

# Chapter 1

## Introduction

**Abstract** This chapter has introductory character and gives the definition and classification of strongly correlated systems. We outline the difference between strongly and weakly correlated systems and show that the former cannot be described adequately in the framework of ubiquitous methods like e.g., band theory of solids. We familiarize the reader with theoretical approaches to strongly correlated systems and to Landau theory of Fermi-liquid in particular. We show that Landau theory is insufficient to describe so-called non Fermi liquid properties of several strongly correlated substances like heavy fermion compounds. For such description, the notion of fermion condensation quantum phase transitions has been introduced. The aims and goals of the book are also discussed.

### 1.1 Introductory Remarks

#### *1.1.1 General Consideration: Strong Versus Weak Correlations*

When we are dealing with an ensemble of particles, which do not interact with each other, the problem can be completely solved analytically. The situation is drastically different, when even weak interparticle interaction is “turned on”: In this case the problem ceases to be single-particle and many body effects enter the scene. As modern physics is dealing primarily with the ensembles of interacting particles, it is not an exaggeration to say, that its central problem is the many-body theory. Indeed, all our surroundings, from cosmic bodies to tiny objects like molecules, are made of many constituents. This statement is also valid for microscopic particles like atoms and nuclei. Several decades ago it became clear that, perhaps, only quarks and leptons can be considered as truly elementary particles, which cannot be splitted into smaller entities.

To form a body of any size, the constituent particles have to interact with each other. Such an interaction is achieved by exchange of these particles by quanta of interaction field—photons, gluons, and mesons. However, if the speed of interacting particles is much less than the speed of light, the interaction can be limited to either some phenomenological potentials, or, for charged objects and not too small distances, to pure Coulomb interaction.

The materials, that are well understood, usually contain the ensemble of free or almost free weakly interacting (or weakly correlated) particles. To understand the latter materials, band theory, which represent electrons in the form of extended plane waves, is a good starting point. That theory helps capture the delocalized nature of electrons in metals. It is valid provided that the Coulomb interaction energy of electrons is much smaller than their kinetic energy. However there are important physical systems for which interactions between the electrons are not weak, and these interactions play a major role in determining the properties of such systems. They are usually called strongly correlated systems. The examples here can be metals with open  $d$ - and  $f$ - electron shells, where electrons occupy narrow bands. There, electrons experience strong Coulomb repulsion because of their spatial confinement in those bands. The effect of correlations on the physical properties of such objects is often profound. The interplay of the  $d$  and  $f$  electrons internal degrees of freedom like spin, charge, and orbital moment can exhibit a lot of exotic phenomena at low temperatures. That interplay makes strongly correlated electron systems extremely sensitive to small variations of external parameters, such as temperature, pressure, or magnetic field.

In materials called heavy fermion systems, mobile electrons at low temperatures behave as if their masses were a hundred times the mass of an electron in a silicon or simple metal. Such systems exhibit a great variety of interesting phenomena like anomalies in electric and thermal conductivity, quantum phase transitions between magnetically ordered state and superconductivity, emergence and dissociation of local magnetic moments etc. This rich variety of the phenomena makes their experimental and theoretical studies all the more difficult. Quantum mechanical study of strongly correlated fermionic systems is done by two approaches: *ab-initio* numerical electronic structure simulations and model theoretical treatment. In the first case real materials can be described with all details of their chemical composition and crystal structure fully taken into account. In model approaches, such subtleties are usually neglected in favor of more rigorous mathematical treatment of the problem. The result yields the dependencies (in graphical and sometimes in analytical form) of system physical properties upon external parameters like temperature, pressure and/or external fields. But nowadays even in latest theoretical treatment, the solutions of derived equations could be obtained by means of numerical calculations only.

In this context we mention so-called optical lattices, consisting of boson atoms ensemble in a periodic potential. At low temperatures such Bose particles can condense: i.e. most of the particles can be found in a state of zero momentum, which helps to minimize their kinetic energy. Below we will see that related phenomenon can occur in the systems with strongly correlated fermions, giving rise to completely new physics, which is the same for many seemingly different systems. We will see also that the notion of fermion condensation permits to elegantly explain the whole bunch of puzzling experimental facts in systems with strongly correlated fermions. At this moment, a good general approach accepted for understanding strongly correlated systems does not exist. For example, certain aspects of systems exhibiting quantum Hall effect or some magnetic materials are already understood. But the other systems are understood very poorly. For instance, the nature of high temperature

superconductivity remains mysterious despite decades of intensive work. Most importantly we do not have a unified view on the fermionic systems for which interparticle interactions not only cannot be neglected but play a decisive role in the formation of their observable properties.

### ***1.1.2 Theoretical Approaches to Strongly Correlated Systems***

A natural question appear: How to solve a many-body problem? In other words, how to describe a system of large number of interacting constituents knowing how to deal with single free particle motion and its interaction with the other particle and environment? This problem is not new and by far not specific to quantum systems. Indeed, this problem existed already at the time when Newton created his mechanics and discovered the law of gravitation. However, in the case of relatively weak gravitational interaction only two-body dynamics is essential so that the rest of particle ensemble could be treated as small perturbation. For instance, the Moon and all other planets of Solar system affect the Earth rotation around the Sun as a small, although noticeable perturbation. Only recently it became clear that in some cases even weak gravitational interaction can lead to prominent many-body effects, so called resonance phenomena.

In quantum mechanics, the many-body problem became essential almost immediately after discovery of the Schrödinger equation [1] in 1926. The motivation was the fact that the potential, in which the given quantum particle (say, electron) moves, is created by the rest of the particles, where this electron resides. At that time it had already been recognized, that the electron-electron interaction in atoms plays less important role than their interaction with the atomic nucleus. This hierarchy is similar to that in Solar system in regard of inter-planet and Sun-planet interactions. Already in 1928 D. Hartree suggested the concept of self-consistent field [2, 3] that permitted to consider many—electron atoms treating their electrons as moving in a field essentially modified as compared to the pure Coulomb field of an atomic nucleus. Tho years later V. A. Fock took into account the fact that all electrons are identical Fermi particles so that their wave function has to be antisymmetric under permutation of any two electrons [4, 5]. As a result, prominent Hartree-Fock equation had been formulated. This equation is in use until now, being applied not only to single atoms, but to multi-atomic objects like molecules, clusters, fullerenes and even bulk solids. The application of the Hartree-Fock equation is not limited to the systems with Coulomb interparticle interaction. The same equation can be successfully applied to nucleus as a system consisting of protons and neutrons. Actually Hartree-Fock equation considers only non-perturbative part of interparticle interaction; it can also be applied to the systems of Bose particles where it is called Gross-Pitaevskiy equation.

