PHYS 563

Renormalization Group and Phase Transitions

Term Paper "Quantum Phase Transitions as Exemplified by Heavy Fermionic Materials"

Abstract

In this term paper I discuss what is meant by a quantum phase transition, as well as its similarities and differences with a conventional thermal phase transition. In order to make the subject concrete the quantum critical point is considered for a model of metallic magnetism and its implications on the phase diagram discussed. To demonstrate the relevance of quantum phase transition to real materials, experimental data on scaling in heavy fermionic materials is presented and universality in this data discussed.

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1 Preface

The scope of the subject of Quantum Phase Transitions (QPT) is vast, complicated, and comprises a wide field of research. Many aspects of this subject are far from being well understood and constitute areas of intense experimental and theoretical investigation. It is for this reason that addressing the entire subject in a term paper would be futile. Thus the main goal pursued in this paper is to answer the question: "What are the fundamental differences between quantum and thermal phase transitions?". What I've discovered for myself is that the scaling behavior near quantum critical points (QCP) provides a useful lens to assess QPTs, which is the very topic we were concerned with in the course "RG and Phase Transitions". To illustrate the relevance of the QPTs in real materials, I discuss experimental data on heavy fermionic materials that cannot be described using the conventional Landau-Ginsburg-Wilson (LGW) paradigm, but is well-modeled by the theory of QPTs. However, before we look at the behavior of heavy fermionic materials, we will follow the historical path by looking at the transverse Ising model as well as the paramagnetic-ferromagnetic transition in interacting electronic systems.

2 Quantum Effects in Phase Transitions

- **Question:** *Fundamentally, what is the driving force behind all differences between quantum and thermal phase transitions?*

Before we proceed to answer this question, I would like to present a definition of quantum phase transition.

- **Def:** *Quantum phase transition is a phase transition that occurs due to a competition of physical effects, the operator representation of which do not commute. For continuous quantum phase transitions, it is synonymous with phase transitions induced by quantum fluctuations* [1].

Such non-commutativity is responsible for Heisenberg uncertainty and can be thought of as the driving force of the QPT via quantum fluctuations. The quantum nature of such fluctuations is intimately linked to the essence of quantum mechanics manifested in the double-slit experiment. Here the probabilistic description comes in as a fundamental feature of nature itself. This is in sharp contrast with the thermal fluctuations responsible for thermal transitions, ultimately stemming from the probabilistic description of macroscopic systems due to "lack of information". The latter description becomes exact only in the thermodynamic limit, enabling non-analyticities in free energy, necessary for phase transitions. In contrast, quantum phase transitions that occur at zero temperature do not require the thermodynamic limit. Comparison of this aspect of thermal transitions to quantum phase transitions reveals one of its distinct features.

- **Remark 1:** The quantum nature of a phase transition does not arise solely from building a statistical theory of quantum degrees of freedom. For instance, manifestly quantum degrees of freedom such as spin-1/2 arranged in a hyper-cubic lattice with a longitudinal magnetic field are described by the Ising model and display perfectly a thermal phase transition. Meanwhile, if we add a transverse magnetic field, the system starts to exhibit a quantum phase transition due to non-commutativity in the spin components.

- **Remark 2:** Similar to regular thermal phase transitions, zero-temperature phase transitions may be classified as either first-order or continuous. Zero temperature forces the system to stay in the ground state so the quantum transition is associated with a transition between different ground states. The difference between the first order and continuous zero-temperature phase transitions has to do with how the rearrangement of the ground state occurs. A sudden jump between the ground states is associated with first order transitions whereas quantum fluctuations are associated with continuous phase transitions. [2]

