Fermions, criticality and superconductivity

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Chapter 1

Introduction

In the early days of quantum physics, the study of many-body systems was regarded as messy, ugly and undignified. The solution of the Schrödinger equation for the hydrogen atom was the hallmark of modern physics. But trying to generalize this procedure to 10^{23} atoms interacting with each other, as is the case in real materials, seems pointless. A huge number of approximations need to be made before one can arrive at any concrete conclusions. Pauli, himself one of the pioneers of the field, had called the study of many-body systems 'dirt physics'.

Thanks to the hard work of several generations of researchers, including the greatest names of all time, such as Lev Landau, John Bardeen, Ken Wilson, Phil Anderson and Bob Laughlin, it has become clear today that many-body physics, under the name *Condensed Matter Physics* replacing the old one *Solid State Physics*, is indeed governed by deep and simple physical principles, which are different from those governing the individual atoms constituting the system. The symmetry of the macroscopic system can be different from that of the microscopic Hamiltonian. The excitations of the macroscopic system can have different charge, spin and statistics as compared to the constituent microscopic particles. These new principles operating at the macroscopic scale are called *emergent*. The appearance of this theme led Anderson to coin the phrase 'More is Different', emphasizing that the study of many-body physics is as equal and fundamental as, say the study of the elementary particles. Sometimes these new principles are written in terms of the sophisticated and beautiful language of higher mathematics, and the Einstein-Dirac type thinking can lead to fruitful discoveries in many-body physics.

The two most important organizing principles that came out of the several decades' investigation of emergent phenomena are spontaneous symmetry breaking (SSB) and adiabatic continuity. SSB refers to the fact that the symmetry of the ground state is different from the symmetry of space or the Hamiltonian describing the system. This is actually something we meet constantly in our everyday life: our desk does not have the translational and rotational symmetry that the Schrödinger equation describing its atomic degrees of freedom possesses. Nevertheless this principle is extremely powerful: instead of describing the system using 10^{23} variables, which is an impossible task, we can now use only one or a few. These few variables are called order parameters (OP). SSB is a quite universal principle, capturing the physics of diverse phenomena, ranging from simple crystals to various density waves, smectic and nematic ordering, from magnetism to superfluidity and superconductivity, even generation of mass. The order parameters can fluctuate in space and time, and field-theoretical methods can be employed. This has opened the door to a whole new world. Later on gauge fields were incorporated, and very recently even gravitational fields have been used to model condensed matter systems.

The prototype of adiabatic continuity is Landau's theory of Fermi liquids. It describes strongly interacting electron systems, for which naive perturbation theory obviously breaks down. The basic insight is that the low energy and low temperature properties of such systems are governed by Fermi-Dirac statistics. The simplest system that possesses this statistics is the free Fermi gas. One can imagine the following process: start from the non-interacting free Fermi gas, and gradually turn on interactions. As long as the system stays away from any phase transitions, the qualitative behavior of the system does not change. For Fermi liquids at low temperature, the specific heat has a linear temperature dependence, the resistivity is quadratic and the spin susceptibility nearly constant, as is the case for free Fermi gas. The main focus here are the excitations. Let us think about the energy levels of the system during this process. There is a shift in each energy level, but they do not cross each other. In other words, the labeling of the energy levels does not change. In this framework, such strongly interacting many-body systems can again be characterized by a rather small number of parameters.

These two principles are so powerful that they have dominated the landscape of condensed matter physics for years, leaving most theorists doing just engineering work: bosonic order parameters + Fermi gas + perturbations around them. However, as always, dark clouds appear in the perfect sky. In 1982, a new state of matter was discovered in the two-dimensional electron gases under a strong magnetic field, the so-called fractional quantum hall states. These states can not be adiabatically continued to free fermions. They do not break any continuous symmetry and can not be described by a conventional order parameter. They are actually topological in nature. Investigations in this direction lead to fruitful outcomes, with groundbreaking wavefunctions, beautiful field theories and even predictions of new states of matter.

The second dark cloud that has develpoed into a serious intellectual crisis over the last twenty years or so is in the condensed matter physics enterprise dealing with strongly interacting electrons in solids. This field is flourishing right now and there is a general perception that after a slump in the 1990's the field has reinvented itself. What is this intellectual crisis about? Substantial progress has been made on the experimental side, both with regard to the discovery of electron systems in solids that behave in very interesting and puzzling ways (high-T_c superconductors [1] and other oxides [2], heavy fermion intermetallics [3], organics [4], 2DEG's in semiconductors [5]), and in the rapid progress of new instruments that make it possible to probe deeper and farther in these mysterious electron worlds (scanning tunneling spectroscopy [6], photoemission [7], neutron- [8] and resonant X-ray scattering [9]). On the theoretical side there is also much action. This is energized by the 'quantum field theory' (QFT) revolution that started in the 1970's in high energy physics, and is still in the process of unfolding its full potential in the low energy realms, as exemplified by topological quantum computation, quantum criticality and so forth. However, the QFT approach still lies within the framework of bosonic order parameters + Fermi gas + perturbations.

We are forced by experimentalists to face the problem of building a theory for the system of strongly interacting fermions that can neither be adiabatically continued to a free Fermi gas, nor be described in terms of bosonic order parameters. And this will be the target of this thesis. In our opinion, the key point that hinders this task is the fermion sign problem. Via the Euclidean path integral, the theory of interacting bosons boils down to exercises in equilibrium statistical physics. It is about computing probabilistic partition sums in euclidean spacetime following the recipe of Boltzmann and this seems to have no secrets left. However, this Boltzmannian path integral logic does not work at all when one wants to describe problems characterized by a finite density of fermionic particles. The culprit is that the path integral is suffering from the fermion sign problem. The Boltzmannian computation is spoiled by 'negative probabilities' rendering the approach to be mathematically ill-defined. In fact, the mathematics is as bad as can be: Troyer and Wiese [10] showed recently that the sign problem falls in the mathematical complexity class 'NP hard', and the Clay Mathematics Institute has put one of its seven one million dollar prizes on the proof that such problems cannot be solved in polynomial time.

Although not always appreciated, the fermion sign problem is quite consequential for the understanding of the physical world. Understanding matter revolves around the understanding of the emergence principles prescribing how a large number of simple constituents (like elementary particles) manage to acquire very different properties when they form a wholeness. The path integral is telling us that in the absence of the signs these principles are the same for quantum matter as they are for classical matter. But these classical emergence principles are in turn resting on Bolzmannian statistical physics. When this fails because of the fermion signs, we can no longer be confident regarding our un-

derstanding of emergence. To put it positively, dealing with fermionic quantum matter there is room for surprises that can be very different from anything we know from the classical realms that shape our intuition. In fact, we have only comprehended one such form of fermionic matter: the Fermi gas, and its 'derivative' the Fermi liquid. The embarrassment is that we are completely in the dark regarding the nature of other forms of fermionic matter, although we know that they exist because the experiments are telling us so.

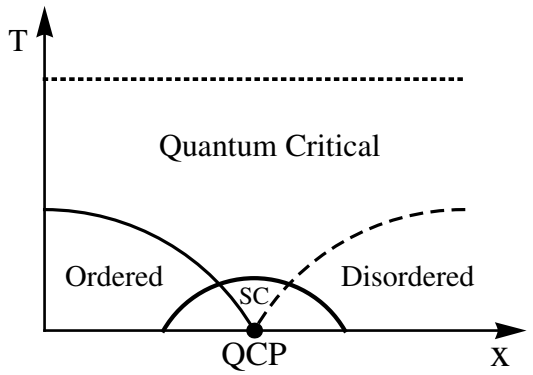

Figure 1.1: Illustration of the interplay of quantum criticality and superconductivity. x is the tuning parameter, which can be pressure, magnetic field or doping. The superconducting temperature usually has the highest value right above the QCP.

This thesis explores the emergent phenomena in the signful fermionic matters. In section 1.1, we introduce the two prototype materials of this thesis: cuprates and heavy fermions. The theme coming out the experimental findings is the phase diagram (1.1). By applying pressure, magnetic field, or doping, a second-order phase transition can be tuned to zero temperature, producing a quantum critical point (QCP). Such a singular point spreads out influence over a wide region in the phase diagram. Anomalous scaling behaviors thus emerge in various finite-temperature properties of the system, such as specific heat, resistivity and magnetic susceptibility, which go far beyond our conventional understanding of metals. Moreover, the QCP is a highly degenerate state. On approach to the QCP, a perturbation that was deemed irrelevant initially, takes over and dominates at low temperature, replacing the QCP by an alternative stable phase. In this way new states of matter that can not be constructed from stable states like normal metals or superconductors can be built. One common way to avoid the critical singularity is that the electrons organize themselves collectively into a superconducting state before they reach the critical point.

In section 1.2, we give a somewhat unconventional discussion of Fermi liq-

uids. To get the problem sharply in focus, we step back from the usual textbook viewpoint and instead consider the Fermi liquid from the perspective of the emergence principles governing classical and bosonic matter. We then proceed in two opposite directions. One direction is to go microscopic and try to deconstruct the existing principles of emergence. We explore the worldline formulation of many particle systems initiated by Feynman. A simple introduction is given in section 1.3. The other direction is to go macroscopic and search for new organizing principles. The keyword here is quantum criticality, which will be introduced in section 1.4. In section 1.5, we outline the basic structure of the remainder of this thesis and summarize the main results.

1.1 The prototype materials of this thesis

1.1.1 Cuprates

Cuprates are a kind of transition metal oxides with layered structure made up of one or more copper oxygen planes. The initial interest in cuprates was triggered by the fact that they can become superconducting at anomalously high temperatures [11]. After more than 20 years' extensive study, with sample preparation sufficiently advanced and nearly all possible experimental tools applied, it has become clear that cuprates means much more than a high transition temperature, a number that can be as large as 160. Their properties in the normal state above the superconducting temperature are even more exotic, and that may also account for the unusually high T_c (see [12] for a comprehensive review).

