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_p = -\frac{1}{V}\frac{\partial^2 f}{\partial T \partial p} \tag{3}$$

The Gruneisen ratio is defined as

$$\Gamma_p = \frac{\alpha_p}{c_p} \tag{4}$$

It is easy to derive the scaling law for Gruneisen ratio when $h = \pm 0$, $t < 0$

$$\Gamma \propto \mathrm{sgn}(h)(-t)^{-1+\alpha+\beta} \tag{5}$$

It is clear that for 2D Ising model ($\alpha = 0$, $\beta = 0.25$) this property diverges at critical point.

Next, they derived a new scaling function for thermal expansivity in the vicinity of critical point. The scaling form of the expansivity can be derived

$$\alpha_p(t,h) \propto \mathrm{sgn}(h)|h|^{-1+(d-y_t)/y_h}\Psi_\alpha(t/|h|^{y_t/y_h}) \tag{6}$$

where, Ψ_α is defined as

$$\Psi_\alpha(x) = \frac{d-y_t}{y_h}\Phi'(x) - \frac{y_t}{y_h}x\Phi''(x) \tag{7}$$

For the 2D Ising universality class, $y_t = 1$, $y_h = 15/8$ and $\Phi(x)$ can be obtained numerically.

The author assumed that in the vicinity of critical point, the scaling law can be expressed by linearly mixing temperature and pressure, i.e. they replace the traditional definition of t and h with $t = (T - T_c - \zeta(p - p_c))/T_0$ and $h = (p - p_c - \lambda(T - T_c))/p_0$. Note that λ, ζ, T_0 and p_0 are parameters to be determined. Assuming that the nonsingular background contribution to the thermal expansivity is linear in temperature, they established the scaling function for thermal expansivity:

$$\begin{aligned} \alpha(T,P) &= A\,\mathrm{sgn}[p - p_c - \lambda(T - T_c)] \times [p - p_c - \lambda(T - T_c)]^{-7/15} \\ &\quad \times \Psi_\alpha\left(B\frac{T - T_c - \zeta(p - p_c)}{[p - p_c - \lambda(T - T_c)]^{8/15}}\right) + C + D[T - T_c - \zeta(p - p_c)] \end{aligned} \tag{8}$$

This new scaling function was used to analyze the data published in Ref.[7]. By adjusting the parameters, the experiment results can be well fitted with their scaling function (Fig.2). The fitting parameters are:
$T_c + \zeta(p - p_c) = 27.5$ K
$(p - p_c)/\lambda = 26.7$ K
$A/\lambda^{7/15} = 874 \times 10^{-6}$ K$^{-8/15}$

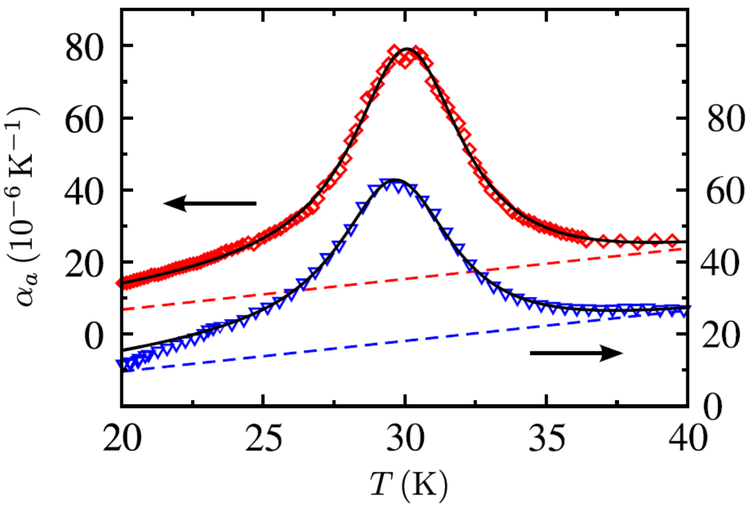

Figure 2: Fit to the expansivity with the scaling form [15].

$B/\lambda^{8/15} = 3.88\ \mathrm{K}^{-7/15}$
$C = 13.2 \times 10^{-6}\ \mathrm{K}^{-1}$
$D = 0.85 \times 10^{-6}\ \mathrm{K}^{-2}$

3. Discussion about Their Methods and Results

The main purpose of the paper is to explain the seemingly unconventional critical exponent discovered in experiment of Ref.[7] by developing a new scaling function. To achieve this goal, two assumptions were made:

- They assume that the system is of 2D Ising universality class as suggested by previous theories. The inconsistency of experiment and theory comes from the wrong belief that Gruneisen ratio is finite near critical point.
- They assume that in the vicinity of critical point, the scaling law can be manipulated by containing small mixing terms in the traditionally defined t and h.

The first assumption has been verified in their paper as shown in the last part. However, the linear mixture of terms in t and h still need consideration. In the paper, they stated that the finite values of λ and ζ represent tilted scaling axes, i.e. approaching to the critical point means sweeping temperature and pressure simultaneously while keeping the ratio of changing rates of the two properties as a constant. Later when they were fitting the data, clearly they regarded p as a constant as can be seen from the fitting parameters listed above. This self-inconsistency makes readers confused.

