TROISIEME CYCLE DE LA PHYSIQUE

EN SUISSE ROMANDE

THEORY OF CORRELATED FERMI SYSTEMS

by

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Foreword

Correlated Fermi Systems are at the forefront of present day research in condensed matter physics. The following nine lectures are intended as an introduction to the problems involved. They do not employ advanced theoretical methods but are rather conceived to stress the basic ideas and models. Part I discusses the effect of disorder on the properties of electrons in metals. Part II introduces Landau's Fermi liquid theory and microscopic models for the description of correlation effects in normal state systems. Part III then concentrates on superconductivity/fluidity in pair correlated Fermi systems and also gives an introduction to the current theoretical problems involved in understanding high-T_c superconductivity.

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Dieter Vollhardt

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Introduction

During the last 15 years condensed matter physics has made particularly important, new contributions to our understanding of physics. There have been numerous discoveries which go far beyond mere quantitative improvements of earlier measurements and which, in fact, concern the fundamental concepts of physics. They have led to significant new insight into the basic properties of many-particle systems.

Below we list some of the most influencial papers on topics in condensed matter physics, which appeared during the last one-and-a-half decades. Each one of them triggered an explosive, new development in condensed matter physics and led to an avalange of hundreds or more papers:

1972: Superfluidity in ^{3}He by Osheroff, Richardson and Lee [1]

1979: (i) Anderson Localization, Metal-Insulator Transition by Abrahams, Anderson, Licciardello and Ramakrishnan [2]

(ii) Interaction effects in disorderd metals by Aronov and Altshuler [3]

(iii) Heavy Fermion Superconductivity by Steglich, Aarts, Bredl, Lieke, Meschede, Franz and Schäfer [4]

1980: (Integer) Quantum Hall Effect by v. Klitzing, Dorda and Pepper [5]

1982: Fractional Quantum Hall Effect by Tsui, Störmer and Gossard [6]

1986: High-T_c Superconductivity by Bednorz and Müller [7]

The relevance of these papers is best illustrated by the number of Nobel prizes connected with them. While Anderson, Mott and van Vleck had already received the Nobel prize in 1977 for work to which the paper by Abrahams et al. [2] relates, the work by v. Klitzing, and that of Bednorz and Müller was an "instant success" - they received their Nobel prizes in 1985 and 1987, respectively.

Browsing through these new discoveries it is obvious that the largest part involves disordered and/or correlated Fermi systems - in particular, of course, electronic systems. This is not so surprising since condensed matter physics itself is predominantly "electron-physics" by nature. However, there are other correlatd Fermi systems, i.e. nuclear matter and neutron stars and - most importantly - liquid ^{3}He, where new discoveries were made, which subsequently enriched our view of the possible states of condensed matter considerably.

Of the four Fermi systems mentioned above, nuclear matter is not really a "many-particle system"(where we usually imply of the order of 10^{23} particles) although it sometimes comes quite close. In fact, in the case of heavy nuclei, the possibility of superfluidity is currently being debated. A neutron star, on the other hand, is a true many-body system and the corresponding techniques of statistical physics do apply very well.The trouble is that direct experimental investigations are difficult for obvious reasons. Therefore not so much is yet known about the details of these super-high-density Fermi

systems, although a lot of information has already been inferred room radiation measurements. This is also a lively area of research [8] .

So we mostly concentrate on electrons and the quantum-(Fermi) liquid ^{3}He. In many respects electrons in metals also behave as a quantum liquid, so that liquid ^{3}He and electrons have a lot in common. This is why in the following we will frequently compare their properties. -

These lectures are thought to present an introduction to the physics of disordered and correlated Fermi systems. We will aim at the discussion of present state-of-art problems in this field and are thus facing the frontiers of physics. Clearly, it is completely impossible to discuss all the relevant topics here. We can only attempt to address some of the problems mentioned above. Besides that, I cannot expect the mathematical techniquesto be generally know, which are necessary to deal with the problems under consideration. Therefore I have to do without them. So I will try to introduce the relevant questions without much mathematics, hoping to create a feeling for the physics behind it. To this end I expect that the audience is familiar with the material from lectures on thermodynamics and statistical mechanics, quantum mechanics (I) and some solid state physics. Second quantization will be needed later and will be recapitulated at the appropriate time.

In these nine lectures three main topics will be discussed

I. Disordered Electronic Systems

II. Correlations in interacting, normal-state Fermi systems

III. Superconductivity/fluidity of Electrons and ^{3}He

We will see that these seemingly disparate topics have a lot in common and that there are many fundamental connections. Many of these links have only been discovered in the last 10 years or so. The development in our understanding of correlated Fermi systems and the discovery of unifying concepts is a particularly exciting and gratifying feature of present day condensed matter physics.

I. Disordered Electronic Systems

Introduction

A metal-insulator transition separates two physical regions, which fundamentally differ in their electrical dc-conductivity $\sigma(\omega = 0)$: while a metal has a finite dc-conductivity $(\sigma(0) > 0)$, an insulator is characterized by $\sigma(0) = 0$.

Such a transition does not only occur in disordered systems. In fact, it can also take place in very clean, purely crystalline materials, in which the particles that are responsible for the current, interact via a Coulomb-interaction. In such systems an overlap of energy bands can lead to a metal-insulator transition. Yet another cause for a transition may be due to a structural change of a crystal leading to a new lattice periodicity. Indeed there exist completely different physical reasons for the occurrence of a metal-insulator transition [9]. We will here confine ourselves to the metal-insulator transition in disordered systems, i.e. where the "disorder" is ultimately responsible for the transition. By "disorder" we mean, e.g. the disturbance of a strict lattice periodicity due to impurities or defects. Our understanding of the physics of disordered systems, in particular of their transport properties and the metal-insulator transition, has greatly changed and substantially deepened since 1978/79[10,11]. These developments especially concern disordered systems in two and three dimensions. The situation in one-dimensional

disordered systems is somewhat special and has its own long history[12].

In the first two lectures of part I we will concentrate on the behavior on non-interacting, quantum mechanical particles in a disordered environment. In the last lecture we will also take into account the effects of a mutual interaction between the particles.

Non-Interacting, Quantum Mechanical Particles in Disordered Systems

Of three-dimensional systems (i.e. those with space dimension $d = 3$) we know, that at temperatures $T = 0$ there exist neither lattice vibrations (phonons) nor any inelastic processes. In fact, in an unbounded, perfect lattice (Fig. 1a) no scattering occurs at all. This is a consequence of quantum mechanics. Consequently such a system has an infinite dc-conductivity. One may equally well say, that the characteristic collision time τ of the particles due to scattering off defects etc. is infinitely long ($\tau = \infty$). In the case of Fermions (and those we only consider here) it follows, that the mean free path $\ell = v_F \tau$ of the particles is also infinite ($\ell = \infty$); here v_F is the Fermi-velocity. The wavefunction of a particle is then characterized by a strict spatial phase coherence.

In a lattice, which is weakly disturbed by impurities or defects (Fig. 1b), the situation is different:

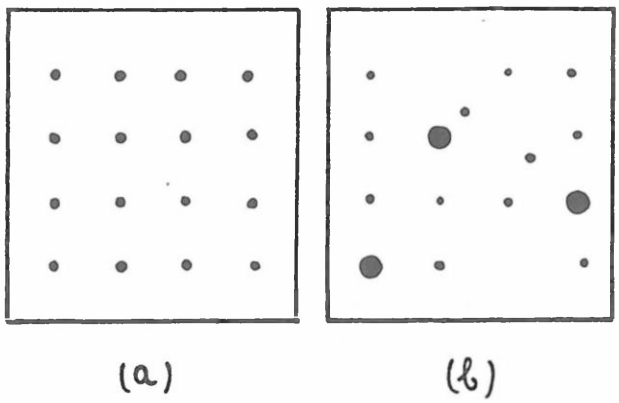

Fig. 1 : (a) perfect lattice, (b) imperfect lattice (presence of defects, impurities etc.)

the scattering of the particles off the defects implies a finite collision time τ and thereby a finite mean free path ℓ . The dc-conductivity is therefore also finite and is given by

$$\sigma(0) = \sigma_0 = \frac{e^2 n}{m} \tau \tag{1}$$

where e and m are the charge and the mass of the particles (e.g. electrons), respectively and n is the density. The quantity σ_0 is often called "Boltzmann - conductivity", because (1) is a direct result of the

Boltzmann transport theory.

The scattering of the particles leads to diffusion (Fig. 2), i.e. to a diffusive motion. The phase coherence of the wave functions is thereby limited;

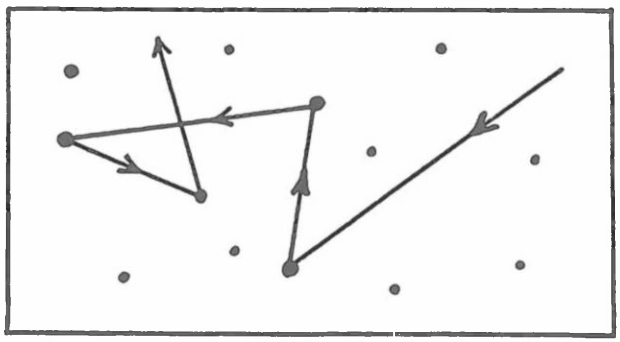

Fig. 2 : Diffusion of a particle in a disordered system

nevertheless the wavefunction $\psi(\vec{r})$ of the particle is still extended, i.e. one has

$$\lim_{r \to \infty} |\psi(\vec{r})|^2 \neq 0 \qquad (2)$$

When the disorder is increased (e.g. by choosing a higher impurity concentration) it may happen that the wave function becomes localized, such that

$$|\psi(\vec{r})|^2 \propto e^{-r/\xi}$$

where ξ is the so-called "localization length". However, it is not a priori clear how to quantify this vague statement. To gain insight, we therefore want to discuss the one-dimensional case ($d = 1$) first [9].

As a model we consider a generalized Kronig-Penney model, namely a chain of δ-function potentials (Fig. 3) at locations x_i with strength V_i and

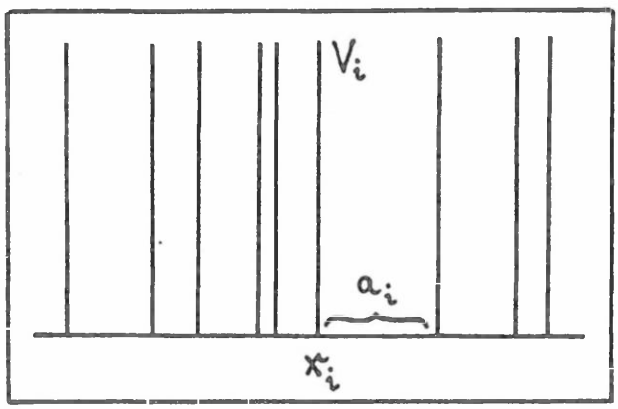

Fig. 3 : One-dimensional model of a disordered system

separations a_i . The potential is then given by

$$V(x) = \frac{\hbar^2}{2m} \sum_i V_i \, \delta(x - x_i) \tag{3}$$

and the Schrödinger equation reads

$$\left[-\vec{\nabla}^2 + \sum_i V_i \, \delta(x - x_i) - k^2 \right] \psi(x) = 0 \tag{4}$$

where $k = (2mE/\hbar^2)^{1/2}$ is the momentum. We first concentrate on a single δ-function at the origin $(x=0)$.

The wave functions $\psi_\pm(x)$ for $x \gtrless 0$ are then given by

$$\psi_\pm(x) = A_\pm e^{ikx} + B_\pm e^{-ikx} \tag{5}$$

The boundary conditions at $x=0$ for the wave functions and their spatial derivative are given by $\psi_+(0) = \psi_-(0)$ and $\psi'_+(0) = \psi'_-(0) + V_0 \psi(0)$. We are now searching for a periodicity in ψ, such that $|\psi_+(a)|^2 = |\psi_-(0)|^2$ for an arbitrary value of $x = a$. In other words we look for the property $\psi_+(a) = e^{i\tilde{k}a} \psi_-(0)$ for arbitrary a and $\tilde{k}$. This leads to the condition

$$\cos \tilde{k}a - \cos ka = \frac{V_0}{k} \sin ka \tag{6}$$

from which $\tilde{k}$ and a can be obtained as functions of k. For a chain of potentials we may conclude from (6) that a wave function will only be periodic (and the state extended) if the separations a_i between the potentials are <u>all</u> equal $(a_i = a)$ and if, at the same time, <u>all</u> potentials V_i also have the same strength $(V_i = V)$. Otherwise all physically sensible wave functions fall off exponentially, i.e. represent localized states. This means that even an arbitrarily small statistical spread of the values of a_i and V_i leads to localized solutions of the Schrödinger equation only.

The first <u>quantitative</u> definition of "localization" dates back to Anderson in 1958 [13]. He investigated a three-dimensional model, namely a regular point lattice, where on each lattice site i an atom with an energy V_i was located (Fig. 4). Now one considers a quantum mechanical particle (e.g. an electron), which (i) hops from one site to the next neighbor site (kinetic energy) and (ii) experiences the potential V_i on site i (potential energy). The question is, how the particles are influenced by these potentials. In the special case that all V_i are equal $(V_i = V)$ one of course obtains a sharply bounded energy <u>band</u>, whose width we characterize by an energy B. This situation is changed when the V_i are statistically distributed (Fig. 5), e.g. with a rectangular distribution

$$P\{V_i\} = \begin{cases} \frac{1}{W} & , |V_i| \leq \frac{W}{2} \\ 0 & \text{else} \end{cases} \tag{7}$$

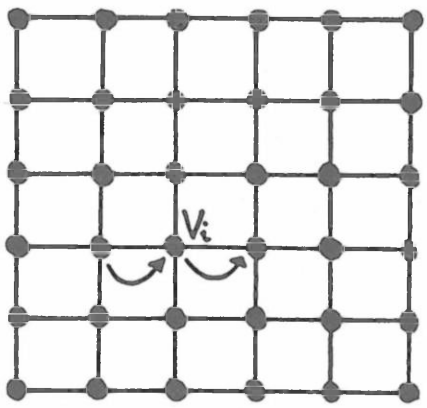

Fig. 4 : Disorder model due to Anderson

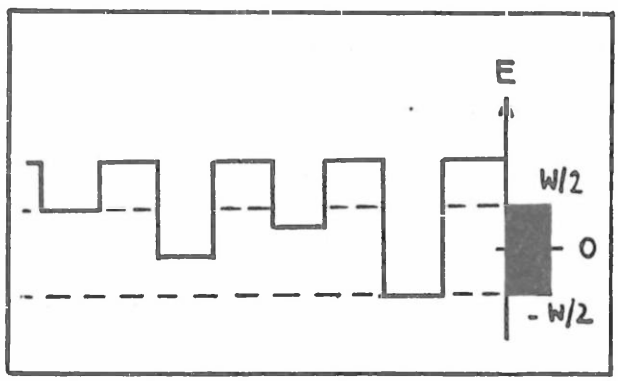

Fig. 5 : Example of the energy distribution of the atoms

For an unbounded system one may now ask: How large is the probability P for a particle to return to a particular lattice site in the limit of long times $(t \to \infty)$? In the case $P = 0$ the particle has "disappeared" in the system; hence it will be characterized by an extended state. In the case $P > 0$, i.e. finite return probability, we speak of "localization", i.e. the particle is described by a localized state.

The answer to the above question depends on the ratio of the maximal energy difference of the atoms, W, to the band width B of the undisturbed system, i.e. on W/B. This number (!) is a measure of the strength of energy fluctuations in the system, i.e. a measure of the <u>disorder</u>. The quantitative answer [13] is, that for $W/B \lesssim 5$ one finds $P = 0$ while for $W/B \gtrsim 5$ one obtains $P > 0$. In between there is a <u>sharp</u> transition, the "Anderson transition". In other words: if the energy E of the particle lies below a certain critical energy E_c (which is determined by the strength of the disorder, $(W/B)_c \simeq 5$), it is localized, while for $E > E_c$ the energy fluctuations of the system will not be able to dominate the particle such that it is described by an extended state. In the first case one deals with an insulator, in the second one with a metal. Since electrons in a metal have a characteristic energy E_F (Fermi energy), the Anderson transition may be induced by changing E_F .

What does the transition actually look like? According to Mott [14] it originally was supposed to be <u>discontinuous</u>. This expectation was based on the following arguments. The dc-conductivity $\sigma_0(\ell)$ of a d-dimensional system can be written as

$$\sigma_0 = \left(\frac{e^2}{\hbar}\right) \frac{a^{2-d}}{\pi} \frac{\ell}{a} = \sigma_c \frac{\ell}{a} \tag{8}$$

where we made use of $\ell = v_F \tau$, $v_F = \hbar k_F / m$ and where the density of a Fermi gas has been expressed as $n = a^{-d}$ (here k_F is the Fermi wave number which is connected with a , the average distance of the particles, by $k_F \simeq \pi/a$) . The conductivity σ_c is an essentially universal quantity — it is independent of the disorder in the system. The disorder-dependence only enters via the mean free path ℓ , i.e. the ratio ℓ/a . When the disorder increases, ℓ and hence σ_0, decrease. On the other hand, (1) and (8) have been derived within the Boltzmann transport theory. So, for these equations to be valid at all, ℓ always has to be greater than the average particle distance a (Ioffe-Regel criterion); shorter ℓ makes no sense. Mott therefore postulated a "minimal metallic conductivity" σ_{min} , which is essentially given by σ_c (more precisely, $\sigma_{min} = C\,\sigma_c$, where $C \simeq 0.08 - 0.3$ is a nonuniversal constant which is due to a reduction of the density of

states of the electrons at the Fermi surface compared to the Fermi gas). He argued that – as the metal-insulator transition was approached from the metallic side — the conductivity σ_0 would decrease proportional to ℓ and then, at $\ell \simeq a$, would drop discontinuously from σ_{min} to zero (Fig. 6). However, already at this point

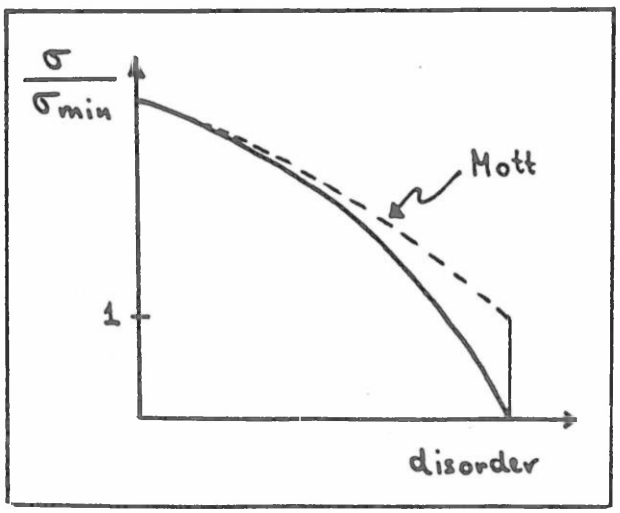

Fig. 6: Possible shape of the conductivity curve as a function of the disorder.

we should like to mention that this concept does not hold — in spite of many experimental results which appeared to support it for a long period of time. Indeed, low temperature experiments have now

measured metallic conductivities much below σ_{min} and have thereby falsified the concept of a minimal metallic conductivity [15]. We will later come back to that problem.

Theoretical Description of Disorder

In the model originally discussed by Anderson, a particle moves on a regular lattice, the energy of the lattice points being statistically distributed (Fig. 7a).

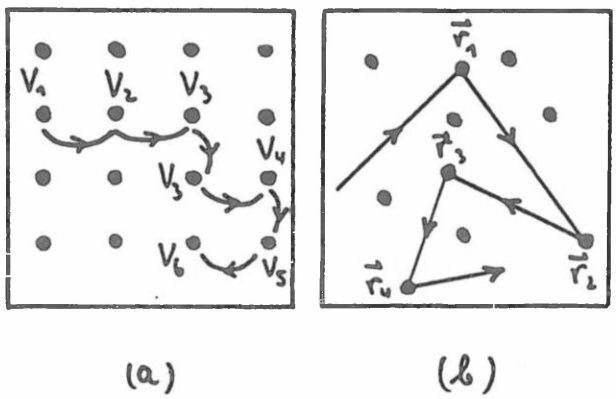

Fig. 7: Disorder and motion of a particle in the model of (a) Anderson, (b) Edwards.

The "disorder" is then exclusively due to the energy state of the lattice sites. An alternative model goes back to Edwards [16]. In his model particles of identical

energy are scattered off randomly distributed scattering centers of equal potential (Fig. 7b). The disorder is then due to the spatial distribution of the scatterers. While the first model starts from the localized regime, the starting point of the Edwards model is the regime of extended states (weak scattering). The latter model is particularly suitable for the formulation of a systematic perturbation theory which starts from the undisturbed, metallic regime and then includes a small impurity concentration, i.e. weak disorder. The following investigations are based on the Edwards model. For this we consider (i) non-interacting particles, which (ii) are scattered by pointlike, randomly distributed scattering centers of equal strength. We are interested in the conductivity σ or the diffusion coefficient D of such a disordered system. The two quantities are actually related by the Einstein relation

$$\sigma = e^2 N_F D \tag{9}$$

where N_F is the density of states at the Fermi surface.

We will measure the disorder by a dimensionless parameter λ with $\lambda \propto n_i V_0^2$, i.e. λ is essentially given by the impurity concentration n_i and the scattering strength V_0^2 of the scatterers. The parameter is often called "coupling constant".

In the case $d = 1$ we saw that even arbitrarily weak disorder $\lambda \to 0$ leads to localization. The "critical" value of the disorder, λ_c, above which one finds localization is therefore given by $\lambda_c = 0$. On the other hand, in the case $d = 3$ λ_c is different from zero $(\lambda_c > 0)$. For $\lambda < \lambda_c$ one finds metallic behavior, which is described by a finite dc-conductivity σ_0 (or diffusion constant D_0). For $\lambda > \lambda_c$ one deals with an insulator. Here $\sigma_0 = 0$; instead, an insulator has a finite polarizability, i.e. dielectric constant ϵ_0. At $\lambda = \lambda_c$ the Anderson transition is located.

Apparently, the case $d = 2$ (very thin films) marks a marginal dimension. The question is now, whether there is an Anderson transition or not in two dimensions, i.e. whether $\lambda_c = 0$ or $\lambda_c > 0$. In other words, one may ask an almost trivially sounding question: "Is there metallic conductivity in very thin films at $T = 0$?" Or is there, for example, a minimal metallic conductivity? The answer to this seemingly simple question has only been found in recent years. It led to unexpected insights into the physics of disordered systems and their transport properties.

