Quantum Phase Transitions and Correlated Electrons

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Abstract

This article is aimed at a pedagogical introduction to the physics of quantum phase transitions that is unique to metallic systems. It has been recognized for some time that quantum criticality can result in a breakdown of Landau’s Fermi liquid theory. Its converse, however, has not been appreciated until very recently: non-Fermi liquid behavior can in turn lead to new classes of quantum phase transition. A concrete example is provided by “local quantum critical points”. I summarize the theoretical reasoning and experimental evidence for local quantum criticality, in the context of heavy fermion metals. The underlying physics is likely to be relevant to other correlated electron systems including doped Mott insulators.
It would seem hopeless to describe the physics of $10^{22}$ or so electrons which are strongly interacting with each other. Yet, for a long time, a remarkably simple theory was considered to be the definite solution. First formulated almost half a century ago, Landau’s Fermi liquid theory was successfully applied not only to simple metals but also to a number of systems in which interaction effects are very strong. For instance, it appears to work even for systems with an effective electron mass that is a few hundreds of the corresponding band-structure value. Over the past decade or so, however, a long list of materials have emerged in which the Fermi liquid description apparently fails. In addition to high temperature superconductors, examples in this category include the $f$-electron-based heavy fermion metals, $d$-electron-based transition-metal compounds (beyond the cuprate oxides), and quasi-one-dimensional materials such as single-walled carbon nanotubes and semiconductor quantum wires. The basic question we are confronted with is when and how electron-electron interactions lead to a breakdown of the Fermi liquid theory.

A number of mechanisms for non-Fermi liquid behavior are currently being pursued. Here we are concerned with one of these, namely proximity to a quantum critical point. In the remainder of this pedagogy-minded article, I will i) briefly introduce quantum phase transitions in correlated electrons and its links to non-Fermi liquid phenomena, ii) summarize some recent progresses in this area, with an emphasis on the notion of local quantum critical points and iii) comment on some broader implications of these results. For further readings, I refer the readers to the following books and articles: Ref. 1 for a recent review on quantum phase transitions in general; Refs. 2–6 for quantum critical points in correlated electrons; Refs. 7, 8 for Fermi liquid theory; Refs. 9, 10 for local moment formation and Kondo effects; Refs. 11–17 for experiments in quantum critical heavy fermions and Refs. 2, 18, which serve as points of departure towards a large literature arguing for quantum criticality in high temperature cuprate superconductors. A recent review (ref. 19) discusses similar issues at a more technical level and contains more references to original works.
I. QUANTUM CRITICALITY MEETS NON-FERMI LIQUIDS

A. Fermi liquid theory and its breakdown

The basic ingredient of the Fermi liquid theory is that the elementary excitations of an interacting many-electron system are quasiparticles. These quasiparticles are sufficiently long-lived at low energies, and have the same intrinsic quantum numbers as a bare electron (spin $\frac{1}{2}$ and charge $\pm e$, with $-e$ for quasiholes – see below).

The meaning of an elementary excitation can be best illustrated by considering a system of $N$ (of the order of $10^{22}$) non-interacting electrons in a periodic potential. The quantum mechanical eigenstates of such an ideal electron system can be specified in terms of those for a single electron in the same periodic potential. The latter, as explained in any elementary solid state textbook, are Bloch states that are characterized by a “crystal wavevector” $k$ and a band index. These parameters specify the bandstructure as illustrated in Fig. 1. The intrinsic quantum numbers of these Bloch states remain charge $e$ and spin $\pm \frac{\hbar}{2}$. The eigenstates of the $N$-ideal-electron system are simply Slater determinants of the Bloch states. The many-body ground state is the Slater determinant of $N$ lowest-energy Bloch states; this is the filled Fermi sea shown in Fig. 1. The many-body excited states can be constructed by moving $m$ ($< N$) electrons from Bloch states in the Fermi sea to those above the Fermi energy. Pictorially, an excited state wavefunction can be constructed by digging $m$ “holes” (an empty circle in Fig. 1 below the Fermi energy) and adding $m$ “particles” (filled dots in Fig. 1 above the Fermi energy). Each “particle” or “hole” is then an elementary excitation. It is obvious from this construction that our elementary excitations have charge $\pm e$ and spin $\pm \frac{\hbar}{2}$. 
FIG. 1. Elementary excitations of a non-interacting electron system. The horizontal dashed line marks the Fermi energy and the vertical dashed lines specify the boundaries of the first Brillouin zone along a particular direction in the wavevector space. For illustrative purposes, only one energy band in the vicinity of the Fermi energy is shown.

