Toptalent Research Proposal
Understanding the Non-Fermi-Liquid Behaviour of MnSi

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1 Introduction

Phase transitions are among the most fascinating phenomena in nature. The transition from a paramagnetic phase to a ferromagnetic one in iron, nickel and cobalt made possible the invention of the compass. Phase transitions come in a wide variety of phenomenologies with no entirely obvious unifying features. In 1965, Landau proposed a unified phenomenological theory of phase transitions [1], introducing the general concept of the order parameter, a thermodynamic parameter that vanishes in one of the two phases separated by the transition and is nonzero in the other. The former is called the disordered phase (without long-range order) and the latter the ordered phase. In the case of a ferromagnet, the order parameter is the magnetization.

The ferromagnet-paramagnet transition is seldomly observed, as the most common ferromagnets lose their magnetic properties only at a Curie temperature far above room temperature. Nevertheless, it is well known that this transition (in the absence of a magnetic field), is second order, or continuous: the magnetization rises continuously from zero as the temperature is lowered below the Curie temperature.

Manganese silicide, one of the most extensively studied transition-metal compounds, crystallizes in a cubic structure that lacks space-inversion symmetry. Its magnetic order is due to itinerant (free) electrons, as is also the case for iron. Strictly speaking, MnSi is a helimagnet, the helical modulation being driven by Dzialoshinski-Moriya chiral interactions. However, since its modulation wavelength of 180 Å is much larger than its lattice constant of only 4.6 Å, MnSi displays ferromagnetic behavior. Interestingly, its Curie temperature is pressure-dependent, decreasing with increasing pressure and actually *vanishing* above a critical pressure p_c of only 14.6 kbar. Thus, by keeping the temperature close to absolute zero and applying pressure, a first order [2] *quantum phase transition* from a helimagnetic to a paramagnetic phase occurs at p_c.

At higher pressures, unusual properties are observed, as depicted in Fig. 1. First, the electri-

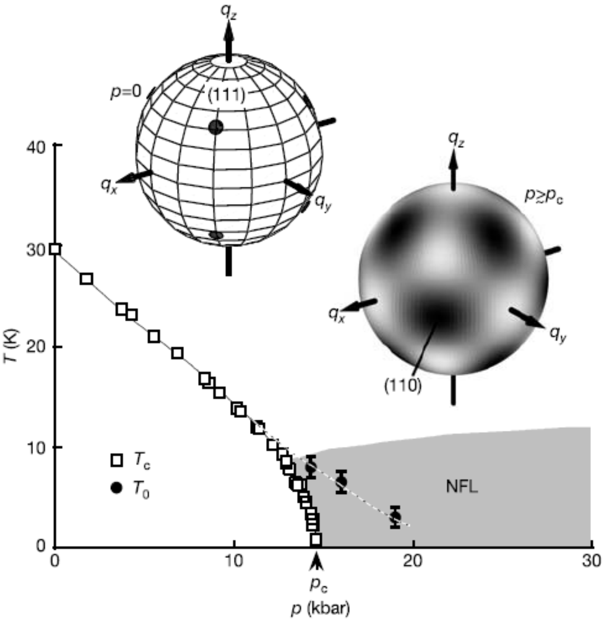

Figure 1: Schematic temperature T versus pressure p phase diagram of MnSi, and qualitative illustration of the scattering intensity characteristic of the magnetic state. The insets show the location and key features of elastic magnetic scattering intensity in reciprocal space at ambient pressure (left) and at high pressure (right). Figure adapted from Ref. [3].

cal resistivity displays an enigmatic $T^{3/2}$ temperature dependence [4]. Landau's Fermi liquid theory [5] – considered to be the "standard model" for metals – predicts a T^2 behavior. Therefore, the high pressure phase of MnSi is generally referred to as a non-Fermi-liquid (NFL). Second, neutron scattering signal is completely changed from the low pressure phase [3]. For temperatures below T_0 (see Fig. 1), enhanced scattering is seen at wave vectors with a length similar to the low pressure phase, but with a different orientation. The intensity is more diffuse over the wave-vector sphere, hence the name "partial order".

Although both of these unusual properties onset at p_c, the NFL persists to pressures far beyond where partial magnetic order is seen. In fact, MnSi is the *only compound* (so far) that shows NFL behavior in such an extended region of the phase diagram, so it recently became a very hot topic in condensed matter physics. The relation between these two puzzles is still unclear, as recent theoretical work has focused almost exclusively on explaining the partially ordered state. Theoretical proposals for the high-pressure state of MnSi have invoked proximity to a quantum multi-critical point [6], magnetic liquid-gas transitions and helical spin crystals reminiscent of the blue phase of liquid crystals [7, 8] and skyrmion-like textures [9]. So far, none of the proposed theories were able to convincingly explain the spectacular NFL behavior of its transport properties.

2 Research questions

A $T^{3/2}$ resistivity is normally observed in spin glasses and amorphous ferromagnets, where it is explained by a diffusive motion of the charge carriers. Most of the theories referred to in Section 1 suggest an explanation of the anomalous resistivity by a very inhomogeneous magnetic state, through comparison with the resistivity of spin glasses. Since the MnSi samples investigated were extremely pure, it was emphasized that this diffusive charge carrier motion would have to be intrinsic (i.e. some kind of spin texture).