The remaining part of interparticle interaction that is neglected in the Hartree-Fock framework is usually called *residual interaction*. This part of interaction leads to so-called *correlation effects*, or *interparticle correlations*. Obviously, the Hartree-Fock equation is able to describe many-body system satisfactorily only if correlations

are negligible. However, as it is known now, there exist a number of many body systems, where correlations lead to decisively important *collective phenomena*.

We note here, that Hartree-Fock approach along with little earlier Thomas-Fermi approach [6, 7] were the first representative of so-called first principle (*ab initio*) methods to incorporate the above collective phenomena in the physical properties of solids and strongly correlated systems in particular. The aim of such methods is to calculate the macroscopic, observable properties of a body having in disposal its microscopic characteristics like its crystalline symmetry and interatomic interaction potentials. If all microscopic details were known, the problem would be solved exactly utilizing (many-particle) Schrödinger equation. Unfortunately, this is not the case for majority of real systems. Only molecules consisting of small number of atoms as well as single atoms can be more or less satisfactorily treated by this straightforward method. In this approach, their wave functions are represented as linear combinations of corresponding Slater determinants.

Further development of *ab-initio* methods was related to the breakthrough, made by Hohenberg-Kohn theorem, which puts a foundation to the Density Functional Theory (DFT) [8–11]. The Hohenberg-Kohn theorem states that a system's wave function is defined uniquely by its charge density. The idea of DFT is a direct generalization of Hartree-Fock self-consistent field approach. Namely, in DFT, the differential equations called Kohn-Sham equation for single-electron wave functions are solved with certain effective potential, which, in turn, is determined self-consistently by that equation's solutions. This Kohn-Sham equation is derived by variation of the energy functional  $E[\rho]$ , depending on the local electronic charge density  $\rho = \rho(\mathbf{r})$ . This functional, expressing the total energy of many-body system, has the form [10]

$$E[\rho] = T[\rho] + \int \rho(\mathbf{r}) V_{ext}(\mathbf{r}) d^3r + \int d^3r d^3r' \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + E_{xc}[\rho], \quad (1.1)$$

where  $T[\rho]$  is kinetic energy,  $V_{ext}(\mathbf{r})$  is the external potential acting on the electrons, third term is the Hartree contribution to the Coulomb interaction between the charges, and the last term is the so-called exchange and correlation energy contributions  $E_{xc}[\rho]$ . The exchange contribution takes into account the partial suppression of Coulomb repulsion between electrons in the same spin state due to Pauli principle. The DFT method would be exact if the explicit form of the term  $E_{xc}$  in (1.1) would be known. However, this is not the case, as for that one needs to solve the system of functional equations exactly [12].

To handle this problem, the DFT self-consistent approach along with approximations (like, for instance, local density approximation (LDA) and its spin counterpart local spin density approximation (LSDA), see [13] for details) for exchange- correlation energy  $E_{xc}$  had been utilized in DFT. Also, as particular representation of wave functions corresponding to  $\rho(\mathbf{r})$  cannot be defined uniquely in DFT, this quantity is expressed usually via single-electron wave functions  $\psi_i(\mathbf{r})$

$$\rho(\mathbf{r}) = \sum_{i=1}^N |\psi_i(\mathbf{r})|^2, \quad (1.2)$$

where  $N$  is the number of electrons in a system.

Minimizing the functional (1.1) over the functions  $\psi_i(\mathbf{r})$  (with respect to the normalization conditions for  $\psi_i$ ) generates Kohn–Sham equations:

$$\left[ -\frac{\nabla^2}{2m} + V_{KS}[\rho(\mathbf{r})] \right] \psi_i = \varepsilon_i \psi_i, \quad (1.3)$$

where  $\varepsilon_i$  are the single-electron eigenvalues, Kohn–Sham potential  $V_{KS}$  represents a static mean field (signifying the explicit neglecting of correlation effects when all electrons feel the same potential) of the electrons and has to be determined in a self-consistent way

$$V_{KS}[\rho(\mathbf{r})] = V_{ext}(\mathbf{r}) + V_{xc}[\rho(\mathbf{r})] + 2 \int \frac{\rho(\mathbf{r}') d^3 r'}{|\mathbf{r} - \mathbf{r}'|}, \quad V_{xc}[\rho(\mathbf{r})] = \frac{\delta E_{xc}[\rho(\mathbf{r})]}{\delta \rho(\mathbf{r})}, \quad (1.4)$$

where  $\delta/\delta\rho$  means the variational derivative. The (1.4) allows one to calculate electronic charge density and total energy for the ground state of a system. The DFT with LDA and/or LSDA approximations for  $E_{xc}[\rho]$  had been successfully applied to describe the electronic properties of atoms, molecules and solids, where correlation effects are not too strong. In the systems with strong correlations like transition metal oxides, the DFT gave incorrect metallic ground state in the absence of long-range magnetic order.

As in 1960-ties the computational power was too feeble to calculate real things by ab initio methods, the so-called model Hamiltonian approach comes into play. Namely, the full many-body Hamiltonian is simplified to account for only a few relevant degrees of freedom—typically, the valence electron orbitals near the Fermi level. One of the simplest models of correlated electrons is the Hubbard Hamiltonian [14], which takes into account the interplay between electron hopping and local on-site repulsion:

$$\mathcal{H} = \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (1.5)$$

where  $c_{i\sigma}$  and  $c_{i\sigma}^\dagger$  are creation and annihilation operators for electron on site  $i$  with spin index  $\sigma = \uparrow, \downarrow$ ,  $n_i = c_{i\sigma}^\dagger c_{i\sigma}$  is the density of electrons at site  $i$ ,  $U$  is a local Coulomb interaction between two electrons occupying the same site  $i$ . The matrix element  $t_{ij}$  describes hopping of electrons with between sites  $i$  and  $j$ . It is usually supposed that hopping is not zero for nearest neighbors (with number  $z_n$ ) only. Such simplified treatment of electron–electron Coulomb repulsion turns out to be very convenient to study the itinerant electron systems, especially their magnetic states. A wide variety of analytical and numerical methods have been utilized to study the

strongly correlated electron systems in the framework of Hubbard model. But despite that, the Hubbard model (1.5) could be solved only for limited number of cases.