The "Weakly" Localized Regime

We first consider the case of very weak disorder $(\lambda \ll 1)$. Therefore the starting point is the metallic regime. We want to understand how a small concentration

of impurities affects the metallic behavior. Since we are far away from the actual Anderson transition itself, these effects can be treated by means of a perturbation theory in the disorder parameter $\lambda \ll 1$. Weak disorder means that the mean free path ℓ is much greater than the average particle distance $a \simeq k_F^{-1}$, i.e. $k_F \ell \gg 1$ or, equivalently, $E_F \tau \gg 1$. We will therefore choose

$$\lambda = \frac{1}{2\pi E_F \tau} \tag{10}$$

as our (small) perturbation parameter. Starting from the metallic regime we want to consider the precursor effects of localization, i.e. the corrections $\delta\sigma$ to the metallic conductivity

$$\sigma = \sigma_0 + \delta\sigma \quad , \quad |\delta\sigma| \ll \sigma_0 \tag{11}$$

These perturbational effects are commonly called "weak localization". Our aim is to calculate $\delta\sigma = f(L, \omega, T, H)$ as a function of several external parameters like the system's size L , the frequency ω , the temperature T or the magnetic field H .

Diffusion of Classical and Quantum Mechanical Particles

As mentioned before, the conductivity σ_0 ,(1)

$$\sigma_0 \propto \frac{1}{\lambda} \tag{12}$$

is a result of the Boltzmann transport theory. In this theory consecutive collisions of particles are assumed to be independent of each other, i.e. collisions are uncorrelated. This implies that multiple scattering of a particle at a particular scattering center is not taken into account. Consequently, if there is a finite probability for the repeated occurrence of such multiple scatterings, the basic assumption of the independence of scattering events breaks down and the validity of the result for σ_0 in (1) becomes, at least, questionable.

To investigate this fundamental point we consider the diffusive behavior of a particle in a d-dimensional disordered system. Let the particle be located at $\vec{r}_0$ at time $t=0$ (Fig. 8a). Due to its diffusive motion the particle moves away from $\vec{r}_0$. At some later time t we will only be able to make a probability statement about its position: it will be located within some smooth volume (Fig. 8b) whose size is determined by the probability distribution $P(\vec{r},t)$, which is the solution of the diffusion equation

$$\frac{\partial P}{\partial t} - D_0 \vec{\nabla}^2 P = 0 \tag{13}$$

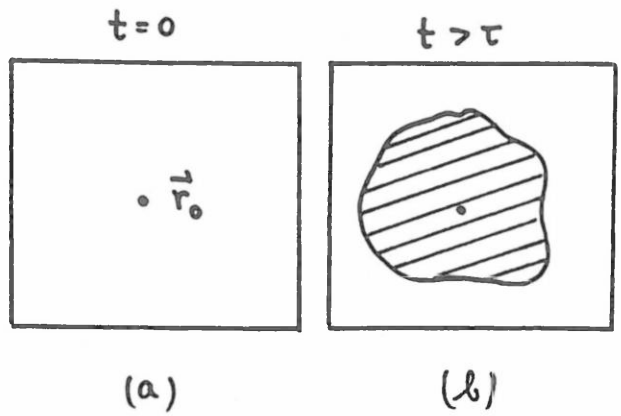

Fig. 8: Probability distribution of a diffusing particle: (a) $t=0$, (b) $t>0$.

The diffusion constant D_0 is given by $D_0 = v_F^2 \tau / d$, where v_F is the characteristic velocity of the particles. The explicit solution of (13) is given by

$$P(\vec{r},t) = \frac{e^{-\frac{|\vec{r}-\vec{r}_0|^2}{4D_0 t}}}{(4\pi D_0 t)^{d/2}} \tag{14}$$

At times $t \gg \tau$ the exponential in (14) is unimportant, so that

$$P(\vec{r},t) \propto \frac{1}{V_{diff}} = \begin{cases} \dfrac{1}{(D_0 t)^{1/2}} & , \quad d=1 \\ \dfrac{1}{D_0 t} & , \quad d=2 \\ \dfrac{1}{(D_0 t)^{3/2}} & , \quad d=3 \end{cases} \tag{15}$$

We observe that $V_{diff} = (D_0 t)^{d/2}$ is the d-dimensional volume into which the particle has diffused after time t .

These considerations are purely classical. To understand the differences in the diffusive behavior of classical and quantum mechanical particles, we take a look at the path of a particle diffusing from point A to point B (Fig. 9) , following the discussion by Khmelnitskii [17].

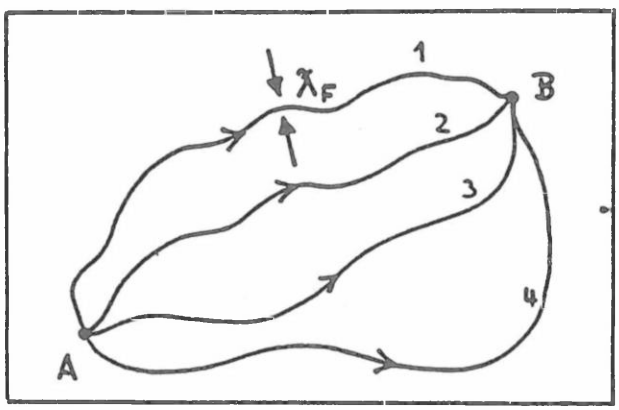

Fig. 9: Possible paths of a particle diffusing from A to B.

This transport can take place via different trajectories (in Fig. 9 four examples are shown). The trajectories, or "tubes", have a typical width given by the Fermi wavelength

$$\lambda\!\!\!^{-}_F = \frac{\hbar}{v_F m} \qquad (16)$$

In the classical case $(\hbar = 0)$ these paths are arbitrarily sharp $(\lambda\!\!\!^{-}_F = 0)$ — in the quantum mechanical case, however, one has $\lambda\!\!\!^{-}_F \simeq k_F^{-1} \simeq a$, i.e. the tubes have a finite diameter. We now assume that (i) the disorder λ is very small $(\lambda\!\!\!^{-}_F / \ell \propto \lambda \ll 1)$ and that (ii) the temperature is low enough such that inelastic processes, characterized by an inelastic scattering time τ_{in} , occur only very rarely $(\tau_{in} \gg \tau)$.

Since the transport from A to B may take place along different trajectories, there is a probability amplitude A_i connected to every path i . The total probability W to reach point B from A is then given by the square of the magnitude of the sum of all amplitudes:

$$W = \left| \sum_i A_i \right|^2 \qquad (17a)$$

$$= \sum_i |A_i|^2 + \sum_{i \neq j} A_i A_j^* \qquad (17b)$$

The first term in (17b) describes separate, i.e. non-

interfering paths — this is the classical case, in which the tubes are infinitely sharp. On the other hand, the second term represents the contribution due to interference of the path-amplitudes,which is therefore an exclusively quantum mechanical effect. In the Boltzmann theory these interference terms had been neglected. In most cases this is in fact justified: since the trajectories have different lengths the amplitudes A_i carry different phases. On the average this leads to destructive interference. Hence the quantum mechanical interferences in Fig. 9 are generally unimportant.

There is, however, one particular exception to this conclusion, namely if point A and B coincide (Fig. 10)!

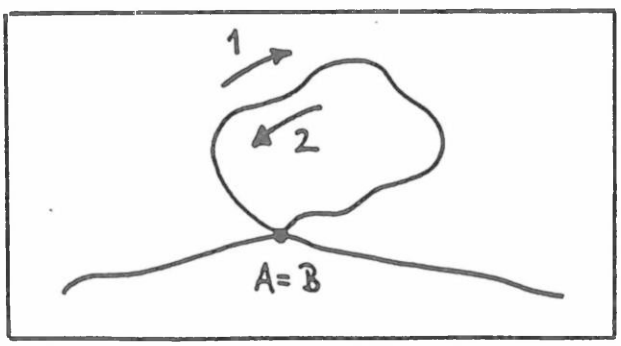

Fig. 10: Return of a particle to its starting point.

In this case starting-point and end-point are identical, such that the path in between can be traversed in two opposite directions: forward and backward. The probability W to go from A to B is then nothing but the <u>return</u>-probability to the starting-point. Since paths 1 and 2 in Fig. 10 are equal, the Amplitudes A_1 and A_2 have a coherent phase relation. This leads to <u>constructive</u> interference, such that the quantum mechanical contribution to W becomes very important. Eq.(17b) then tells us that for $A_1 = A_2 \equiv A$ the classical return probability (due to the neglect of the interference terms) is given by $W_{class} = 2|A|^2$, while the quantum mechanical case yields $W_{qm} = 2|A|^2 + 2A_1A_2^* = 4|A|^2$. Hence one obtains

$$W_{qm} = 2\, W_{class} \tag{18}$$

The probability for a quantum mechanical particle to return to some starting point is hence seen to be <u>twice</u> that of a classical particle. One might say "quantum-diffusion" is slower than classical diffusion because in the first case there exists a more effective back scattering effect. In other words: quantum mechanical particles in a disordered medium are (at low temperatures) less mobile than classical particles. This in turn leads to a correspondingly lower conductivity σ.

It should be stressed that the factor of 2 in (18) is simply a consequence of constructive wave interference of the two time reversed paths in Fig. 10. In the case of electrons its origin is quantum mechanical only because the wave nature of electrons is an inherently quantum mechanical effect. In general, any wave propagation in a disordered medium will lead to a qualitatively identical result. Any wave will do. For example, shouting into a forest(we assume a naturally grown forest, where trees are irregularly spaced ...) will yield the same kind of enhancement ("echo") into the backward direction as will result from shining light into white paint [18]. Localization involving classical wave propagation has been discussed by Anderson [18], who also gave a number of examples for related electromagnetic and acoustic phenomena.

Indeed, inspired by the weak localization effects known from disordered elctronic system, it was convincingly shown that coherent backscattering equally applies to the propagation of light in a disordered medium[19,20]. Shining light into a highly concentrated aqueous suspension of submicron size polystyrene spheres, the scattered intensity was measured and a striking enhancement in the backscattering direction within a narrow cone was found. This enhancement comes from the constructive interference of light-waves travelling on closed, time-reversed

paths just as explained in the case of weak localization. Note that the explicit condition of static disorder necessary for weak localization is fulfilled even in these experiments, since the thermal motion in the liquid is much slower than the propagation of the light wave along any relevant closed path in the medium. Ideally, i.e. assuming isotropic scattering and scalar waves, the backscattered intensity should be enhanced by the factor of 2 in(18) relative to the incoherent background. This would require that the starting and endpoint of the loops really coincide (A = B in Fig. 10). Otherwise interference cannot be complete, resulting in a reduced enhancement. A theoretical calculation of the intensity of the reflected relation to the incident light[21,22], which takes all these effects into account, has found a truely remarkable quantitative agreement with the experimental results.

The localization of light, sound and other kinds of wave-like entities in disordered media has also been studied; for a discussion see ref.[23].

Estimate of the Correction to the Conductivity

To estimate the size of the interference effects on σ, we consider the change $\delta\sigma$ relative to the metallic conductivity σ_0, i.e. $\delta\sigma/\sigma_0$. Because of the expected lowering of σ, the sign of $\delta\sigma/\sigma_0$ will be negative. Furthermore, the change will be proportional to the probability that during diffusion a closed path as in Fig. 10 occurs at all. (This is the probability to find a particle in a closed tube, i.e. the probability for the trajectory to intersect itself during the diffusion.) Let us therefore have a look at a d-dimensional tube (Fig. 11) with diameter λ_F, i.e. cross-section λ_F^{d-1}. During

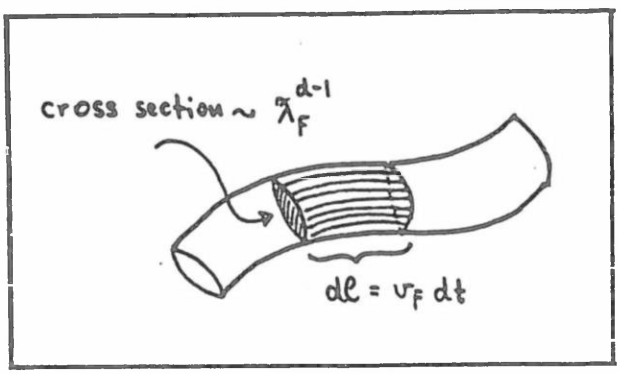

Fig. 11: Enlarged section of a quantum mechanical trajectory.

the time interval dt the particle moves a distance $dl = v_F\, dt$, such that the corresponding volume-

element of the tube is given by $dV = v_F\, dt\, \lambda_F^{d-1}$.
On the other hand, the maximally attainable volume for the diffusing particle is given by (15), i.e. by $V_{diff} = (D_0 t)^{d/2}$. The above mentioned probability for a particle to be in a closed tube is therefore given by the ratio of these two volumes. We find

$$W = \int_{\tau}^{\tau_{in}} \frac{dV}{V_{diff}} = v_F\, \lambda_F^{d-1} \int_{\tau}^{\tau_{in}} \frac{dt}{(D_0 t)^{d/2}} \tag{19}$$

where we have integrated over all times $\tau \leq t \leq \tau_{in}$: τ is the microscopic time for a single elastic collision (shorter times are not sensible), while τ_{in} is the shortest inelastic relaxation time in the system. It determines the maximal time during which coherent interference of the path-amplitudes is possible.
Because of $D_0 \propto 1/\lambda$ and $\lambda_F \propto \hbar$ we obtain

$$\frac{\delta\sigma}{\sigma_0} \propto -\lambda \times \begin{cases} \left(\frac{\tau_{in}}{\tau}\right)^{1/2} , & d=1 \\ \hbar \ln\left(\frac{\tau_{in}}{\tau}\right) , & d=2 \\ \hbar^2 \left(\frac{\tau_{in}}{\tau}\right)^{-1/2} , & d=3 \end{cases} \tag{20}$$

If we assume, that for $T \to 0$ the inelastic relaxation rate vanishes with some power of T , i.e. $1/\tau_{in} \propto T^p$, where p is a constant, (20) is given by

$$\frac{\delta\sigma}{\sigma_0} \propto -\lambda \cdot \begin{cases} T^{-p/2} & , \; d=1 \\ \hbar \frac{p}{2} \ln\left(\frac{\hbar\tau}{k_B T}\right) & , \; d=2 \\ \hbar^2 T^{p/2} & , \; d=3 \end{cases} \tag{21}$$

We observe the following: (i) the conductivity decreases for decreasing temperature, (ii) the relative correction $\delta\sigma/\sigma_0$ is linear in the disorder parameter $\lambda \ll 1$ (lowest order in λ), (iii) except for $d=1$, these corrections are of quantum mechanical origin, i.e. they disappear for $\hbar \to 0$. (In the case $d=1$ the "tube" in Fig. 11 has no finite diameter — just as in the classical situation; furthermore, since in $d=1$ there is only forward and backward scattering all paths are trivially "closed".)

In $d=2$ one therefore obtains a <u>logarithmic</u> temperature dependence of the conductivity correction $\delta\sigma$. We note that the elastic scattering due to the disorder in principle leads to a <u>divergent</u> temperature behavior of $\delta\sigma$ in $d \leq 2$. For the initial assumption $|\delta\sigma| \ll \sigma_0$ to remain valid, the results in (21) for $d \leq 2$ may therefore not be used at too low temperatures. In particular, (21) does not allow to draw conclusions about $\delta\sigma$ at exactly $T=0$!

Finally, it should be pointed out that the results in (21) have been derived with a tacit assumption:

namely that the path-amplitudes A_1 and A_2 in Fig. 9 were perfectly coherent $(A_1 = A_2)$. So we actually took for granted that particle states with momentum $\vec{k}$ and $-\vec{k}$ are equivalent. Such a "time reversal invariance" is given if there are no external magnetic fields and if the impurities are non-magnetic. Otherwise a new situation arises which we will discuss later.

We should like to stress once more, that (20) and (21) are based on the explicit consideration of backscattering effects, i.e. multiple scattering and the correlation of consecutive collisions. Thus they cannot be obtained within the framework of the Boltzmann transport theory. Also CPA ("coherent potential approximation" [24]), an almost classical approximation method in problems involving disorder, is not able to obtain these results because it makes similar assumptions as the Boltzmann theory ("single site approximation", etc.).

Systematic Calculation of Corrections to the Conductivity

The arguments leading to (21) already contain the essential physics. They enabled us to understand the temperature dependence of $\delta\sigma$. On the other hand, we cannot deduce more than proportionality relations from them. For example, the precise prefactors in (20) can thereby not be determined. Furthermore, the perturbation theory cannot be extended beyond first order in λ.

For this we need a systematic approach. This involves calculational methods which can only be formulated within a certain mathematical framework which we cannot discuss here. To obtain a precise calculation of we will therefore "use" methods without really explaining their theoretical background. The necessary concepts and terms will thus only be mentioned by appealing to their plausibility.

In spite of all quantum mechanical effects the functional form of the results expressed in (21) are due to the diffusive behavior of the particles. Their probability distribution $P(\vec{r},t)$, (14), is determined by the diffusion equation (13). Fourier-transforming (13), or $P(\vec{r},t)$, leads to $P(\vec{q},\omega)$. Using (13) plus proper boundary conditions one can easily convince oneself that one finds

$$P(\vec{q},\omega) \propto \frac{1}{-i\omega + D_0 q^2} \tag{22}$$

This is called a "diffusion pole", because $P(\vec{q},\omega)$ diverges for $|\vec{q}|, \omega \to 0$. Its origin is exclusively due to particle conservation during the diffusion.

The knowledge of $P(\vec{r},t)$, which is a local quantity describing a density distribution, or of $P(\vec{q},\omega)$ is not sufficient, however, if we want to know a dynamical quantity like the conductivity

or the diffusion coefficient $\mathcal{D}(\vec{q},\omega)$. For this one needs a more general function, e.g. the so-called "density-density correlation function" $\chi(\vec{r},t)$. It describes the dependence of a density distribution at one point in space and time on that at some other point in space and time. Its Fourier transform has the general structure [25]

$$\chi(\vec{q},\omega) = \frac{\mathcal{D}(\vec{q},\omega)\, q^2}{-i\omega + \mathcal{D}(\vec{q},\omega)\, q^2}\, \chi(\vec{q},0) \tag{23}$$

i.e. it also has a diffusion pole, where $\mathcal{D}(\vec{q},\omega)$ is now a $\vec{q}$ and ω -dependent diffusion coefficient. Once we know $\chi(\vec{q},\omega)$ we of course also know $\mathcal{D}(\vec{q},\omega)$. This quantity is therefore of fundamental importance for a systematic calculation of corrections $\delta\sigma$, $\delta\mathcal{D}$ to σ_0, $\mathcal{D}_0$ due to the impurity scattering. It can be derived within a perturbation theory using a diagrammatic "sign language" (Feynman diagrams) [26]. In this way the microscopic scattering processes are described graphically: (i) the motion of a particle is characterized by a line with an arrow ("propagator"), while (ii) the scattering at an impurity is symbolized by a dashed line with a cross. An example is shown in Fig. 12. The upper line, pointing to the right, describes a "particle" with energy $E_F + \omega$ and momentum $\vec{p} + \frac{\vec{q}}{2}$, while the lower line, pointing to the left, describes

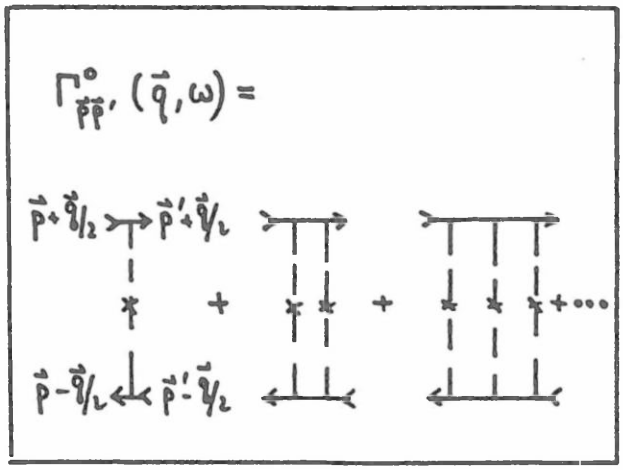

Fig. 12: Particle-hole ladder diagrams describing diffusion.

a "hole" with energy E_F and momentum $\vec{p}-\frac{\vec{q}}{2}$.
In this way the density-density correlation of a particle-hole pair due to the usual diffusion (namely a sequence of independent collisions) is described by means of intuitively appealing diagrams. It should be pointed out that the dashed line describes only a correlation and not an interaction (which so far has not been considered at all) between particle and hole. The arrows carry the initial and final momenta of the particle and the hole.

The diagrams in Fig. 12 can easily be summed up. In the case of small energy - and momentum differences between particles and holes (i.e. $\hbar\omega \ll E_F$, $|\vec{q}| \leq p_F = \hbar k_F$) one finds

$$\Gamma^{0}_{\vec{p}\vec{p}'}(\vec{q},\omega) = \frac{V_0 \tau}{-i\omega + D_0 q^2} \tag{24}$$

where V_0 is the potential energy of the scatterers. So, as expected, we have obtained a diffusion pole.

To understand the properties of the correlation leading to (24) we note that a particle-hole pair with small energy - and momentum difference can be graphically represented in momentum space as shown in Fig. 13.

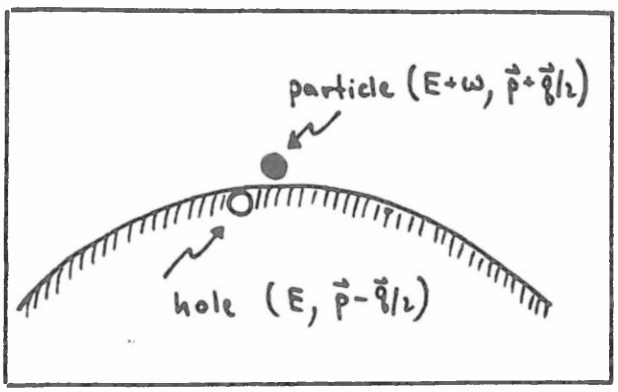

Fig. 13: Particle-hole excitation at the Fermi surface

The partners of such a pair always propagate in the same direction, experience the same collisions and are hence correlated for all time. This is a consequence of particle number conservation and this is the reason why the diffusion pole (24) always exists — even in the case of inelastic processes.