Real electrons in solids of course do interact with each other. Once these interactions are included, the many-body spectrum becomes hard to construct exactly (except for simplified models in one spatial dimension). The assumption of the Fermi liquid theory is that, the low-lying many-body excited states can still be constructed from the many-body ground state by simply adding quasiparticles and quasiholes. Compared to the dots and holes of Fig. 1, a quasiparticle is much more complex. It can be pictured as a bare electron with a polarization cloud attached. Nonetheless, in many ways a quasiparticle/quasihole behaves just like a bare electron/hole in a non-interacting electron system: it has charge $\pm e$ and spin $\pm \frac{1}{2}$, and it obeys Fermi statistics. The lower the energy, the more precise this construction is, as reflected in the quasiparticle lifetime that goes to infinity as the wavevector approaches the Fermi surface.
These phenomenological statements can be proven by treating the electron-electron interactions perturbatively, to infinite orders. (Unless special bandstructure effects such as nesting come into play, the only perturbative instability occurs when the effective interaction in some pairing channel is attractive; the resulting state is the celebrated, and well-understood, BCS superconductor.) In this sense, the Fermi liquid theory is internally consistent when the interactions are not too strong.

But how strong is too strong? The answer to this question is a priori unknown.

**B. Quantum phase transitions**

Just like ice melts as the thermal fluctuations are increased with increasing temperature, an ordered state (such as an antiferromagnet) at zero temperature can become disordered as the zero-point motion is tuned. The latter can be achieved through varying an external parameter such as pressure. The vanishing of the order parameter characterizes a quantum phase transition. For definiteness and also with the heavy fermion metals in mind, we will take the ordered state to be an antiferromagnetic metal; the corresponding order parameter is the staggered magnetization. With appropriate modifications, the discussions below would apply to other types of ordered states. There are also quantum phase transitions for which neither of the phases has an obvious order parameter, as exemplified by the metal-insulator transitions in disordered interacting electron systems; we will not consider such situations here.

A quantum critical point arises when the zero-temperature transition is continuous. Here, the order parameter fluctuations are critical. In the magnetic case, the spin susceptibility diverges in the limit of zero frequency and zero temperature and as the wavevector approaches the ordering wavevector.
C. The connection between a quantum critical point and non-Fermi liquid

Quantum critical points are especially complex in correlated electron systems. Besides the order parameter fluctuations, we also have to deal with the electronic excitations near the Fermi energy. A key observation, known since the original work of John Hertz, is that the effective interactions between the electrons can be infinite due to the divergence of the order parameter susceptibility. Such a divergence invalidates the aforementioned condition of internal consistency for the Fermi liquid theory, opening the door to a non-Fermi liquid critical state.

The effective electron-electron interactions become finite away from the quantum critical point. In principle, Fermi liquid theory may break down before the onset of magnetic order. For the systems under discussion, it is generally believed theoretically and supported experimentally that the system remains a Fermi liquid on the paramagnetic side and turns into a non-Fermi liquid only at the quantum critical point. In other words, the emergence of non-Fermi liquid behavior coincides with the onset of magnetic ordering.

Such a linkage between quantum critical points and non-Fermi liquids has two important sides to it. On the one hand, it already says that quantum criticality provides a mechanism for non-Fermi liquid behavior. Experimentally, the situation is especially clear-cut in heavy fermion metals. In the quantum critical regime, the electrical resistivity is linear (or close to being linear) in temperature; the specific heat divided by temperature either diverges as temperature goes to zero or at least has a non-analytic dependence on temperature. Away from the quantum critical regime, both the electrical resistivity and specific heat coefficient recover the Fermi liquid form ($T^2$ and constant, respectively).

On the other hand, the fact that the Fermi liquid - non-Fermi liquid transition coincides with the magnetic phase transition raises a more drastic possibility: the non-Fermi liquid physics can in turn change the universality class of the quantum phase transition itself. This converse effect has not been discussed until recently.
II. GAUSSIAN QUANTUM CRITICAL METALS