It had been observed in 1989 [15] that the consideration of the electron correlations on the lattices with large (actually infinite) number of nearest neighbors  $z_n$ , simplifies the problem essentially so that it can be solved exactly for any strength of Coulomb repulsion. The simplification at  $z_n \rightarrow \infty$  occurs due to the fact that in this case one can neglect the spatial fluctuations leaving only time dependent on-site fluctuations. This fact laid the foundation of Dynamical Mean-Field Theory (DMFT), which mapped lattice models (like Hubbard one [16, 17]) to effective impurity problem with correlated electrons feeling mean field which this time is dynamic, i.e. time or energy dependent. Solution of the latter effective impurity problem can be further used to construct the self-energy for lattice Green's function  $G$  that, in turn, gives new approximation for above dynamic mean-field. The DMFT solutions become exact as the number of neighbors increases. Similar to DFT, the DMFT also relies on energy functional  $E_{DMFT}[\rho(\mathbf{r}), G]$ , which in this case depends on the above local Green's function  $G$ :

$$E_{DMFT}[\rho(\mathbf{r}), G] = T[\rho(\mathbf{r}), G] + \int \rho(\mathbf{r}) V_{ext}(\mathbf{r}) d^3 r + \int d^3 r d^3 r' \frac{\rho(\mathbf{r}) \rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + E_{xc}[\rho(\mathbf{r}), G], \quad (1.6)$$

where  $G = G_{i\sigma}(t - t') = - \langle c_{i\sigma}(t) c_{i\sigma}^\dagger(t') \rangle$  specifies the probability to create an electron with spin index  $\sigma$  at a site  $i$  at time  $t'$  and annihilate it at the same site at a time  $t > t'$ . In practical calculations this function is found self-consistently from the above effective single-impurity problem, where the rest of the electrons are considered as the bath for given impurity one. The theory is called “dynamic” as Green's function depends explicitly on time or frequency argument. Also, the approximations for  $E_{xc}[\rho(\mathbf{r}), G]$  are provided.

Although dynamical mean-field methods clearly represent a new advance in many-body physics, they are still unable to capture many effects in strongly correlated systems, e.g., the divergent behavior of the effective mass. That is why generalizations of DMFT to account for real materials is an active area of research. The above consideration shows that only ab-initio methods in principle cannot give sufficient insights in the physics of strongly-correlated systems because of their computational complexity, still beyond reach of modern computer's possibilities. The more insight has been achieved on the way of model assumptions and simplification of initial many-body Hamiltonian, leaving in them only the most essential terms, which, on the other hand, could be assessed both analytically and numerically. Nonetheless, these methods meet with enormous difficulties while being applied to consideration of excitation spectra of a many-body system, while these spectra define the thermodynamic, transport and relaxation properties.

The complimentary approach essential break-through in the understanding of many-body systems was the introduction of so-called *quasiparticles*. Namely, the real interacting (with potential  $V$ ) particle ensemble is substituted by quasiparticles, that interact via some *effective* interaction  $V_{\text{eff}}$  and represent the excitation on top of some vacuum ground state.

Then the question appears how to construct the quasiparticles and their effective interaction. At a first glance, this is a simple problem, if the interaction is weak. But what is the meaning of weakness if, roughly speaking, the effect of interaction includes in some cases a large number generated by the corresponding phase transition. So, the weakness can be overwhelmed by the large number, leading to macroscopic correlated coherent phenomena like superfluidity and/or superconductivity.

The first attempt in this direction was undertaken by Landau in 1956 [18], when he assumed the existence of quasiparticles, and afterwards, when he, together with his colleagues gave a proof of the developed approach on the general grounds of many-body theory [19]. He suggested that for systems where the interaction is strong, quasiparticles can be introduced as well defined objects. The ground state energy  $E$  in that case is assumed to be a functional of the quasiparticle distribution function  $n(\mathbf{p})$ ,  $E[n(\mathbf{p})]$ , with the single particle spectrum (or the dispersion law)  $\varepsilon(\mathbf{p}) = \delta E[n(\mathbf{p})]/\delta n(\mathbf{p})$ . According to conventional usual practice a quasiparticle is presumed to be well-defined until proven not to be. The textbook picture of quasiparticles as long-living excitations weakly interacting with each other works very well for many objects. This system of quasiparticles forms the Landau quasiparticle paradigm. Nevertheless, in a number of recently studied strongly correlated systems the above quasiparticles neither interact weakly nor remain well-defined even at zero temperature. As we shall see in Chap. 2, this paradigm is to be substituted by an extended one. As an example, Landau treated the liquid  $^3\text{He}$ , which is a liquid, whose constituents are Fermi particles—two-electron atoms with  $^3\text{He}$  nuclei. He demonstrated that at low temperatures the excitations of such a system could be described as those of a quasiparticle gas.

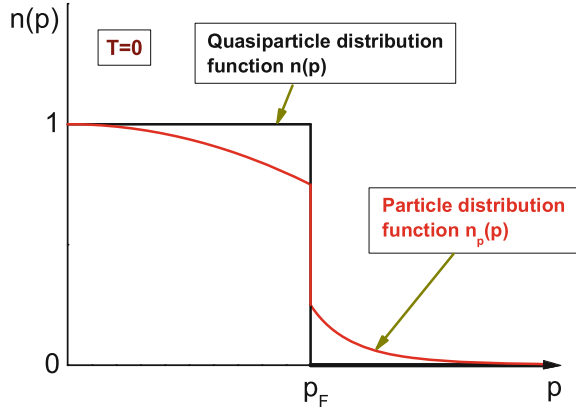
It is worth noting, that at temperature  $T = 0$  in spite of strong interparticle interaction the distribution of quasiparticles  $n(\mathbf{p})$  as a function of their momentum  $p$  can be presented as a Fermi-step of noninteracting fermions:

$$n(\mathbf{p}) = \begin{cases} 1, & p \leq p_F \\ 0, & p > p_F, \end{cases} \quad (1.7)$$

where  $p_F$  is the so-called Fermi-momentum of the system. It is essential that the densities (i.e. total numbers per unit volume) of particles and quasiparticles coincide. E.g., in three dimensional (3D) case they both equal to

$$\rho = \frac{p_F^3}{3\pi^2}. \quad (1.8)$$

**Fig. 1.1** Quasiparticle  $n(\mathbf{p})$  and particle  $n_p(\mathbf{p})$  distribution functions at  $T = 0$  are shown by the arrows.  $n(\mathbf{p})$  is given by (1.7) and  $n_p(\mathbf{p})$  by (1.9) with the jump at  $p = p_F$



Throughout, if otherwise do not stated, we adopt the atomic system of units, where  $\hbar = c = 1$ , where  $c$  is the speed of light. In this book, we consider a different branches of the condensed matter physics. As a result, in some chapters we use those systems of units which are commonly accepted in the considered area. For example, as it is done in Chap. 12.