In the presence of time reversal invariance (which, by the way, does not refer to a global invariance of the whole system but to that of single-particle states!), particle states with momenta $\vec{k}$ and $-\vec{k}$ are equivalent. It means that we may invert the momentum of one of the arrows ("propagators"), i.e. replace $\vec{k}$ by $-\vec{k}$, without changing anything. To understand its consequences we now consider the particle-hole ladder in Fig. 11: we first turn around all the lower propagators and at the same time invert all the momenta as mentioned $\left(\vec{p}-\frac{\vec{q}}{2} \rightarrow -\vec{p}+\frac{\vec{q}}{2}\text{, etc.}\right)$. In this way (Fig. 14) we again arrive at a diagrammatic ladder but this time both arrows point into the same direction ("particle-particle ladder"). To obtain the usual particle-hole picture we merely have to turn around the total lower half of all diagrams, thereby arriving at strangely looking, seemingly complicated, "maximally crossed", i.e. fan-like, diagrams [27]. Their contribution [28] is easily obtained once we remember that they originated from a particle-hole ladder (24) in which, however, the momentum transfer is now given by

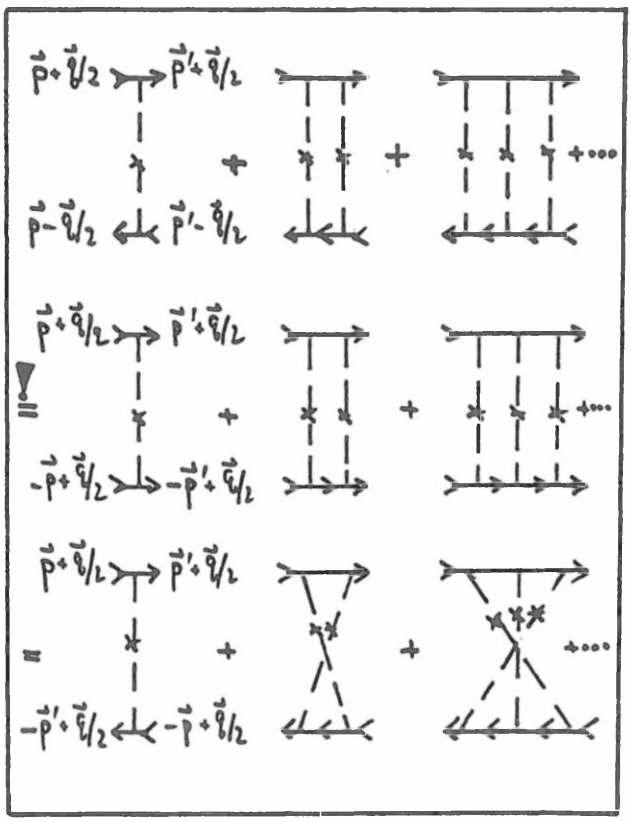

Fig. 14: Application of time reversal invariance for calculating the "maximally crossed" diagram.

$\left(\vec{p} + \frac{\vec{q}}{2}\right) - \left(-\vec{p}' + \frac{\vec{q}}{2}\right) = \vec{p} + \vec{p}'$ instead of $\vec{q}$ [29].

Their sum $\Lambda^{0}_{\vec{p}\vec{p}'}(\vec{q}, \omega)$ is then found to be

$$\Lambda^{0}_{\vec{p}\vec{p}'}(\vec{q}, \omega) = \frac{V_0 \tau}{-i\omega + D_0 (\vec{p} + \vec{p}')^2} \tag{25}$$

The essential difference to the particle-hole diffusion pole in (24) is, that the diffusion pole in (25) is no longer due to particle number conservation. This implies that, for example, inelastic processes (during which particles change their energy state) will destroy ("cut off") the pole structure in (25). This property will later become very important.

The contribution to the conductivity due to the scattering processes described by the diagrams in Fig. 14 is given by the "Kubo-formula" [26], i.e. by an integral over (25); more precisely by

$$\delta\sigma \propto \int d\vec{p} \int d\vec{p}' \, \frac{\vec{p}\cdot\vec{p}'}{-i\omega + D_0 (\vec{p}+\vec{p}')^2} \tag{26}$$

(Note, that the particle-hole diffusion pole, (24), when integrated over as in (26), does not contribute because the integrand is then odd in $\vec{p}$ and $\vec{p}'$! The main contribution of the integrand in (26) comes from the region $\vec{p}+\vec{p}' \simeq 0$, i.e. $\vec{p}' \approx -\vec{p}$ and is hence due to <u>backscattering</u>. The contribution considered here is in fact identical to one previously discussed, which we had obtained by calculating the return probability of a particle to its starting point. Clearly, a pronounced back scattering will favor localization. Since all scattering processes take place very close to the Fermi-surface $(|\vec{p}| \simeq \hbar k_F)$

backscattering means that one deals with a momentum change of $2\hbar k_F$. One therefore often speaks of "$2k_F$ - scattering". Here we encounter an essential similarity with Cooper pairing in superconductors, where particles with momenta $\vec{k}$ and $-\vec{k}$ couple, i.e. where one also has a particle correlation across the whole Fermi sphere. For this reason the particle-particle diffusion pole in (25) is often called "Cooper-pole" or "Cooperon", while the particle-hole diffusion pole in (24) is simply referred to as "diffuson".

Taking into account all prefactors in (26) and using the substitution $\vec{p}+\vec{p}'=\vec{k}$ one obtains a frequency dependent correction to the conductivity [30]

$$\frac{\delta\sigma(\omega)}{\sigma_0} = -\frac{k_F^{2-d}}{\pi m}\int_0^{1/\ell} dk\, \frac{k^{d-1}}{-i\omega + D_0 k^2} \tag{27}$$

The negative sign, indicating a lowering of the conductivity, is due to the minus sign in $\vec{p}'=-\vec{p}+\vec{k}$, i.e. is due to the back scattering. In $d=2$ one finds

$$\delta\sigma(\omega) = -\frac{1}{2\pi^2}\left(\frac{e^2}{\hbar}\right)\ln\frac{1}{\omega\tau} \tag{28}$$

For $\omega\to 0$ the conductivity indeed decreases.

Equations (27) and (28) are valid for an unbounded system at $T=0$. In the case of a finite system (e.g. a d-dimensional hyper-cube of side length L) the integration in (27) must be cut off from below at momenta $k = 1/L$, because smaller momenta do not exist. In that case the frequency ω can be put to zero [28] and one obtains a <u>length</u> dependent conductivity correction:

$$\delta\sigma\,(L) = -\left(\frac{e^2}{\hbar}\right) c_d \frac{\ell^{d-2}}{d-2} \left[1 - \left(\frac{L}{\ell}\right)^{2-d} \right] \tag{29a}$$

where $c_d = (2/\pi)\, S_d / (2\pi)^d$ and S_d is the surface of the d-dimensional sphere. In $d=2$ we have

$$\delta\sigma\,(L) = -\frac{1}{\pi^2}\left(\frac{e^2}{\hbar}\right) \ln\left(\frac{L}{\ell}\right) \tag{29b}$$

We note, that the prefactor of the logarithm in (28) and (29b) is given by a <u>universal</u> constant, where $(e^2/\hbar)^{-1} \simeq 4k\,\Omega$ is a universal resistance. Using $\sigma = \sigma_0 + \delta\sigma$ we also recognize that (28) and (29b) are indeed the lowest-order corrections to σ_0 in λ:

$$\sigma = \sigma_0 \left\{ 1 - \lambda (k_F \ell)^{2-d} \frac{d}{d-2} \left[1 - \left(\frac{L}{\ell}\right)^{2-d} \right] \right\} \tag{30a}$$

and in $d=2$

$$\sigma = \sigma_0 \left[1 - 2\lambda \ln\left(\frac{L}{\ell}\right) \right] \tag{30b}$$

i.e. the correction $\delta\sigma/\sigma_0$ is linear in $\lambda \ll 1$ and has a negative sign. The conductivity thus decreases when the system's size is increased — this is the precursor effect of localization.

How can one check these results experimentally? Well, we first have to bear in mind that all experiments are performed at finite temperatures. So, besides the elastic impurity scattering, one will also always have inelastic processes, which are described by some inelastic scattering time τ_{in} and for which we again assume that $\tau_{in}^{-1} \propto T^p$. In this way a new energy scale $\hbar/\tau_{in}$ enters the problem. As a consequence the energy $-i\omega$ in (27) is replaced by $-i\omega + \tau_{in}^{-1}$ The particle-particle diffusion pole is then cut off, such that $\omega \to 0$ does not lead to a divergence anymore. In turn, the frequency dependence in (28), $\ln(1/\omega\tau)$ is replaced by $\ln(\tau_{in}/\tau) \propto \ln(\hbar/k_B\tau T)$, i.e. by a temperature dependence just as in (20), (21). Alternatively one may say, that the inelastic processes introduce a new length scale, an "inelastic diffusion length", $L_{in} = (D_0 \tau_{in})^{1/2}$, the so-called "Thouless-length" [31]. It provides the length scale on which a particle suffers an inelastic process and is scattered

out of its energy state. For $L_{in} < L$ the size of the system is quite irrelevant: a particle will then only experience L_{in} as the relevant length. In this way L has to be replaced by in (29), (30) which leads to exactly the same temperature dependence of $\delta\sigma$ as in (20),(21).

A decrease of the conductivity $(\delta\sigma < 0)$ is equivalent to an increase of the resistance $(\delta R > 0)$. The corresponding logarithmic temperature dependence of the resistance of very thin films $(d = 2)$, as shown in Fig. 15, has been found in numerous experiments (for a

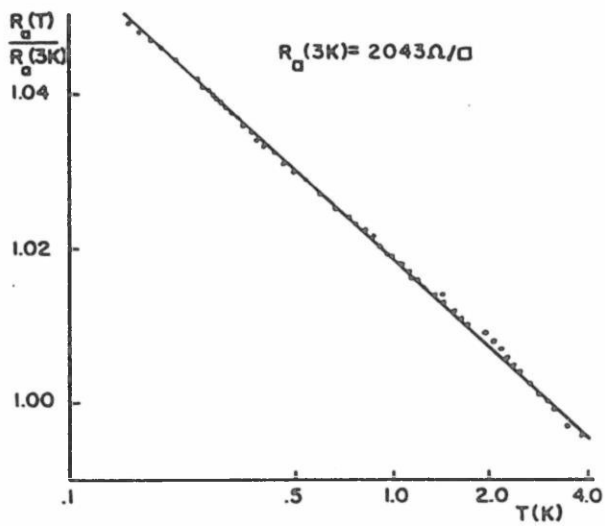

Fig. 15: Logarithmic temperature dependence of the resistivity of a thin palladium film[32].

review see [33]).

The preceding discussion was limited to the so-called "normal" scattering, i.e. scattering by non-magnetic impurities. Therefore the spin of the particles was unimportant. However, in the case that the impurities carry a magnetic moment, spin scattering will occur, causing the spin of the particles to flip. Therefore the particles experience something similar to a fluctuating magnetic field. The time reversal invariance is then lifted so that the Cooperon (25) does not diverge any longer (the pole is cut off by a constant term $1/\tau_s$, where τ_s is a characteristic collision time for spin scattering [34]). Field theoretical investigations [35,36], which we cannot discuss here in spite of their fundamental importance [37], have shown, that nevertheless even in this new situation one finds a logarithmic correction in $d=2$ just as in (30b). However, now the prefactor goes like λ^2 instead of λ, i.e. the correction is even smaller than in the case of normal scattering. Since Cooperons no longer yield a divergent contribution, these logarithmic corrections must be due to diffusons only, i.e. due to the usual diffusion process. It has not yet been possible to understand this result by means of the simple probability arguments used before in the case of normal scattering.

Impurities with a heavy nucleus lead to yet another type of scattering, namely to spin-orbit scattering of the particles. Theoretical investigations [36,38]

have again predicted a logarithmic correction for as in (30b) – but this time with a positive sign. The conductivity therefore increases with decreasing temperature! A simple quantum mechanical explanation, and experimental results fully supporting these findings, can be found in [33].

The Influence of a Magnetic Field on Localization

In the case of normal impurity scattering the localization effects originate from the quantum coherence of paths 1 and 2 in Fig. 10, i.e. from their ability to interfere. Therefore they are very sensitive to any kind of disturbance of time reversal invariance of the momentum states $\vec{k}$ and $-\vec{k}$. Such a perturbation is, for example, caused by a magnetic field. In its presence a state is no longer characterized by a momentum $\vec{k}$, but rather by the electromagnetic momentum $\vec{k} - 2e\vec{A}$. Here, $\vec{A}$ is the vector potential and the factor $2e$ (instead of simply e) is due to the correlation of two particles just as in superconductivity. If we now let $\vec{k}$ go into $-\vec{k}$, the momentum states, i.e. the paths 1 and 2 in Fig. 10, are no longer equivalent. Mathematically speaking this is a consequence of the fact, that now the amplitudes A_1 and A_2 carry field dependent phase factors [17].

$$A_1 \rightarrow A\, e^{\frac{ie}{\hbar c}\oint d\vec{\ell}\cdot\vec{A}}$$

$$= A\, e^{i\varphi} \quad , \quad \varphi = 2\pi \frac{\Phi}{hc/e} \tag{31}$$

$$A_2 \rightarrow A_1^*$$

The phases are given by the line integral over the vector potential $\vec{A}$, i.e. by the magnetic flux $\Phi = H\cdot S$, where H is the magnetic field and S is the area of the closed path in Fig. 10 (c = velocity of light). Since the motion of the particles is diffusive, S is given by $S = D_0 t$. The return probability W_H of a particle to its starting point in the presence of a magnetic field is again given by (17). One therefore obtains

$$W_H = 2|A|^2 \left[1 + \cos\left(\frac{2e}{c\hbar} H D_0 \cdot t \right) \right] \tag{32}$$

If $H = 0$ we find the old result $W_{H=0} = 4\,|A|^2$. The conductivity correction in the presence of a magnetic field, $\delta\sigma(H)$, is again determined by the return probability W_H . The <u>total</u> change of the conductivity due to a magnetic field, $\Delta\sigma(H) = \delta\sigma(H) - \delta\sigma(0)$, therefore depends on the probability <u>difference</u> $\Delta W = W_H - W_{H=0}$, such that

$$\Delta\sigma(H) = \int_{\tau}^{\tau_{in}} v_F \lambda_F^{d-1} \frac{dt}{(D_0 t)^{d/2}} \left[1 - \cos\left(\frac{2e}{c\hbar} H D_0 t\right) \right] \tag{33}$$

In $d=2$ (33) can be written as $\Delta\sigma(H) = e^2 F(x)$, where $x = \frac{2e}{c\hbar} H D_0 \tau_{in}$. The function $F(x)$ has the limits

$$F(x) = \begin{cases} x^2 & , x \ll 1 \\ \ln x & , x \gg 1 \end{cases} \tag{34}$$

For weak magnetic fields $(x \ll 1)$ one therefore finds

$$\Delta\sigma(H) \propto H^2 \tau_{in}^2 \tag{35}$$

while stronger fields $(x \gg 1)$ (34) give rise to a logarithmic field dependence

$$\Delta\sigma(H) \propto \ln(H \tau_{in}) \tag{36}$$

In any case, $\Delta\sigma$ is always <u>positive</u> $(\Delta R < 0)$, so the resistance <u>decreases</u> with increasing magnetic field ("anomalous magnetoresistance")[36]. The reason lies in the disturbance of the phase coherence by the magnetic field, leading to a weakening of the localization

effects. The "critical" field H_c, determined by $x = 1$, at which the change from the H^2 to the $\ln H$ behavior occurs, depends on τ_{in} and thus on temperature. At temperatures commonly used in experiments, H_c is of the order $H_c \simeq 100 - 500$ Gauss $(= 10 - 50\ mT)$. This should be contrasted with the classical result $\Delta\sigma(H)/\sigma_0 \simeq -(\omega_L \tau)^2$, which is not only many orders of magnitude smaller but also has a different sign (ω_L is the Larmor frequency)! So we see that even very small magnetic fields have a drastic influence on localization.

Oscillation effects

As first observed by Altshuler et al [39] the phase dependence of the electron wave function leads to a novel kind of quantum oscillation in the magnetoresistance of a multiply connected geometry, e.g. a torus made by wrapping up a thin, disordered metallic film (Fig. 16). The total change in phase, $\Delta\varphi_{loc}$, of the two oppositely traversed paths in the cylinder (Fig.17(b)), is given by (see (31))

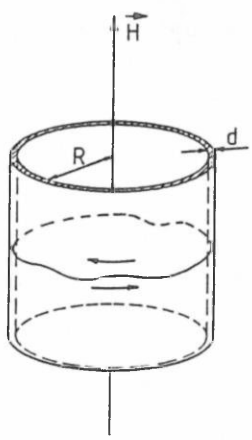

Fig. 16: Geometry used for detecting quantum oscillations in the magnetoresistance with period hc/2e.

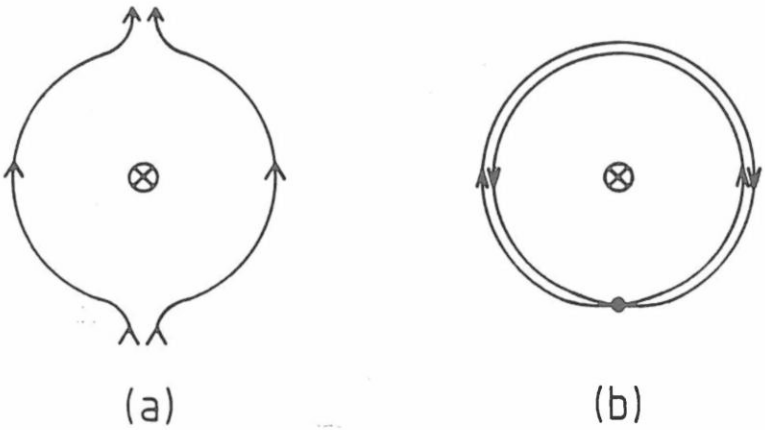

Fig. 17: Paths of interfering waves around screend magnetic field(⊗); (a) Usual Aharonov-Bohm effect, (b) geometry of Altshuler et al [39].

$$\Delta \varphi_{loc} = 2\varphi = 2\pi \frac{\Phi}{\Phi_0} \tag{37}$$

where $\Phi_0 = hc/2e$ is the flux quantum known from superconductivity (although we are here in a normal-conducting situation!). The weak localization correction to the conductivity is thus given by a straightforward extension of Eq. (33), i.e. [17]

$$\Delta\sigma(H) = \int_{\tau}^{\tau_{in}} dt \left[W_0 + 2 \sum_n W_n(t) \cos\left(2\pi n \frac{\Phi}{\Phi_0}\right)\right] \tag{38}$$

where the W_n are the return-probabilities for an electron after having traversed the loop n times. Clearly, $\Delta\sigma$ is an oscillatory function of the flux with periodicity Φ_0.
This finding must be contrasted with the well-known Aharonov-Bohm effect (Fig. 17(a)) where electrons passing a coil enclosing a magnetic field will only acquire a phase change

of half the change given by Eq. (31). This is so because in the Aharonov-Bohm effect each electron only samples half the flux Φ, because it only passes through half the loop (Fig. 17(a)). This yields a total phase change of

$$\Delta \varphi_{AB} = 2 \cdot \frac{\varphi}{2} = 2\pi \frac{\Phi}{hc/e} \tag{39}$$

leading to oscillations of the flux with period hc/e = 2 Φ_0. While the Aharonov-Bohm effect in a cylinder geometry is similar to Dingle-oscillations [40], the effect predicted in [39]with period Φ_0 is reminiscent of Parks-Little oscillations [41]in a superconducting geometry.

To observe the effect it is important that the inelastic diffusion length

$$L_{in} = \sqrt{D_0 \tau_{in}} \tag{40}$$

be larger than the circumference $2\pi R$ of the cylinder (Fig. 16), because otherwise the coherence is destroyed. (Note that both L_{in} and R can be much larger than the mean free path!).

The predicted oscillations were indeed measured [42](Fig. 18), and full agreement with theory was found. These experiments were done on thin Mg-films; other experiments used Li (where spin-orbit scattering is negligible) and also yielded very good agreement with theory[43]. For

a review see ref.[44].Subsequently, oscillations of the conductance with period hc/e in very small one-dimensional disordered metal rings when there is a magnetic flux through the center of the ring, have also been predicted [45, 46]. These authors used the Landauer formula[47]to connect the transmission coefficient through such a device to its conductance.

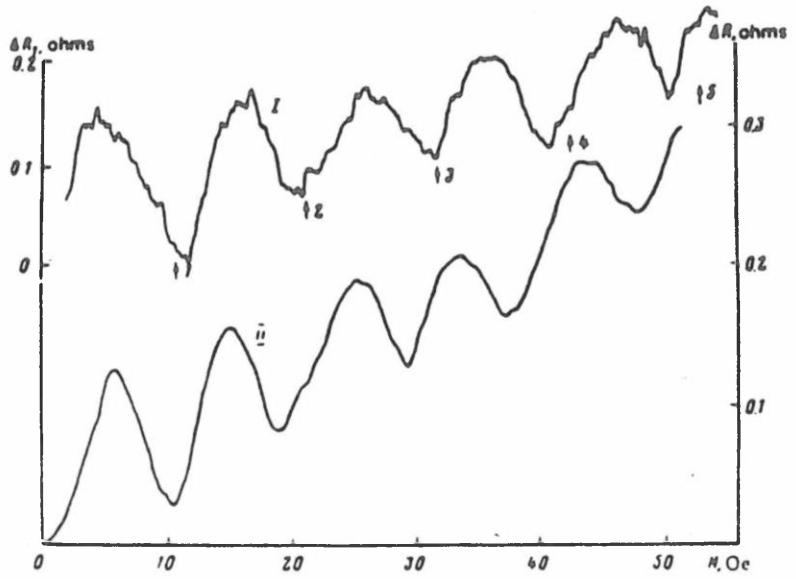

Fig. 18: Oscillations of the magnetoresistance of two different cylindrical Mg-films[42].

Networks

In the attempt to reproduce the experiments of ref.[42] other multiply-connected geometries than a single hollow cylinder where studied. This led to the investigation of networks of loops, e.g. of samples containing about 2.7×10^6 identical hexagonal loops forming a regular, two-dimensional honeycomb-network[48], or of ladders of 1000 little squares in series with 50 ladders in parallel[49]. The magnetoresistance of these new geometries were measured, and oscillations with period $\Phi_0 = hc/2e$ were found. A detailed theory of interference effects and quantum oscillations in the magnetoresistance of normal metal networks (loops, ladders, lassos, fractal networks, etc.) was worked out by Doucot and Rammal[50,51]who also found remarkable agreement with the experiment (Fig. 19). This work is

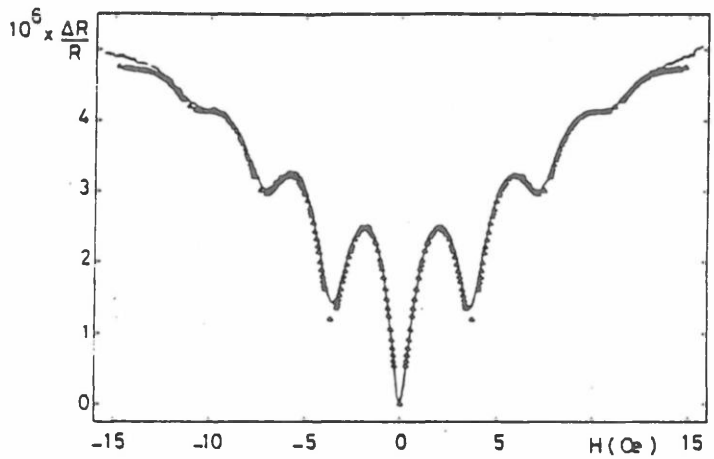

Fig. 19: Comparison between the theoretical results[50,51] and experimental data[50]for magnetoresistance oscillations measured with a copper network with honey comb structure.

closely related to similar investigations of superconducting networks[52], where fascinating physics is known to occur (frustration, fractional number of flux quanta per unit cell of the network, fractal fine structure of the upper critical field line due to interference effects between adjacent loops, etc.). In contrast, static properties of normal-conducting networks do not show such a fine structure because of an inherent regularization of the otherwise complicated spectrum[50,51].

hc/e versus hc/2e Oscillations

Both from an experimental and theoretical point of view a single ring should be about the simplest geometry to observe the above-mentioned oscillations in the magnetoresistance. Experimentally, the opposite was true since, at first, the Φ_0 -oscillations could not be found. Later, both $2\Phi_0$ = hc/e and Φ_0= hc/2e-oscillations were detected in individual, micron size, normal metal rings[53]. The different temperature and field dependence clearly distinguishes between the two effects and their physical origin. At low fields the localization induced hc/e-effect is visible. Most recently both types of oscillations were also measured in samples made up of N such rings in series[54]. It was found that, on averaging, the amplitude of the hc/e oscillations showed a $1/\sqrt{N}$ decrease, while the hc/2e-effect was indepen-

dent of N. This has also been verified theoretically[55]. It clarifies the role of ensemble averaging in calculating corrections to the conductivity. This kind of averaging is canonically employed in the framework of weak localization (yielding hc/2e-oscillations) but not in the calculation of the transmission coefficient[46]in metal rings, where only the hc/e-effect is found. So, to obtain the hc/2e-effect, ensemble averaging is necessary.