It is now generally agreed that the active physics of cuprates lies in the CuO_2 plane, and the effect of the c-axis is basically to tune the electronic structure of the CuO_2 plane. For the parent compound without doping, each copper is surrounded by 4 oxygens in the planes, with the copper ion in the d^9 configuration, providing per unit cell a single 3d hole, and the oxygen ion in the p^6 configuration. The tetragonal environment promotes the $d_{x^2-y^2}$ orbital of the copper ions to higher energy level, which further mixes with the oxygen p_x and p_y orbitals, forming a strong covalent bond. The question is then where the holes reside. A crucial insight is that there is a strong repulsion when two electrons or two holes are placed on the same ion. The energy to doubly occupy the copper d orbital is actually the largest energy scale in the problem. It also costs more energy for the holes to be placed at the oxygen p orbitals than at the copper d orbitals. When this energy difference is large enough, as is the case for cuprates, the holes will mainly just stay at the lattice sites of copper atoms, forming a charge transfer insulator with localized moments [13]. Virtual hopping to nearby oxygen p orbitals induces an exchange interaction between these local moments, and the insulator is actually in an antiferromagnetic ground state.

When replacing, say some La by Sr, more holes are added to the CuO_2 plane. These extra holes will occupy the oxygen p orbitals at the first place. A metallic

state is formed when these holes hop around among the oxygen p orbitals. However, the Cu-O hybridization creates a new low lying resonate state, in which the local moment on the copper lattice site forms a local spin singlet with the spin of the doped hole residing on the neighboring square of the oxygen atoms [14]. These singlets can hop from one site to another, and the low energy physics is captured by a one-band tight-binding model on the square lattice. This way, cuprates present an almost perfect realization of the simple single-band Hubbard model, with the energy difference between the oxygen p orbital and copper d orbital playing the role of the Hubbard U. When this energy difference is large, the problem is further reduced to the t-J model,

$$H = -P\left[\sum_{<ij>,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{i\sigma}\right] P + \sum_{<ij>} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j, \tag{1.1}$$

where $c^{\dagger}_{i\sigma}$ and $c_{i\sigma}$ are the fermion creation and annihilation operators, and $\mathbf{S}_i$ the spin operator. The crucial part is the Gutzwiller projection operator P which eliminates double occupancies. The essential physics of the t-J model is encapsulated by the trial wavefunctions proposed by Anderson: $\Psi_{tJ}(\mathbf{r}_1, \cdots, \mathbf{r}_N) = P\Phi_{\mathrm{HF}}(\mathbf{r}_1, \cdots, \mathbf{r}_N)$, with Φ_{HF} a Hatree-Fock wavefunction for either conventional Fermi liquid or BCS superconductor. The projection operator is a singular transformation. Thus Ψ_{tJ} and Φ_{HF} can not be adiabatically continued to each other.

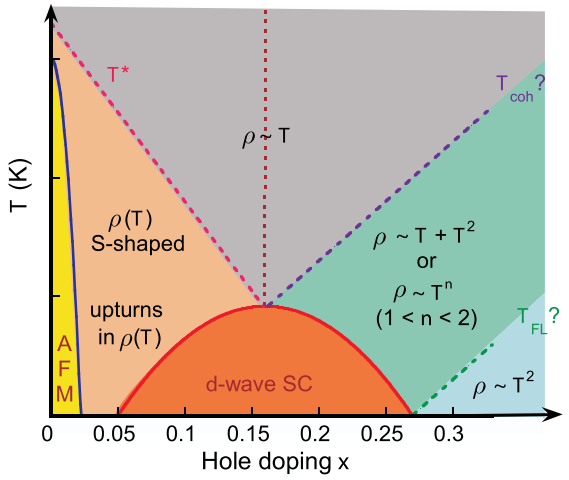

Figure 1.2: Phase diagram of cuprates as determined by transport measurements (from Hussey [15]).

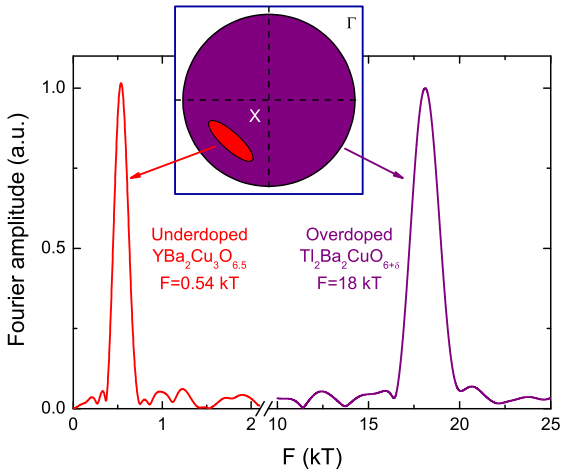

Figure 1.3: Change of the cuprate Fermi surface between the overdoped and underdoped regions deduced from quantum oscillation (from Jaudet et al. [16]).

Now let us look at the phase diagram of cuprates [15]. A large variety of emergent phenomena flourish in the underdoped region, such as stripes, vertex liquids, quantum liquid crystals and the intra-unit cell spontaneous diamagnetic currents. This part of the phase diagram is still attracting most of the attentions of the researchers in the field. There is ample evidence that at large doping (the so-called overdoped region), cuprates gradually conform to the laws of Landau Fermi liquid, with the T^2 component of the resistivity dominating over the T-linear component.

The arguably most mysterious part of the phase diagram is the strange metal phase above the superconducting dome. The behavior in this region is actually extremely simple and universal, of mathematical purity. The defining property of such states is the linear temperature dependence of the resistivity for a wide temperature range. The optical conductivity measurement (in optimally doped $Bi_2Sr_2Ca_{0.92}Y_{0.08}Cu_2O_{8+\delta}$) also shows clear scaling behavior. The absorptive and reactive parts combine to produce a nearly perfect power law behavior in the complex optical conductivity, with $\sigma(\omega) \sim (-i\omega)^{\gamma-2}$, where the exponent is determined to be $\gamma \simeq 1.35$.

So one would suspect that the strange metal phase is in some critical state. And with temperature the most prominent energy scale in this regime, one would be tempted to further associate this state with a zero temperature quantum critical point near optimal doping. We notice that, different from the quantum critical states in many heavy fermion systems, which will be the topic of the next subsection, the electronic specific heat of this state displays an ordinary Fermi liquid type behavior, $C = \gamma T$, with γ nearly constant for a wide range of

temperature and doping. There is no evidence for quasiparticle mass divergence. Neither is it inconsistent with quantum criticality. Anyhow, it is clear that the stange metal phase is not a conventional Fermi liquid. It is well established by ARPES measurements that in the normal state at optimal doping, although there is well defined Fermi surface in momentum space, sharp quasi-particle peaks cease to exist near the $(\pi, 0)$ point of the Brillouin zone.

An immediate question would be what is changing across such a QCP. In the overdoped regime, a large closed Fermi surface characteristic of a normal metal is observed. In the underdoped regime, ARPES sees only disconnected arcs shape residues of Fermi surface, while quantum oscillations reveal small closed pockets of Fermi surface. It has also been proposed by Zaanen and Overbosch that such QCP actually corresponds to a statistics changing transition [17]. The crucial insight is that in the underdoped regime, the t-J model actually encodes a completely different quantum statistical principle, which is fundamentally different from the Fermi-Dirac statistics governing the overdoped regime. It is a great theoretically challenge to reconcile such abrupt change with the second order nature of the transition as expected from the scaling behavior in the normal state. To our knowledge, up to now, we do not even have a simple proof-of-principle model demonstrating such compatibility.

1.1.2 Heavy fermions

The term 'heavy fermions' stands for a class of rare earth or actinide compounds, the electronic excitations of which can be as much as thousand times heavier than that in copper. These systems show a diversity of orderings, including ferromagnetism, antiferromagnetism and unconventional superconductivity. The conventional wisdom of mutual exclusion of magnetism and superconductivity was invalidated by the discovery of superconductivity in such f-electron systems, first in the compound $CeCu_2Si_2$ by Steglich, Aarts et al. in 1976 [18] and confirmed in 1983 in UBe_{13} [19]. In 1994, von Lohneyson et al. discovered that by changing pressure or the gold concentration, the heavy fermion alloy $CeCu_{6-x}Au_x$ can be tuned through an antiferromagnetic quantum phase transition [20]. The finite temperature properties of the system above the critical point show pronounced deviations from the predictions of conventional Landau Fermi liquid theory (for a comprehensive review see [21]).

The basic picture of the heavy fermion systems is that of a dense lattice of magnetic moments immersed in the sea of conduction electrons. The f-electrons associated with the rare earth or actinide ions have strong on-site Coulomb repulsion and they localize into magnetic moments, as in the Mott insulators. The local moments interact antiferromagnetically with the spin density of the conduction electron fluid, generating a lattice analog of the single ion Kondo effect. A heavy electron band is thus formed out of the resonances created in each unit cell. Resistivity drops down at low temperature when coherence develops. The f-electrons are effectively dissolved in the conduction electron fluid, with the net

effect that the Fermi surface volume counts the number of both conduction electrons and f-electrons.

The local moments also induce Friedel oscillations in the spin density of the conduction electron liquid. These oscillations again couple to the other local moments, resulting in an effective magnetic interaction between the local moments. Such conduction-electron-mediated interactions between magnetic moments are called RKKY interactions, named after Ruderman, Kittel, Kasuya and Yosida. The RKKY interaction favors an antiferromagnetic ground state for the local moments. When the f-electrons are locked into the local moments, the Fermi surface volume just counts the number of conduction electrons.