As to the momentum dependence of the *particle* distribution function  $n_p(\mathbf{p})$ , it has, according to Migdal [20], a tail at  $p > p_F$ , in contrast to the distribution function of quasiparticles. This tail decreases as  $p$  increases. This decrease is fast, but not exponential. In the same paper [20], it had been demonstrated that at  $p = p_F$  the function  $n_p(\mathbf{p})$  has a step:

$$0 < n_p(p_F) = z < 1. \quad (1.9)$$

It is seen from (1.7), (1.9) and Fig. 1.1, that both the quasiparticles and the particles distribution functions have jumps at the Fermi momentum  $p_F$ .

The single-particle spectrum  $\varepsilon(\mathbf{p})$  for Landau quasiparticle at  $(p - p_F)/p_F \ll 1$  is similar to that of an excitation of a gas of non-interacting Fermi-particles at low temperatures  $T$

$$\varepsilon(p) - \mu = \frac{p_F(p - p_F)}{M^*}, \quad (1.10)$$

where  $\mu$  is the chemical potential and  $M^*$  is the effective mass that, from case to case, differs from the mass  $M$  in a different degree. Here  $M$  is the bare mass of the particles constituting the many-body system under consideration. In the many-body theory, one usually investigates systems consisting of single-particle type, having the same mass, spin and charge. Generalization to multi-component systems is very often not a simple and straightforward task.

A quasiparticle excitation can decay by creating two and more quasiparticles. If this decay proceeds sufficiently fast, the concept of quasiparticle as well defined



system's excitation faces difficulties. More precisely, before the decay process quasiparticle lives for time (so-called *quasiparticle lifetime*), which is reciprocal to its width  $\gamma$ . It had been also demonstrated by Migdal [20], that the quasiparticle width can be estimated by the following relation

$$\gamma \sim \frac{(p - p_F)^2}{2M^*}. \quad (1.11)$$

Note that  $\gamma \ll \varepsilon(p) - \mu = p_F(p - p_F)/M^*$  at  $(p - p_F)/p_F \ll 1$  and therefore quasiparticle can be considered to be reasonably stable, if they are close enough to the Fermi-surface at any inter-particle interaction strength. The simplest excitation of a Fermi-system, which interacts strongly with an external field, can be viewed as an absorption of its quanta with low excitation energy  $\omega$  and small (as compared to  $p_F$ ) momentum  $k$  by a combination of a quasi-particle of energy  $\varepsilon(p)$  (with  $p > p_F$ ) and quasi-hole  $\varepsilon(p')$  (with  $p' \leq p_F$ ). Note that the energy and momentum conservation is valid:

$$\omega(k) = \varepsilon(p) - \varepsilon(p'), \quad \mathbf{k} = \mathbf{p} - \mathbf{p}'. \quad (1.12)$$

The presence of effective interaction, transforming one electron-hole pair into the second, third and so on, leads to collective response of the Fermi-system on the external field. Due to the presence of  $V_{eff}$ , so-called coherent collective excitations in the Fermi-system are formed. One of examples is a sound-like excitation with  $\omega = c_t k$  termed *zero sound* with propagation velocity  $c_t \geq p_F/M^*$  [19]. General expressions to determine the dependence of excitation energy  $\omega$  upon momentum  $k$  had been derived in [19, 21]. It is essential to have in mind that there exists a profound analogy between quasi-hole in condensed matter and antiparticle in elementary particles theory.

The concept of relatively weakly interacting quasiparticles permits to express the low-temperature thermodynamic and electrodynamic properties of the Fermi-system under consideration via several numbers characterizing the quasiparticles and their effective interaction. For instance, the specific heat  $C$  turned out to be simply proportional to  $M^*$ , which in turn generates its proportionality to the system's temperature  $T$

$$C \propto M^* T. \quad (1.13)$$

At some parameters of the effective interaction a Fermi-liquid can undergo *phase transitions* to other states like ferromagnetic and antiferromagnetic. This corresponds to solutions of Landau equation determining collective excitations that have zero or pure imaginary energy for non-zero momentum. I. Ya. Pomeranchuk derived the conditions [22] yielding the value and sign of  $V_{eff}$ , which is necessary for the susceptibility towards a fictitious external field to become infinite. This means that the system is unstable with respect to transition to certain fundamentally different (than the initial one) ground state, which is already stable for above  $V_{eff}$ . The phase

transitions are of particular interest, since they describe possible system evolution under the action of above weak perturbations. The stability conditions itself can only signal on possible instability of initially chosen system's ground state. But they are not enough for finding the state of a system formed after instability has been developed.

It was common wisdom for many years, that if we augment the above Pomeranchuk conditions by the one, determining the transition to the superconducting state, we are able to describe all possible phase transitions of a Fermi-system. However, for  $^3\text{He}$  the experimental situation is not that clear. The investigation of the heat capacity  $C$  at temperature dropping from tenths of Kelvins down to millikelvin start to contradict the linear law (1.13). The data, instead of temperature independence, demonstrated a more complex law like  $M^* = a + b \ln T$  with very strange at that time possibility of diverging in the limit  $T = 0$  [23]. Starting from millikelvin, new phases, including a superfluid one, were discovered in liquid  $^3\text{He}$  [24]. Arguments appear that for any system a superfluidity is inevitable for sufficiently low  $T$  and therefore strictly speaking the above presented quasiparticle concept in liquid  $^3\text{He}$  is not valid at low temperatures.