To put these considerations on a firmer footing consider the aforementioned Ising model with transverse magnetic field:

$$\mathcal{H} = -J\sum_i S_i^z S_{i+1}^z - h\sum_i S_i^x = \mathcal{H}_0 + \mathcal{H}_1 \tag{1}$$

where S_i^z and S_i^x are spin components, J the coupling constant that describes nearest neighbor spin interaction, and h the transverse magnetic field. The statistical information about the model is encoded in its partition function $Z = Tr\{e^{-\beta\mathcal{H}}\}$, which can be rewritten as:

$$Z = \lim_{\delta\tau\to 0}(1-\delta\tau\mathcal{H})^{\beta/\delta\tau} = \lim_{\delta\tau\to 0}\prod_i(1+h\delta\tau S_i^z)e^{K\sum_i S_i^z S_{i+1}^z} = Tr\Big\{e^{-\mathcal{H}_0}T\{e^{-\int_0^\beta \mathcal{H}_1(\tau)d\tau}\}\Big\} \tag{2}$$

where $\mathcal{H}_1(\tau) = e^{\tau\mathcal{H}_0}\mathcal{H}_1 e^{-\tau\mathcal{H}_0}$. It is precisely the non-commutativity of $\mathcal{H}_0$ and $\mathcal{H}_1$ that forces us to introduce the imaginary-time ordering operator T that generates "dynamics" in quantum phase transitions. It turns out that the inextricable nature of "statics" and "dynamics" constitutes another feature of quantum phase transitions.

3 The Paramagnet to Ferromagnet Phase Transition in Metals

- **Goal:** *Provide an arena for theoretical and experimental investigation of quantum critical phenomena.*

For concreteness we will describe a QPT supported by a the Hubbard model, following Hertz [3] and Mills [4], with Hamiltonian

$$\mathcal{H} = -t\sum_{i,j} c_i^\dagger c_j + U\sum_i n_{i\uparrow}n_{i\downarrow} = \mathcal{H}_0 + \mathcal{H}_1 \tag{3}$$

where $\mathcal{H}_0$ represents hopping between the nearest neighbor sites and $\mathcal{H}_1$ stands for the on-site repulsive interaction. Such a Hamiltonian describes a non-interacting electron gas perturbed by local repulsive repulsion. Since we will be interested in a magnetic transition, it is convenient to separate the interaction term into charge- and spin-dependent parts:

$$\mathcal{H} = \mathcal{H}_0 + \frac{U}{4}\sum_i (n_{i\uparrow} + n_{i\downarrow})^2 - \frac{U}{4}\sum_i (n_{i\uparrow} - n_{i\downarrow})^2 \tag{4}$$

Since we expect charge density to be irrelevant at the magnetic transition, we will neglect the charge density part and focus on the spin density. We can write down a partition function for this model analogous to Eq. 2:

$$Z = Tr\Big\{e^{-\mathcal{H}_0} T\{e^{-\int_0^\beta \mathcal{H}_1(\tau)d\tau}\}\Big\} = Z_0 \Big\langle T\{e^{-\int_0^\beta \mathcal{H}_1(\tau)d\tau}\}\Big\rangle_0 \tag{5}$$

and use the Hubbard-Stratonovich transformation:

$$e^{\frac{a^2}{2}} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-\frac{x^2}{2} - ax} dx \tag{6}$$

to turn the quartic term into quadratic at the cost of introducing a new variable:

$$Z = Z_0 \int D\psi \; e^{-\frac{1}{2}\int_0^\beta \sum_i \psi_i(\tau)^2 d\tau} \Bigg\langle T\Big\{exp\Big(- \sum_{i\sigma}\int_0^\beta \sigma V_i(\tau) n_{i\sigma}(\tau)d\tau\Big)\Big\}\Bigg\rangle_0 \tag{7}$$

where $V_i(\tau) = \sqrt{\frac{U}{2}}\psi_i$. It is important to mention how we have introduced the field ψ, since it serves as an order parameter of the transition, representing local magnetisation field. The expectation value in Eq. 7 can be expressed in terms of non-interacting electron Green's function $G^0_{ij}(\tau\tau')$ leaving us with the expression for Z solely in terms of the order parameter ψ:

$$Z = Z_0 \int D\psi \; e^{-\frac{1}{2}\int_0^\beta d\tau \left(\sum_i \psi_i(\tau)^2 + \sum_\sigma Tr\left\{ln(1-\sigma V G^0)\right\}\right)} \tag{8}$$