All these ingredients can be grouped together into the following Hamiltonian, usually called the Kondo lattice model,

$$\mathcal{H} = \sum_{\mathbf{k}\alpha} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha} + \frac{J_K}{2} \sum_i \mathbf{S}_i \cdot c^{\dagger}_{i\alpha} \sigma_{\alpha\beta} c_{i\beta} + \sum_{i,j} J^{\mathrm{RKKY}}_{ij} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{1.2}$$

where $c_{\mathbf{k}\alpha}$ represents the conduction electrons and $\mathbf{S}_i$ the local moments. J_K parameterizes the Kondo coupling between the conduction electrons and the local moments, and J^{RKKY}_{ij} the RKKY interaction between the local moments. The Kondo coupling is proportional to the square of the hybridization matrix element V between the conduction electrons and f-electrons, $J_K \sim V^2$, and the RKKY interaction is proportional to the conduction electron density of states and the square of the Kondo coupling, $J^{\mathrm{RKKY}} \sim J_K^2 \rho$.

The canonical picture of Kondo lattice, due to Doniach, is that the competition between the Kondo coupling and RKKY interaction governs the phase diagram [22]. Daniach's reasoning is based on a comparison of energy scales. There are two characteristic energy scales in such system: the single ion Kondo temperature $T_K = De^{-1/(2J_K\rho)}$ with D the bandwidth and the RKKY temperature $T_{\mathrm{RKKY}} = J_K^2 \rho$. For $J_K\rho$ large, the Kondo temperature is the larger one and the ground state is the heavy Fermi liquid with a large Fermi surface. For $J_K\rho$ small, the RKKY temperature is larger, resulting in an antiferromagnetic ground state with a small Fermi surface.

Let us look at one example: the heavy fermion alloy $CeCu_{6-x}Au_x$. The parent compound $CeCu_6$ is a heavy fermion metal showing no long-range magnetic order above 5 mK. Antiferromagnetic fluctuations have been observed in inelastic neutron scattering. By replacing some copper atoms by gold atoms, the lattice expands, leading to a reduction in the hybridization between the Ce 4f electrons and the conduction electrons. And the RKKY interaction becomes more important. Actually in the doping range $0.1 \leqslant x \leqslant 1$, the Neel temperature is linear in x, $T_N \propto (x - 0.1)$. By decreasing x or adding pressure, the Neel temperature can be tuned to essentially zero, where we get a continuous phase transition at zero temperature. Such phase transitions will be dominated by quantum mechanical fluctuations, and are thus called quantum phase transitions (QPTs).

There are two aspects of such transitions. One is that the system goes from a

magnetically ordered state to a magnetically disordered state, for which an order parameter can be asigned that captures such a transition. The other aspect is that the Fermi surface also changes across the transition. One would expect that the Fermi surface changes continuously from the phase with a large Fermi surface to the other phase with a small Fermi surface. A spin density wave transition would give rise to such a result. However de Haas-van Alphen measurements have shown that at least for some QPTs, e.g. the pressure-tuned QPT in $CeRhIn_5$, there is a sudden change in the Fermi surface area right at the transition point (see Fig.1.4). How to reconcile the second-order nature of the phase transition with the sudden change in the Fermi surface area is a serious challenge to theorists, which obviously goes beyond the conventional paradigm of spontaneous symmetry breaking.

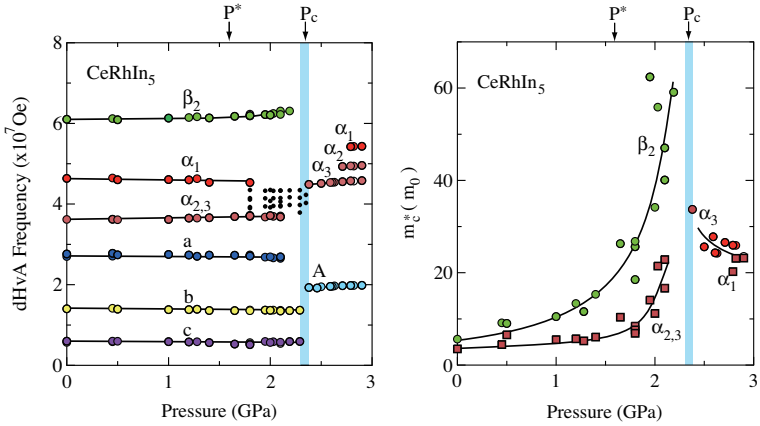

Figure 1.4: Pressure dependence of the de Haas-van Alphen frequency and cyclotron mass in $CeRhIn_5$. P_c denotes the critical pressure (from Gegenwart et al. [23], measurement by Shishido et al. [24]).

Associated with such unconventional zero-temperature phase transitions are the various exotic behaviors in the finite temperature properties of the system above the QCPs, widely known as the non-Fermi liquid behavior (see [25] and references therein), signaling our ignorance of such states. In various systems, the specific heat coefficient shows an upturn at low temperature, which is usually best fitted by a logarithmic divergence, $C_V/T \sim -\log T$, e.g. $CeCoIn_5$, $CeCu_{6-x}Au_x$, U_2Pt_2In, $U_xTh_{1-x}Cu_2Si_2$, $YbRh_2Si_2$, YbAgGe, and sometimes equally well or even better fitted by a power-law divergence, $C_V/T \sim T^{-1+\lambda}$ with $0 < \lambda < 1$, e.g. $Ce_{1-x}Th_xRhSb$, $UCu_{4-x}Pd_{1+x}$, $U_xY_{1-x}Pd_3$. Thinking Fermi liquid, this would mean that the quasiparticle effective mass diverges $m^*/m \to \infty$. The transport properties of such systems are also quite different from that of Fermi liquid. For $CeCoIn_5$ (along the c-axis), $CeCu_2Ge_2$,

$CeCu_{6-x}Au_x$, $UCu_{4-x}Pd_{1+x}$, $UCu_{4+x}Pt_{1-x}$, $U_2Cu_{12}Al_5$, $YbRh_2Si_2$, YbAgGe and $YbRh_2Si_{2-x}Ge_x$, the resistivity has a (quasi-)linear temperature dependence, reminiscent of the strange metal phase of cuprates. In many other systems, the resistivity obeys the power law $\rho = \rho_0 + AT^\alpha$, with the power α obviously smaller than 2, e.g. $CeCu_2Si_2$, $CePd_2Si_2$, $CeNi_2Ge_2$, $Ce(Ru_{1-x}Rh_x)_2Si_2$, $CeIrIn_5$, $CeRu_4Sb_{12}$, $U_2Co_2Sn_5$, UBe_{13}, UPt_{13}, UCoAl, $U_xTh_{1-x}Cu_2Si_2$ and $YbCu_{3+x}Al_{2-x}$. The Fermi-liquid-type scattering can not account for such behavior. The critical fluctuations evade the locking of the Fermi-Dirac statistics.

Another important feature of the quantum critical state in heavy fermion systems, which is also observed in cuprates, is the so-called locality. For example, for $CeCu_{6-x}Au_x$, the scale-invariant part of the dynamical spin susceptibility shows the same ω/T scaling for different momenta, which implies that the critical excitations are local.

It is surprisingly universal that as one lowers temperature, new phases appear near the QCP. Most commonly observed to date is the superconducting phase (see [26] and references therein). The phenomenon of a superconducting dome enclosing the region near the QCP is quite general (see Fig.1.1). The prototype material in heavy fermions with such a phase diagram is the intermetallic compound $CePd_2Si_2$. At ambient pressure, $CePd_2Si_2$ orders antiferromagnetically below about 10 K. Applying pressure reduces the Neel temperature, and at about 28 kbar, the Neel temperature vanishes, where one expects the existence of a QCP. However, in the immediate vicinity of the critical pressure, superconductivity appears, with highest T_c about 0.4 K. Above the superconducting dome, the electrical resistivity shows anomalous scaling behavior, with quasi-linear temperature dependence over almost two orders of magnitude in temperature. Other materials with a similar phase diagram include $CeIn_3$, $CeCu_2Si_2$, $CeCu_2Ge_2$, UGe_2, URhGe and UCoGe.

1.2 Fermions: the main target of this thesis

The new experimental findings in cuprates and heavy fermions clearly indicate the breakdown of the old paradigm of Landau. At this time, it is helpful to go back to basics, deconstruct the old laws, and get detoxified from the stubborn beliefs of the traditional way of thinking, which we have been following for decades.

The experimentalists measure systems formed from electrons and electrons are fermions. The only exactly solvable many Fermion problem is the non-interacting Fermi gas. Surely, every student in physics knows the canonical solution. Introduce creation and annihilation operators that anti-commute,

$$\{c^\dagger_{\vec{k}}, c_{\vec{k}'}\} = \delta_{\vec{k},\vec{k}'}, \tag{1.3a}$$

$$\{c^\dagger_{\vec{k}}, c^\dagger_{\vec{k}'}\} = \{c_{\vec{k}}, c_{\vec{k}'}\} = 0, \tag{1.3b}$$

and the Hamiltonian is

$$H_0 = \sum_{\vec{k}} \varepsilon_k c^\dagger_{\vec{k}} c_{\vec{k}}, \tag{1.4}$$

where $\vec{k}$ is some set of single particle quantum numbers; a representative example is the spinless gas in the continuum where $\vec{k}$ represents single particle momentum and $\varepsilon_k = \hbar^2 k^2/2m$. It follows from standard manipulations that its grand canonical free energy is

$$F_G = -\frac{1}{\beta} \sum_{\vec{k}} \ln\left(1 + e^{-\beta(\varepsilon_{\vec{k}} - \mu)}\right), \tag{1.5}$$

where $\beta = 1/(k_B T)$ and μ the chemical potential, tending to the Fermi-energy E_F when $T \to 0$. The particle number is

$$N = \sum_{\vec{k}} n_{\vec{k}}, \tag{1.6a}$$

$$n_{\vec{k}} = \frac{1}{e^{\beta(\varepsilon_{\vec{k}} - \mu)} - 1}, \tag{1.6b}$$

where $n_{\vec{k}}$ is recognized as the momentum distribution function. At zero temperature this momentum distribution function turns into a step function: $n_{\vec{k}} = 1$ for $|\vec{k}| \leq k_F$ and zero otherwise where the Fermi-momentum $k_F = \sqrt{2mE_F/\hbar^2}$. The step smears at finite temperature, and this is another way of stating the fact that only at zero temperature one is dealing with a Fermi-surface with a precise locus in single particle momentum space separating occupied- and unoccupied states.