Since the experiment was usually conducted at a fixed pressure or temperature, the linea mixture of the two makes no sense. Actually it is not necessary to derive such a complicated scaling function to fit the data. The beauty of scaling law lies in its simplicity. As pointed out by the authors, the fits is almost independent on the parameter λ. This is because as T goes to T_c, the term with λ is negligible compared with $p - p_c$. Since the experiment was performed near critical temperature, it is reasonable to set $\lambda = 0$. By redefining parameters according to their fitting parameters, the scaling function eq.(9)can be simplified as

$$\alpha(T,P) = \frac{A}{\lambda^{7/15}} \operatorname{sgn}(p') \times (p')^{-7/15} \times \Psi_\alpha \left(\frac{B}{\lambda^{8/15}} \frac{T - T_c'}{(p')^{8/15}} \right) + C + D(T - T_c') \quad (9)$$

with $p' = \frac{p-p_c}{\lambda}$, $T_c' = T_c + \zeta(p - p_c)$. It is just the traditional scaling law, so their "new" scaling function is essentially the same as the traditional one.

On the other hand, we can obtain the critical exponent of thermal expansivity directly. Make some changes to Eq.(6), we obtain

$$\alpha_p(t,h) \propto |t|^{-7/8} \Psi_\alpha'(t/|h|^{8/15}) \quad (10)$$

where $\Psi'(x) = x^{7/8}\Psi(x)$. Because $\Psi(x) \propto (-x)^{-7/8}$ as $x \to -\infty$ [15], when $h = 0$, the scaling law is

$$\alpha_p(t,0) \propto |t|^{-7/8} \quad (11)$$

It is valid when $|t| \gg |h|^{8/15}$.

From Eq.(11), the critical exponent for expansivity of 2D Ising model is 7/8, which is in agreement with the experimental result 0.8 ± 0.15 in Ref.[7]. The reason that authors of Ref.[7] reached the wrong conclusion that the system did not belong to 2D Ising universality class is that their analysis is based on the proportionality of thermal expansion to specific heat. They compared their result with the critical exponent α which is zero in 2D Ising model. Therefore, the experiment confirmed that Mott transition is in Ising universality class.

4. Ising or not

Although the work done by Bartosch *et al.* is inconsistent and overcomplicated, it gave the correct fitting to the experimental data. This paper together with Ref.[7] (I believe they are come from the same research group) supports the statement that Mott transition is in the Ising universality class.

However, the experimental results need further discussion. Eq.(11) is only valid when $|t| \gg |h|^{8/15}$. According to Ref.[7], the experiment was performed at a pressure far away from critical pressure. This indicates $|t| < |h|^{8/15}$ especially when $T \to \infty$. Considering the crossover effect, the authors obtained the critical exponent by assuming a Gaussian distribution for T_c [7].

There are two other experiments also studied the critical behavior at the end of first order Mott transition [4][6]. Instead of measuring thermal expansivity, they chose conductivity as the order parameter and obtained critical exponents (δ,β,γ). Both the experiments on Cr-doped V_2O_3 [4] and organic charge-transfer salts κ-(BEDT-TTF)$_2$X with X=Cu[N(CN)$_2$]Cl [6] exhibit good data collapse, indicating the existence of scaling law. The experiment on V_2O_3 obtained mean field value $\delta = 3$, $\beta = 0.5$, $\gamma = 1$ in the vicinity of critical point and 3D Ising value $\delta \approx 5$, $\beta \approx 0.34$, $\gamma = 1$ at the region closer to critical point [4]. The experiment on κ-(BEDT-TTF)$_2$X obtained $\delta = 2$, $\beta = 1$, $\gamma = 1$ which fits to no universality class [6].

Although the scaling law is only valid before crossover, It is interesting to realize that the critical exponents obtained after crossover are in agreement with Ising universality class in both Ref.[4] and Ref.[7] despite the fact that they measured different properties in different systems. Whether this is coincidence or has physical meaning still needs exploration. The critical exponents obtained before crossover should be the correct critical exponents, but they are either mean-field value [4] or unconventional [6].

Note that the critical exponents of κ-(BEDT-TTF)$_2$X is $\delta = 2$, $\beta = 1$, $\gamma = 1$ [6]. From the relation $\alpha + 2\beta + \gamma = 2$, we get $\alpha = -1$, but α is supposed to be positive. Therefore, the experimental results still need detailed analysis.

The reason for inconsistency between theory and experiments may be that Hubbard model is too simple to describe realistic systems. Recent theoretical works show that including new correlations may change the properties near critical point [13] and subleading corrections can lead to the unconventional exponent $\delta = 2$. As most theoretical work were based on half filled Hubbard model, it is true that systems described by this model are in Ising universality class, but whether this model can describe realistic systems or whether it can represent the symmetry of real systems still needs more discussion.

5. Summary

This essay discusses the critical behavior of Mott transition. After a short review of previous works on Mott transition and its critical properties, we analyze the work of Ref.[15]. Their theory is convincing in the sense that it provides a good fit to the experimental data. However, their analysis is a little self-inconsistent and overcomplicate.

Their results together with other two experiments are used to discuss the universality class that Mott transition belongs to. These experimental results are at odds with previous predictions derived from Hubbard model, indicating that Mott transition may not be in the Ising universality class.

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