Mesoscopic Systems and Universal Fluctuations

As an unexpected byproduct, the investigations of quantum oscillations in (sub-)micron structures("mesoscopic" systems) led to the discovery of anomalously large, universal fluctuations [56-58]. These fluctuations, known from experiment[59]and numerical simulations[60], are not due to time dependent noise or finite-size effects. They only occur if the temperature is low enough such that the inelastic diffusion length L_{in} ,(40), exceeds the sample dimension. In this case "pure"quantum mechanical interference of the electronic wave function occurs. The resulting stochastic fluctuations of the magnetoresistance are sample-dependent, but are reproducible for every sample and hence yield the "magneto-finger print" of a sample. As such they characterize the individual impurity configuration of a sample.

This implies in particular, that these samples do not show some kind of "average" behavior.

To understand this behavior we return to the discussion of the probability W for going from one point to another one by the diffusion of quantum mechanical particles (see below (17(b)). The sum $\sum_{i \neq j} A_i A_j^*$ in (17b) is clearly configuration dependent, but the <u>ensemble average</u> is not - in fact, it vanishes. By contrast, in the case of the paths shown in Fig. 10, this sum is configuration <u>independent</u>, since it involves a priori coherent paths.

An important quantity to look at is the "conductance" G

$$G = \frac{1}{R} \quad [\mho] \tag{41}$$

i.e. the inverse of the resistance R of a d-dimensional system. For a d-dimensional hypercube of side length L, R is given by

$$R = \rho \frac{L}{A} \tag{42}$$

with ρ the "resistivity" and $A = L^{d-1}$ the cross-section of the conductor. Since ρ is the inverse of the conductivity σ ($\rho = 1/\sigma$), the conductance is given by

$$G = \sigma \, L^{d-2} \tag{43}$$

In the ohmic regime σ is independent of L. Note that one may write

$$G = \frac{e^2}{\hbar} g \tag{44}$$

where g is a dimensionless conductance in units of $e^2/\hbar$, i.e. is just a number.

When one calculates the r.m.s. value of the relative variance of G for a mesoscopic system in d dimensions at very low temperatures one obtains[56,57]

$$\frac{\sqrt{\langle G^2\rangle - \langle G\rangle^2}}{\langle G\rangle} \propto \frac{1}{L^{d/2}} \cdot \frac{1}{L^{(d-4)/2}} \tag{45a}$$

$$\propto \frac{1}{L^{d-2}} \tag{45b}$$

where $\langle\rangle$ stands for the ensemble average. This should be contrasted with the wellknown classical, thermodynamic result $1/L^{d/2}$, which implies <u>self-averaging</u> in the system. Obviously, the quantum mechanical result (45a) shows that in d = 1,2 there is no longer self-averaging. Even in d = 3 the relative variance vanishes much slower than in the classical case. The second factor in (45a) represents the effect of quantum interference in the diffusion (the exponent (d-4)/2 is due to the integral over the <u>square</u> over the diffusion poles, which describe the fluctuations).

The absence of self-averaging is due to spatial correlations in the system building up during the random walk of the quantum mechanical particle, which in d = 1,2 may visit essentially all scatterers.

The absolute variance of G is then given by $(\langle G \rangle \propto L^{d-2})$

$$\sqrt{\langle G^2 \rangle - \langle G \rangle^2} \propto \frac{e^2}{\hbar} \qquad (46)$$

i.e. is found to be <u>independent</u> of the system's size, implying a universal behavior! The effect depends only weakly on dimensionality and the strength of (weak) disorder and is, of course, much larger than expected classically. It has clearly been observed in the experiment[61]. The quantum interference of randomly diffusing electrons, which leads to the large fluctuations, implies an extraordinarily large sensitivity of the conductance on the impurity configuration. Indeed, the displacement of a single impurity by only λ_F (de Broglie wave length) affects essentially all quantum mechanical paths and hence changes the conductance by a universal, i.e. sample size independent amount [62,63]. A comprehensive discussion of the effects of finite temperatues, interactions, and magnetic fields on the universal conductance fluctuations, as well as of the physical assumptions underlying the ergodic hypothesis has been presented by Lee et al [64].

The Anderson transition

We have so far calculated small corrections to the metallic conductivity σ_0 due to the elastic impurity scattering. These corrections are the result of a perturbation theory and are lowest order in the disorder parameter $\lambda \ll 1$. On the other hand, for $d \leq 2$ we found that, in spite of the smallness of λ, the corrections diverge in the limits ω or $T \to 0$ or $L \to \infty$. In this situation the perturbation theory breaks down, i.e. fails because the condition $|\delta\sigma| \ll \sigma_0$ is no longer fulfilled. What now? One could try to calculate higher order corrections in λ, but that doesn't get us very far and is also very complicated. Besides that, a phase transition and the critical behavior can never be obtained by a finite order perturbation theory. Since an exact solution of the problem does not a priori appear to be possible, one has to use other methods. Two such possibilities will be discussed here: (i) a scaling theory, which is based on renormalization group ideas and which determines and (ii) a self-consistent approach which calculates $\sigma(\omega)$.

Scaling Theory

A very successful scaling theory of the Anderson localization problem was introduced in 1979 by Abrahams et al. [13]. These authors developed a one-parameter scaling theory for the conductance g, (44),

of a d-dimensional system and connected it to a perturbation theory, in which the previously discussed length dependence of the correction was calculated for the first time. The conductance g is a <u>number</u>, i.e. a dimensionless parameter, whose relevance for the localization problem (particularly that of its length dependence) had first been recognized and discussed by Thouless [23] in several very important papers. In the metallic regime where Ohm's law holds, the conductivity is by definition length independent, so that the conductance is given by $g \propto L^{d-2}$. On the other hand in the insulating regime the wave functions fall off exponentially; one would therefore also expect an exponential length dependence of σ and thus of g , i.e. $g \propto \sigma \propto e^{-L/\xi}$, where ξ is an unknown "localization length". What now is the length dependence of g in between these limiting cases? To answer this question, we take hypercubes of side length L and build up a larger hypercube with side length b·L . Now we ask how the conductance of the larger system, $g(bL)$, depends on the conductance of the initial cube, i.e. $g(L)$. In principle $g(bL)$ could be a function of $g(L), b, L$ and also all kinds of non-universal properties of the material (ℓ, k_F, m etc.). The heart of the argument proposed by Abrahams et al. now is, to assume that the old g was in fact the <u>only</u> relevant parameter of the system that would determine the <u>new</u> g , i.e. to have a relation

$$g(bL) = f[b, g(L)] \tag{47a}$$

or, equivalently,

$$g(L) = f\left[b, g\left(\frac{L}{b}\right)\right] \tag{47b}$$

where f is some, yet unknown, function. In this way microscopic details are assumed to be unimportant. Eq. (47b) may be called a "scaling equation". Since the relation is supposed to hold for any value of b, we differentiate (47b) by b and then set $b = 1$. Then we obtain

$$\frac{dg(L)}{d\ln L} = \tilde{f}\left[g(L)\right] \tag{48}$$

where $\tilde{f}$ is a function involving f. The logarithmic derivative of g with respect to L therefore turns out to be a function of only g itself. To take a logarithmic instead of the usual derivative is indeed a convenient trick: one thereby achieves that length <u>scales</u> of L (e.g. ℓ or ξ in L/ℓ, L/ξ) which we do not know anyhow, drop out! Abrahams et al. [28] now defined a so-called "β-function"

$$\beta \equiv \frac{1}{g}\frac{dg}{d\ln L} = \frac{d\ln g}{d\ln L} = F\left[g(L)\right] \tag{49}$$

which is essentially given by (48) and which is also only a function of $g(L)$. Its behavior under a change

of $g(L)$ determines the conductivity behavior of the system.

Starting from what we already know, we can easily calculate the limiting cases of β. In the localized regime $g \ll 1$, with $g \propto e^{-L/\xi}$, we find

$$\beta \simeq \ln g \tag{50}$$

while in the metallic regime $g \gg 1$ we have $\sigma = \sigma_0 + \delta\sigma$, where $\delta\sigma$ is given by (29a). Combining (43) and (49) one arrives at

$$\beta = d-2 - \frac{c_d}{g} + O\left(\frac{1}{g^2}\right) \tag{51}$$

The first term in (51), i.e. $d-2$, represents Ohm's law (purely metallic conductivity) while the $1/g$ correction term follows from the perturbation theory for the conductivity.

By means of (50),(51) which describe β in the limits $g \ll 1$ and $g \gg 1$ we may try to draw conclusions about the shape of β for <u>all</u> g. This is shown in Fig. 20, where $\beta(g)$ has been plotted versus $\ln g$. The calculated limits of β for the insulating and the "metallic" regime are shown by full curves. Note the important fact, that for $g \gg 1$ all β-curves are smoothly bending upward — a consequence of the negative

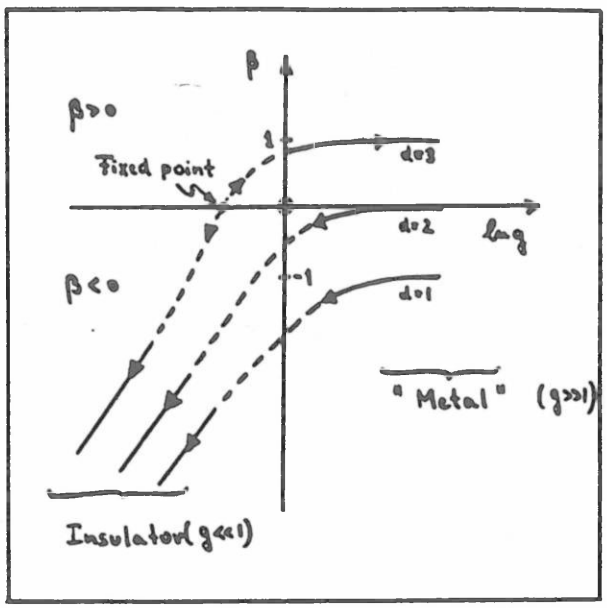

Fig. 20: The β-function for d = 1,2,3 dimensions

sign of the 1/g correction in (51). So, as g becomes smaller, the β-curves move away from the limiting value $d-2$. One may therefore make a sensible assumption about the unknown region in between: namely, that also there the β-curves have a smooth and monotonous shape as shown by the dashed curves in Fig. 20. This figure corresponds to a "flow diagram", which reflects the behavior of the system under changes of the system's size. For $d \leq 2$ this behavior is characteristically

different from the one for $d>2$: (i) $\underline{d \leq 2}$; in this case β is always negative. Since β describes the change of the conductance g with the system's size L, this implies $dg/d\ln L < 0$. An enlargement of the system therefore always leads to a decrease of g: the curves in Fig. 20 always "flow" to the left into the insulating regime. This tells us that for $d \leq 2$ and $L \to \infty$ all states are localized. The system is always an insulator. Of the curves that always have a negative β the case $d=2$ is obviously special ("marginal"): the curve approaches $\beta = 0$ for $g \gg L$ but never reaches $\beta = 0$ at finite g ; so even here the states of the infinite system are always localized. This provides the answer to our initial question about the possibility of metallic conductivity of very thin films $(d=2)$ at $T = 0$: we now find that a truely metallic conductivity in $d=2$ is never possible! (ii) $\underline{d > 2}$; here two possibilities, $\beta < 0$ and $\beta > 0$, exist since the β-function has a zero at $g = g_c$. For systems with an initial value of the conductance $g < g_c$ (i.e. with a disorder $\lambda > \lambda_c$, where $g(\lambda_c) \equiv g_c$) we find $\beta < 0$. Therefore an enlargement of the system again leads to an insulating behavior (flow of the curve to the left). However, for an initial value $g > g_c$ (i.e. $\lambda < \lambda_c$) one has $\beta > 0$, such that increasing the size of the system drives it to the right, i.e. into the <u>metallic</u> regime. The point $\beta(g_c) = 0$ is called "fixed point", because g stays

fixed when L is changed. This point represents the Anderson transition. So we find that for d > 2 there exists a transition at a finite g_c, i.e. at a finite value of the disorder, λ_c. Depending on the disorder $(\lambda \lessgtr \lambda_c)$ states are either extended (metal) or localized (insulator).

In the vicinity of the transition, $\beta(g) \simeq 0$, the β-function may be linearized:

$$\beta = \frac{1}{\nu} \frac{g-g_c}{g_c} \tag{52}$$

where $1/\nu$ is the slope of β at $g = g_c$ in Fig. 20. Eq. (52) can be integrated and yields

$$\frac{L}{L_0} = \left(\frac{g-g_c}{g_0-g_c}\right)^{\nu} \tag{53}$$

where $g_0 = g(L_0)$.

In the localized regime $(g, g_0 < g_c)$ one finds

$$g = g_0 \left[1 - \left(\frac{L}{\xi}\right)^{1/\nu}\right] \tag{54}$$

where ξ has been introduced as a "localization length". If we define a parameter $t = (g_0 - g_c)/g_c \propto (\lambda - \lambda_c)/\lambda_c$, which measures the disorder of the system relative to the corresponding critical value, i.e. the distance from the critical

point, then (53), (54) imply

$$\xi \propto |t|^{-\nu} \tag{55}$$

Thus the number ν turns out to be the critical exponent of the localization length ξ. Eq.(55) says that ξ diverges as the disorder approaches the critical value λ_c and is then the only relevant length in the problem.

In contrast, the metallic side $(g, g_0 > g_c)$ is characterized by a finite dc-conductivity $\sigma(0)$. Using (43) and (53) we find

$$\sigma(0) \propto t^{\nu(d-2)} \tag{56}$$

The critical exponent of $\sigma(0)$, which is usually referred to as s, is therefore given by

$$s = (d-2)\nu \tag{57}$$

This relation connects two critical exponents, one of which describes the behavior on the metallic side (s), while the other one determines the critical behavior on the insulating side (ν). This scaling relation was first derived by Wegner [66] already in 1976, who showed (in a paper of fundamental importance for the Anderson localization problem) that there exists a close connection to the problem of critical phenomena.

Integration of (51) leads to an explicit value for s, namely $s=1$. Within the approximations used, this result is valid at least close to 2 dimensions ($\epsilon \equiv d-2 \ll 1$). In particular, in d = 3 (57) implies $s = \nu$ and therefore $s, \nu = 1$.

Numerical calculations of the conductance in d = 1,2,3 apparently confirm the one-parameter scaling hypothesis[67], and obtain $s = \nu$. On the other hand, in d = 3 the actual value of s is found to be significantly higher than s = 1, i.e. yield $s \simeq 1.5-1.7$[67].

Field theoretical methods have also led to a scaling theory in the case of magnetic impurities [35-38]. The results are qualitatively very similar to the ones obtained in the previously discussed case. In particular, one again expects an Anderson transition for $d>2$, while for $d \leq 2$ all states are localized. The fact that the perturbational corrections due to the spin scattering are proportional to λ^2 (instead of λ as for normal scattering) is also reflected in the critical properties: the conductivity exponent s is here found to be $s=1/2$ instead of $s=1$.

Eq. (56) implies that the dc-conductivity goes to zero continuously as the transition is approached. This finding contradicts Mott's concept of a "minimal metallic conductivity" and the related discontinuous transition. The experimental confirmation of the continuous behavior will be discussed later.

The Method of Selfconsistency

The theoretical approach[28]as described above is based on the assumption of a one-parameter scaling relation (49), whose validity cannot be further proven within this very framework.

Quite a different theoretical concept, which may be used to describe the conductivity behavior as well as the transition and the critical properties and which does not rely on a scaling assumption, is that of "selfconsistency" [68]. Within this method one attempts to express the frequency dependent conductivity (or the diffusion coefficient by means of a non-trivial, generally approximate, relation which itself involves this quantity. So one wants to find an equation of the form

$$\mathcal{D}(\omega) = \mathcal{F}\{\mathcal{D}(\omega)\} \tag{58}$$

whose "self-consistent" solution then yields $\mathcal{D}(\omega)$ for all ω and all disorder-parameters λ. For this to be successful it is necessary to start from known limiting cases (e.g. (58) has to agree with perturbation theory for $\lambda \ll 1$) such that the theory can be anchored to an exact result [29]. The selfconsistency is then used to go beyond perturbation theory, i.e. to the transition itself (and even beyond). It is therefore used as a substitute for an (infeasible) perturbation theory to infinite order.

Since $\mathcal{D}(\omega)$ vanishes at the transition, its inverse $\mathcal{D}_0/\mathcal{D}(\omega)$ correspondingly diverges at that

point. Using a diagrammatic theory Vollhardt and Wölfle [29,69] showed that a selfconsistent calculation of the latter quantity can be performed by summing up the largest (i.e. most divergent) contributions of perturbation theory. In this way one can indeed derive a selfconsistent equation. It has the simple structure

$$\frac{D_0}{D(\omega)} = 1 + \frac{1}{\pi N_F} \int \frac{d\vec{k}}{(2\pi)^d} \frac{1}{-i\omega + D(\omega) k^2} \tag{59}$$

where $D_0 / D(\omega)$ is given by the integral over a diffusion pole involving the diffusion coefficient itself rather than the diffusion constant D_0. This relation can also be obtained by other methods [70-73]. Its solution can easily be obtained: one finds that for $d \leq 2$ the dc-conductivity $\sigma(0)$ is always zero, irrespective of how small the disorder is (insulating behavior). However, in dimension $d=2$ the localization length ξ is exponentially large for $\lambda \ll 1$ [29]:

$$\xi \propto e^{1/2\lambda} \tag{60}$$

For $d > 2$ there exists a critical value of the disorder below which $\sigma(0)$ is finite (metallic regime), while for larger values it vanishes (insulating regime). Since the limit $\omega \to 0$ can be explicitly performed within this theory one obtains results which go beyond

the range of applicability of the scaling theory described above ($\omega \to 0$ means, that one leaves the critical regime). Besides that one obtains complete agreement with the results of the scaling theory. In particular one also finds the scaling relation (57) and the value $S=1$ for dimensions $2 < d < 4$. In fact one can show that (59) itself possesses scaling properties and therefore naturally leads to a scaling theory [69,71,74,75]. Performing the integral in (59) and choosing appropriate units such that one obtains dimensionless quantities G and z instead of D and ω , (59) can be written as [69]

$$\frac{d-2}{r_d} G = \pm z^{\frac{2-d}{d}} + G^{\frac{2-d}{2}} \tag{61}$$

where the plus (minus)-sign corresponds to the metallic (insulating) regime and r_d is a dimension-dependent constant. In (61) no material dependent parameters (k_F , m , λ etc.) are explicitly involved. It is therefore indeed a "scaling equation" which establishes a <u>universal</u> dependence of the conductivity or frequency. Its solution determines a complete and smooth curve for the β-function (49) [75].

A field theoretical analysis [73] of the present problem shows that, if a perturbational treatment is valid at all, (59) is an <u>exact</u> relation — at least close to two dimensions.

A full renormalisation-group treatment of the density-density correlation function[76]yielded the scaling behavior of the diffusion coefficient $D(\omega,\vec{q})$. For $v_F q < \omega$ the result is again identical to the self-consistent equation (59).

Interacting, Quantum Mechanical Particles in Disordered Systems

The theory discussed so far only involved the elastic scattering of non-interacting, quantum mechanical particles due to impurities. If, on the other hand, one wants to check the results experimentally, one always deals with systems, in which the particles also mutually interact. The most important example is that of electrons in a disordered metal. Even if one was always allowed to assume the Coulomb interaction between the electrons to be strongly screened, one would still have to know about its actual qualitative and quantitative influence compared with the effects of localization [11,37].

Pure electron-electron interaction is strictly momentum conserving and therefore does not contribute to the metallic resistance. So, as much as before, the momentum change of particles due to impurity scattering is essential. To understand the combined effects, we

take a look at the inelastic interaction among the electrons themselves [78]. It is characterized by a momentum transfer q (with $q\ell \ll 1$) and an energy transfer $\hbar\omega$ (with $\omega\tau \ll 1$), where ℓ and τ are the mean free path and the average collision time of the electrons due to the impurities. One may then define an "interaction time" $t_0 = 2\pi/\omega$; obviously $t_0 \gg \tau$. This means that during the time t_0 many scatterings between electrons and impurities occur, leading to a qualitative change of the interaction itself. The "bare" interaction therefore becomes an "effective" interaction whose character depends on the energy transfer $\hbar\omega$. These effects lead to corrections $\delta\sigma$ and δN of the (metallic) conductivity and of the density of states close to the Fermi surface, respectively.

Estimating the Corrections

Calculating the corrections to σ to lowest order in the disorder λ , Altshuler and Aronov [78], found the surprising result, that they had the <u>same</u> structure as those in the non-interacting case. In particular, there is again a logarithmic temperature dependence of $\delta\sigma$ in $d = 2$, although the quantum mechanical interference processes that led to (19),(21) had not been considered by these authors at all! If initially one perhaps believed in an obscure coincidence,

we now know that these results are solely due to the disorder in the system. It leads to a diffusive behavior of the particles and thereby to a change of the interaction due to density fluctuations. In this way the naked, long range interaction between the electrons becomes an effective interaction of short range.