To appreciate how non-Fermi liquid behavior can modify the quantum critical physics, we first outline the standard theory of metallic quantum critical points. This picture was introduced in the modern form by John Hertz in 1975. It can be traced back even further, to the literature on paramagnons in the 1960’s; the field theoretical formulation most commonly used today is referred to as the Hertz-Millis theory. In spite of its non-Fermi liquid nature, the electronic states are not considered as a part of the critical theory; instead, they are treated as bystanders. The only critical modes are the long-wavelength fluctuations of the magnetic order parameter - the paramagnons. The critical theory describes the non-linear couplings of such paramagnons, and assumes the form of the standard “$\phi^4$” theory with an effective dimensionality of $d_{eff} = d + z$. The effective dimensionality is raised from the spatial dimension $d$ by $z$, the dynamic exponent, reflecting the mixing of statics and quantum dynamics. The primary effect of the bystanding electrons is to provide extra channels for the critical spin fluctuations to decay into, leading to an over-damped situation: the spin-damping term is the strongest term in the frequency dependence. This makes the dynamic exponent $z$ larger than one – $z = 2$ for the antiferromagnetic case. As a result, in three or two spatial dimensions $d_{eff}$ is larger than or equal to 4, the upper critical dimension of the $\phi^4$ theory. The critical theory is then Gaussian, and physical properties are expected to have a very simple mean-field behavior. For instance, the dynamical spin susceptibility is expected to be linearly dependent on the frequency $\omega$.

Can the non-Fermi liquid electronic excitations really be taken as bystanders? And would such electronic excitations directly participate in the critical theory leading to a breakdown of the Gaussian picture? These turned out to be not just academic questions. The past few years has witnessed a systematic experimental test of the Gaussian picture. The experiments have become possible because quantum critical points have been explicitly identified in a number of heavy fermion metals, including YbRh$_2$Si$_2$, CeCu$_{6-y}$Au$_y$, CePd$_2$Si$_2$ and CeIn$_3$. Inelastic neutron scattering experiments, particularly those of Almut Schröder and co-workers, have raised the most striking puzzles:
• The frequency and temperature dependences of the dynamical spin susceptibility display an anomalous exponent, $\alpha < 1$, as well as $\omega/T$ scaling. The critical theory cannot be Gaussian.

• The same anomalous exponent $\alpha$ is seen essentially everywhere in the wavevector space, suggesting new local physics.

The non-Gaussian and local nature calls for new critical physics beyond the paramagnons.

III. LOCAL QUANTUM CRITICAL METALS

To address the interplay between the onset of magnetic ordering and the development of non-Fermi liquid behavior, we have to go into some microscopics about the electronic excitations. Our focus is on the heavy fermion metals, though the discussion may be extended to other strongly correlated electron systems as well. The name “heavy fermions” itself refers to the fact that materials containing partially-filled $f$-orbitals often behave as though the electrons have a very heavy mass (typically a few hundred times of the value given by bandstructure calculations).

On the paramagnetic side, the formation of a heavy Fermi liquid – and the associated heavy quasiparticles – is an intricate many-body process. A microscopic Hamiltonian, appropriate for heavy fermions at low energies (typically 100 K and below) is the Kondo lattice model: a lattice of spin-$\frac{1}{2}$ local magnetic moments, which are only weakly coupled to a separate conduction electron band. (There are seven $f$-orbitals, but at the energy scale of interest we can focus on only one of them – the lowest Kramers doublet.) The formation of local magnetic moments itself is the result of very strong Coulomb interactions between two electrons occupying the same $f$-orbital. Double occupancy of an $f$-orbital is excluded as a result of a microscopic Coulomb blockade. The empty orbital is also unfavorable when the $f$-orbital is a deep level (i.e. its energy is much lower than the chemical potential). Only spins are left as the low-lying degrees of freedom, as illustrated in Fig. 2.
The electronic excitations of a heavy Fermi liquid are composed of Kondo resonances. The notion of Kondo resonance is most clearly understood in the case of a single-impurity Kondo problem. The Kondo resonance appears in the $f$-electron spectral function as a peak in the vicinity of the Fermi energy. The width of this peak is of the order of $kT_K^0 \sim k\rho_0^{-1} e^{-1/\rho_0 J}$, where $\rho_0$ is the conduction electron density of states at the Fermi energy and $J$ the antiferromagnetic Kondo exchange coupling between the magnetic moment and spin of the conduction electrons. The center of the peak is in the vicinity of the Fermi energy, with a separation that is smaller than $kT_K^0$.