The simplicity of the Fermi gas is deceptive. This can be highlighted by a less familiar but illuminating argument. As Landau guessed correctly [27], the Fermi gas can be adiabatically continued to the interacting Fermi liquid. The meaning of this statement is that when one considers the system at sufficiently large times and distances and sufficiently small temperatures('scaling limit') a state of interacting fermionic matter exists that is physically indistinguishable from the Fermi gas. It is characterized by a sharp Fermi surface and a Fermi energy but now these are formed from a gas of non-interacting quasiparticles that have still a finite overlap ('pole strength' $Z_{\vec{k}}$) with the bare fermions, because the former are just perturbatively dressed versions of the latter, differing from each other only on microscopic scales [27]. This is the standard lore, but let us now consider these matters with a bit more rigor. The term describing the interactions between the bare fermions will have the general form,

$$H_1 = \sum_{\vec{k},\vec{k}'\vec{q}} V(\vec{k},\vec{k}',\vec{q}) c^\dagger_{\vec{k}+\vec{q}} c_{\vec{k}} c^\dagger_{\vec{k}'-\vec{q}} c_{\vec{k}'}. \tag{1.7}$$

It is obvious that single particle momentum does not commute with the interaction term,

$$\left[c^{\dagger}_{\vec{k}}c_{\vec{k}}, H_1\right] \neq 0, \tag{1.8}$$

henceforth, single particle momentum is in the presence of interactions no longer a quantum number and single particle momentum space becomes therefore a fuzzy, quantum fluctuating entity. But according to Landau we can still point at a surface with a sharp locus in this space although this space does not exist in a rigorous manner in the presence of interactions!

In the textbook treatments of the Fermi liquid this obvious difficulty is worked under the rug. Since the above argument is rigorous, it has to be the case that the Fermi-surface does not exist when one is dealing with any finite number of particles! Since we know empirically that the Fermi liquid exists in the precise sense that interacting Fermi-systems are characterized by a Fermi-surface that is precisely localized in momentum space in the *thermodynamic limit* it has to be that this system profits from the singular nature of the thermodynamic limit, in analogy with the mechanism of spontaneously symmetry breaking that rules bosonic matter.

We refer to the peculiarity of bosonic- and classical systems that (quantum) phases of matter acquire a sharp identity only when they are formed from an infinity of constituents [28]. Consider for instance the quantum crystal, breaking spatial translations and rotations. Surely, one can employ a STM needle to find out that the atoms making up the crystal take definite positions in space but this is manifestly violating the quantum mechanical requirement that 'true' quantum objects should delocalize over all of space when it is homogeneous and isotropic. The resolution of this apparent paradox is well known. One should add to the Hamiltonian an 'order parameter' potential $V(\mathbf{R})$ where $\mathbf{R}$ refers to the dN dimensional configuration space of N atoms in d dimensional space, having little potential valleys at the real space positions of the atoms in the crystal. It is then a matter of order of limits,

$$\lim_{N\to\infty}\lim_{V\to 0}\langle\sum_i \delta(\vec{r}_i - \vec{r}_i^{\,0})\rangle = 0, \tag{1.9a}$$

$$\lim_{V\to 0}\lim_{N\to\infty}\langle\sum_i \delta(\vec{r}_i - \vec{r}_i^{\,0})\rangle \neq 0, \tag{1.9b}$$

where $\vec{r}_i$ and $\vec{r}_i^{\,0}$ are the position operator and the equilibrium position of the i-th atom forming the crystal. Henceforth, the precise positions of the atoms in the solid, violating the demands of quantum mechanical invariance, emerge in the thermodynamic limit – we know that a small number of atoms cannot form a crystal in a rigorous sense.

Returning to the Fermi liquid, the commonality with conventional symmetry breaking is that in both cases non existent quantum numbers (position of atoms in a crystal, single particle momentum in the Fermi liquid) come into existence

via an 'asymptotic' emergence mechanism requiring an infinite number of constituents, at least in principle. But this is as far the analogy goes. In every other regard, the Fermi liquid has no dealings with the classical emergence principles, that also govern bosonic matter.

Although it is unavoidable that the Fermi liquid needs the thermodynamic limit it is not at all clear what to take for the order parameter potential V. In this regard, the Fermi liquid is plainly mysterious. The textbook treatises of the Fermi liquid, including the quite sophisticated 'existence proofs', share a very perturbative attitude. The best treatments on the market are the ones based on functional renormalization and the closely related constructive field theory [29]. Their essence is as follows: start out with a Fermi gas and add an infinitesimal interaction, follow the (functional) renormalization flow from the UV to the IR to find out that all interactions are irrelevant operators. Undoubtedly, the conclusions from these tedious calculations that the Fermi gas is in a renormalization group sense stable against small perturbations are correct. The problem is that these perturbative treatments lack the mighty general emergence principles that we worship when dealing with classical and bosonic matter.

To stress this further, let us consider a rather classic problem that seems to be more or less forgotten although it was quite famous a long time ago: the puzzle of the ^{3}He Fermi liquid. The ^{3}He liquid at temperatures in the Kelvin range is not yet cohering and it is well understood that it forms a dense van der Waals liquid. Such liquids have a bad reputation; all motions in such a classical liquid are highly cooperative to an extent that all one can do is to put them into a computer and solve the equations of motions by brute force using molecular dynamics. When one cools this to the millikelvin range, quantum coherence sets in and eventually one finds the impeccable textbook version of the Fermi liquid: the macroscopic properties arise from dressed helium atoms that have become completely transparent to each other, except that they communicate via the Pauli principle, while they are roughly ten times as heavy as real ^{3}He atoms. When one now measures the liquid structure factor using neutron scattering one finds out that on microscopic scales this Helium Fermi liquid is more or less indistinguishable from the classical van der Waals fluid! Hence, at microscopic scales one is dealing with the same 'crowded disco' dynamics as in the classical liquid except that now the atoms are kept going by the quantum zero-point motions. On the microscopic scale there is of course no such thing as a Fermi surface. For sure, the idea of renormalization flow should still apply, and since one knows what is going on in the UV and IR one can guess the workings of the renormalization flow in the ^{3}He case: one starts out with a messy van der Waals ultraviolet, and when one renormalizes by integrating out short distance degrees of freedom one meets a 'relevant operator creating the Fermi-surface'. At a time scale that is supposedly coincident with the inverse renormalized Fermi-energy this relevant operator takes over and drags the system to the stable Fermi liquid fixed point. How to construct such a 'Fermi-surface creation operator'? Nobody seems to have a clue!

Although the microscopic details are quite different, the situation one encounters in interesting electron system like the ones realized in manganites [2, 30], heavy fermion intermetallics [3] and cuprate superconductors [1] is in gross outlines very similar as in ^{3}He. In various guises one finds coherent quasiparticles (or variations on the theme, like the Bogoliubons in the cuprates) only at very low energies and low temperatures. Undoubtedly the UV in these systems has much more to do with the van der Waals quantum liquid than with a free Fermi gas. Still, the only activity the theorists seem capable off is to declare the UV to be a Fermi gas that is hit by small interactions. It is not because these theorists are incompetent: humanity is facing the proverbial brick wall called the fermion sign problem that frustrates any attempt to do better.

The other 'anomaly' of the Fermi liquid appears again as rather innocent when one has just worked oneself through a fermiology textbook. However, giving this a further thought, it is actually the most remarkable and most mysterious feature of the Fermi liquid. Without exaggeration, one can call it a 'UV-IR connection', indicating the rather unreasonable way in which microscopic information is remembered in the scaling limit. It refers to the well known fermiology fact that by measuring magneto-oscillations in the electrical transport (De Haas-van Alphen, and Shubnikov- de Haas effects) one can determine directly the average distance between the microscopic fermions by executing measurements on a macroscopic scale. This is as a rule fundamentally impossible in strongly interacting classical- and sign free quantum matter. Surely, this is possible in a weakly interacting and dilute classical gas, as used with great effect by van der Waals in the 19-th century to proof the existence of molecules. But the trick does not work in dense, strongly interacting classical fluids: from the hydrodynamics of water one cannot extract any data regarding the properties of water molecules. Surely, the weakly interacting Fermi gas is similar to the van der Waals gas but a more relevant example is the strongly interacting ^{3}He, or either the heavy fermion Fermi liquid. At microscopic scales it is of course trivial to measure the inter-particle distances and the liquid structure factor of ^{3}He will directly reveal that the helium atoms are apart by 4 angstroms or so. But we already convinced the reader that there is no such thing as a Fermi surface on these scales. Descending to the scaling limit, a Fermi-surface emerges and it encloses a volume that is protected by the famous Luttinger theorem [31,32]: it has to enclose the same volume as the non-interacting Fermi gas at the same density. Using macroscopic magnetic fields, macroscopic samples and macroscopic distances between the electrical contacts one can now measure via de Haas van Alphen effect, etcetera, what k_F is and the Fermi momentum is just the inverse of the inter-particle distance modulo factors of 2π. This is strictly unreasonable. We repeat, on microscopic scales the system has knowledge about the inter-particle distance but there is no Fermi-surface; the Fermi surface emerges on a scale that is supposedly in some heavy fermion systems a factor 100 or even 1000 larger than the microscopic scale. But this emerging Fermi-surface still gets its information from somewhere, so that it knows to fix its volume satisfying Luttinger's rule! In Chapter 3 we hope to

shed some light on the 'mysteries' addressed here using Ceperley's path integral but we are still completely in the dark regarding this particular issue. It might well be that there are even much deeper meanings involved; we believe that it has dealings with the famous anomalies in quantum field theories [33]. These are tied to Dirac fermions and the bottom line is that these process in rather mysterious ways ultraviolet (Planck scale) information to the infrared, with the effect that a gauge symmetry that is manifest on the classical level is destroyed by this 'quantum effect'.