To study the implications we now investigate the inelastic scattering of two electrons (more precisely: of a particle-hole pair) with energy ϵ (relative to the Fermi surface) in which an energy transfer $\hbar\omega \simeq \epsilon$ is assumed to occur [79]. According to the uncertainty principle the particle and the hole remain in mutually coherent states up to times $t \lesssim \hbar/\epsilon$, during which interference is possible. However, in the case of a short range interaction it is necessary that the particles actually meet at the same position during that time. The probability for this to happen we call $W(\epsilon)$. The short range interaction Λ is thereby changed to

$$\Lambda_{eff} = \Lambda\left(1 + W(\epsilon)\right) \tag{62}$$

To estimate $W(\epsilon)$ we observe once more that the motion of the particles is diffusive, i.e.

$$W(\epsilon) \propto \int_{\tau}^{\hbar/\epsilon} \frac{dt}{(D_0 t)^{d/2}} \tag{63}$$

The integrand is thus given by $1/V_{diff}$, (15), just as in the localization problem. Consequently the integral leads to the same dimension dependent expression as in ( ). In $d = 2$ one obtains

$$W(\epsilon) \propto \ln(\hbar/\epsilon\tau) \quad . \tag{64}$$

We now assume that the relative corrections of physical quantities to lowest order in λ due to these effects are given by the change in the interaction, i.e. by

$$\frac{\delta\sigma}{\sigma_0}, \frac{\delta N(\epsilon)}{N_F} \propto \delta\Lambda_{eff} = \Lambda \cdot W(\epsilon) \tag{65}$$

For example, the correction to the density of states in $d = 3$ is then given by

$$\delta N(\epsilon) \propto \Lambda \sqrt{|\epsilon|} \tag{66}$$

In the case of repulsive interaction $(\Lambda > 0)$ the density of states is hence found to <u>decrease</u> in the vicinity of the Fermi surface, having a downward, non-analytical cusp at E_F (i.e. $\epsilon = 0$). This behavior has in fact been observed in tunnel experiments [80] where the tunnel conductance dI/dV , which is proportional to the density of states, is measured as a function of the voltage V (instead of the energy ϵ); see Fig. 21 .

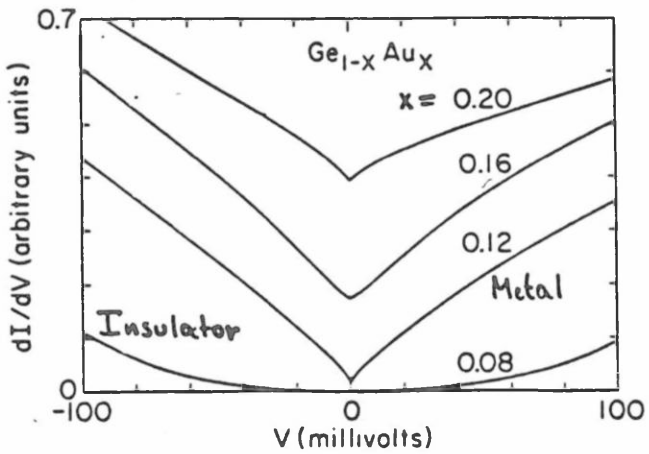

Fig. 21: Behavior of the density of states close to the Fermi energy in d = 3 [80].

To obtain the conductivity correction at finite temperatures the energy ϵ is replaced by T in (63):

$$\frac{\delta\sigma}{\sigma_0} \propto \Lambda = \begin{cases} \ln\left(\frac{\hbar/\tau}{k_B T}\right) & , d=2 \\ T^{\frac{d-2}{2}} & , d \neq 2 \end{cases} \tag{67}$$

The temperature dependence of $\delta\sigma$ is therefore identical to the one previously found in the localization problem, although the quantum mechanical interference due to backscattering (67) is not involved at all. Only

the diffusive behavior of the electrons is of importance. In fact, inclusion of the "Cooperons" only leads to an insignificant change of the results in (67) [81].

The singularities in the density of states and other physical quantities show that, in fact, the disorder leads to essential changes of the properties of a Fermi liquid, thus disproving long held, opposite views.

In the meantime there even exists an exact solution of the interaction problem to lowest order in $\lambda \ll 1$ [82] which can also be understood within Fermi liquid theory [83]. Therefore, in the case of weak disorder, again a satisfactory situation has been reached.

The Metal-Insulator Transition

To go beyond perturbation theory and to be able to study the metal-insulator transition (including its critical properties), one needs a scaling theory or some other high-power mathematical method. Such a scaling theory of the transition close to d = 2 dimensions has, in fact, been formulated [82,84,85], whereby the relevant scaling variables in the problem have been identified. However, only in a few special cases (strong external magnetic field and magnetic spin scattering, respectively) have they led to definite conclusions. In these cases one finds that, just as in the localization problem, a

transition will only occur above $d = 2$ dimensions. Close to the transition the dc-conductivity is expected to vanish linearly in $\lambda_c - \lambda$ (i.e. with critical exponent $s=1$, like in Anderson localization without magnetic field or spin scattering). However, the general behavior is still unknown. In fact, in the case of zero external magnetic field the renormalization-group analysis breaks down before the transition is reached since scaling go towards strong coupling[84,85]. This is due to the appearance of local magnetic moments (strong spin fluctuations) which lead to a divergence of the spin susceptibility for $T \to 0$. Furthermore, the quantum interference effects due to backscattering which are responsible for the transition in the non-interacting system have not yet been fully considered. Nevertheless, it has been noted that the results of the renormalisation group approach [84]for physical quantities like the compressibility, spin susceptiblity and specific heat show a similarity to those known from Landau's Fermi liquid theory (for a detailed discussion of the latter see part II of these lectures). This correspondence allowed for the formulation of an effective Landau theory for disordered electrons close to the metal-insulator transition and has yielded predictions, e.g. for the low temperature behavior of the specific heat and the spin susceptibility in various experimental situations [82,84-87]. Nevertheless, the general problem of the metal-insulator transition for interacting, disordered systems is not yet understood.

Experimental Results and Theoretical Conjectures

In an experiment the transition is usually not approached by increasing the disorder λ to λ_c but rather by decreasing the particle density n . In semi-conductors this can be achieved by a change of the doping concentration; in this way the energy of the particles

$$E = \frac{\hbar^2}{2m} (3\pi^2 n)^{2/3} \tag{68}$$

is lowered. If the critical energy at which the transition takes place is denoted by $E_c = E(n_c)$, the system will be in the metallic regime for $n > n_c$ (i.e. $E > E_c$) and in the insulating regime for $n < n_c$ (i.e. $E < E_c$).

As the details of the transition have not yet been understood, the corresponding experiments have also not been explained conclusively [88]. In three-dimensional samples one finds for example that there is one group of systems (e.g. amorphous $Nb_x Si_{1-x}$ or compensated $Ge:Sb$) where $\sigma(0)$ vanishes linearly with $n-n_c$ (i.e. $s=1$; see Fig. 22a) while in another group (e.g. $Si:P$ or uncompensated $Ge:Sb$) one finds a root-behavior (i.e. $s=\frac{1}{2}$; see Fig. 22b). (Note, that in both cases the conductivity goes to zero continuously; furthermore, in both cases conductivities significantly below the postulated minimal metallic conductivity σ_{min} (see the arrows in Fig. 22a,b)

have been measured.) The reason for this different critical behavior is still not clear. However, the two groups of materials differ in one essential point and this has led to certain conjectures concerning the underlying physics [90,91]. The systems exhibiting

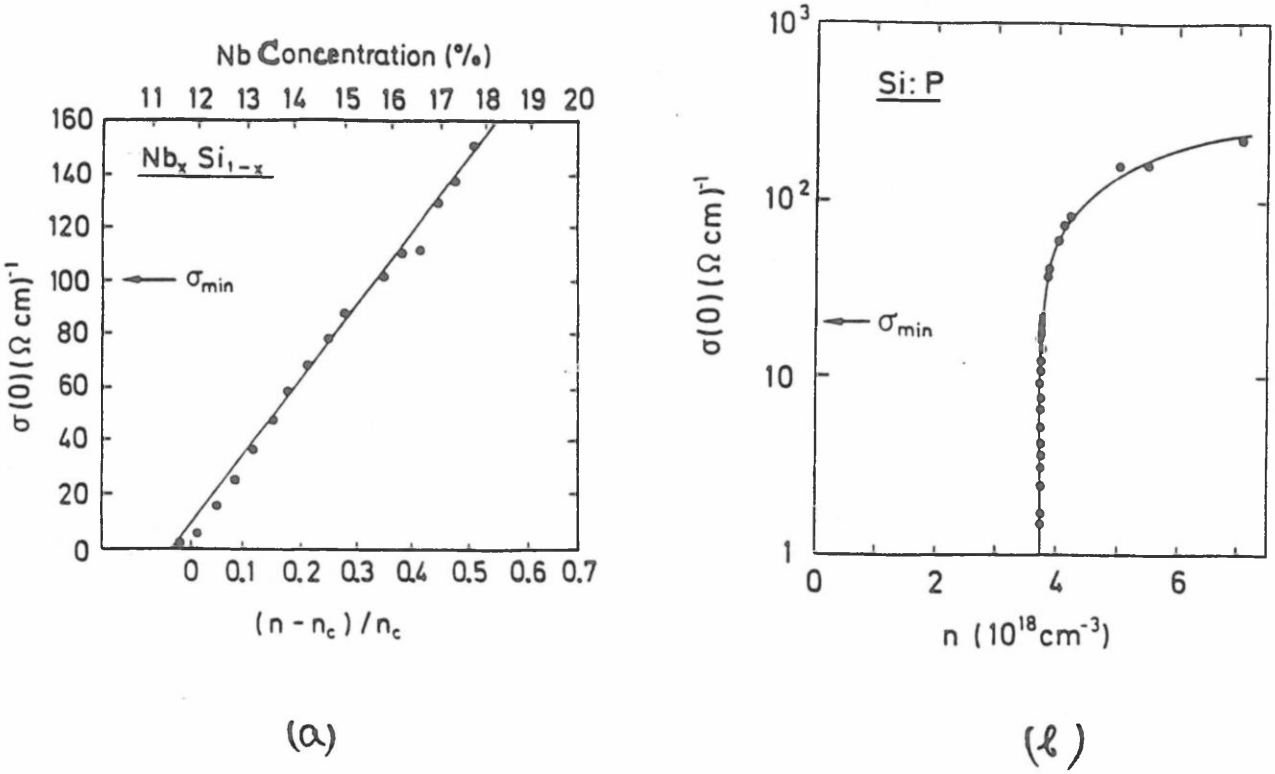

Fig. 22: Dc-conductivity of different systems close to the metal-insulator transition: (a) Exponent $s=1$ [89], (b) $s=1/2$ [88].

$s=\frac{1}{2}$ possess one valence electron per scattering center. (In the case of Si:P every P-atom contributes one additional valence electron to the electronic system, while the remaining P-ions represent the random potentials by which the electrons are scattered). In contrast to this, in the systems with $s=1$ there are several electrons per scattering center. (In the case of compensated Ge:Sb equal amounts of Sb and B are added, which then

exchange an electron; so they do not contribute additional charge carriers but only scattering centers.) One may now speculate that these additional scatterers lead to an increased scattering of the electrons and that therefore the conductivity behavior with $S=1$ is essentially that of the Anderson transition. On the other hand $S=1$ is also compatible with the interaction theory for systems with strong spin scattering.

The situation in the group of materials with $S=\frac{1}{2}$ is even more unclear. The behavior $S=\frac{1}{2}$ has so far only been found for non-interacting systems with strong spin scattering. However, in $Si:P$ only the electrons carry a spin. Now, it might just be so that the local magnetic moments (spin fluctuations), which the renormalization group calculations for the interacting system come across (and which lead to their ultimate breakdown) act as spin scattering centers themselves [90]. The interaction would then, through a collective behavior of the electrons, provide magnetic moments on which the electrons themselves scatter. Apart from that the electrons would "feel" a non-interacting system. Within this concept one would be able to obtain $S=\frac{1}{2}$. In fact this picture is supported by measurements of the specific heat and the spin susceptibility of these systems [88]. In the limit $T \to 0$ one finds that both quantities strongly increase. – In particular, ESR measurements of $Si:P$

just on the metallic side of the transition[91], as well as NMR results taken through the transition [92], clearly indicate spin localization, i.e. slowing down of spin diffusion. At present it is not clear whether this behavior is similar to that known from the theory of strongly correlated ("almost localized") Fermi systems such as normal liquid ^{3}He [93]. In the latter systems correlation effects are known to enhance both the specific heat and the spin susceptibility via an enhancement of the effective mass, leaving their ("Wilson"-) ratio essentially unaffected.

In any case, there are remarkable connections between seemingly very different areas of condensed matter physics: between the problem of disordered systems, of Fermi liquid theory, of the theory of strongly correlated Fermi systems and also of superconductivity. We can be sure that a great deal of new and unexpected physics will evolve from the combination of these concepts.

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II. Correlations in Interacting Fermi Systems

Correlated Fermi systems play a particularly important role in physics. However, they are also notoriously difficult to tackle. Even in the non-interacting case the Pauli-principle implies spatial correlations between fermions. Interactions, especially those of short range, further enhance these complications since they introduce additional subtle phase relations among the fermions in real space. In condensed matter physics these difficulties are well-known from the investigations of narrow band metals [1] or liquid [2] and solid ^{3}He [3]. The theoretical developments in new areas like heavy fermion systems [4] , disordered electronic systems close to the metal insulator transition [5,6] and, most recently, high temperature superconductivity, [7,8] have once again drawn attention to these problems and have further challenged our understanding of strongly correlated fermions.

As already mentioned in the introduction of these lectures there are only two genuine many-particle Fermisystems available in a terrestrial laboratory: electrons and ^{3}He. While electrons are the "standard" Fermions, it is not so obvious that ^{3}He-atoms obey Fermi statistics, too. Nevertheless, they <u>are</u> Fermions owing to the nuclear spin: the nucleus consists of two protons and

one neutron which add up to a nuclear spin $I = -\frac{1}{2}$. The two electrons in the atomic shell on the other hand, have a total spin zero and are completely irrelevant concerning quantum statistics. They are only important to the extent that they make a ^{3}He-atom a perfectly spherical particle, thus causing ^{3}He-atoms to interact via a short-range, hard-core interaction. At 3.2K ^{3}He-gas condenses into a high density liquid and, below $\sim$100mK, this turns out to be the prototype of a "Fermi liquid". As such it is extremely pure and only consists of a single species of particles (in contrast to electrons which are always confined to a lattice and where electrons of different bands may interact). At zero external pressure ^{3}He does not solidify even at the lowest temperatures: the mass of a ^{3}He-atom is so small that even at T=0 the quantum mechanical zero point motion always wins over the omnipresent van-der Waals interaction and this prevents solidification. Hence ^{3}He is a quantum(Fermi)-liquid.

To understand and appreciate the complexity of interacting Fermi systems it is essential to have a firm understanding of the Fermi gas. On such a basis correlation effects, the notion of quasiparticles and the essence of Landau's Fermi liquid theory are relatively easy to comprehend.

Fermions are ruled by the Fermi-Dirac statistics and, hence, by the Pauli exclusion principle. Free fermions

may be represented by plane waves for which a momentum representation is particularly suited.- At zero temperature the ground state of a many-fermion system forms a "Fermi-body" in $\vec{k}$-space, which - depending on the dispersion $\epsilon_{\vec{k}}$ - may be very complicated.Only for a parabolic dispersion $\epsilon_{\vec{k}} = \frac{(\hbar k)^2}{2m}$ (valid for free fermions in a continuum or for fermions on a lattice when the density is low enough) does this body have the shape of a sphere. In most cases we will consider the latter case. States in this Fermi-sphere with $|\vec{k}| \leq k_F$ are occupied, where k_F is the Fermi momentum and

$$E_F = \frac{\hbar^2 k_F^2}{2m} \tag{1a}$$

is the Fermi energy. The corresponding temperature

$$T_F = \frac{E_F}{k_B} \tag{1b}$$

is called "Fermi-" or "Degeneracy-Temperature". Hence the momentum distribution at T = 0 is given by (see Fig. 1)

$$n_{\vec{k}\sigma}\Big|_{T=0} = \Theta\left(k_{F\sigma} - |\vec{k}|\right) = \begin{cases} 1 \ , & \epsilon_{\vec{k}} \leq E_F \\ 0 \ , & \epsilon_{\vec{k}} > E_F \end{cases} \tag{2}$$

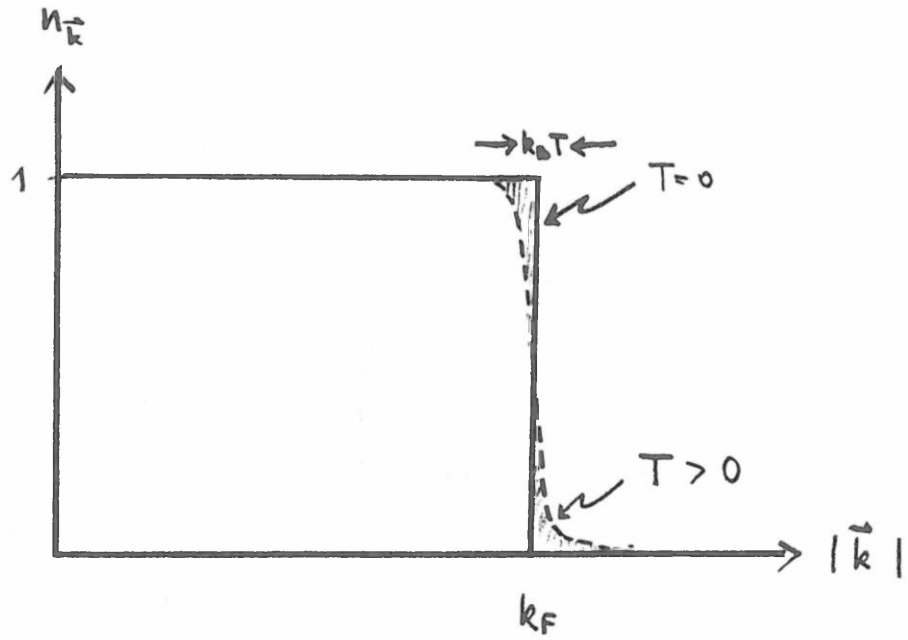


Fig.1

The total particle number N is given by

$$N_\sigma = \sum_{\vec{k}} n_{\vec{k}\sigma} \quad , \qquad N = \sum_\sigma N_\sigma = N_\uparrow + N_\downarrow \tag{3a}$$

$$N = V \frac{k_F^3}{3\pi^2} \tag{3b}$$

where (3b) applies to d = 3 dimensions. Here V is the volume and we assumed $N_\uparrow = N_\downarrow$; furthermore we made use of

$$\sum_{\vec{k}} \xrightarrow{N\to\infty} V \int \frac{d\vec{k}}{(2\pi)^3}$$

Hence $k_F = (3\pi^2 n)^{1/3}$, where $n = N/V = n_\uparrow + n_\downarrow$ is the density with $n = 1/a^3$; this defines an average particle distance a. The Fermi energy is thus found to vary as

$$E_F \propto n^{2/3} \tag{4}$$

This dependence is in fact also obeyed by many mono-valent metals (e.g. Li, Na, K,...). For a system with electronic density ($a \simeq 3\mathring{A}$, $m_e = 9 \times 10^{-31}$kg) the Fermi temperature is about 50000K, while for liquid ^{3}He, which has about the same particle separation but where $m \simeq 6000m_e$, T_F=6K.

Thermal Properties of the Fermi Gas

At finite temperatures thermal excitations of particles from below the Fermi surface, ($E < E_F$), to $E > E_F$ occur, leading to a smearing of the sharp cut-off in momentum-space (see Fig. 1). This is reflected in the Fermi-Dirac distribution at T > 0 for fermions

$$n_{\vec{k}} = \frac{1}{e^{\frac{\epsilon_{\vec{k}}-\mu}{k_B T}} + 1} \tag{5}$$

where μ is the chemical potential. The entropy S is then finite and is composed of contributions from "particles" and "holes"

$$S = -k_B \sum_{\vec{k}} \left[n_{\vec{k}} \ln n_{\vec{k}} + (1-n_{\vec{k}}) \ln (1-n_{\vec{k}}) \right] \tag{6}$$

It is crucial to note that for low temperatures ($T \ll T_F$) the states deep inside the Fermi surface are not

involved in these excitations at all. At these temperatures only a thin shell of states close to E_F with volume $\sim T$ is affected. In particular, metal-physics, where $T \lll T_F$, only deals with phenomena very close to the Fermi surface. This surface is no longer mathematically sharp but is nevertheless still very pronounced: In particular, the <u>change</u> of $n_{\vec{k}}$, i.e. $\partial n_{\vec{k}} / \partial \epsilon_{\vec{k}}$, is a strongly peaked function at $\epsilon_{\vec{k}} = E_F$. Introducing the density of states (DOS)

$$N(E) = \sum_{\vec{k}} \delta(\epsilon_{\vec{k}} - E) \tag{7}$$

with

$$N(E_F) \equiv N(0) = \frac{3}{2} \frac{n}{E_F} \tag{8}$$

(here N(0) is the DOS for both spin species, $N(0) = mk_F/\pi^2$) this fact implies

$$\sum_{\vec{k}} \mathcal{F}(\epsilon_{\vec{k}}) = \int_{-\infty}^{\infty} dE \; N(E) \; \mathcal{F}(E) \tag{9a}$$

$$\simeq N(0) \int_{-\infty}^{\infty} dE \; \mathcal{F}(E) \tag{9b}$$

where (9b) applies for any function $\mathcal{F}(E)$ which is strongly peaked at $E = E_F$.

Using (5), the internal energy U

$$U = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} n_{\vec{k}\sigma} \tag{10}$$

at low temperatures is given by

$$\frac{U}{V} = \frac{3}{5} n E_F + \frac{\pi^2}{6} N(0) (k_B T)^2 + O\left[\frac{(k_B T)^4}{E_F^3}\right] \tag{11}$$

The T^2-correction can easily be understood: it is simple the <u>number</u> of excited particles ($N(0) \times k_B T$) times the excitation energy ($k_B T$).

<u>Specific heat</u>

The specific heat at low temperatues

$$c_V = \frac{1}{V} \left(\frac{\partial U}{\partial T}\right)_N \tag{12}$$

follows as

$$c_v = \gamma_0 T + O(T^3) \tag{13a}$$

$$= \frac{\pi^2}{2} n k_B \frac{T}{T_F} + O(T^3) \tag{13b}$$

where

$$\gamma_0 = \frac{\pi^2}{3} N(0) k_B^2 \tag{14}$$

(Note, that $\gamma_0 \neq 0$ only because N(0) > 0, i.e. there are states at the Fermi energy). This should be compared with the classical result

$$c_v|_{class} = \frac{3n}{2} k_B$$

The linear T-dependence of c_v is one of the most important results of the quantum mechanical nature of fermions. Simple <u>metals</u> (i.e. interacting systems) do indeed show such a behavior; see below). The entropy

$$S = V \int dT \frac{c_v}{T} \tag{15}$$

hence also goes linearly with T at low T.

In a crystal lattice vibrations contribute a term $A_{ion}T^3$ to c_v which is much larger than that of the (free) electrons. Hence, the quantity

$$\frac{c_v}{T} = \gamma + AT^2 \tag{16}$$

plotted vs. T, allows one to determine the prefactor γ of a real system by taking the intercept a T = 0, as well as A, i.e. the contribution of lattice vibrations, by taking the slope.