The Fermi liquid approach along with quasiparticles paradigm have been successfully applied to studies of electrons in solids and in metals in particular [19, 21]. It appeared that vast majority of properties of electron liquid in metals can be well understood in the framework of the temperature independent Landau-type quasiparticles so that this approach becomes almost universal in quantum liquids description in condensed matter. However, further development of the condensed matter physics shows convincingly that more and more properties of solids either cannot be satisfactorily described by the ordinary Fermi-liquid picture and/or require complete revision of the quasiparticle paradigm. It turned out that latter revision is highly nontrivial task. It appeared, however, that additionally to above Fermi liquid instabilities (i.e. those related to Pomeranchuk's conditions and to transition to superfluid (superconducting) state, another instability was overlooked. Indeed, it has never been discussed what happens to the system if some interparticle interaction generates the divergence of the effective mass  $M^* \rightarrow \infty$  rather than the susceptibility. In this case, as we will see in Chap. 2, all quasiparticle excitation energies equal to zero so that the system resembles a condensate of Fermi particles or Fermi condensation/condensate (FC) [12, 25–28]. Numerous studies has confirmed the possibility of the FC state that exists for certain interparticle interaction potentials and demonstrates its unusual properties. The possibility of the fermion condensation quantum phase transition (FCQPT), preceding FC, does not abandon the concept of quasiparticles. On the contrary, it demonstrates that during this phase transition the quasiparticle effective mass  $M^*$  become dependent on external parameters like temperature, pressure and/or external field. This situation opposes the Landau Fermi-liquid picture, where the effective mass never depend on the above external parameters, being a constant, determined by particle density and their interaction. The above consideration makes it clear that FCQPT has a quantum nature, determining a non-Fermi liquid (NFL) behavior or quantum criticality in strongly correlated systems.

At the beginning, the idea of FC has not been considered by the community too seriously. It was interpreted as a mathematical trick rather than an approach to describe real phenomena. It turns out, however, that above idea is capable to deliver the adequate description of a huge body of otherwise unexplained experimental data. It has been demonstrated several times that classical Landau theory of Fermi liquid is insufficient and too narrow to encompass many experimentally important cases. A variety of these effects appeared in a number of newly discovered systems, including those, explained in the framework of FC picture (see e.g., [26–28]). Abundance of data stimulates to present these results in a form of a book, what makes data better accessible to not only to experts, but also to graduate students who will, hopefully, use this approach in their future research. This approach can be considered as complimentary, but also in many case as an unique tool to treat and describe real systems, exhibiting the quantum criticality.

The physics of quantum matter occupies a substantial part of modern physics. In contrast to the general belief, a quantum matter can show up even at room temperature, as it takes place for electrons in metals, which behave in accordance with the above the famous Landau Fermi liquid (LFL) theory based on the quasiparticle paradigm [18, 19, 24]. We consider the quantum criticality in HF compounds begotten by quantum phase transitions with their quantum critical points located at  $T = 0$ . The quantum criticality describes a new quantum state of matter which exhibits a universal behavior, and can hardly be understood within the framework of the LFL theory. Thus, quantum criticality in materials of significant theoretical and practical interest requires a new theoretical input. Furthermore, there are indications that the relevant new physics demands a departure from the quasiparticle paradigm of LFL theory. One could also expect that we have to confine our consideration to ultra low temperatures. This is not the case since HF compounds, for instance, reveal significant deviation from LFL properties, termed as NFL behavior, for the temperatures as high as tens of Kelvins. On the other hand, as we shall see, HF compounds at their quantum criticality can exhibit a quasi-classical behavior.

From now on, we call HF compounds “strongly correlated Fermi systems” as well. Strongly correlated Fermi-systems, represented by HF compounds, high- $T_c$  superconductors, strongly correlated insulators with spin liquid, quasicrystals, and two-dimensional (2D) Fermi liquids, are among the most intriguing and best experimentally studied fundamental systems in physics, however until very recently these lacked theoretical description [26–28]. The properties of these materials differ dramatically from those of ordinary Fermi-systems [26–39]. For instance, in the case of HF metals, the strong electron-electron correlations lead to a renormalization of  $M^*$ , which may exceed the ordinary, so called “bare” electron mass by several orders of magnitude or even become infinitely large. The effective mass strongly depends on temperature, pressure, or applied magnetic field. HF metals exhibit NFL behavior and unusual power laws of the temperature dependence of the thermodynamic properties at low temperatures. To describe this NFL behavior, the ideas based on the concept of quantum, thermal fluctuations, and Kondo lattice in a quantum critical point (QCP) have been utilized, see e.g., [29, 31, 40–43]. These ideas, however, could not provide a universal description of NFL properties. This generated a real

crisis in physics of HF systems and to overcome this crisis, a new quantum phase transition, responsible for the observed behavior was suggested [26–28, 34–38, 40, 44]. Below we will show that FCQPT based concept of quantum criticality permits to resolve many puzzles of physics of strongly correlated fermion systems, and HF metals in particular.

### ***1.1.3 Quantum Phase Transitions and NFL behavior of HF compounds***

The unusual properties and NFL behavior observed in high- $T_c$  superconductors, HF metals, 2D Fermi-systems and other HF compounds, such as novel insulators and quasicrystals, are assumed to be determined by various magnetic quantum phase transitions [26–36, 38–41]. Since a quantum phase transition occurs at  $T = 0$ , the control parameters are all but temperature, i.e. composition, electron (hole) number density  $x$ , pressure, magnetic field strength  $B$ , etc. A quantum phase transition occurs at a quantum critical point, which separates the ordered phase (emerging as a result of quantum phase transition) from disordered one. It is usually assumed that magnetic (e.g., ferromagnetic and antiferromagnetic) quantum phase transitions with the corresponding critical fluctuations are responsible for the NFL behavior. The critical point of such a phase transition can be shifted to  $T = 0$  by varying the above control parameters.

Universal behavior can be expected only if the system under consideration is sufficiently close to a quantum critical point, e.g., when the correlation length is much larger than the microscopic length scale, so that critical quantum and thermal fluctuations determine the anomalous contribution to the thermodynamic functions of a substance. Quantum phase transitions of this type are so widespread [30–32, 36–40] that we call them ordinary quantum phase transitions [45]. In this case, the physics is determined by thermal and quantum fluctuations of the critical state, while quasiparticle excitations are destroyed by these fluctuations. Conventional arguments that quasiparticles in strongly correlated Fermi liquids “get heavy and die” at a quantum critical point commonly employ the well-known formula based on the assumptions that the  $z$ -factor (the quasiparticle weight in the single-particle state, see above) vanishes at the points of second-order phase transitions [44]. However, it has been shown that this scenario is problematic, see Chap. 3, Sect. 3.2 [46, 47].