The main result of Ref. [4] is that the resistivity in the grey region of Fig. 1 exhibits a temperature dependence of the form $\rho(T) = \rho_0 + AT^{3/2}$ over a wide temperature range. This behavior also extends up to pressures of $3p_c$, and persists in magnetic fields of up to 1 T. All this data points towards the fact that we are dealing with a very stable and extended phase. As stated above, this behavior cannot result from impurity scattering because it is observed in very clean samples. The coefficient A is only weakly dependent on the residual resistivity ρ_0, but it depends on pressure and scales approximately as $1/p$. The "conventional" T^2 form of the resistivity is observed in MnSi only at low temperatures in (i) the helimagnetic state and (ii) the normal state at pressures far above p_c.

Non-Fermi liquid behavior was also observed in other materials [10] (high-temperature superconductors, heavy fermion antiferromagnets etc), but only in the vicinity of the quantum critical point and never in such an extended portion of the phase diagram.

The main research question of my thesis would be to explain the peculiar properties of this novel state of matter. Doing so could contribute towards a better understanding of electron behavior in metallic systems.

3 Approach

It is quite obvious that the disorder experienced by electrons in MnSi can only be caused by intrinsic magnetic fluctuations.

Since MnSi is an *itinerant* magnet, the "local" spins on which electrons scatter are just a mean-field description of the magnetization created by the itinerant electrons. In other words, electrons scatter on the spin background created by themselves! This implies that the magnetic fluctuations and the electron dispersion (and scattering) have to be calculated self-consistently. However, deriving the full self-consistent solution is difficult to achieve in practice, so it seems reasonable to separate the problem into three steps.

As a first step, I propose to model the dynamic magnetic fluctuations by static (frozen) magnetic disorder, which however is temperature-dependent. The description of disorder can be greatly simplified by using Landau theory.

The low temperature behavior of the resistivity is governed by large scale magnetic fluctuations. The system effectively averages over large volumes, rendering the microscopic details of the Hamiltonian unimportant. Therefore, at this stage, I can use a simplified, phenomenological description of frozen disorder. Landau theory provides a convenient way to describe magnetic fluctuations, in terms of a single variable, called the order parameter[1]. This reduced description is significantly simpler than considering the microscopic structure of a spin texture.

The method that allows one to connect the magneto-resistance to magnetic correlations is known [11] and moreover, it was conveniently cast into the form of the memory-function formalism [12]. Thus, knowing the form of the magnetic correlations (they result directly from Landau theory), one can deduce the temperature dependence of the resistivity.

In practice, Landau theory can be tailored to describe various phenomenological models (skyrmions, blue phases, etc). The memory-function formalism will then provide a way to compute the temperature dependence of the resistivity. For instance, for the skyrmion model, one can describe phenomenologically a skyrmion liquid and then see what the properties of this liquid should be (how the density of defects and spin correlations should scale with temperature) in order to reproduce the observed NFL transport properties. More than one model will probably lead to the correct result by fine-tuning, but in most of them this tuning would imply physically unreasonable assumptions. The model that gives the correct behavior of the resistivity *and* is also physically reasonable will be the relevant one.

Secondly, once the correct model is identified, I can then fix the coefficients of the Landau expansion of free energy by numerical Monte Carlo simulations. There are of course symmetry considerations which tell one how many terms there should be in this expansion, but the coefficients in front of these terms are largely unknown. The values of these coefficients are important for *quantitative* comparison to experiment.

The third and final step is a self-consistent microscopical description of the magnetic fluctuations (which are collective excitations) and the single-particle electron excitations. One way to proceed would be to expand on the self-consistent theory of Moriya [13].

4 Innovation

The high-pressure phase of manganese silicide shows a non-Fermi liquid behavior, implying the existence of a novel state of matter.

The main advantage of the approach sketched here is that it could work in the whole NFL region of the phase diagram, unlike previously proposed models.

Furthermore, people have so far only looked at energetically favorable ground states for this NFL phase, but the present proposal also includes a way to model its peculiar transport properties.

[1] In our case, the mean-field magnetization.

Developing such a theory could ultimately lead to a deeper understanding of many-electron systems and especially of their critical behavior.

5 Relevance for science

The itinerant electron helimagnet MnSi presents a novel type of behavior, namely critical behavior in an extended region of the phase diagram, and understanding its origin is a fundamental problem in the field of condensed matter physics. Actually, one of the most exciting topics in this field is understanding novel states of matter and here we clearly have something that defies our conventional wisdom.

The NFL phase of MnSi can also be thought of as a particular case of the formation of liquid-like states in magnetically frustrated systems[2] which do not have any quenched disorder. Furthermore, a long-standing question in the field of condensed matter physics was whether a glassy state could be generated spontaneously in very clean systems.

In a broader sense, the realization of my proposal could also contribute towards understanding glass-like type of order in systems without impurities.

A myriad of quantum critical phenomena recently came under scrutiny and the search is on for new interesting materials.

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