where $V_{ij}(\tau,\tau') = V_i(\tau)\delta_{ij}\delta(\tau,\tau')$. Finally, we move to the frequency domain both in space and imaginary time and keep only the quadratic and quartic terms of the ln expansion, which nevertheless capture all the essential physics:

$$Z = Z_0 \int D\;\psi e^{-\frac{1}{\beta}\Phi[\psi]}$$

$$\Phi[\psi] = -\frac{1}{2}\sum_{q\omega}\Big(\delta + |q|^2 + \frac{|\omega|}{\Gamma q}\Big)|\psi|^2 + \frac{u}{4}\sum_{q_i\omega_i}\psi(q_1,\omega_1)\psi(q_2,\omega_2)\psi(q_3,\omega_3)\psi(q_4,\omega_4) \tag{9}$$

This expression Eq. 9 for the partition function in terms of magnetization will serve as a starting point for our discussion of the QCP. Note that the scalar form of the order parameter can be easily generalized to vectorial form, but this does not result in new physics.

4 Quantum Criticality

- **Goal 1:** *Analyze the behavior of the the model presented in the previous section near the the QCP using the RG approach in momentum space.*

- **Goal 2:** *Explore some of the differences between quantum critical and thermal critical behavior.*

To understand the quantum critical behavior we can use the renormalization group approach, in particular its momentum space implementation. The momentum integration cut-off is naturally given by lattice spacing a: $\Lambda = 1/a$. We will not describe here the whole procedure of renormalization, but rather state the results and discuss their significance for the topic at hand. However, several remarks are in order before we do so. First, it is important to note that the scaling of the Matsubara frequencies, or equivalently scaling of imaginary time τ, is intertwined with momentum scaling. The way how they are intertwined depends on the actual details of the system and are summarized by *dynamical exponent* z defined through the scaling relations

$$\tau' = b^z \tau \ , \ r' = br \ , \ q' = q/b \tag{10}$$

The dynamical exponent modifies the well known relations between critical exponents by means of introducing a "correction" to the *effective dimensionality* of the system:

$$d_{eff} = d + z \tag{11}$$

For instance, the hyperscaling law becomes:

$$2 - \alpha = \nu d_{eff} = \nu(d + z) \tag{12}$$

Such "correction" is not accidental. It is a reflection of the fact that the quantum mechanical phase transition may be treated as a classical one with effective dimensionality. Having stressed the special role of the dynamical exponent, it goes without saying that integration over the fast modes happens not only in the momentum space, but also over the Matsubara frequencies. Furthermore, it turns out that integrating out momentum and Matsuabra frequency results in a fairly complicated recursion relations. Much simpler relations are obtained if we treat the frequency cut-off as momentum-dependent:

$$\frac{\Lambda^2}{b^2} < \frac{\omega^2}{q} + q^2 < \Lambda^2 \tag{13}$$

as illustrated by the Fig. 1. To study the QCP we first look at the behavior of the model at $T = 0$. In this case the corresponding classical theory acquires an infinite extent in the imaginary-time direction and Matsubara frequency becomes a continuous variable. The recursion relations in this limit are:

$$\frac{d\delta(b)}{d(lnb)} = 2\delta(b) + \frac{3K(d)u(b)}{\delta + 1} \tag{14}$$

$$\frac{du(b)}{d(lnb)} = (4 - d - z)u(b) - \frac{9K(d)u^2}{(\delta + 1)^2} \tag{15}$$

where $K(d)$ is only a function of dimensionality. These equations have two fixed points: (1) Gaussian fixed point at $u = 0$ and $\delta = 0$, and (2) non-trivial fixed point. Above the upper critical dimension $d_u = 4 < d + z$, quantum criticality is thus defined by the Gaussian exponents with interaction being an irrelevant variable.