To summarize, in this section we have discussed the features of the Fermi liquid that appear to be utterly mysterious to a physicist believing that any true understanding of physics has to rest on Boltzmannian principle:
(i) What is the order parameter and order parameter potential of the zero temperature Fermi liquid?
(ii) How to construct a 'Fermi-surface creation operator', which is supposed to be the relevant operator associated with the IR stability in the renormalization group flow?
(iii) Why is it possible to retrieve microscopic information via the Luttinger sum rule by performing macroscopic magneto-transport measurements, even in the asymptotically strongly interacting Fermi liquid?

1.3 Feynmanian deconstruction of the order parameter

A better way to understand symmetry breaking is to inspect the dual representation in terms of the worldline path integral [34, 35], which will be the task of Chapters 2 and 3 of this thesis. In such first-quantized formalism, the order parameter is deconstructed, in the sense that the condensate can be expressed directly in terms of the microscopic constituents of the system. The indistinguishability of the bosons and fermions translates into the recipe that one has to trace about all possible ways the worldlines can wind around the periodic imaginary time axis. For a bosonic system, at the temperature where the average of the topological winding number w becomes macroscopic, $\lim_{N\to\infty}\langle w\rangle/N \neq 0$, a phase transition occurs either to the BEC or the superfluid. Bose condensation means that a macroscopic number of particles 'share the same worldline' and the only difference between a BEC and a superfluid is that in the latter this condensate is somewhat depleted.

What is more attractive to us is that the worldline formalism has also the merit of making the fermion sign most transparent. Fermionic worldlines with an even winding number have positive signs, while those having an odd winding number carry negative signs, and they are the origin of the fermion sign problem. It is in this formalism that a partial solution of the sign problem is proposed [Chapter 3]. The basic idea is to discard the worldlines with odd winding numbers and in compensation, some of the even winding worldlines also need to be thrown

away.

Feynman's worldline path integral formulation of many body system is now a textbook problem, although we are aware of only one textbook where it is worked out in detail: Kleinert's Path integral book [36]. Consider the partition function for Bosons or Fermions; this can be written as an integral over configuration space $\mathbf{R} = (\mathbf{r}_1, \ldots, \mathbf{r}_N) \in \mathbb{R}^{Nd}$ of the diagonal density matrix evaluated at an imaginary $\hbar\beta$,

$$\mathcal{Z} = \mathrm{Tr} e^{-\beta H} = \int \mathrm{d}\mathbf{R} \rho(\mathbf{R}, \mathbf{R}; \beta). \tag{1.10}$$

The path integral formulation of the partition function rests on a formal analogy between the quantum mechanical time evolution operator in real time $e^{-i\hat{H}t/\hbar}$ and the finite temperature quantum statistical density operator $\hat{\rho} = e^{-\beta\hat{H}}$, where the inverse temperature $\beta = 1/k_B T$ has to be identified with the imaginary time $it/\hbar$. The partition function defined as the trace of this operator and expression (1.10) simply evaluates this trace in position space. More formally this can viewed as a Wick rotation of the quantum mechanical path integral, and requires a proper analytic continuation to complex times. This rotation tells us that the path integral defining the partition function lives in D-dimensional Euclidean space, with $D = d + 1$ and d the spatial dimension of the equilibrium system. This analogy tells us that to study the equilibrium statistical mechanics of a quantum system in d space dimensions, we can study the quantum system in a Euclidean space of dimension $d + 1$, where the extra dimension is now identified as a 'thermal' circle of extent β. At finite temperature this circle is compact and world-lines of particles in the many-body path integral (1.10) then wrap around the circle, with appropriate boundary conditions for bosons or fermions. The discrete Matsubara frequencies that arise from Fourier transforming modes on this circle carry the idea of Kaluza-Klein compactification to statistical mechanics.

For distinguishable particles interacting via a potential V the density matrix can be written in a worldline path integral form as,

$$\rho_D(\mathbf{R}, \mathbf{R}'; \beta) = \int_{\mathbf{R}\to\mathbf{R}'} \mathcal{D}\mathbf{R} \exp(-\mathcal{S}[\mathbf{R}]/\hbar), \tag{1.11a}$$

$$\mathcal{S}[\mathbf{R}] = \int_0^{\hbar\beta} d\tau \left(\frac{m}{2} \dot{\mathbf{R}}^2(\tau) + V(\mathbf{R}(\tau)) \right), \tag{1.11b}$$

but for indistinguishable bosons or fermions one has also to sum over all $N!$ permutations $\mathcal{P}$ of the particle coordinates,

$$\rho_{B/F}(\mathbf{R}, \mathbf{R}; \beta) = \frac{1}{N!} \sum_{\mathcal{P}} (\pm 1)^p \rho_D(\mathbf{R}, \mathcal{P}\mathbf{R}; \beta), \tag{1.12}$$

where p is he parity of the permutation. For the bosons one gets away with the positive sign, but for fermions the contribution of a permutation with uneven

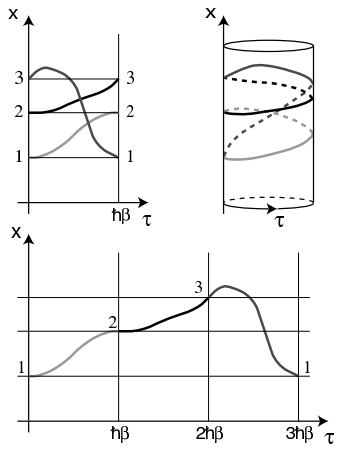

Figure 1.5: Worldline configuration corresponding to a cyclic exchange of three particles, $1 \to 2$, $2 \to 3$, and $3 \to 1$, or in short notation (123) (upper left). On a cylinder (upper right), the worldlines form a closed loop winding $w = 3$ times around the cylinder. In the extended zone scheme (bottom), the exchange process of three particles can be identified with a worldline of a single particle at an effective inverse temperature 3β.

parity to the partition sum is a 'negative probability', as required by the anti-symmetry of the fermionic density matrix. This is the origin of the fermion sign problem, which will be discussed in more detail in section 2.

The partition sum describes worldlines that 'lasso' the circle in the time direction. Every permutation in the sum is composed out of so called permutation cycles. For instance, consider three particles. One particular contribution is given by a cyclic exchange of the three particles corresponding with a single worldline that winds three times around the time direction with winding number $w = 3$ (see Fig. 1.5), a next class of contributions correspond with a 'one cycle' with $w = 1$ and a two-cycle with $w = 2$ (one particle returns to itself while the other two particles are exchanged), and finally one can have three one cycles (all particles return to their initial positions).

The crucial insight of Feynman was that quantum mechanics actually renders a strongly interacting Bose or Fermi liquid to act like a system of free particles, with renormalized parameters ([34], [35]). The main task here is to characterize the important trajectories for the partition sum. One can neglect the contributions from configurations $\mathbf{R}(0)$ and motions $\mathbf{R}(\tau)$ which give small contributions. Let us consider the contribution from moving a single particle i from its initial position $\mathbf{r}_i(0)$ to a final position $\mathbf{r}_i(\beta)$. $\mathbf{r}_i(\beta)$ might be the same as $\mathbf{r}_i(0)$, or $\mathbf{r}_j(0)$ for another particle j. As a simple model that captures the essence of the

problem, imagine the interaction to be of very short range. So the important initial configurations are those for which particles are far apart. There may be other particles in the way of the path $\mathbf{r}_i(\tau)$, and they will interact with particle i due to the potential energy V. It is also possible that as particle i moves, the other particles move out of its way, avoiding to interact with it. For some special paths $\mathbf{R}(\tau)$, it can be that the particles have adjusted their motions so well that during the whole motion, the total potential energy of all the particles is nearly equal to the potential energy of the original configuration $\mathbf{R}(0)$. Instead of increasing their potential energy, for which the time integral is proportional to β, the particles just need to pay an increase of kinetic energy for the readjustment of their coordinates, which varies as the square of the velocity of particle i and has time integral inversely proportional to β. The change in kinetic energy can be accounted for by assigning a larger mass to particle i. The net effect is that for every trajectory, the particle behaves like a free particle with a shifted effective mass.