The order parameter fluctuations, developing an infinite correlation range, and the vanishing of quasiparticle excitations are considered to be the main reason for the NFL behavior of heavy-fermion metals, 2D fermion systems and high- $T_c$  superconductors [31, 32, 36, 39, 40, 48]. However, this approach faces certain difficulties. Critical behavior in HF metals is observed experimentally at high temperatures comparable to the effective Fermi temperature  $T_k$ . For instance, the thermal expansion coefficient  $\alpha(T)$ , which is a linear function of temperature for normal LFL,  $\alpha(T) \propto T$ , demonstrates the experimental  $\sqrt{T}$  temperature dependence in  $\text{CeNi}_2\text{Ge}_2$  as the temperature decreases from 6 K to at least 50 mK (i.e. varies by two orders

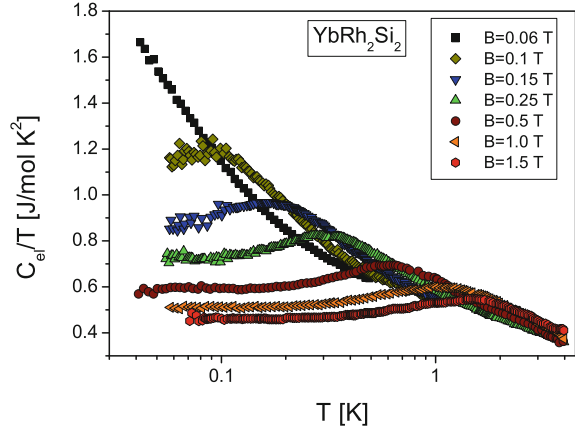
of magnitude) [41]. Such behavior can hardly be explained within the framework of the above critical fluctuation theory. Obviously, such a situation is realizable only at a low-temperature regime,  $T \rightarrow 0$ , when the critical fluctuations make the leading contribution to the entropy and when the correlation length is much longer than the microscopic length scale. At a certain temperature  $T_k$ , this macroscopically large correlation length must be destroyed by ordinary thermal fluctuations and the corresponding universal behavior must disappear.

Another difficulty is in explaining the restoration of the LFL behavior under the application of magnetic field  $B$ , as observed in HF metals and in high- $T_c$  superconductors [29, 41, 49]. At  $T \rightarrow 0$  for the LFL state the following relations are valid for the electric resistivity  $\rho(T) = \rho_0 + AT^2$ , the heat capacity  $C(T) = \gamma_0 T$ , and the magnetic susceptibility  $\chi = \text{const}$ . It turns out that the coefficients in the above laws depend on the magnetic field strength  $B$ . Namely,  $A = A(B)$ , the Sommerfeld coefficient  $\gamma_0(B) \propto M^*$ , and the magnetic susceptibility  $\chi = \chi(B)$ . These quantities depend on  $B$  in such a way that  $A(B) \propto \gamma_0^2(B)$  and  $A(B) \propto \chi^2(B)$ , which implies that the Kadowaki-Woods relation  $K = A(B)/\gamma_0^2(B)$  [50] is  $B$ -independent and is preserved [41]. Such universal behavior, quite natural when quasiparticles with the effective mass  $M^*$  play the main role, can barely be explained within the framework that assumes the absence of quasiparticles or Kondo lattice. We emphasize here, that quasiparticles are absent in ordinary quantum phase transitions in the vicinity of QCP. Indeed, there is no reason to expect that  $\gamma_0$ ,  $\chi$  and  $A$  are affected by the fluctuations in a such a correlated fashion that preserves the Kadowaki-Woods ratio.

For instance, the Kadowaki-Woods relation does not agree with the spin density wave scenario [41] and with the results of research in quantum criticality based on the renormalization-group approach [51]. Moreover, measurements of charge and heat transfer have shown that the Wiedemann-Franz law holds in some high- $T_c$  superconductors [49, 52] and HF metals [53–56]. All this suggests that quasiparticles do exist in such metals, and this conclusion is also corroborated by photoemission spectroscopy results [57, 58]. The inability to explain peculiarities of behavior of HF metals mentioned above in the framework of theories based on ordinary quantum phase transitions implies that another important concept introduced by Landau, the order parameter, also ceases to operate (see, e.g., [36, 38, 40, 44]). Thus, we are left without the most fundamental principles of many-body quantum physics [18, 19, 24], and many interesting phenomena associated with the NFL behavior of strongly correlated Fermi-systems remain unexplained.

NFL behavior manifests itself in the power-law behavior of the physical quantities of strongly correlated Fermi-systems located close to their QCPs, with exponents different from those of ordinary Fermi liquids [59, 60]. It is common belief that the main output of theory is the explanation of these exponents which are at least dependent on the magnetic character of QCP and dimensionality of the system. On the other hand, the NFL behavior cannot be captured by these exponents as seen from Fig. 1.2. Indeed, the specific heat  $C/T$  exhibits a behavior that is to be described as a function of both temperature  $T$  and magnetic  $B$  field rather than by a single exponent. One can see that at low temperatures  $C/T$  demonstrates the LFL behavior which is changed by the transition regime at which  $C/T$  reaches its maximum and finally

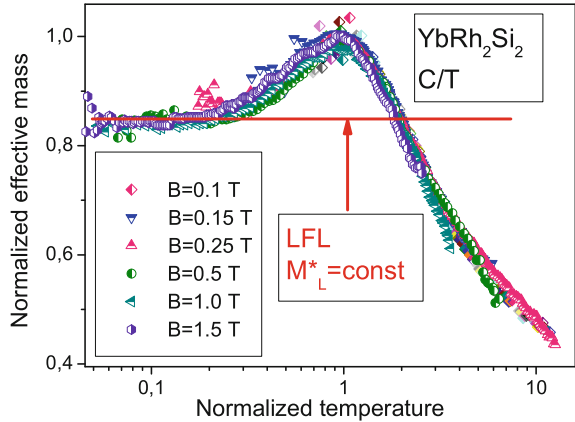
**Fig. 1.2** Electronic specific heat of  $\text{YbRh}_2\text{Si}_2$ ,  $C/T$ , versus temperature  $T$  as a function of magnetic field  $B$  [59] shown in the legend