The key to the existence of a Kondo resonance is the singlet nature of the ground state. This can already be seen in a simple atomic Kondo problem. Consider a spin-$\frac{1}{2}$ local moment (call it $S$) coupled to a single conduction electron orbital (call it $a$), as specified by the Hamiltonian:

\[ H = -J_S a \cdot S. \]
\[
H = JS \cdot \sum_{\sigma, \sigma'} a_\sigma^\dagger \vec{\tau}_{\sigma, \sigma'} a_{\sigma'} + \epsilon_a \sum_{\sigma} a_\sigma^\dagger a_\sigma,
\]

where \(\vec{\tau}\) represents the Pauli matrices. Such a Kondo Hamiltonian arises by projecting the Hilbert space of the impurity \(f\)-orbital to the low-energy local-moment subspace as already shown in Fig. 2. This projected atomic problem has a reduced Hilbert space, of eight dimensions. For our illustrative purpose, it suffices to consider the case \(\epsilon_a = 0\). (The Kondo lattice model we will be considering is particle-hole asymmetric; but this distinction is unimportant at the moment.) The ground state is a singlet:

\[
|0\rangle = \frac{1}{\sqrt{2}}(|\uparrow_f\rangle |\downarrow_a\rangle - |\downarrow_f\rangle |\uparrow_a\rangle)
\]

The ket with a subscript \(f\) (a) acts in the local-moment (conduction electron) space. The first low-lying exited states are two doublets,

\[
|\sigma >_1 = |\sigma >_f |0 >_a \\
|\sigma >_2 = |\sigma >_f |2 >_a
\]

To determine the \(f\)-electron spectral function, we need to know the form of the \(f\)-electron operator in the projected local-moment subspace (again, c.f. Fig. 2). A relatively straightforward calculation (through the same Shrieffer-Wolff canonical transformation that leads to the Kondo Hamiltonian Eq. 1) shows that this projected operator reads

\[
F_\sigma = -\sqrt{\frac{2J}{U}}[\sigma S_z a_\sigma + (S_x - \sigma i S_y)a_{-\sigma}]
\]

The parameter \(U\) is the original on-site Coulomb interaction between two \(f\)-electrons; this parameter also characterizes the spacing between the singly-occupied and doubly occupied levels shown in Fig. 2. It is easily seen that \(F_\sigma|0\rangle = \sigma \frac{3}{2} \sqrt{\frac{J}{U}}|\sigma >_1 \) and \(F_\sigma^\dagger|0\rangle = \frac{3}{2} \sqrt{\frac{J}{U}}|\sigma >_2\).

This finite matrix element of the \(f\)-electron creation/annihilation operator between the singlet ground state and the first excited doublets establishes the existence of a small amount of the \(f\)-electron spectral weight at low energy, of order \(J\) as opposed to \(U\). This excitation is precisely the Kondo resonance as manifested in this atomic model; when we go beyond the atomic limit, the scale \(J\) turns into the Kondo scale \(T_K^0\). Such low-lying excitations would be absent if the ground state were not a singlet.
B. Destruction of the Kondo resonance

On the paramagnetic side, every local moment is fully screened. The ground state is a global singlet. Each local moment would contribute one Kondo resonance, as inferred from the discussion of the previous subsection. Since they have the quantum numbers of an electron, these Kondo resonances would combine with the conduction electron band. The result is a heavy quasiparticle band, with a “large” Fermi surface: the volume that the Fermi surface encloses counts the number of both the local moments and conduction electrons.

The necessary condition for the Kondo resonances to form is that the local moments are fully screened by the spins of the conduction electrons, as we saw in the previous subsection. This condition is equivalent to saying that the local spin susceptibility must have a Pauli form. In other words, the zero-temperature and zero-frequency limit of the local spin autocorrelation function must be finite.

Can this local spin susceptibility remain finite as the system approaches the magnetic quantum critical point? To address this question, we note that in a translationally-invariant system the local spin susceptibility is equal to the average of the wavevector-dependent dynamical spin susceptibility $\chi(q, \omega, T)$. Now, at an antiferromagnetic QCP, by construction the peak susceptibility $\chi(Q, \omega, T)$ is divergent (where $Q$ is the antiferromagnetic ordering wavevector). When the peak susceptibility diverges, the average susceptibility can either stay finite or become divergent as well. If the average susceptibility is finite, then the local Kondo physics proceeds without much modification. On the other hand, a divergent average susceptibility would be incompatible with the expected Pauli form of the local spin susceptibility of a fully developed Kondo state.

This consideration already raises the possibility of two classes of quantum critical metals. For the more exotic type, the local spin susceptibility is divergent and fully developed Kondo resonances are absent at the quantum critical point. The heavy fermion physics then becomes a part of the critical theory. This is a concrete example in which the emergence of non-Fermi liquid must be treated on an equal footing with the onset of magnetic ordering: fermions cannot simply be taken as innocent bystanders.
C. Local quantum critical points

Since the Kondo effect and Kondo resonance formation are largely spatially local phenomena, we have treated the interplay between the Kondo resonance formation and onset of magnetic ordering within an extended dynamical mean field theory of the Kondo lattice model. The more exotic type of quantum critical behavior arises when the magnetic fluctuations are two-dimensional. The schematic phase diagram is shown in Fig. 3. The vanishing of the energy scale $E^*_{loc}$ at the QCP signals the destruction of Kondo resonances in the quantum critical regime: the local susceptibility is Pauli only below $E^*_{loc}$. If the magnetic fluctuations are three dimensional, and if there is no magnetic frustration, then $E^*_{loc}$ would be finite at the QCP corresponding to a crossover scale towards the eventual Gaussian behavior.