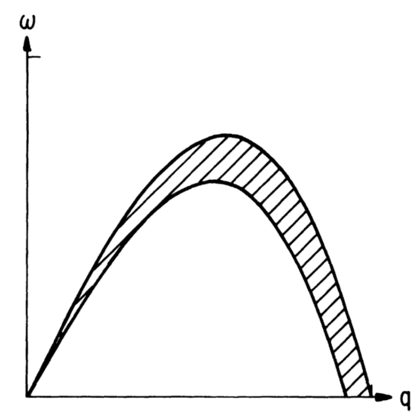

Figure 1: Shaded region depicts the fast modes simultaneously integrated out in the renormalization group analysis of the system near quantum critical point.

Extending our analysis to the finite temperature focusing again on the case $d_{eff} > 4$ we look at the recursion relations for the temperature T, control parameter δ and the interaction coupling constant u:

$$\frac{dT(b)}{dlnb} = zT(b) \tag{16}$$

$$\frac{d\delta(b)}{dlnb} = 2\delta(b) + 12u(b)f^{(2)}[T(b)] \tag{17}$$

$$\frac{du(b)}{dlnb} = (4 - d - z)u(b) \tag{18}$$

with $f^{(2)}$ being a dimensionless function of temperature. As a first step in our analysis of this recursion relations I would like to note that they simplify to a ϕ^4 theory in the high temperature limit. However, in the low temperature limit the critical behavior is influenced by the quantum fluctuations, which we expect to greatly modify the behavior of the system. As we mentioned before, the relevant unstable fixed point is Gaussian so the small u approximation is appropriate. Solving the recursion relations in this approximation results in the expression for the critical temperature as a function of δ and u:

$$T_c = \Big(\frac{\delta_c - \delta}{(B + C)u}\Big)^{\frac{z}{d+z-2}} \tag{19}$$

This equation describes a critical line with an ordered phase (ferromagnet) on the low temperature (low interaction) side (Fig. 2). Furthermore, the requirement for the coupling u to remain small under RG iteration results in the Ginzburg criterion:

$$\frac{uT^{(d+z-3)/z}}{\left(\delta_c - \delta + (B+C)uT^{(d+z-2)/z}\right)^{1/2}} \ll 1 \tag{20}$$

that defines the region on the phase diagram (between dotted lines on Fig. 2) within which the critical behavior is defined by critical fluctuations.

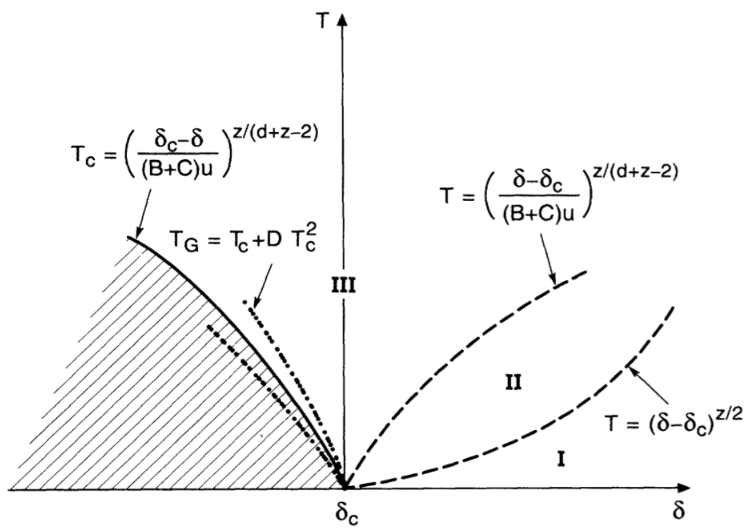

Figure 2: Phase diagram around the quantum critical point for the metallic paramagnet-ferromagnet transition.

There is another piece of phenomenology that may be derived from the recursion relations Eq.(16,17,18) by analyzing the neighborhood of the QCP. To stay within scaling regime we need to require $\delta(b) < 1$. Depending on the interplay of the scaling of T and u, we may recognize several regimes of scaling that correspond to regions I, II, and III in Fig. 2. The region I corresponds to the quantum disordered phase ($T \ll 1$) where thermal fluctuations are negligible and the scaling is defined by the $T = 0$ fixed point. The regions II and III are characterized by $T \gg 1$, but differ in the scaling of u. While the region III is Gaussian classical (interaction stays small), in the region II the non-Gaussian fluctuations may have a significant contribution (u grows to be ~ 1).