So we can proceed by considering as fixed point theory the non-interacting Bose and Fermi gas, keeping in mind that mass m is now a renormalized quantity. The evaluation of their path integrals reduces to a combinatorial exercise. Let us first illustrate these matters for the example of $N = 3$ particles. It is straightforward to demonstrate, that the identity permutation gives a contribution $Z_0(\beta)^3$ to the partition function (here $Z_0(\beta)$ denotes the partition function of a single particle), whereas an exchange of all three particles contribute as $Z_0(3\beta)$. The meaning is simple: in the absence of interactions the 3-cycle can be identified with a single particle worldline returning to its initial position at an effective inverse temperature 3β (see Fig. 1.5). Further on, a permutation consisting of a $w = 1$ and a $w = 2$ cycle contributes with $Z_0(\beta)Z_0(2\beta)$. To write down the canonical partition function for $N = 3$ non-interacting bosons or fermions we only have to know the combinatorial factors (e.g. there are 3 permutations made out of a $w = 1$ and a $w = 2$ cycle) and the parity of the permutation to obtain

$$Z_{B/F}^{(N=3)}(\beta) = \frac{1}{3!}[Z_0(\beta)^3 \pm 3Z_0(\beta)Z_0(2\beta) + 2Z_0(3\beta)]. \tag{1.13}$$

This result can easily be generalized to N particles. We denote the number of 1-cycles, 2-cycles, 3-cycles, ... N-cycles the permutation is build of with C_1, C_2, C_3,..., C_N and denote the combinatorial factors counting the numbers of permutations with the same cycle decomposition $C_1, \dots C_N$ with $M(C_1, \dots C_N)$. For N particles we have to respect the overall constraint $N = \sum_w C_w$ and obtain

$$Z_{B/F}^{(N)}(\beta) = \frac{1}{N!} \sum_{C_1,\dots C_N}^{N=\sum_w C_w} M(C_1, \dots C_N)(\pm 1)^{\sum_w (w-1)C_w} \prod_{w=1}^{N} [Z_0(w\beta)]^{C_w}. \tag{1.14}$$

Although the combinatorial factors can be written down in closed form,

$$M(C_1, \dots C_N) = \frac{N!}{\prod_w C_w! w^{C_w}}, \tag{1.15}$$

the canonical partition function (1.14) is very clumsy to work with because of the constraint acting on the sum over cycle decompositions. The constraint problem can be circumvented by going to the grand-canonical ensemble. After simple algebraic manipulations we arrive at the grand-canonical partition function

$$\begin{aligned} Z_G(\beta,\mu) &= \sum_{N=0}^{\infty} Z_{B/F}^{(N)}(\beta) e^{\beta\mu N} \\ &= \exp\left(\sum_{w=1}^{\infty} (\pm 1)^{w-1} \frac{Z_0(w\beta)}{w} e^{w\beta\mu}\right), \end{aligned} \tag{1.16}$$

corresponding to a grand-canonical free energy

$$F_G(\beta) = -\frac{1}{\beta} \ln Z_G(\beta,\mu) = -\frac{1}{\beta} \sum_{w=1}^{\infty} (\pm 1)^{w-1} \frac{Z_0(w\beta)}{w} e^{\beta w\mu}, \tag{1.17}$$

with the $\pm$ inside the sum referring to bosons $(+)$ and fermions $(-)$, respectively. This is a quite elegant result: in the grand-canonical ensemble one can just sum over worldlines that wind w times around the time axis; the cycle combinatorics just adds a factor $1/w$ while $Z_0(w\beta)\exp(\beta w\mu)$ refers to the return probability of a single worldline of overall length $w\beta$. In the case of zero external potential we can further simplify

$$Z_0(w\beta) = \frac{V^d}{\sqrt{2\pi\hbar^2 w\beta/M}^d} = Z_0(\beta)\frac{1}{w^{d/2}}, \tag{1.18}$$

to obtain for the free energy and average particle number N_G, respectively,

$$F_G = -\frac{Z_0(\beta)}{\beta} \sum_{w=1}^{\infty} (\pm 1)^{w-1} \frac{e^{\beta w\mu}}{w^{d/2+1}}, \tag{1.19a}$$

$$N_G = -\frac{\partial F_G}{\partial \mu} = Z_0(\beta) \sum_{w=1}^{\infty} (\pm 1)^{w-1} \frac{e^{\beta w\mu}}{w^{d/2}}. \tag{1.19b}$$

To establish contact with the textbook results for the Bose and Fermi gas one just needs that the sums over windings can be written in an integral representation as,

$$\sum_{w=1}^{\infty} (\pm 1)^{w-1} \frac{e^{\beta w\mu}}{w^{\nu}} = \frac{1}{\Gamma(\nu)} \int_0^{\infty} d\varepsilon \frac{\varepsilon^{\nu-1}}{e^{\beta(\varepsilon-\mu)} \mp 1}, \tag{1.20}$$

and one recognizes the usual expressions involving an integral of the density of states ($N(\varepsilon) \sim \varepsilon^{d/2}$ in d space dimensions) weighted by Bose-Einstein or Fermi-Dirac factors.

For bosons, by using the worldline path integral formalism, the quantum mechanical problem is reduced to a purely classical equilibrium ring polymer problem. At the transition $\mu \to 0$, one directly infers from Eq. (1.19) that very long

worldlines corresponding with winding numbers $w \sim N$ are no longer penalized, while there are many more long winding- than short winding contributions in the sum. It is straightforward to show that in the thermodynamic limit worldlines with w between $\sqrt{N}$ and N have a vanishing weight above the BEC temperature, while these infinite long lines dominate the partition sum in the condensate [37]. One starts with a summation over a finite number of winding worldlines and take the infinite winding limit, or equivalently the infinite particle number limit, at the end of the day.

The number of particles contained in worldlines with winding number w is

$$N_w = \frac{e^{w\beta\mu}}{w^{d/2}} \left[\frac{D}{\lambda} W\left((\frac{D}{\lambda})^2 \frac{\pi}{w} \right) \right]^d , \tag{1.21}$$

where $W(x) = \sum_{n=-\infty}^{\infty} e^{-xn^2}$ comes from a summation over all discrete momentums, and $\lambda = \hbar\sqrt{2\pi\beta/m}$ is the de Broglie thermal wavelength. It is easy to show that for $d = 3$ the fraction of particles contained in the long loops is

$$\lim_{N\to\infty} \frac{1}{N} \sum_{w=\sqrt{N}}^{N} N_w = \begin{cases} 0 & \text{for } T > T_c \\ 1 - \left(\frac{T}{T_c}\right)^{3/2} & \text{for } T \leqslant T_c. \end{cases} \tag{1.22}$$

while for $d = 2$ the result is

$$\lim_{N\to\infty} \frac{1}{N} \sum_{w=\sqrt{N}}^{N} N_w = \begin{cases} 0 & \text{for } T > 0 \\ 1 & \text{for } T = 0. \end{cases} \tag{1.23}$$

A related issue is the well known fact that the non-interacting Bose-Einstein condensate and the superfluid that occurs in the presence of finite repulsions are adiabatically connected: when one switches on interactions the free condensate just turns smoothly into the superfluid and there is no sign of a phase transition. This can be seen easily from the canonical Bogoliubov theory. Again, although the algebra is fine matters are a bit mysterious. The superfluid breaks spontaneous $U(1)$ symmetry, thereby carrying rigidity as examplified by the fact that it carries a Goldstone sound mode while it expels vorticity. The free condensate is a non-rigid state, that does not break symmetry manifestly, so why are they adiabatically connected? The answer is obvious in the path-integral representation [38, 39]. The superfluid density ρ_S can be written in terms of the mean-squared winding number in the spatial direction,

$$\rho_S = \frac{m}{\hbar^2} \frac{\langle W^2 \rangle L^{2-d}}{d\beta}. \tag{1.24}$$

Here periodic boundary condition is imposed. d is the dimensionality, L is the size of the periodic cell, which is assumed to be the same for all spatial directions. The winding number W describes the net number of times the paths of the N

particles have wound around the periodic cell, $\mathbf{W}L = \sum_{i=1}^{N}(\mathbf{r}_{\mathcal{P}_i} - \mathbf{r}_i)$. Although interactions will hinder the free meandering of the polymers, a lot of this hindrance is required to make it impossible for worldlines to become infinitely long below some temperature. The fraction of infinitely long worldlines is just the condensate fraction ρ_S/ρ and even in the very strongly coupled ^{4}He superfluid these still make up for roughly 30% of all worldlines! The only way one can get rid of the infinite windings in the interacting system is to turn it into a static array of one cycles - the ^{4}He crystal.

1.4 Quantum criticality: a new organizing principle

Quantum criticality is an important concept that has dominated the landscape of modern condensed matter physics for the last decade [40]. The idea behind quantum criticality is simple and powerful. Imagine competing interactions that typically drive the transitions between different phases. Logically one has to allow for the possibility that the relative strength of these competing interactions is tunable as a function of the external control parameters such as pressure, magnetic field or doping; we deliberately omit temperature as a control parameter since quantum phase transitions (QPTs) will occur at T=0. The simplest route to arrive at a QPT is to consider a line of finite temperature phase transition as a function of some control parameter, such as pressure P, magnetic field B or doping x. At $T = 0$ this line will indicate a critical value of the control parameter. This specific value of the control parameter, where one expects a precise balance between tendency to different phases or states, is called a quantum critical point (QCP). Near this point, competing interactions nearly compensate each other. It is often asserted that it is the physics of frustration and competition which leads to the finite temperature transition, and that also controls and enables the interesting properties of materials as they are brought to the $T = 0$ QCP.

In this section, we intend to give a short introduction to the theoretical idea of quantum criticality. In the previous section, we have seen the experimental evidence that by applying pressure, magnetic field, or doping, a second-order phase transition can be tuned to zero temperature, producing a quantum critical point. Associated with such a singular point, ordinarily anomalous scaling behaviors emerge in various finite-temperature properties of the system, such as specific heat, resistivity and magnetic susceptibility, which goes far beyond our conventional understanding of metals. One of the basic questions arising from the experimental findings is how the zero temperature phase transition point is related to the finite temperature behavior of the system. The theoretical idea of quantum criticality states that the zero temperature QCPs actually profoundly modify finite temperature properties of the quantum critical metals.