In the quantum-critical regime, the local susceptibility is neither Pauli nor Curie (the Curie behavior is recovered only above some cut-off scale $T^0$). It diverges logarithmically,

FIG. 3. Local quantum critical point. Here $\delta$ is a tuning parameter.
\[ \chi_{\text{loc}}(\omega) = \frac{1}{2\Lambda} \ln \frac{\Lambda}{-i\omega} \]  

where \( \Lambda \approx T^0_K \). One can also introduce a “spin self-energy”, which captures the spin damping. It has the following form,

\[ M(\omega) \approx -I_Q + A (-i\omega)^\alpha \]

Our recent numerical work for a Kondo lattice model with an Ising anisotropy (done in collaboration with D. Grempel) yields a nearly universal value for \( \alpha \) that is close to 0.7.

At finite temperature, the spin self-energy displays an \( \omega/T \) scaling. Both the fractional exponent and \( \omega/T \) scaling reflect the non-Gaussian nature of the fixed point. The corresponding critical theory captures both the spatially-long-ranged fluctuations corresponding to the onset of magnetic ordering, and spatially local fluctuations reflecting the destruction of Kondo resonances. Based on Ginzburg-Landau considerations, we have also argued that the results are robust beyond the extended dynamical mean field theory.

**D. Experiments in heavy fermion metals**

The above analysis leads to a dynamical spin susceptibility with \( \omega/T \) scaling and, for every wavevector, a fractional exponent (\( \alpha < 1 \)). The results are consistent with the inelastic neutron scattering experiments of Schröder and co-workers mentioned earlier.

There is also a prediction that the NMR relaxation rate contains a temperature-independent component. Recent NMR experiments in YbRh\(_2\)Si\(_2\), by Kenji Ishida and co-workers, have provided evidence for this.

Finally, the destruction of the Kondo resonance at the quantum critical point implies that the Fermi surface undergoes a reconstruction at the QCP, from being “large” (enclosing a volume that counts the local moments) to being “small” (counting only the conduction electrons and with a different topology) as the system orders. There are de Haas-van Alphen experiments in heavy fermions by Yoshichika Onuki’s group which are suggestive of such a Fermi-surface reconstruction. Additional evidence is also emerging from the Hall-coefficient measurements of Silke Paschen and co-workers.
IV. SUMMARY AND OUTLOOK

We have emphasized the important role electronic excitations play in the quantum critical phenomena of correlated metallic systems. Due to their non-Fermi liquid nature, these electronic excitations may not simply serve as bystanders as traditionally assumed in the Gaussian quantum critical metal picture. Instead, they can become a part of the critical degrees of freedom. The critical theory is then much richer than the $\phi^4$ theory of paramagnons, opening the door to non-Gaussian quantum critical metals.

Concrete progresses have been made in the context of quantum critical heavy fermions. Here, the electronic excitations are in fact the Kondo resonances. In the local quantum critical picture, these Kondo resonances are part of the critical theory along with the paramagnons: a destruction of the Kondo resonances accompanies an onset of magnetic ordering. The non-Gaussian nature of the critical theory allows fractional exponents and $\omega/T$ scaling. This picture is largely consistent with existing and emerging experiments.

Some aspects of the heavy fermion phenomenology, such as $\omega/T$ scaling, have also been reported in high temperature cuprate superconductors, including in the angle resolved photoemission spectra over a wide range of wavevectors. Microscopically, a common feature between the cuprates and heavy fermions is the strong Coulomb interaction, as manifested through the formation of local magnetic moments in heavy fermions and by the emergence of Mott insulating phase in the cuprates. While quantum critical points in the cuprates have yet to be explicitly identified, it appears hard to understand the scaling aspects of the phenomenology without invoking quantum critical physics. In any event, to the extent that quantum criticality plays a role in the cuprates, the photoemission results would suggest that the non-Fermi liquid electronic spectrum are also a part of the critical theory. As in the locally critical quantum phase transitions, this can in turn make the quantum critical point non-Gaussian.

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