5 Heavy Fermions

To provide an example of quantum critical behavior in nature, we will consider the topic of heavy fermionic materials. Before we discuss the influence of QCP on their behavior, I will provide a brief summary of features of these materials relevant to our discussion. Structurally, heavy fermionic materials are compounds that contain metallic elements with partially filled f-shells, which results in partially filled f-bands. The electrons in f-shells partially behave as localized magnetic moments and partially itinerant. This behavior may considered as a source of rich physics, and will be further formalized below. There are several competing points of view on the microscopic behavior of heavy fermionic materials [5] and we will choose here the one that most simply illustrates the point. The Hamiltonian that describes the aforementioned behavior is:

$$\mathcal{H} = \sum_{q,\sigma} \epsilon_q c^\dagger_{q\sigma} c_{q\sigma} + J \sum_{i \neq j} S_i \sigma_j \ , \ \sigma_j = \sum_{\sigma} \sigma c^\dagger_{j\sigma} c_{j\sigma} \tag{21}$$

where ϵ describes the conduction band and the second term provides coupling between conduction electrons and localized f-electron magnetic moments (S_i) (Fermi-liquid coupled to spin-density). This Hamiltonian describes the essential physics of competing RKKY interaction, which favors a magnetic ground state, and the Kondo effect, producing local magnetic moments. Thus the system can sustain multiple ground states due to competition of the terms, which as we explained in the Section 1 is the prerequisite for quantum critical behavior. In our discussion we will be concerned with the (paramagnetic) Fermi liquid state and anti-ferromagnetic state (Fig. 3).

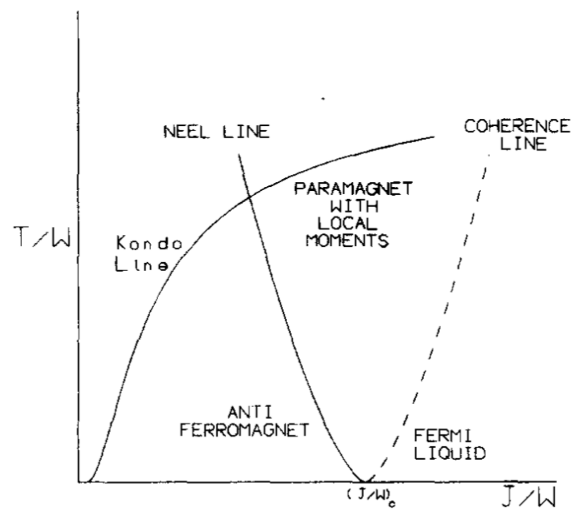

Figure 3: Phase diagram of the heavy fermionic material in the coordinates of temperature and coupling strength, both normalized by the bandwidth of the conduction band.

- **Remark:** Although the RG analysis in the previous section was performed for the ferromagnetic interaction, most of the results can be translated on the ferromagnetic case (relevant in the context of heavy fermionic materials) with slight changes, for instance in the dynamic exponent.

It is also worthwhile to note that the unusual properties of the heavy-fermion state is what spawned its name. In particular, the interaction renormalizes the electronic mass up to 1000 times. One could say that the electrons start to move very slowly due to great amount of scattering that they experience.

- **Goal:** *Demonstrate universal behavior in a range of heavy fermionic materials associated with proximity to QCP by studying its scaling behavior.*

Much insight into the scaling behavior of some heavy fermionic materials can be obtained by assuming that they are near the QCP. The relevant degrees of freedom are magnetic excitations, since the system is near the magnetic instability. The picture that we need to keep in our head is the following. At zero temperature when $J/W < (J/W)_C$, the RKKY interaction prevails producing anti-ferromagnetic state. In contrast, when $J/W > (J/W)_C$ the Kondo effect is dominant and the system prefers the non-magnetic state. We can thus use $g = (J/W) - (J/W)_C$ as a measure of proximity to the QCP. This continuous transition extends into finite temperature and represented by Neel Line on Fig. 3. The experimental probe that we will describe approaches the QCP from the non-magnetic (Fermi-liquid) side utilizing the dependence of the J/W on pressure [6].