The basic concepts of quantum criticality is best illustrated by a simple model: the 1+1-dimensional Ising chain in a transverse field. This model can be solved

exactly and it is the hydrogen atom of quantum phase transitions. One can find a comprehensive introduction to this model in Sachdev's book [40]. We will summarize the essential points here. The Hamiltonian is of the form,

$$H_I = -J \sum_i \left(\hat{\sigma}_i^z \hat{\sigma}_{i+1}^z + g \hat{\sigma}_i^x \right). \tag{1.25}$$

Here the overall coefficient $J > 0$ is an exchange constant. It sets the microscopic energy scale of the system. When temperature is much larger than J, the properties are nonuniversal. In the following, we consider temperature within the range $T \ll J$. $\hat{\sigma}$'s are the Pauli matrices. $g > 0$ is a dimensionless coupling. When $g = 0$, the ground state is a product of eigenstates of $\hat{\sigma}_i^z$. It is a ferromagnetic state, with all the spins aligned up, either all in the spin up state or all in the spin down state. The Z_2 symmetry, $\hat{\sigma}_i^z \to -\hat{\sigma}_i^z, \hat{\sigma}_i^x \to \hat{\sigma}_i^x$, is broken. For $g \to \infty$, the ground state is a product of eigenstates of $\hat{\sigma}_i^x$, $|\to\rangle_i = (|\uparrow\rangle_i + |\downarrow\rangle_i)/\sqrt{2}$. This state restores the above Z_2 symmetry. Then the question is what happens in-between the two limits.

This quantum model can be mapped to a classical model in 2 dimension. Temperature in the quantum model corresponds to the total length of the classical system in the time direction, and gap in the quantum model is mapped to the correlation length along the time direction. One can introduce the concept of dynamical critical exponent z, which relates the scaling in the time direction to the space direction, and frequency scales with momentum as $\omega \sim k^z$. In the quantum Ising model, $z = 1$.

The immediate consequence of this mapping is that the zero temperature phase transition in the quantum Ising model is second order. The Hamiltonian is invariant under the above Z_2 transformation. So this symmetry can only be broken spontaneously, which also points to a second order phase transition. For $g \gg 1$, the correlation in $\hat{\sigma}_i^z$ is short-ranged, decaying as $\langle 0|\hat{\sigma}_i^z \hat{\sigma}_j^z|0\rangle \sim \exp(-|x_i - x_j|/\xi)$ at long distance, with ξ the correlation length. For $g \ll 1$, there is spontaneous symmetry breaking, with $\langle 0|\hat{\sigma}_i^z|0\rangle$ finite.

This model can be mapped to a free fermion problem and solved exactly. By making the Jordan-Wigner transformation, with the spin axes rotated by $\pi/4$ about the y axis, $\hat{\sigma}_i^x = 1 - 2c_i^\dagger c_i$, $\hat{\sigma}_i^z = -\prod_{j<i}(1 - 2c_j^\dagger c_j)(c_i + c_i^\dagger)$, the Hamiltonian reads in momentum space

$$H_I = J \sum_k \left(2[g - \cos(ka)] c_k^\dagger c_k - i \sin(ka)[c_{-k}^\dagger c_k^\dagger + c_{-k} c_k] - g \right), \tag{1.26}$$

where a is the lattice spacing. A Bogliubov transformation $c_k = u_k \gamma_k + i v_k \gamma_{-k}^\dagger$ brings the above quadratic Hamiltonian into the simple form, $H_I = \sum_k \varepsilon_k (\gamma_k^\dagger \gamma_k - \frac{1}{2})$, with $\varepsilon_k = 2J\sqrt{1 + g^2 - 2g\cos k}$. For $g \neq 1$, there is an energy gap at $k = 0$, with amplitude $2J|1 - g|$, which vanishes at $g = 1$. So $g = 1$ is expected to be the phase transition point, at which fermions dominate the low energy properties.

Near this point, the system is described by a universal continuum field theory, with partition function

$$\begin{aligned} \mathcal{Z} &= \int \mathcal{D}\Psi\mathcal{D}\Psi^\dagger \exp\left(-\int_0^\beta d\tau dx \mathcal{L}_I\right) \\ \mathcal{L}_I &= \Psi^\dagger \frac{\partial \Psi}{\partial \tau} + \frac{c}{2}\left(\Psi^\dagger \frac{\partial \Psi^\dagger}{\partial x} - \Psi \frac{\partial \Psi}{\partial x}\right) + \Delta \Psi^\dagger \Psi, \end{aligned} \tag{1.27}$$

with higher order terms all irrelevant. Here the continuum Fermi field $\Psi(x_i) = c_i/\sqrt{a}$, and coupling constants $c = 2Ja, \Delta = 2J(1-g)$. At the critical point, $g = 1$ and $\Delta = 0$. We also notice that above the energy scale J, lattice effects will be important, and the above critical field theory is no longer adequate to describe the system. So J is the ultraviolet cutoff ω_c of the critical theory. Here Δ is the most relevant perturbation about the QCP and it has scaling dimension 1. The correlation length scales as $\xi \sim |g - g_c|^{-\nu}$, and one can read off the critical exponent $\nu = 1$.

The two-point correlation functions read for $\tau > 0$,

$$\begin{aligned} \langle \Psi(x,\tau)\Psi^\dagger(0,0)\rangle =& \frac{T}{4c}\left(\frac{1}{\sin(\pi T(\tau - ix/c))} + \frac{1}{\sin(\pi T(\tau + ix/c))}\right), \\ \langle \Psi(x,\tau)\Psi(0,0)\rangle =& i\frac{T}{4c}\left(\frac{1}{\sin(\pi T(\tau - ix/c))} - \frac{1}{\sin(\pi T(\tau + ix/c))}\right). \end{aligned} \tag{1.28}$$

The $T = 0$ result and $T > 0$ result is connected by the conformal mapping from a plane to a cylinder,

$$c\tau \pm ix \to \frac{c}{\pi T}\sin\left(\frac{\pi T}{c}(c\tau \pm ix)\right). \tag{1.29}$$

The central object of this model is the order parameter correlation function $C(x_i, t) = \langle \hat{\sigma}^z(x_i, t)\hat{\sigma}^z(0,0)\rangle$. The equal-time correlation function can be calculated from the fermion representation. At long distance, it has the scaling form

$$\lim_{|x|\to\infty} C(x,0) = ZT^{2s} G_I\left(\frac{\Delta}{T}\right)\exp\left[-\frac{T|x|}{c}F_I\left(\frac{\Delta}{T}\right)\right]. \tag{1.30}$$

The operator $\hat{\sigma}^z$ has dimension $s = 1/8$. F_I and G_I are universal scaling functions, and they are smooth across the critical point $\Delta = 0$. One can see clearly from the above expression that there is only long-range order at zero temperature. At any finite temperature, the correlation decays exponentially, with correlation length $\xi = c/(TF_I)$. With ξ behaving qualitatively differently in different regions of the parameter space, the phase diagram is divided into several different regions. This can already been seen by just comparing the two energy scales Δ and T. And the crossover lines are at $\Delta \sim T$. When $\Delta > 0, T \ll \Delta$, one has $\xi^{-1} = (2|\Delta|T/\pi c^2)^{1/2}\exp(-|\Delta|/T)$. For $\Delta < 0, T \ll |\Delta|$, the correlation length

is given by $\xi^{-1} = |\Delta|/c + (2|\Delta|T/\pi c^2)^{1/2} \exp(-|\Delta|/T)$ and reaches a finite value as $T \to 0$. In the region with $T \gg |\Delta|$, the correlation length is $\xi = 4c/\pi T$, which has the quantum critical scaling form $T^{-1/z}$, and this region is called the quantum critical region (see Fig. (1.6)).

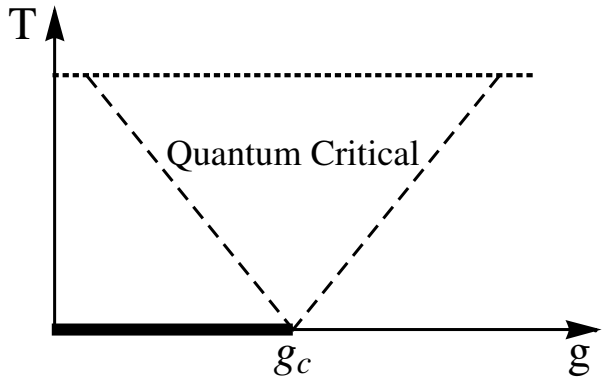

Figure 1.6: Theoretical phase diagram of the 1+1-dimensional quantum Ising model. The dashed lines are the crossover lines $|\Delta| = 2J|g - g_c| \sim T$, with the critical coupling $g_c = 1$. The dotted line represents the ultraviolet cutoff energy scale $T \sim J$. The thick solid line at $T = 0, 0 < g < g_c$ is the region in the phase diagram with long-range order. The ground state at $T = 0, g > g_c$ is a quantum paramagnet. The triangular region in the center is the quantum critical region.