The linear behavior of c_v, i.e. the saturation of c_v/T for $T \to 0$ obtained for the Fermi gas, is in fact found in many, very different Fermi systems such as simple metals, heavy fermion systems and liquid ^{3}He shown in Fig. 2-4.

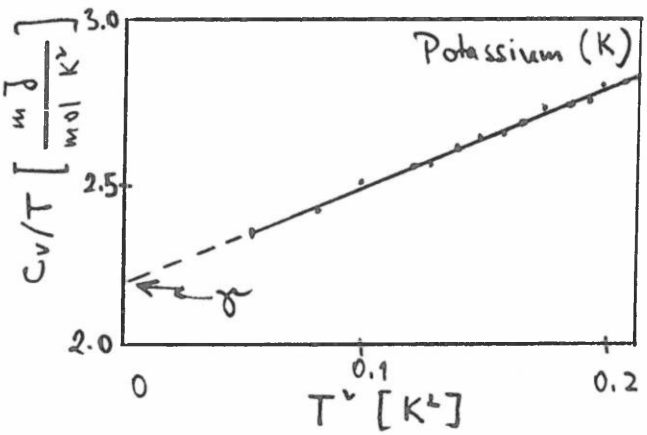


Fig. 2

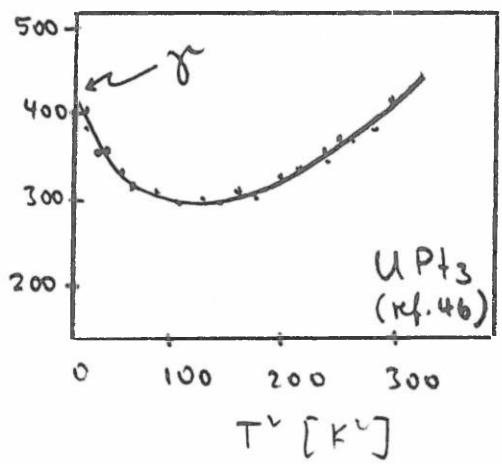
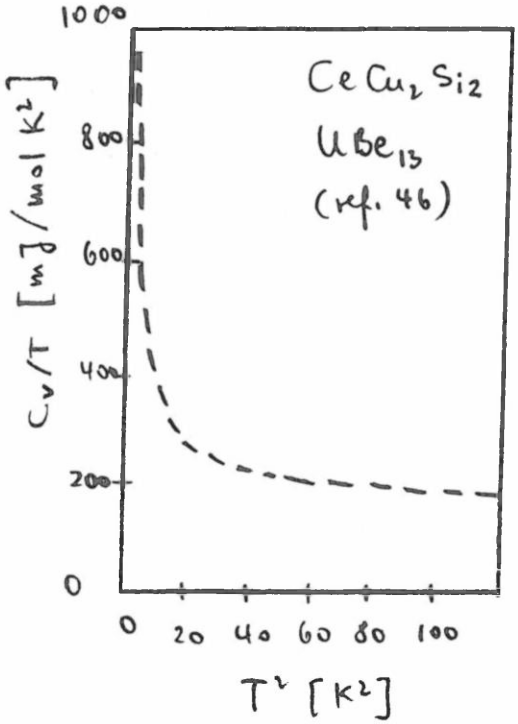


Fig. 3a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0
C_v/T [mJ/mol K²]
$CeCu_2Si_2$
UBe_{13}
(ref. 46)
0
20
40
60
80
100
T^2 [K²]

Fig. 3b

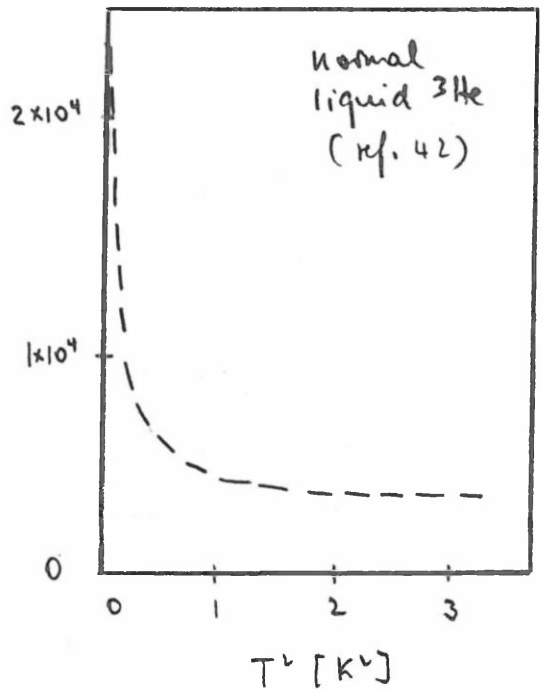
2×10⁴
1×10⁴
0
normal
liquid ³He
(ref. 42)
0
1
2
3
T^2 [K²]

Fig. 4

This is very surprising: After all there exist strong interactions in these systems which will destroy the independence of $\vec{k}$-states of the particles. Therefore one would have to expect that the low-T behavior of <u>interacting</u> fermions does not resemble that of the Fermi <u>gas</u> at all. The qualitative similarity has indeed a very subtle origin and will be discussed in the context of Fermi liquid theory.

<u>Spin Susceptibility</u>

A magnetic field $\vec{H}$ acts on the magnetic moments $\vec{\mu} = \gamma \hbar \vec{J}$ of the Fermions and shifts the energy levels by $\pm |\vec{\mu}| H$; here $\gamma = 2\mu/\hbar$ is the gyromagnetic ratio of the fermions (e.g. electrons or ^{3}He-nuclei). The magnetization density is given by

$$M = \mu (n_\uparrow - n_\downarrow) \tag{17}$$

where n_σ is the density of σ-spin (see (3b)). At low fields ($\mu H \ll E_F$) we have

$$M = \chi_s H \tag{18}$$

The susceptibility χ_s of the Fermi gas is given by

$$\chi_s(T) = \mu^2 N(0) \left[1 - O\left(\frac{T}{T_F}\right)^2\right] \tag{19}$$

At T = 0 this is the "Pauli susceptibility":

$$\begin{aligned} \chi_{s,\,\mathrm{Pauli}} &= \mu^2 N(0) = \mathrm{const} \\ &= \mu^2 \frac{3n}{2} \frac{1}{k_B T_F} \end{aligned} \tag{20}$$

Hence the Fermi gas is paramagnetic and has a <u>finite</u> susceptibility, in contrast to the classical result

$$\chi_{s,\mathrm{Curie}} = \mu^2 n \frac{1}{k_B T} \tag{21}$$

which is the "Curie susceptibility" and which diverges for $T \to 0$. Clearly, for $T \ll T_F$ only the electrons close to the Fermi surface contribute to χ_s. Hence the temperature T in (21) is replaced by T_F, yielding essentially (20). The T-dependence of χ_s is shown in Fig. 5. For $T \to 0$ $\chi_{s,\mathrm{Pauli}} \ll \chi_{s,\mathrm{Curie}}$ as seen in metals. In Fig. 6

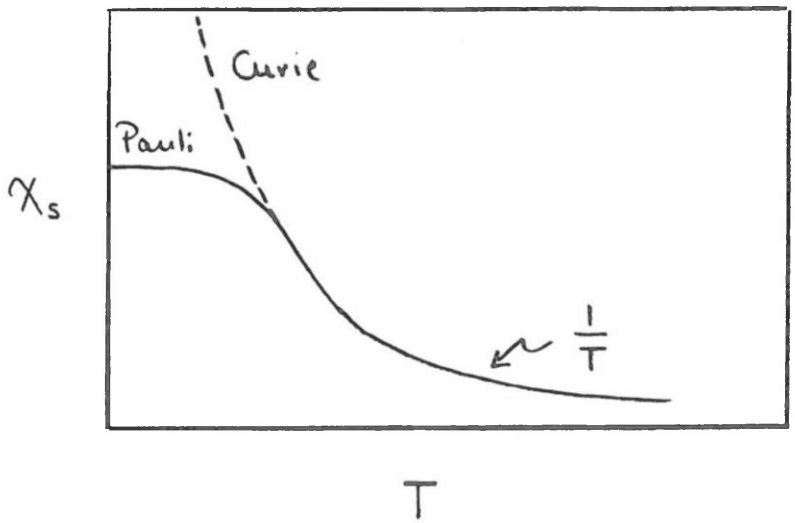

Fig. 5

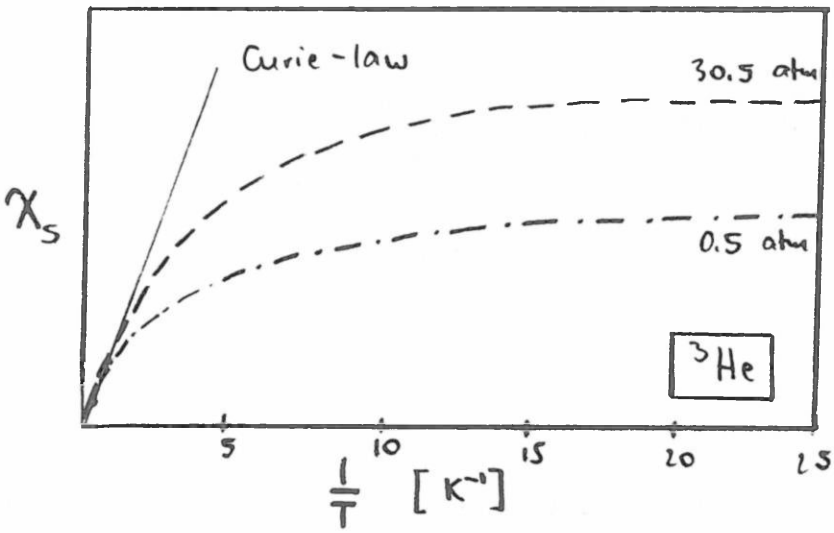

Fig. 6

we show the temperature dependence of $\chi_s(T)$ of normal liquid ^{3}He versus 1/T. At T $\gg T_F$ the T-independence indicates the Curie-behavior, while for $T \ll T_F$ the linear T-dependence indicates Pauli paramagnetism. Again it is surprising that a result derived for the Fermi gas holds for a strongly interacting system such a ^{3}He.

Compressibility

The compressibility κ (or "density susceptibility") is given by

$$\kappa = -\frac{1}{V}\frac{\partial V}{\partial p} \tag{22}$$

Since $P = -(\partial U/\partial V)_N$ we find from (11) that

$$\kappa(T) = \frac{1}{n^2} N(0) \left[1 - O\left(\frac{T}{T_F}\right)^2 \right] \tag{23}$$

At T = 0 κ assumes a finite value

$$\kappa(0) = \frac{1}{n^2} N(0) \tag{24}$$

which has the same form as that for the spin suceptibility $(\mu \to \frac{1}{n})$, (19). In Fig. 7

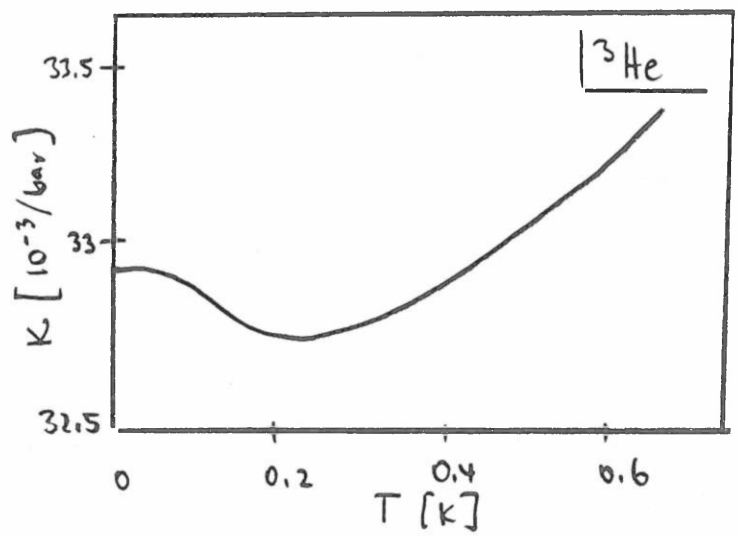

Fig. 7

we show the T-dependence of κ for normal liquid ^{3}He which indeed reproduces this feature. The density dependence of K(0) in (24) is obeyed by many simple metals such as Li, Na, K,..., Cu, Ag, Al. Below we summarize the low temperature properties ($T \ll T_F$) of a Fermi gas

$$\boxed{\begin{aligned} C_V &= \frac{\pi^2}{3} N(0)\, T + O(T^3) \\ \chi_s &= \mu^2 N(0) + O(T^2) \\ K &= \frac{1}{\mu^2} N(0) + O(T^2) \end{aligned}} \qquad (25)$$

<u>The Validity of the Picture of Independent Particles</u>

Although the above results were obtained for <u>non-interacting</u> particles, we have seen that several dense and <u>strongly interacting</u> Fermisystems, e.g. (heavy fermion) metals and liquid ^{3}He, show a qualitatively identical behavior. Why don't the interactions modify those dependences completely? Why is the concept of independent fermions for an interacting Fermi system not a priori absurd? A partial answer is provided by [9]

(i) Screening

(ii) Fermi statistics

<u>Screening:</u> Even strong, longrange interactions such as the Coulomb-interaction among electrons will be substantially weakened by <u>screening</u>, i.e. by polarization effects in the interacting medium. Thus the Coulomb potential due to a charge Q

$$V_{coul}(r) = \frac{Q}{r} \tag{26}$$

will be screened to

$$V_{coul}^{screen}(r) = \frac{Q}{r}\, e^{-r/\lambda} \tag{27}$$

and becomes essentially <u>short-ranged</u> and "soft". Here λ is the "screening length". The Fourier transforms then behave as

$$\tilde{V}_{coul}(q) = 4\pi \frac{Q}{q^2} \rightarrow \tilde{V}_{coul}^{screen}(q) = 4\pi^2 \frac{Q}{q^2 + \lambda^{-2}} \tag{28}$$

such that the screened potential approaches an undangerous <u>constant</u> for $q \rightarrow 0$ and no longer diverges.

<u>Fermi statistics:</u> Let us start with free Fermions and let us slowly switch on a (repulsive) interaction. Let us assume(!) that the interaction leads to scattering of the fermions into and out of one-particle states(which of course are no longer stationary). Question: Will the scattering be so strong that the picture of independent particles becomes invalid? The answer is: No! At low temperatures the Pauli-principle reduces the scattering rate drastically owing to energy- and momentum conservation in the scattering event. Initial and final states have to be <u>available</u> for scattering. At low T, where scattering

only takes place in a thin shell of energies of width T around E_F, this is then a very severe restriction. Hence close to the Fermi surface the scattering rate $1/\tau$ (with τ as a scattering time) is given by the product of two probabilities, each of which is of order T, i.e.

$$\frac{1}{\tau} \propto T^2 \tag{29}$$

which can be arbitrarily small. The life time of a fermionic state and thereby the mean free path $\ell = v_F \tau$, with v_F as the Fermi velocity, can then be <u>arbitrarily long</u> . So, although in liquid ^{3}He the density of particles is very high, the mean free path can be macroscopically long, since scattering simply cannot take place. This implies that for energy levels close to E_F interactions <u>play essentially no role</u> and therefore the picture of independent particles does not loose it validity! Astonishing...

<u>Landau Fermi Liquid Theory</u>

As a starting point for the above arguments we <u>assumed</u> that - in spite of interactions - the picture of independent fermions did not loose its meaning. We then convinced ourselves that electron-electron interaction - processes etc. did not invalidate this starting point. But, if the interaction is really strong, why should the picture

of independent particles be a good starting point in the first place? [9]

This puzzling situation was brilliantly clarified by Landau [10,11]. He concluded that the above starting point was indeed wrong for the actual fermions in the system (i.e. the electrons, ^{3}He-atoms) but that it was correct for something else, a somewhat abstract entity named "Quasiparticle"(QP). This picture then provides at least a consistent framework to understand the low-T properties of certain Fermi systems.

Landau-theory is phenomenological in nature but of the most exquisite sort. It involves parameters which cannot be determined within the theory itself but - using these parameters - one can make predictions about measurable quantities. For details we refer to refs. [12,13].

Elementary Excitations, Quasiparticles

In a noninteracting Fermi system an "elementary excitation" is obtained by lifting a particle from below the Fermi surface ($k < k_F$) to above the Fermi surface ($k < k_F$). This leaves us with a "particle-like" excitation above the Fermi surface and a "hole-like" excitation below the Fermi surface. Their energies are best measured from

the Fermi surface, i.e. "particles" and "holes" have energies ξ_p and ξ_h respectively

$$\xi_p = \frac{k^2}{2m} - \frac{k_F^2}{2m} \simeq v_F\,(k - k_F) \tag{30a}$$

$$\xi_h = -\xi_p \tag{30b}$$

Every excited state may thus be generated by bringing particles successively from below to above the Fermi surface. In a non-interacting system such an excited state is stationary and has infinite life time. How is the situation changed if the interaction is swith on? Are there still elementary excitations as in the non-interacting case?

Landau's theory applies to "normal Fermi systems", in which the exact ground state of the interacting system may evolve adiabatically from an eigenstate of the non-interacting system. In other words: there must be a one-to-one correpondence between the eigenstates of the free Fermi gas and that of the interacting system. This is not automatically fulfilled, i.e. there is no a-priori reason to assume that by switching on the interaction <u>all</u> eigenstates of the interacting system are generated. There might be an energy gap appearing. For example, an attractive interaction will lead to pair correlations (c.f. superconductivity!); the latter state is not in direct

relation to the non-interacting system. For this reason we only consider repulsive interactions. One does not know whether a Fermi system is "normal" or not. Note, that the <u>strength</u> of the interaction is quite unimportant here.

It can be shown by microscopic methods [14,15], that the momentum distribution $n_{\vec{k}}$ of an interacting, "normal" Fermi system still has a <u>finite discontinuity at k_F</u> (Fig.8). This is very astonishing!

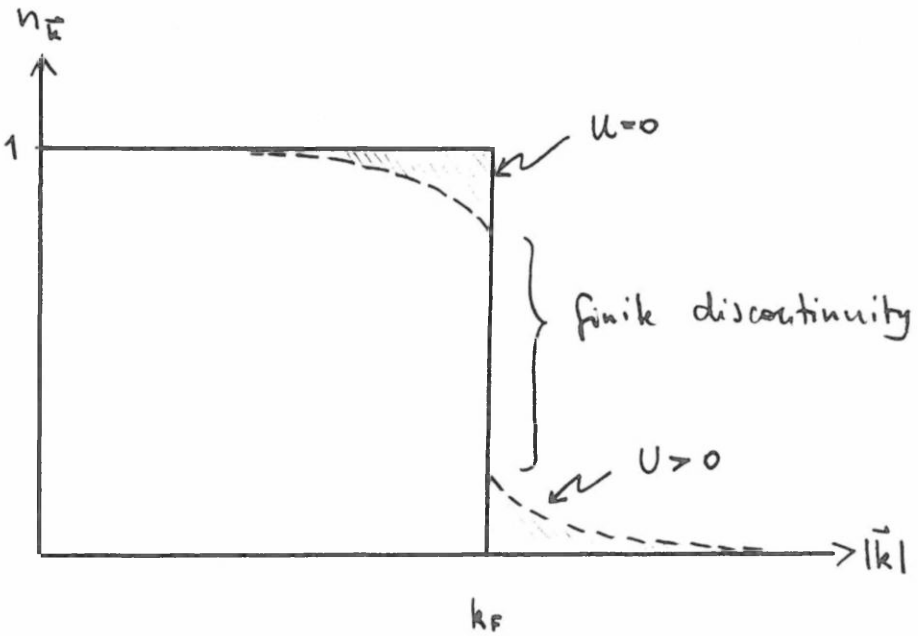

Fig. 8

Since there is still a sharp Fermi surface, one may excite particles as in the non-interacting case. Thereby one creates "quasiparticles" (QP) and "quasiholes" with the same linear dispersion as in (30a,b). These QPs are

fermions and obey the Pauli-principle, they interact, and - in the case of electrons - they carry a charge e .

In the interacting system $\vec{k}$-states are no longer <u>stationary</u> states of the system. Hence QPs have a <u>finite lifetime</u> . However, the concept of "elementary excitations" only makes sense if the damping is small compared to the energies. But since QPs are fermions their lifetime $\tau \propto 1/T^2$ can become arbitrarily long. So for sufficiently <u>small</u> excitation energies or temperatures QP-state are well-defined. The QP-concept is thus only relevant for <u>low</u> temperatues $T \ll T_F$.

Because of the one-to-one correspondence the Fermi momentum k_F of the QP-systems is that of the <u>non-</u>interacting system

$$k_F^* = k_F = (3\pi^2 n)^{1/3} \tag{31}$$

This may be <u>interpreted</u> as if the number of QP was equal to the actual number of particles. However, this is dangerous since QP only have a meaning close to the Fermi surface, which only involves very few QPs.

Let the QP-distribution function be $n_{\vec{k}\sigma}$. The deviation

$$\delta n_{\vec{k}\sigma} = n_{\vec{k}\sigma} - n^0_{\vec{k}\sigma} \tag{32}$$

with $n^{0}_{\vec{k}\sigma}$ as the ground state distribution is a measure of the degree of excitation of the system. Only $\delta n_{\vec{k}\sigma}$ is a meaningful quantity, and

$$\sum_{\vec{k}\sigma} \delta n_{\vec{k}\sigma} = 0 \tag{33}$$

QPs are assumed to interact via a self-consistent field which acts on a QP, and which is produced by the surrounding QPs. Adding a QP in a state $\{\vec{k},\sigma\}$ to the system increases the energy by $\epsilon_{\vec{k}\sigma}\{n_{\vec{k}\sigma}\}$, the "QP-energy", which is a functional of $n_{\vec{k}\sigma}$ and is thus very complicated. $\epsilon_{\vec{k}\sigma}$ consists of, (i), a one-particle energy $\epsilon^{0}_{\vec{k}\sigma} = \epsilon_{\vec{k}\sigma}\{n^{0}_{\vec{k}\sigma}\}$ relative to the ground state $n^{0}_{\vec{k}\sigma}$ and, (ii), an interaction energy due to the change of $n_{\vec{k}\sigma}$, i.e. $\delta n_{\vec{k}\sigma}$, caused by the presence of the new QP. The change of the total energy is

$$\delta E\{n_{k\sigma}\} = \frac{1}{V}\sum_{\vec{k}\sigma} \epsilon_{\vec{k}\sigma}\delta n_{\vec{k}\sigma} + \text{higher terms} \tag{34}$$

In thermodynamic equilibrium $\delta E = \frac{1}{V}\left[T\delta S + \mu\,\delta N\right]$. Now, the <u>entropy</u> of the QPs has the same form as for free fermions, (6) and their number N is given by (2). Hence the distribution $n_{\vec{k}\sigma}$ has the same form as in (5). But this is now a very <u>complicated</u> expression since $\epsilon_{\vec{k}\sigma} = \epsilon_{\vec{k}\sigma}\{n_{\vec{k}\sigma}\}$.