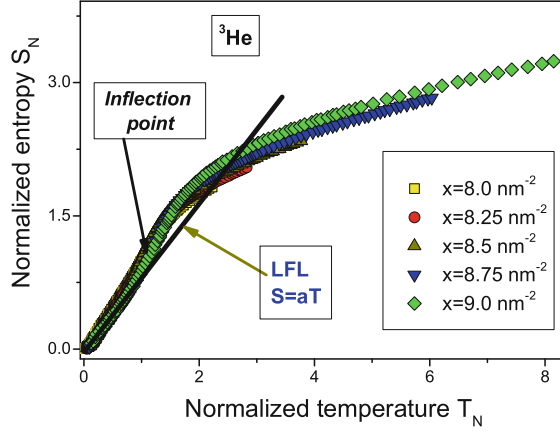
$C/T$  decays into NFL behavior as a function of  $T$  at fixed  $B$ . It is clearly seen from Fig. 1.2 that, in particularly in the transition regime, these exponents may have little physical significance.

To show that the behavior of  $C/T$  reported in Fig. 1.2 is of generic character, we recollect that in the QCP vicinity it is helpful to use “internal” scales to measure the effective mass  $M^* \propto C/T$  and temperature  $T$  [26–28, 61, 62]. As it is seen from Fig. 1.2, a maximum structure in  $C/T \propto M_M^*$  at temperature  $T_M$  appears under the application of magnetic field  $B$  and  $T_M$  shifts to higher  $T$  as  $B$  is increased. The value of the Sommerfeld coefficient  $C/T = \gamma_0$  is saturated towards lower temperatures decreasing at elevated magnetic field. To obtain the normalized effective mass  $M_N^*$ , we use  $M_M^*$  (maximal value of the effective mass) and  $T_M$  as above “internal” scales: The maximum value of  $C/T$  has been used to normalize  $C/T$ , and  $T$  was normalized by  $T_M$ . In Fig. 1.3 the obtained  $M_N^* = M^*/M_M^*$  as a function of normalized

**Fig. 1.3** The normalized effective mass  $M_N^*$  versus normalized temperature  $T_N$ .  $M_N^*$  is extracted from the measurements of the specific heat  $C/T$  on  $\text{YbRh}_2\text{Si}_2$  in magnetic fields  $B$  [59] listed in the legend. Constant effective mass  $M_L^*$  inherent in normal Landau Fermi liquids is depicted by the *solid line*



**Fig. 1.4** The normalized entropy  $S_N$  versus normalized temperature  $T_N$ .  $S_N$  is extracted from the measurements of the entropy  $S$  on  $^3\text{He}$  at different number densities  $x$  [63] shown in the legend. The behavior of the entropy  $S \propto T$  inherent in normal Landau Fermi liquids is represented by the *solid line*



temperature  $T_N = T/T_M$  is shown by symbols. Note that we have excluded the experimental data for magnetic field  $B = 0.06$  T. In that case, as will be shown,  $T_M \rightarrow 0$  and the corresponding  $T_M$  and  $M_M^*$  are unavailable. It is seen that the LFL and NFL states are separated by the transition (or crossover) regime (or region) where  $M_N^*$  reaches its maximal value. Figure 1.3 reveals the scaling behavior of the normalized experimental curves—the curves at different magnetic fields  $B$  merge into a single one in terms of the normalized variable  $y = T/T_M$ . As it is seen from Fig. 1.3, the normalized effective mass  $M_N^*(y)$  extracted from the measurements is not a constant, as would be for LFL, and shows the scaling behavior over three decades in normalized temperature  $y$ . It is seen from Figs. 1.2 and 1.3 that the NFL behavior and the associated scaling extend at least to temperatures up to few Kelvins. Scenario, where order parameter fluctuations with infinite (or sufficiently large) correlation length and time develop the NFL behavior, can hardly occur at such high temperatures. We now briefly discuss how the scaling behavior of the normalized entropy, reported in Fig. 1.4 and revealing the quantum criticality observed in 2D  $^3\text{He}$  [63]. This quantum criticality is extremely significant as it allows us to detect the scaling behavior in the 2D system formed by  $^3\text{He}$  atoms which are essentially different from electrons. As we shall see, the dependence of some observable like the entropy, obviously, do not have “peculiar points” like maxima. The normalization is to be performed in the other points like the inflection point at  $T = T_{inf}$  shown in Fig. 1.4 by the arrow, for details see Chap. 18 and Sect. 18.4. It is seen from Fig. 1.4 that the normalized experimental curves  $S(T)$  taken at different values of the number densities  $x$  merge into single curve  $S_N(T_N) = S(T/T_{inf})/S(T_{inf})$ . The observed behavior of  $S_N$  strongly deviates from that of the LFL one, and cannot be described by a function  $S_n(T_N) \simeq T_N^\beta$ .

Thus, we conclude that the proper explanation of scaling behavior of both  $M_N^*(y)$  and  $S_N(y)$  shown in Figs. 1.3 and 1.4 is a challenge for theories of critical behavior of HF metals. While the existing theories are primarily dealing with calculations of so-called critical exponents  $\beta$  that characterize  $M_N^*(y)$  and  $S_N$  at  $y \gg 1$ , they overlook the regime, signifying transition from LFL to NFL behavior, and are unable



to explain both the LFL and scaling behavior, emerging under the application of magnetic field. As we mentioned above, this transition regime is indeed related to the quantum criticality of systems located near FCQPT. Another part of the problem is the remarkably large temperature ranges over which the NFL behavior is observed. Thus, we conclude that the influence of the critical point extends over a wide range in  $T > 0$ . This is the regime of quantum criticality, which is crucial for interpreting a wide variety of experiments. As we will see below, the above large temperature ranges are precursors of the quantum critical point related with FCQPT and the emergence of new quasiparticles. The latter fact, in turn, generates the scaling behavior of the normalized effective mass that allows to explain the thermodynamic, transport and relaxation properties of HF compounds at the LFL, transition and NFL regimes.