In the quantum critical region, the order parameter susceptibility can be easily derived from the universal two-point correlator at an imaginary time τ. One starts from the equal-time correlator at $T = 0, \Delta = 0$,

$$C(x, 0) \sim \frac{1}{(|x|/c)^{2s}}. \tag{1.31}$$

The consideration here is quite general, not just restricted to the Ising model, which has $s = 1/8$. Due to Lorentz invariance, the time direction can be included simply,

$$C(x, \tau) \sim \frac{1}{(\tau^2 + x^2/c^2)^s}. \tag{1.32}$$

The finite temperature result can be obtained through the transformation (1.29),

$$C(x, \tau) = \tilde{Z} \frac{T^{2s}}{(\sin[\pi T(\tau - ix)] \sin[\pi T(\tau + ix)])^s}. \tag{1.33}$$

The analytical continuation to real time $\tau \to it$ yields the real time two-point

correlation function

$$C(x,t) = \tilde{Z}\frac{T^{2s}}{(i\sinh[\pi T(t-x)]i\sinh[\pi T(t+x)])^s}, \tag{1.34}$$

with a Fourier transform corresponding to the dynamic structure factor

$$S(k,\omega) = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dt C(x,t) e^{-i(kx-\omega t)}. \tag{1.35}$$

A convenient way to perform the Fourier transform is by factorizing $C(x,t)$ into left-moving and right-moving modes, $C(x,t) = C_-(t-x)C_+(t+x)$, to subsequently integrate over $t \pm x$. The result is

$$S(k,\omega) = Ze^{\frac{\omega}{2T}}\frac{1}{T^{2(1-2s)}}B(s+i\frac{\omega+k}{4\pi T}, s-i\frac{\omega+k}{4\pi T})B(s+i\frac{\omega-k}{4\pi T}, s-i\frac{\omega-k}{4\pi T}), \tag{1.36}$$

where B is the beta function, and the overall numerical coefficient $Z = 2^{4s-3}\pi^{2(s-1)}\tilde{Z}$. The fluctuation-dissipation theorem

$$S(k,\omega) = \frac{2}{1-e^{-\omega/T}}\chi''(k,w) \tag{1.37}$$

then yields the imaginary part of the order parameter susceptibility,

$$\chi''(k,\omega) = Z\frac{\sinh(\frac{\omega}{2T})}{T^{2(1-2s)}}B(s+i\frac{\omega+k}{4\pi T}, s-i\frac{\omega+k}{4\pi T})B(s+i\frac{\omega-k}{4\pi T}, s-i\frac{\omega-k}{4\pi T}). \tag{1.38}$$

Indeed $\chi''(\omega) \to 0$ in a linear fashion with ω with a slope set by $1/T$, while for $\omega >> T$ the temperature dependence drops out, recovering the power law. The crossover occurs at $\omega \simeq 2k_BT/\hbar$ where $\chi''(\omega)$ has a maximum. This result will be used in the later chapters when we consider superconductivity in quantum critical metals. The real part can be computed from the Kramers-Kronig transform,

$$\chi'(k,\omega) = \frac{Z'}{T^{2(1-2s)}}\left(\frac{-i\pi}{s-i\frac{\omega+k}{4\pi T}}\frac{\sin(2s\pi-\frac{ik}{2T})}{\sinh(\frac{k}{2T})}\frac{\Gamma(2s)\Gamma(2s-\frac{ik}{2\pi T})}{\Gamma(1-\frac{ik}{2\pi T})}\right.$$
$$\left.{}_3F_2(2s, s-i\tfrac{\omega+k}{4\pi T}, 2s-\tfrac{ik}{2\pi T}; 1+s-i\tfrac{\omega+k}{4\pi T}, 1-\tfrac{ik}{2\pi T}; 1) + (k \to -k)\right) \tag{1.39}$$

where F is the generalized hypergeometric function.

In summary, we have shown that for the 1+1-dimensional quantum Ising chain in the quantum critical region $|\Delta| \ll T \ll J$, the finite temperature properties of the system are related to its property at the zero temperature critical point $\Delta = 0, T = 0$ simply by conformal mapping (1.29). As one approaches the QCP, the correlation length scales as $\xi \sim |g - g_c|^{-\nu}$, and the correlation time scales as $\xi_\tau \sim \xi^z$. Here the critical exponents are $z = 1, \nu = 1$. For higher dimensional systems, the mapping will be more complex. But the basic idea of finite size scaling in the temporal direction is the same. The critical exponents are different for different universal classes. The fact that there is only long-range order at zero temperature is the special property of 1+1 dimension. In higher dimensional systems, the ordered phase can extend to finite temperature, occupying a finite region in the phase diagram.

1.5 This thesis

This thesis is divided into two parts. The first part (Chapters 2 and 3) is about worldline path integrals and the fermion nodal structure. The second part (Chapters 4, 5, 6) is about quantum criticality and its interplay with superconductivity. There are actually intrinsic connections between the two, though they look far apart at first glance. The study of the nodal structure of the fermionic wavefunctions and density matrices serves as an antidote to the conventional Fermi gas way of thinking. What we learn from exploring the nodes is that the world of condensed matter systems is not just about the single particle Green's functions, and the many-body entanglement perspective is crucial for the understanding of emergent phenomena. Nature has already revealed this to us when the FQHE was discovered: Laughlin's wavefunction contains much more information than a single particle Green's function, or even earlier, when Schrieffer wrote down the simple wave function for the superconducting ground state. A simple step going beyond the Fermi gas way of thinking would be to consider the two particle correlation functions, e.g. charge susceptibility, spin susceptibility and pairing susceptibility, to be as fundamental as the single particle Green's functions, which is the basic idea of Chapter 5.

We start in Chapter 2 with the signful worldline path integrals. The Feynmanian deconstruction of the order parameter is shown explicitly by calculating, in the first quantized path integral formalism, the effect of the condensation of a gas of charged particles in the background magnetic field. Coupling to a bosonic condensate generates a mass term for the background magnetic field, leading to the Anderson-Higgs effect. The value of the mass is determined by the number density of the condensed particles. In this formalism, the fermionic statistics are encoded via the inclusion of additional Grassmann coordinates in a manner that leads to a manifest worldline supersymmetry. This extra symmetry is key in demonstrating the absence of the Anderson-Higgs effect for charged fermions.

In Chapter 3, we study the fermion sign problem in the worldline path integral formalism. The insightful work of Ceperley in constructing fermionic path integrals in terms of constrained world-lines is reviewed. In this representation, the minus signs associated with Fermi-Dirac statistics are self consistently translated into a geometrical constraint structure, the nodal hypersurface, acting on an effective bosonic dynamics. Working with the path integral in momentum space, we then show that the Fermi gas can be understood by analogy to a Mott insulator in a harmonic trap. Going back to real space, we discuss the topological properties of the nodal cells, and suggest a new holographic conjecture relating Fermi liquids in higher dimensions to soft-core bosons in one dimension.

We turn to the exploration of quantum criticality in Chapter 4. In this chapter, we consider the dynamics of the bosonic order parameters around the QCPs, assuming that the fermionic degrees of freedom can be integrated out. We are interested in the stability of QCPs in the presence of two competing phases. These phases near QCPs are assumed to be either classical or quantum and as-

sumed to repulsively interact via square-square interactions. We find that for any dynamical exponents and for any dimensionality strong enough interaction renders QCPs unstable, and drives transitions to become first order. We propose that this instability and the onset of first-order transitions lead to spatially inhomogeneous states in practical materials near putative QCPs. Our analysis also leads us to suggest that there is a breakdown of Conformal Field Theory (CFT) scaling in the Anti de Sitter models, and in fact these models contain first-order transitions in the strong coupling limit.

In particular, we carry out the renormalization group (RG) analysis of two coupled order parameters with different dynamical exponents, and we find a line of fixed points in such theories. The RG analysis of such models is not an easy task. The conventional picture is that in d spatial dimensions, the quantum field theory of a bosonic field with dynamical exponent z is equivalent to a classical field theory in d + z dimensions. This picture still holds when there are more than one field, but all the fields have the same dynamical exponent. However, when the coupled fields have different dynamical exponents, this picture is no longer valid: the fields are frustrated in choosing their effective dimensions. Technically, this problem arises in the RG analysis for example when one calculates the loop diagrams containing internal lines corresponding to fields with different dynamical exponents. If we think more carefully about how one arrives at the conventional way of counting effective dimensions, we will find that one has to rescale the parameters to absorb the generally dimensionfull coefficient in the frequency dependent terms, the presence of which ensures these terms to have the right dimensions. We will show explicitly such rescaling. With distinct dynamical exponents, one can no longer rescale out these coefficients. They actually lead to dramatically different scaling behavior in the RG structure.

In Chapter 5, we present a simple phenomenological scaling theory for the pairing instability of a quantum critical metal. It can be viewed as a minimal generalization of the classical BCS theory of superconductivity for normal Fermi liquid metals. We assume that attractive interactions are induced in the fermion system by an external bosonic glue that is strongly retarded. Resting on the small Migdal parameter, all the required information from the fermion system needed to address the superconductivity enters through the pairing susceptibility. Asserting that the normal state is a strongly interacting quantum critical state of fermions, the form of this susceptibility is governed by conformal invariance and one only has the scaling dimension of the pair operator as free parameter. Within this scaling framework, conventional BCS theory appears as the marginal case but it is now easily generalized to the (ir)relevant scaling regimes. In the relevant regime an algebraic singularity takes over from the BCS logarithm with the obvious effect that the pairing instability becomes stronger. However, it is more surprising that this effect is strongest for small couplings and small Migdal parameters, highlighting an unanticipated important role of retardation. Using exact forms for the finite-temperature pair susceptibility from 1+1D conformal field theory as models, we study the transition temperatures, finding that the gap

to transition temperature ratios is generically large compared to the BCS case, showing, however, an opposite trend as a function of the coupling strength compared to the conventional Migdal-Eliashberg theory. We show that our scaling theory naturally produces the superconducting domes surrounding the quantum critical points, even when the coupling to the glue itself is not changing at all. We argue that hidden relations will exist between the location of the crossover lines to the Fermi liquids away from the quantum critical points and the detailed form of the dome when the glue strength is independent of the zero-temperature control parameter. Finally, we discuss the behavior of the orbital-limited upper critical magnetic field as a function of the zero-temperature coupling constant. Compared to the variation in the transition temperature, the critical field might show a much stronger variation pending the value of the dynamical critical exponent.

In Chapter 6, we propose to use the second order Josephson effect as a direct probe of the Cooper channel of quantum critical metals, to shed light on the problem of unconventional superconductivity in such systems. We review the idea of Ferrell and Scalapino who suggested a superconductor-insulator-normal (SIN) tunneling setup in which a strong superconductor acts as an effective external probe for a normal metallic state above its superconducting transition temperature T_c. The fluctuating pair field of the metal is coupled to the rigid pair-field of the strong superconductor, and this leads to an additional contribution to the total tunneling current, on top of the well-known SIN-junction quasiparticle current. This additional tunneling current is proportional to the imaginary part of the pair(ing) susceptibility in the metallic state. We calculate the pair susceptibility for several different scenarios of the pairing mechanism for quantum critical metals, to provide templates for experimentalists. We find that different models differ qualitatively.