QPs have an "effective mass" m^{*} defined by

$$v_F^{*} = \left|\vec{\nabla}_{\vec{k}}\,\epsilon^{0}_{\vec{k}\sigma}\right|_{k_F} = \frac{\hbar k_F}{m^{*}} \tag{35}$$

which is an unknown parameter. Their density of states (DOS) at the Fermi surface is

$$N(0) = \frac{1}{V} \sum_{\vec{k}\sigma} \delta\left(\epsilon^{\circ}_{\vec{k}} - E_F\right)$$

$$= \frac{m^* k_F}{\pi^2 \hbar^2} \tag{36}$$

$$= \frac{m^*}{m} N_0(0)$$

where $N_0(0)$ is the DOS of the free fermions.

The interaction energy between two QPs, i.e. the energy change of a particle with $\{\vec{k},\sigma\}$ due to the presence of another QP with $\{\vec{k}'\sigma'\}$, is given by

$$\frac{1}{V} f_{\vec{k}\sigma,\vec{k}'\sigma'}$$

and hence there is a contribution to $\epsilon_{\vec{k}\sigma}$:

$$\delta\epsilon_{\vec{k}\sigma} = \frac{1}{V} \sum_{\vec{k}'\sigma'} f_{\vec{k}\sigma,\vec{k}'\sigma'}\, \delta n_{\vec{k}'\sigma'} \tag{37}$$

The change in total free energy $F = E - \mu N$ due to a variation of $n_{\vec{k}\sigma}$ is then given by

$$\delta F = \frac{1}{V} \sum_{\vec{k}\sigma} (\epsilon^{\circ}_{\vec{k}\sigma} - \mu)\, \delta n_{\vec{k}\sigma} \tag{38}$$

$$+ \frac{1}{2} \frac{1}{V^2} \sum_{\vec{k}\sigma,\vec{k}'\sigma'} f_{\vec{k}\sigma,\vec{k}'\sigma'}\, \delta n_{\vec{k}\sigma}\, \delta n_{\vec{k}'\sigma'} + O(\delta n^3)$$

and the QP-energy is

$$\epsilon_{\vec{k}\sigma} = \epsilon^{\circ}_{\vec{k}\sigma} + \frac{1}{V} \sum_{\vec{k}'\sigma'} f_{\vec{k}\sigma,\vec{k}'\sigma'} \, \delta n_{\vec{k}'\sigma'} \tag{39}$$

These are the central equations of the phenomenological Landau-theory, where the interaction term in (38), (39) is of particular importance.

Note, that the two terms in (38) are of the <u>same</u> order $(\delta n)^{\sim}$, since $\epsilon^{\circ}_{\vec{k}\sigma} - \mu \propto \delta n$. Only Landau realized that for consistency the second term in (38) had to be included. Restricting ourselves to the simplest kind of interactions, i.e. exchange forces between the σ , σ' -spins, the QP-interaction may be parametrized as

$$f_{\vec{k}\sigma,\vec{k}'\sigma'} = f^{s}_{\vec{k}\vec{k}'} + f^{a}_{\vec{k}\vec{k}'} \, \vec{\sigma}\cdot\vec{\sigma}' \tag{40}$$

which has the correct rotation properties and where s,a mean "symmetric" and "anti-symmetric". If the spins of the QP are in an eigenstate w.r.t. to one direction we have

$$f_{\vec{k}\uparrow,\vec{k}'\uparrow} = f_{\vec{k}\downarrow,\vec{k}'\downarrow} = f^{s}_{\vec{k}\vec{k}'} + f^{a}_{\vec{k}\vec{k}'} \tag{41a}$$

$$f_{\vec{k}\uparrow,\vec{k}'\downarrow} = f_{\vec{k}\downarrow,\vec{k}'\uparrow} = f^{s}_{\vec{k}\vec{k}'} - f^{a}_{\vec{k}\vec{k}'} \tag{41b}$$

Since scattering essentially takes place <u>on</u> the Fermi surface we have $|\vec{k}| = |\vec{k}'| \approx k_F$ and

$$\vec{k} \cdot \vec{k}' = k_F^2 \cos\theta \tag{42}$$

This allows for the decomposition in Legendre polynomials

$$f^{s,a}_{\xi\xi'} = \sum_{\ell=0}^{\infty} f_\ell^{s,a} P_\ell(\cos\theta) \tag{43}$$

which defines the dimensionless "Landau parameters"

$$F_\ell^{s,a} \equiv N(0) f_\ell^{s,a} \tag{44}$$

Landau theory therefore contains the following phenomenological parameters

(i) m^* for the one-particle energy spectrum

(ii) $\{F_\ell^s\}, \{F_\ell^a\}$ for the QP interaction.

For a neutral, one-component system such as ^{3}He the $F_\ell^{s,a}$ are connected via the "forward-scattering sum rule"

$$\sum_\ell (A_\ell^s + A_\ell^a) = 0 \tag{45}$$

where

$$A_\ell^{s,a} \equiv \frac{F_\ell^{s,a}}{1 + \frac{F_\ell^{s,a}}{2\ell+1}} \tag{46}$$

The Landau parameters enter directly in experimentally measurable quantities like the specific heat, spin susceptibility and compressibility.

Specific heat

To obtain

$$C_v = T \left(\frac{\partial S}{\partial T} \right) \tag{47}$$

from the entropy we calculate S from (6) and find

$$\delta S = \frac{\pi^2}{3} N(0) \, k_B \, \delta T \tag{48}$$

where N(0) contains the effective mass m^* . Hence, to linear order in T (higher orders go beyond Landau theory!) one finds

$$C_V = \frac{m^*}{m} C_V^\circ \tag{49}$$

$$= \frac{\pi^2}{2} n k_B \frac{T}{T_F^*} \tag{50}$$

Here c_V° is the specific heat of the Fermi gas and $T_F^* = (k_F^2/2m^*)/k_B$ is the "effective" Fermi temperature. So for $T \to 0$ the leading T-dependence of the specific heat of the <u>interacting</u> Fermi system has the same form as that of the <u>gas</u> with a renormalized particle mass; in particular it is still linear in T. By measuring the specific heat the effective mass can be determined. For example, in normal liquid ^{3}He $2.8 \lesssim m^* \lesssim 5.8$ for pressures $0 \lesssim P \lesssim P_{melt}$, i.e. m^* is considerably larger than in the non-interacting system.

It is very interesting that the next order contribution in T to the linear dependence of C_V is no longer a T^3-term as in the case of the Fermi gas. Rather is is of order $T^3 \ln T$ [13]. This is due to the fact that the QP-interaction depends on

$$\frac{\epsilon_{\vec{k}} - \epsilon_{\vec{k}'}}{|\vec{k} - \vec{k}'|}$$

(owing to the exchange of phonon-like, i.e. <u>bosonic</u>, modes) which has no well-defined limit. The logarithmic correction requires a new temperatures or energy scale, which goes beyond Landau theory.

Compressibility

Since (22) is equivalent to

$$\kappa = \frac{1}{n^2} \frac{\partial n}{\partial \mu} \tag{51}$$

we have to calculate the variation of μ w.r.t. $n_{\vec{k}\sigma}$. Using

$$\delta n = \sum_{\vec{k}\sigma} \delta n_{\vec{k}\sigma} = \sum_{\vec{k}\sigma} \left(- \frac{\partial n_{\vec{k}\sigma}}{\partial \epsilon_{\vec{k}\sigma}} \right) \left[\delta\mu - \delta\epsilon_{\vec{k}\sigma} \right] \tag{52}$$

with

$$\delta \epsilon_{\vec{k}\sigma} = \frac{1}{V} \sum_{\vec{k}'\sigma'} f_{\vec{k}\sigma, \vec{k}'\sigma'} \, \delta n_{\vec{k}'\sigma'} \tag{53}$$

we find

$$\delta n = N(0) \left[\delta\mu - f_0^s \, \delta n \right] \tag{54}$$

because the variation of $n_{\vec{k}\sigma}$ should be isotropic and spin-independent. Then κ is obtained as

$$\kappa = \frac{1}{n^2} \frac{N(0)}{1+F_0^s} \tag{55}$$

which is the results for the Fermi gas of particles with mass m^* but with a renormalization factor $(1+F_0^s)^{-1}$ due to the QP-interaction. Measuring κ (or the sound velocity $c=1/\sqrt{\kappa m n}$) and the specific heat, allows one to determine F_0^s.

In ^{3}He $F_0^s \simeq 10$-100 depending on pressure, i.e. the compressibility is much smaller than that of a Fermi gas with particles of mass m^*; the QP-interaction makes the liquid much"stiffer".

Spin suceptibility

In an external magnetic field the change fo QP-energy is

$$\delta \epsilon_{\vec{k}\sigma} = -\sigma_z \left(\frac{\gamma \hbar}{2}\right) H + \frac{1}{V} \sum_{\vec{k}'\sigma'} f_{\vec{k}\sigma,\vec{k}'\sigma'} \, \delta n_{\vec{k}'\sigma'} \tag{56}$$

Employing (52) (neglecting $\delta\mu \propto H^2$) and taking the variation of $n_{\vec{k}\sigma}$ to be isotropic ($\ell = 0$) and to be only due to the spin part of f, the spin polarization is found as

$$\delta n_\uparrow - \delta n_\downarrow = \mu^2 \frac{N(0)}{1+F_0^a} H \tag{57}$$

where $\mu = \gamma\hbar/2$. The spin susceptibility is hence given by

$$\chi_s(0) = \mu^2 \frac{N(0)}{1+F_0^a} \tag{58}$$

The result is similar to that for the compressibility (55) but with $F_0^s \to F_0^a$. In ^{3}He $F_0^a \simeq -3/4$ and hence χ_s is much <u>larger</u> than that of a Fermi gas with mass m^*; the interacting liquid is magnetically much "softer".

Effective mass

As noted by Landau, m^* may be related to $f_{k\sigma,k'\sigma'}$. If we set the liquid in motion by giving it a momentum $\hbar\vec{k}$ (i.e. velocity $\hbar\vec{k}/m$) and observing Galilei invariance one finds from the change in QP-energy

$$\frac{1}{m} = \frac{1}{m^*} + \frac{1}{m^*}\,\frac{F_1^s}{3} \tag{59}$$

and hence the exact relation

$$\frac{m^*}{m} = 1 + \frac{1}{3}F_1^s \tag{60}$$

The second term in (59) is due to "backflow" in the system, generated by pulling a particle through the liquid. In ^{3}He this effect is strong ($F_1^s \simeq 5$-14).

So, besides (60) there are exactly <u>three</u> measurable quantities which may be expressed in terms of Landau parameters: eqs. (49), (55) and (58):

$$\begin{aligned} C_v &= \frac{m^*}{m}\,C_v^0 \\ \chi_s &= \frac{m^*/m}{1+F_0^a}\,\chi_s^0 \\ \kappa &= \frac{m^*/m}{1+F_0^s}\,\kappa^0 \end{aligned} \tag{61}$$

where the superscript zero indicates the Fermi gas result. These results are <u>qualitatively</u> similar to those for a Fermi gas and this behavior is indeed found in many systems where fermions are known to interact. We refer to it as "Fermi liquid behavior". <u>Hence in the case of a Fermi liquid only a few numbers ($F_\ell^{s,a}$) are necessary for a complete low-T description.</u>

The results for χ_s and κ may be understood by interpreting the QP-interaction in terms of "molecular fields" [16]. For example, F_0^a produces a molecular field as in the Weiss-theory of ferromagnetism.

<u>Electrons in a metal</u>

Electrons are charged. The Coulomb interaction is <u>long</u>-ranged and the long range part cannot be described by the QP interaction f (it is given by the macroscopic, selfconsistent crystal field). In fact, the q^{-2}-divergence in (28) for $q \to 0$ implies an "incompressibility" of the electron liquid. The sum rule (45), valid for neutral system, is then modified [17]

$$\sum_\ell \left(A_\ell^s + A_\ell^a\right) = A_0^s - 1 \tag{62}$$

i.e. A_0^s is replaced by $A_0^s = 1$ (or $F_0^s = \infty$).

On the other hand, if we think of compressing the electron liquid <u>plus</u> the crystal then K makes perfect sense and a finite F_0^s may be defined.

In contrast to liquid ^{3}He electronic systems are much more complicated since the Fermi surface is no longer spherical. Furthermore, the lattice breaks translational invariance, so that (60) is no longer valid. Instead one may write [18]

$$\frac{m^*}{m_\lambda} = 1 + \frac{1}{3} F_1^s \tag{63}$$

where m_λ is a "dynamical mass" with contributions from band structure, phonons etc. Eq. (63) may be written as

$$\frac{m^*}{m} = \frac{m_\lambda / m}{1 - \frac{1}{3} \bar{F}_1^s} \tag{64}$$

with $\bar{F}_1^s = (k_F m_\lambda / \pi^2) f_1^s$.

For electrons (58) also becomes more complicated, since the magnetic moment is no longer simply given by $\gamma \hbar/2$; it has to be replaced by some μ_{eff} . Spin-orbit interactions also have to be included. -

It should be stressed that Fermi liquid theory not only explains the qualitative behavior of the above mentioned experimental quantities (this would be very much already!). In the case of ^{3}He Landau was also able to make

quantitative predictious on the basis of the QP-picture, e.g. of the existence of a collective mode called "zero sound" which was later found experimentally.

Microscopic Models; the Hubbard model

If one wants to calculate low temperature properties of interacting Fermi systems without introducing phenomenological parameters (or, else, calculate the Landau parameters themselves) one has to employ microscopic models and methods. In this case the full complexity of correlations in Fermi systems shows up. These difficulties are well-known in condensed matter physics, since they are shared by all dense, strongly interacting Fermi systems and they have thus appeared again and again in condensed matter physics (see ref. 1-8).

These problems are very well exemplified by those involved in the investigation of the Hubbard-model [19-21]. This is perhaps the simplest of all interaction models for up- and down-spin electrons on a lattice. Originally it was introduced to describe transition metals with narrow bands [1] (which have only a small overlap of atomic wave functions). The Coulomb interaction is then assumed to be strongly screened and - to obtain the simplest possible form - the interaction is taken as purely local, i.e. on-site, and therefore only between electrons with opposite spin ("cell-model"). The Hubbard model has the form

$$\hat{H} = \hat{H}_0 + \hat{H}_1 \tag{65a}$$

$$\hat{H}_0 = \sum_{ij} \sum_{\sigma} t_{ij} \, \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} \tag{65b}$$

$$\hat{H}_1 = U \sum_{i} n_{i\uparrow} n_{i\downarrow} \tag{65c}$$

where $\hat{c}_{i\sigma}$ ($\hat{c}^{\dagger}_{i\sigma}$) are the destruction (creation) operators of an electron with spin σ at site i and $\hat{n}_{i\sigma} = \hat{c}^{\dagger}_{i\sigma} \hat{c}_{i\sigma}$ is the density operator. $\hat{H}_0$, (65b), describes hopping from site to site (kinetic energy), which is usually assumed to involve only next-neighbors ("tight-binding model"). This term yields pure band behavior and is quantum mechanical in origin. $\hat{H}_1$ (65c), describes the purely on-site interaction between different spins ("Hubbard interaction"). It is essentially classical and counts the number of doubly occupied sites of a spin configuration, i.e. it favors <u>single</u> occupancy of a lattice site, i.e. localization, if the interaction is repulsive. Hence the two terms are seen to compete against each other. In $\vec{k}$-representation (65) reads

$$\hat{H} = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} \hat{n}_{\vec{k}\sigma} + U \sum_{\vec{k}} \hat{\rho}_{\vec{k}\uparrow} \hat{\rho}_{-\vec{k}\downarrow} \tag{66}$$

where $\hat{n}_{\vec{k}\sigma} = \hat{a}^{\dagger}_{\vec{k}\sigma} \hat{a}_{\vec{k}\sigma}$ and

$$\hat{a}_{\vec{k}\sigma} = \frac{1}{\sqrt{L}} \sum_i e^{i\vec{k}\cdot\vec{R}_i} \hat{c}_{i\sigma} \tag{67a}$$

$$\epsilon_{\vec{k}} = \frac{1}{L} \sum_{ij} t_{ij} e^{i\vec{k}\cdot(\vec{R}_i - \vec{R}_j)} \tag{67b}$$

$$\hat{\rho}_{k\sigma} = \frac{1}{L} \sum_{\vec{k}'} \hat{a}^{\dagger}_{\vec{k}'\sigma} \hat{a}_{\vec{k}'+\vec{k},\sigma} \tag{67c}$$

and L is the number of lattice sites in the system. While the kinetic part in (66) is very simple, the interaction which was so simple in position space, is now seen to be very complicated since there is no $\vec{k}$-space restriction (U = const). Therefore one almost always writes the Hubbard interaction in position space.

Because of its simplicity the Hubbard model has been widely used in condensed matter physics. At present it is again being studied with great vigor because it is hoped to provide insight into the pairing mechanism of high-T_c superconductivity [7,8]. The Hubbard model is a quantum mechanical model and an eigenstate is always a complicated superposition of many (if not all) different spin configurations. To understand its basic properties let us solve the two-site model with one up-spin and one down-spin with periodic boundary conditions. There a four different spin configurations on the two sites possible

$$
\begin{aligned}
|1\rangle &= |\uparrow, \downarrow\rangle \\
|2\rangle &= |\downarrow, \uparrow\rangle \\
|3\rangle &= |\uparrow\downarrow, 0\rangle \\
|4\rangle &= |0, \uparrow\downarrow\rangle
\end{aligned}
\tag{68}
$$

and the total wave function is

$$
|\psi\rangle = \sum_{n=1}^{4} a_n |n\rangle \tag{69}
$$

Application of $\hat{H}$ to $|\psi\rangle$ (with $t_{ij} \equiv -t$ and nearest neighbor hopping) yields

$$
\begin{aligned}
\hat{H}_0 |\psi\rangle &= -2t\left[(a_1 + a_2)(|3\rangle + |4\rangle) + (a_3 + a_4)(|1\rangle + |2\rangle)\right] \\
\hat{H}_1 |\psi\rangle &= U\left[a_3 |3\rangle + a_4 |4\rangle\right]
\end{aligned}
\tag{70}
$$

The energy eigenvalues E as found from

$$
\begin{aligned}
E_\pm &= \tfrac{1}{2} U \pm \left[\left(\tfrac{U}{2}\right)^2 + (4t)^2\right]^{1/2} \\
E_1 &= 0 \\
E_2 &= U
\end{aligned}
\tag{71}
$$

For a repulsive interaction ($U > 0$) E_- corresponds to the

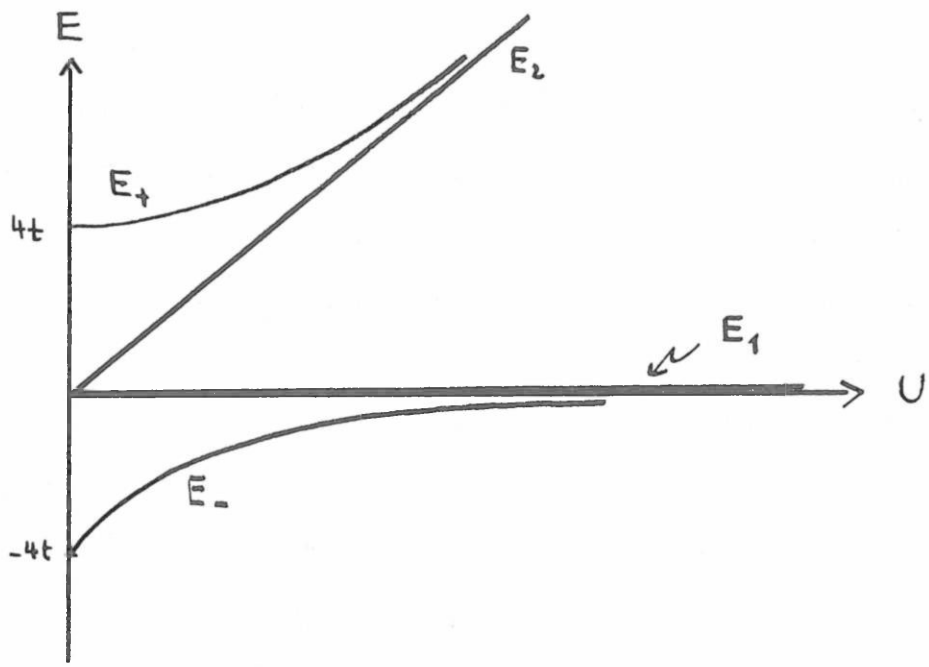

Fig. 9

ground state (see Fig. 9). The ground state wave function then has the form

$$|\psi_-\rangle = |\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle + \frac{|E_-|}{4t}\left(|\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle\right) \tag{72}$$

For $U \to \infty$ the configurations with simply occupied sites (antiferromagnetic configuration) become more and more probable, but only for $U = \infty$ are they really eigenstates.

For a larger number of lattice sites the difficulty of diagonalizing H increases catastrophically. -

In spite of 25 years of work and thousands of papers on the Hubbard model [22,23] only very few exact results are known. In d = 1 dimensions and T = 0 Lieb and Wu [24] found the exact solution by means of a Bethe-ansatz. They

find that U = 0 and n = $(N_\uparrow + N_\downarrow)/L$ = 1 (half-filled band) is a singular point: for any finite U > 0 and n = 1 is the system an insulator and only at U = 0 is it a conductor. The ground state energy E(here t = 1) [24]

$$\frac{E}{L} = -4\int_0^\infty dz \; \frac{J_0(z)\, J_1(z)}{z\,(1+e^{zU/2})} \tag{73}$$

is indeed non-analytic at U = 0 and is a discontinuous function of n at n = 1; see Fig. 10

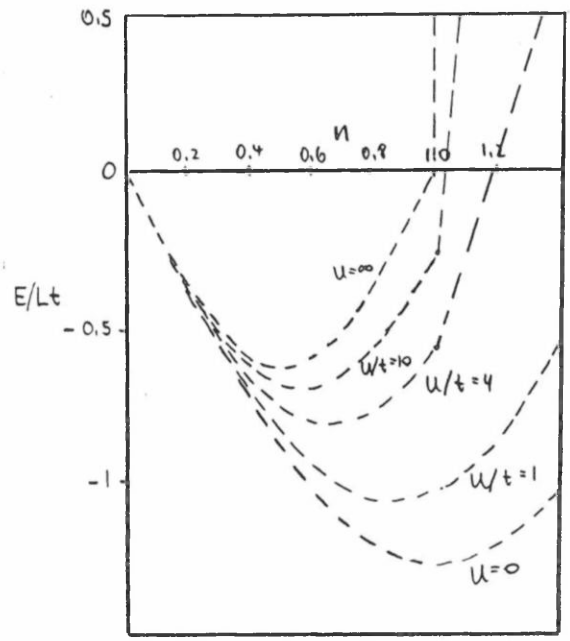

Fig. 10

Unfortunately the exact result for E does not yield the momentum distribution $n_{\vec{k}}$ of the interacting system; it is still unknown: However, <u>most</u> probably it has a smooth shape, i.e. has no discontinuity at k_F, for all U = 0. If it had a discontinuity for some U < U , Fermi liquid theory

would apply and the system would be conducting. Since this is not the case we conclude that $U_c = 0$. So the interaction effects may not be obtained in perturbation theory. Indeed for next-neighbor hopping and A-B type ("bi-partite") lattices (e.g. simple cubic, bcc), where a next-neighbor site to A(B) is always on B(A) (see Fig. 11)

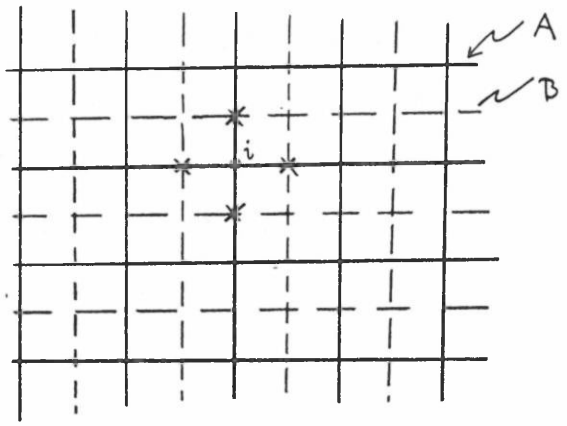

Fig. 11

the energy has the "perfect nesting" property

$$\epsilon_{\vec{k}} + \epsilon_{\vec{k}+\vec{Q}} = 0 \tag{74}$$

where $\vec{Q}$ is half a reciprocal lattice vector (e.g. $\vec{Q}$ = (1,1,1) for a d = 3 simple cubic lattice). We will see below that this leads to an <u>anti-ferromagnetic</u> divergence of the spin susceptibility already in lowest order perturbation theory in U. So the Migdal/Luttinger conditions [14,15] do

not hold and Fermi liquid theory is not applicable. Furthermore, for $t/U \to 0$ it has been shown [25] that

$$n_{\vec{k}} = 1 - \frac{\alpha \varepsilon_{\vec{k}}}{U} + \mathcal{O}\left(\left(\frac{\varepsilon_k}{U}\right)^2\right) \tag{75}$$

i.e. $n_{\vec{k}}$ is continuous.