Taking into account the simple behavior shown in Figs. 1.3 and 1.4, we ask the question: what theoretical concepts can replace the Fermi-liquid paradigm with the notion of the effective mass in cases where the LFL theory breaks down? So far such a concept within the framework of ordinary quantum phase transitions approach is not available [26–28, 31]. Therefore, here in this book we focus on the FCQPT concept that preserves the notion of quasiparticles and is intimately related to the unlimited growth of the effective mass  $M^*$ . We shall show that this approach is capable to reveal the scaling behavior of the effective mass and to deliver an adequate theoretical explanation of a vast majority of experimental results collected on strongly correlated Fermi systems like HF metals, quasicrystals, quantum spin liquids, 2D fermi-systems, etc. As we shall see, all these HF compounds exhibit a universal scaling behavior at their quantum criticality, and constitute a new state of matter. Thus whichever mechanism drives the system to FCQPT, the system demonstrates the universal behavior, while there are lot of such mechanisms or tuning parameters like the pressure, number density, magnetic field, chemical doping, frustration and etc.

In contrast to the Landau paradigm based on the assumption that  $M^*$  is a constant as shown by the solid line in Fig. 1.3, in FCQPT approach the effective mass  $M^*$  of new quasiparticles depends strongly on  $T$ ,  $x$ ,  $B$  etc. Therefore, to explain numerous experimental data, the extended quasiparticles paradigm is to be introduced. The main point here is that the new well-defined quasiparticles (with  $M^*$  depending on external parameters) determine, as before, the thermodynamic, relaxation and transport properties of strongly correlated Fermi-systems in wide temperature range. The FCQPT approach had been already successfully applied to describe the thermodynamic properties of such different strongly correlated systems as  $^3\text{He}$  on the one hand and complicated HF compounds and insulators with spin liquid on the other [26–28, 46, 64–67].

### ***1.1.4 Limits and Goals of the Book***

This monograph presents a theory of strongly correlated compounds, i.e. HF metals, high-  $T_c$  superconductors, substances with quantum spin liquids, quasicrystals, and 2D systems like  $^3\text{He}$ . As we have seen above, this extremely wide diversity of strongly



correlated fermion systems represents, or introduces a new state of matter, demonstrating in many cases the universal scaling behavior. Our aim is to show that diverse strongly correlated Fermi-systems such as 3D HF metals, 2D Fermi liquids, compounds with spin liquid and quasicrystals exhibit the quantum criticality, which can be described within a unified approach based on FCQPT theory [12, 25–28]. We discuss the construction of the theory and show that it is capable to explain the vast majority of experimental facts in strongly correlated Fermi-systems. Our analysis is in the context of salient experimental results. Our calculations of the non-Fermi liquid behavior, the scales and thermodynamic, relaxation and transport properties are in good agreement with experimental facts. We shall focus on the scaling behavior of the thermodynamic, transport and relaxation properties that can be revealed both from experimental facts and theoretical analysis. We do not discuss, however, the specific features of strongly correlated systems in full; instead, we focus on the universal behavior of such systems. We also do not discuss the physics of Fermi-systems, that are not related to condensed matter. Namely, these are neutron stars, atomic clusters and nuclei, quark plasma, and ultra-cold gases in traps, where, according to our views, the fermion condensate induced by FCQPT can also exist [68–73]. Ultra-cold gases in traps are interesting because their easy tuning allows selecting the values of the parameters required for observations of quantum critical point and FC. We also do not discuss the specific microscopic mechanisms of quantum criticality related to the emergence of FCQPT in a specific compound. Such mechanisms rely heavily on crystalline structure of a specific substance and development of these mechanisms seems not feasible in a near future. In contrast, we consider general mechanisms leading to the formation of flat bands, and analyze the common properties of strongly correlated Fermi-systems in close connection with accessible experimental facts. For example, the mechanism of quantum criticality, observed in f-electron materials, can take place in the systems when the centers of merged single-particle levels “get stuck” at the Fermi surface. One observes that this could provide a simple mechanism for pinning narrow bands in solids to the Fermi surface [73]. Also, we consider high- $T_c$  superconductors within a coarse-grained model based on the FCQPT theory just to illuminate their generic relationships with HF metals. When studying quasicrystals, quantum spin liquids and 2D systems, we propose the corresponding mechanisms as well. To stress the ubiquitous features of FCQPT, in Chap. 16 we consider its possible role in the emergence of the Universe.

Experimental studies of the properties of quantum phase transitions and their quantum critical points are very important for understanding the physical nature of strongly correlated Fermi-systems. The experimental data, gathered on different strongly correlated Fermi-systems, complement each other. In the case of high- $T_c$  superconductors, only few experiments dealing with their QCPs have been conducted. This is because the corresponding QCPs are in the superconductivity range at low temperatures and the physical properties of the respective quantum phase transition are altered by the superconductivity. As a result, high magnetic fields are needed to destroy the superconducting state. Such experiments can be conducted for HF metals. Experimental research provides data for HF metals behavior, shedding light on the nature of their critical points and phase transitions [41, 49, 52, 54].

Hence, a complete understanding of unusual physical properties related to NFL behavior, can be achieved on the base of simultaneous and comparative experimental studies of high- $T_c$  superconductors, HF metals and other correlated Fermi-systems [55, 57, 58].

Since we are concentrated on the properties that are non-sensitive to the detailed crystalline structure of the system, we avoid difficulties associated with the anisotropy generated by the crystal lattice of solids, its special features, defects, etc., We study the universal behavior of high- $T_c$  superconductors, HF metals, quasicrystals, quantum spin liquids, and 2D Fermi-systems at low temperatures using the model of a homogeneous HF liquid [26–28, 61, 62]. The model is quite meaningful as we consider the low-temperature scaling behavior of these compounds. This behavior is closely related to the scaling of quantities like effective mass, heat capacity, thermal expansion coefficient, etc. The aforementioned scaling is determined, primarily, by long wave length properties of corresponding compound. In other words, they are dealing with transfers of momenta with wave vectors, that are small compared to those of the reciprocal lattice constant. The high momentum contributions can therefore be ignored by substituting the lattice for the jelly model.

We analyze the universal properties of HF compounds systems using the FCQPT theory [12, 25–28, 74], because the behavior of HF metals already suggests that their unusual properties can be associated with the QPT related to the infinite increase in the effective mass at the critical point. Moreover, we shall see that both the scaling behavior and the quantum criticality displayed in Figs. 1.3 and 1.4 can be quite naturally captured within the framework of the above FCQPT related extended quasiparticle paradigm, which gives explanations of the NFL behavior observed in wide range of HF compounds.

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Theory of Heavy-Fermion Compounds

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