Consider a physical parameter X that scales near the QCP with pressure P as:

$$X(P) = A|(V(P) - V_c)/V_c|^{-x}$$

Now we introduce the reference pressure P_0 and assume that the change of volume $\Delta V = V - V_0$ caused by the change of pressure $\Delta P = P - P_0$ is small. Then we can arrive at the semi-logarithmic dependence:

$$ln\Big(\frac{X(P)}{X(P_0)}\Big) = x\frac{\kappa_0 V_0}{V_0 - V_c}\Delta P \ , \ \kappa_0 = -\frac{1}{V}\frac{\partial V}{\partial P} \tag{22}$$

Note that such critical behavior can be tested experimentally and indeed has been verified for several different heavy-fermionic materials (Fig. 4, [6]). We observe the data collapse on one line for each separate material, which implies the relation between the critical exponents:

$$2 - \alpha = \nu z \tag{23}$$

There are several conclusions that we can draw from this. First of all, we note that there is an apparent violation of the hypersaling relation. This phenomenon may be interpreted as a result of localization $d = 0$ (analogous to single impurity problem). But more importantly the data demonstrates the universality in scaling relations for this class of materials, which can be attributed to the presence of quantum phase transition between anti-ferromagnetic and Kondo states. Such universality is one of the many experimental hints on the universal state of matter - *quantum critical matter*[7], which analogously to the classical critical state is oblivious to the microscopic details of the system.

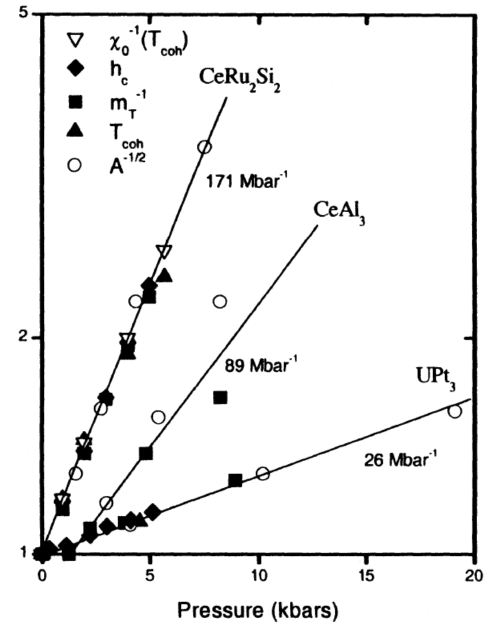

Figure 4: Semi-logarithmic plot of thermal mass $m_T \sim |g|^{2-\alpha-2\nu z}$, susceptibility $\chi \sim |g|^{2-\alpha-2\phi_h}$, coherence temperature $T_{coh} \sim |g|^{\nu z}$, pseudo-magnetic field $h_c \sim |g|^{\phi_z}$ and T^2 term of resistivity as a function of pressure.

6 Conclusion

In this term paper we discussed only one example of a quantum critical point and how it influences the behavior of real materials. Since the original work in the '70s by Hertz, Young, et al., research in this area has grown to be a vast field of investigation. Just like many other subjects in condensed matter physics, it enjoys the luxury of simultaneous developments on both fronts of experiment and theory. Our understanding of quantum phase transitions has expanded greatly, and many connections to other areas of research have been made. Among these are entanglement in many-body systems, topological order, and fractionalization. Meanwhile, quantum phase transitions have been observed in many new real systems, ranging from engineered ones such as quantum dots, cold atomic traps, and 2D electron gases to neutron stars and quark gluon plasmas. However, despite many achievements in the field of quantum phase transitions, it remains at the forefront of research in physics and in the focus of many lively debates.

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