Nevertheless, for lattices <u>without</u> perfect nesting a Fermi surface is expected to exist even at a finite U. Note, therefore, that the above results for the d = 1 case (in particular the absence of a Mott-transition and the singularity at U = 0) is somewhat pathological. It is a consequence of the lattice type which in d = 1 is neccessarily of the A-B type.

<u>Approximate Solutions of the Hubbard Model</u>

<u>Random Phase Approximation (RPA):</u> Here the dynamic spin susceptibility $\chi_s(\vec{q},\omega)$ of the interacting system is calculated in perturbation theory by summing a certain class of diagrams, i.e. the most divergent diagrammatic contributions; see ref. 26. This yields the well-known RPA result

$$\chi_s(\vec{q},\omega) = \mu^2 \frac{\Pi_0(\vec{q},\omega)}{1 - U\Pi_0(\vec{q},\omega)} \tag{76}$$

where $\Pi_0(\vec{q},\omega)$ is the Lindhard function

If we set

$$\langle \hat{n}_{i\sigma} \rangle = n_\sigma \tag{84}$$

i.e. assume a spatially homogeneous field, we obtain the naive Hartree-Fock result

$$\langle \hat{H}_{HF} \rangle_{naive} = L \left[\bar{\epsilon}_0 + U n_\uparrow n_\downarrow \right] \tag{85}$$

where $\bar{\epsilon}_0 = L^{-1} \sum_{|\vec{k}| < k_F} \epsilon_{\vec{k}}$ is the energy of the free particles. This is only acceptable for $U n_\uparrow n_\downarrow \ll |\bar{\epsilon}_0|$.

To improve on (85) we make use of the fact that in lattices with AB-symmetry and for $n_\uparrow = n_\downarrow = \frac{1}{2}$ anti-ferromagnetic behavior is favored [27-29]. Therefore we expect $\langle \hat{n}_{i\sigma} \rangle$ to be spatially <u>varying</u>, depending on whether $i \in A$ or $i \in B$. We assume

$$\langle \hat{n}_{i\sigma} \rangle = \frac{1}{2} \left[1 + \sigma m \, e^{i \vec{Q} \cdot \vec{R}_i} \right] \tag{86}$$

where m is the sublattice magnetization and $\vec{Q}$ is a reciprocal lattice vector such that

$$e^{i \vec{Q} \cdot \vec{R}_i} = \begin{cases} 1, & \vec{R}_i \in A \\ -1, & \vec{R}_i \in B \end{cases} \tag{87}$$

$\hat{H}_{HF}$, (85), then reduces to

$$\hat{H}_{HF} = \sum_{ij,\sigma} t_{ij}\, \hat{c}^{\dagger}_{i\sigma}\, \hat{c}_{j\sigma} + \frac{UL}{4} + \sum_{i,\sigma} \mu_{i\sigma}\, \hat{n}_{i\sigma} \tag{88}$$

where

$$\mu_{i\sigma} = -\sigma \Delta\, e^{i\vec{Q}\cdot\vec{R}_i} \tag{89a}$$

$$\Delta = \frac{1}{2} U m \tag{89b}$$

is the self-consistent potential (a number!). Rewriting (88) in $\vec{k}$ -representation, this Hamiltonian is diagonalized by the canonical transformation

$$\hat{b}_{\vec{k}\sigma} = u_{\vec{k}\sigma}\, \hat{a}_{\vec{k}\sigma} + v_{\vec{k}\sigma}\, \hat{a}_{\vec{k}+\vec{Q},\sigma} \tag{90}$$

where

$$u_{\vec{k}\sigma} = \frac{1}{\sqrt{2}} \left[1 + \left| \frac{\epsilon_{\vec{k}}}{E_{\vec{k}}} \right| \right]^{1/2} \tag{91}$$

$$v_{\vec{k}\sigma} = -\sigma s_{\vec{k}} \frac{1}{\sqrt{2}} \left[1 - \left| \frac{\epsilon_{\vec{k}}}{E_{\vec{k}}} \right| \right]^{1/2} \tag{92}$$

and $s_{\vec{k}} = -\mathrm{sgn}\, \epsilon_{\vec{k}}$, $E_{\vec{k}} = -s_{\vec{k}} \sqrt{\epsilon^2_{\vec{k}} + \Delta^2}$. The perfect nesting property (74) has been explicitly used. Here $u^2_{k\sigma} + v^2_{k\sigma} = 1$ and $v_{\vec{k}+\vec{Q},\sigma} = -v_{\vec{k},\sigma}$

The generalized Hartree-Fock ground state is build up by

$$|\psi_{HF}\rangle = \prod_{|\vec{k}|<k_F} \hat{b}^{\dagger}_{\vec{k}\uparrow}\, \hat{b}^{\dagger}_{\vec{k}\downarrow}\, |0\rangle \tag{93}$$

and the ground state energy is given by

$$\langle \hat{H}_{HF} \rangle = L \left[\frac{2}{L} \sum_{|\vec{k}|<k_F} E_{\vec{k}} + m\Delta + \frac{U}{4}(1-m^2) \right] \tag{94}$$

For m = 0 we obtain (85). Eq. (94) has to be minimized w.r.t. Δ, which yields the self-consistent equation

$$\Delta = \frac{U}{L} \sum_{|\vec{k}|<k_F} \frac{\Delta}{|E_{\vec{k}}|} \tag{95}$$

with a solution $\Delta \neq 0$. Hence a state with a finite sublattice magnetization is energetically preferred. Note, that the correction in U to (85) is exponentially small for small U ($\sim \exp(-|\bar{\epsilon}_0|/U)$) but that for $U \to \infty$ one finds

$$\langle \hat{H}_{HF} \rangle \propto - \frac{|\epsilon_0|^2}{U} \tag{96}$$

in excellent agreement with exact results.

This approach can be generalized to finite temperature [30,31] and non-AB lattices. In particular, Cyrot [32] obtained a mean-field phase diagram for a non-AB lattice (see Fig. 12)

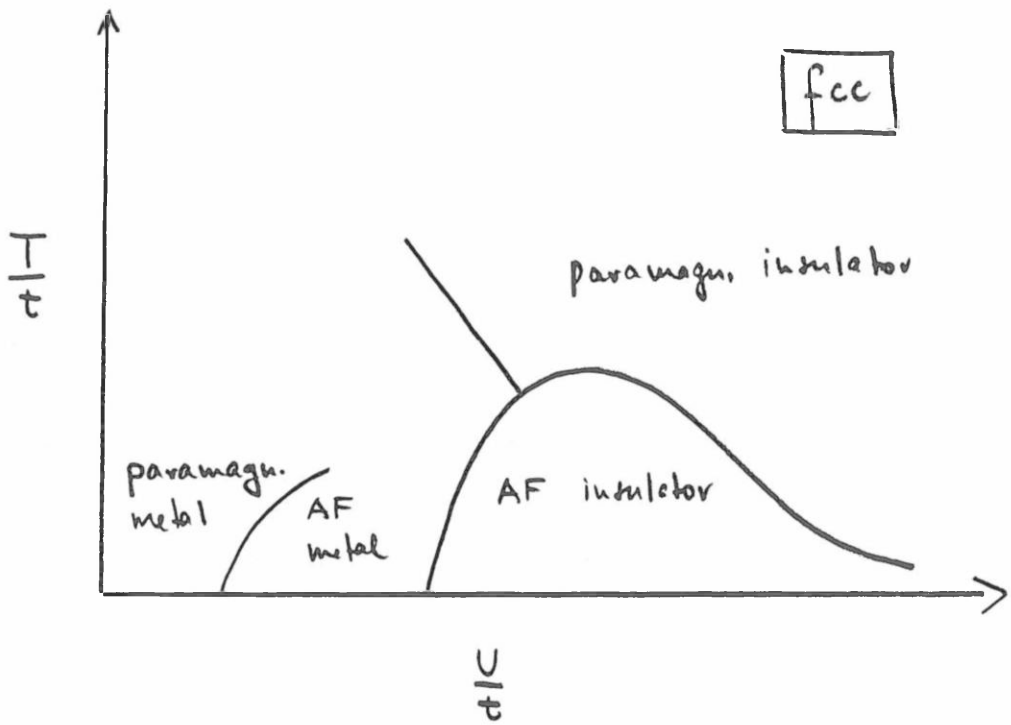

Fig. 12

showing a succession of phase transitions for increasing U from a paramagnetic to an antiferromagnetic metal and further to an antiferromagnetic insulator. Experimental candidates are, for example, V_2O_3.

Improvements of the above approach may in principle be achieved by using functional integral approaches [33]. For this the Hubbard interaction is written as

$$\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} = \frac{1}{4}\left[(\hat{n}_{i\uparrow}+\hat{n}_{i\downarrow})^2 - (\hat{n}_{i\uparrow}-\hat{n}_{i\downarrow})^2\right] \tag{97}$$

where the first term on the r.h.s. of (97) describes local density (or charge) fluctuations and the second one local spin fluctuation. For $U\to\infty$ one assumes the former to be suppressed ($\langle(\hat{n}_{i\uparrow}+\hat{n}_{i\downarrow})^2\rangle \simeq 1$) such that (65) reads

$$\hat{H} \simeq \hat{H}_0 - \frac{U}{4} \sum_i (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})^2 \tag{98}$$

which has a suitable form for a functional integral approach owing to the quadratic form of the interaction operator. Namely, one can investigate the partition function

$$\mathcal{Z} = \mathrm{Tr}\, e^{-\beta \hat{H}} \tag{99}$$

and use the identity for an operator

$$e^{\alpha \hat{\sigma}^2} = \int d\mu \; e^{-\alpha \mu^2 + 2\alpha \hat{\sigma} \cdot \mu} \tag{100}$$

where $\hat{\sigma} \cdot \mu$ describes a coupling of $\hat{\sigma}$ to an external, effective field μ. In the case of (98)

$$\frac{U}{4} (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})^2 \rightarrow \frac{U}{2} \mu_i(\tau) (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}) \tag{101}$$

in the exponent,

where $\mu_i(\tau)$ is a space and time dependent effective magnetic field. Neglecting the time dependence ("static approximation" [33]) brings us back to the Hartree-Fock Hamiltonian (83).

Variational approaches

Methods employing variational wave functions for the investigation of interacting Fermi systems, as in the case of liquid ^{3}He, have many attraction features and have a long, quite successful history by itself [2,34]. In the spirit of Jastrow/Feenberg (see [34]) a variational wave function $|\psi\rangle$ is constructed from a simple starting wave function $|\psi_0\rangle$ (e.g. a Slater determinant in the case of fermions) by letting a correlation operator $\hat{\mathcal{F}} = \exp(-\hat{f})$ act on $|\psi_0\rangle$

$$|\psi\rangle = \hat{\mathcal{F}}\,|\psi_0\rangle \tag{102}$$

so as to suppress those (spin-) correlations in $|\psi_0\rangle$ which are energetically unfavorable in the interacting system. The operator $\hat{\mathcal{F}}$ depends on the interaction and contains variational parameters which have to be determined by minimizing the ground state for a given Hamiltonian $\hat{H}$

$$E = \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} \tag{103}$$

The variational principle yields an exact, upper limit for E.

To study the Hubbard model by a variational method, Gutzwiller [35,36] introduced the simplest possible non-trivial correlation operator

$$\hat{\mathcal{F}} = g^{\hat{\mathcal{D}}} \tag{104}$$

$$\hat{\mathcal{D}} = \sum_i \hat{\mathcal{D}}_i$$

where $\hat{D}_i = \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$, $\hat{D} = \hat{H}_1/U$ is the on-site interaction operator (65c) and $0 \leq g \leq 1$ is a variational parameter. Note that this is the <u>only</u> single-site operator in the model. Clearly, $\hat{D}$ counts the number of doubly occupied sites $\hat{D}_i$ (where the interaction takes place) of a given spin configuration. Eq. (104) may be written as

$$g^{\hat{\mathcal{D}}} = \prod_i \left[1 - (1-g)\,\hat{\mathcal{D}}_i\right] \tag{105}$$

owing to the property

$$\hat{\mathcal{D}}_i^2 = \hat{\mathcal{D}}_i \tag{106}$$

The Gutzwiller variational wave function (GWF) is then

$$|\psi_G\rangle = g^{\hat{\mathcal{D}}}\,|\psi_0\rangle \tag{107}$$

where $|\psi_0\rangle$ is ground state wave function of non-interacting fermions and the correlation factor attributes a factor g to every doubly occupied site of a spin configuration in $|\psi_0\rangle$. Thereby it reduces the amplitude of spin configuration in $|\psi_0\rangle$ with too many doubly occupied sites.

In principle the correlation operator may be improved by including next-neighbor density and/or spin correlations [37].

Note that $\hat{\mathcal{F}}$ in (102) must not be an eigen-operator of $|\psi_0\rangle$ to make $|\psi\rangle$ non-trivial. Indeed $\hat{D}$ (a classical quantity) is <u>not</u> an eigen-operator of $|\psi_0\rangle$.

In the limit g = 1 $|\psi_G\rangle$ in (107) describes the non-interacting case (U = 0). On the other hand for g = 0 , $|\psi_G\rangle$ is only defined if $\langle\hat{D}\rangle = 0$ (only then is $g^{\hat{D}}$ still finite). This is the case if the spins are localized $(U\to\infty)$. Using $|\psi_G\rangle$ the energy E, (103), has to be minimized by

$$\frac{\partial E}{\partial g} = 0$$

In spite of the simplicity of $|\psi_G\rangle$ in (107), exact evaluations of expectation values of operators in terms of $|\psi_G\rangle$ (and hence of E) where not possible until recently. Instead, various kinds of approximations were made. The most famous (because of its physically appealing results) is the "Gutzwiller approximation" (GA) [36]. Its physical meaning was not very clear for a long time. Later it was shown [23,38] that the GA is in fact equivalent to the evaluation of matrix elements by calculating the <u>classical</u>, statistical weights of different spin configurations in $|\psi_0\rangle$. Thereby the GA neglects spatial correlations (and the relative phases between different configurations). Such an

approach, where the correlation operator $\hat{\tilde{f}}$ is treated classically, is known to be a good approximation in the case of Bosons [24].

<u>The Gutzwiller approximation (GA)</u>

The results of the GA may be obtained by purely classical, combinatoric considerations, i.e. by simple counting (for a detailed derivation see [23]). In the Hubbard model a lattice site may be occupied in four different ways (Fig. 13): empty (a "hole"), singly occupied

Fig. 13

($\uparrow,\downarrow$) and doubly occupied. Introducing the symbols

L = No. of lattice sites

N_σ = No. of σ-spins (108)

D = No. of doubly occupied sites

$L_\sigma = N_\sigma - D$ = No. of sites with a single spin σ

$H = L - N_\uparrow - N_\downarrow + D$ = No. of holes

and the densities $d = D/L$, $n_\sigma = N_\sigma/L$ etc. and <u>neglecting</u> all spatial correlations , we obtain the following two quantities:

(i) $N_D(L, N_\uparrow, N_\downarrow)$ = No. of spin configurations of $N_\uparrow$, $N_\downarrow$ spins on L lattice sites, where D sites are doubly occupied

$$= \frac{L!}{L_\uparrow!\, L_\downarrow!\, D!\, H!} \tag{109}$$

(ii) $P(L,N_\sigma)$ = Prob. to find a <u>particular</u> spin configuration of σ-spins

$$= \frac{1}{\binom{L}{N_\sigma}} \simeq n_\sigma^{N_\sigma} (1-n_\sigma)^{L-N_\sigma} \tag{110}$$

Attributing a factor g^D with every spin configuration, the norm of $|\psi_G\rangle$ is then given as the sum over all configurations with different D

$$\langle\psi_G|\psi_G\rangle = \sum_D g^{2D} N_D(L, N_\uparrow, N_\downarrow) P(L, N_\uparrow) P(L, N_\downarrow) \tag{111}$$

where $\uparrow,\downarrow$-spins are taken as spatially uncorrelated. The matrix element for $\hat{D}$ is obtained similarly as

$$\langle \psi_G | \hat{D} | \psi_G \rangle = \sum_{D} g^{2D+2} N_D(L-1, N_\uparrow-1, N_\downarrow-1)\, P(L,N_\uparrow) P(L,N_\downarrow) \tag{112}$$

To calculate the kinetic energy $\langle \psi_G | \hat{H}_0 | \psi_G \rangle$ one has to distinguish between <u>four</u> different possibilities (Fig. 14)

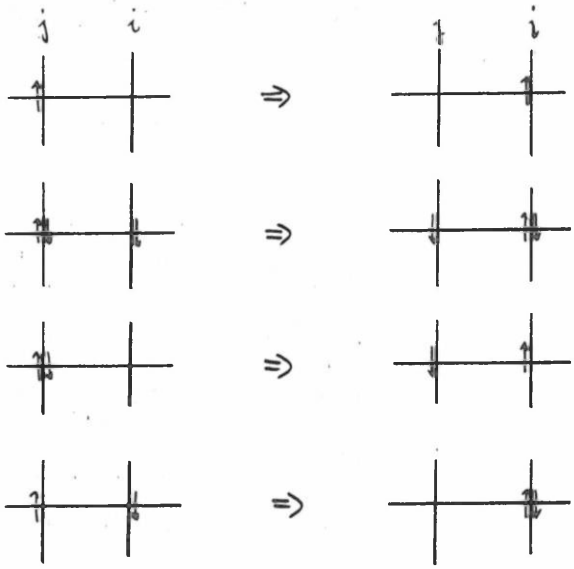

Fig. 14

for a spin to hop from one site to another. For a $\uparrow$-spin this yields

$$\langle \psi_G | \hat{H}_0 | \psi_G \rangle = \sum_{D} \Big[g^{2D} N_D(L-2, N_\uparrow-1, N_\downarrow) + 2g^{2D-1} N_D(L-2, N_\uparrow-1, N_\downarrow-1) + g^{2D-2} N_D(L-2, N_\uparrow-1, N_\downarrow-2) \Big] \times P(L-2, N_\uparrow-1)\, P(L, N_\downarrow)\, \bar{\epsilon}_{0\uparrow} \tag{113}$$

where $\bar{\epsilon}_{0\sigma} = L^{-1} \sum_{|\vec{k}|<k_{F\sigma}} \epsilon_{\vec{k}}$ is the average energy of the free σ-spins. In the thermodynamic limit the $\sum_D$-sums are

given by their largest term (obtained by taking the derivative w.r.t. D, e.g. $\partial[g^{2D} N_D(L, N_\uparrow, N_\downarrow)]/\partial D = 0$ in the case of (111)). This determines $\bar{D}$, the "optimal" no. of doubly occupied sites, as a function of g

$$g^2 = \frac{\bar{d}(1-n+\bar{d})}{(n_\uparrow - d)(n_\downarrow - d)} \tag{114}$$

Clearly, g^2 plays the role of a Boltzmann factor. The energy of the Hubbard model is then found as [36]

$$\frac{E}{L} = \sum_\sigma q_\sigma(d, n_\sigma)\, \bar{\epsilon}_{0\sigma} + Ud \tag{115}$$

where $0 \leq q_\sigma \leq 1$ determines the reduction of the hopping of σ-spins caused by the interaction. In fact, q_σ is the <u>discontinuity</u> in the momentum distribution function $\langle \hat{n}_{\vec{k}\sigma} \rangle$ at $k_{F\sigma}$ [36]. This shows that, in contrast to the Hartree-Fock result (94), the GA affects the distribution function not only in the vicinity of k_F but implies a drastic rearrangement of $\vec{k}$-states. Furthermore, it obeys Luttinger's theorem [15] concerning the conservation of Fermi surface volume.

For $n_\uparrow = n_\downarrow$, $n = 1 - \delta$, the discontinuity is given by

$$q_\uparrow = q_\downarrow \equiv q = 2\,\frac{1-\delta-2d}{1-\delta^2}\left[\sqrt{d+\delta} + \sqrt{d}\,\right]^2 \tag{116}$$

In particular, for n = 1

$$q = 8d(1-2d) \tag{117}$$

Minimization of (115) yields

$$\begin{aligned} d &= \tfrac{1}{4}(1-\bar{U}) \\ q &= 1-\bar{U}^2 \\ \frac{E}{L} &= -|\bar{\epsilon}_0|\,(1-\bar{U})^2 \end{aligned} \tag{118}$$

where $\bar{U} = U/8|\bar{\epsilon}_0|$. At $\bar{U} = 1$ the system is seen to localize ($d = 0$) and the discontinuity vanishes ("Brinkman-Rice transition" [39]) such that the system becomes an <u>insulator</u>. This localization transition only occurs at $n = 1$.

One can also calculate the spin susceptibility and compressibility of the system within the GA [39]. The result may be understood within the concept of a simplified Landau theory [23] where the change of the ground state energy due to an external perturbation is calculated as

$$\delta E = \frac{1}{V}\sum_{\vec{k}\sigma} q_\sigma \epsilon^{0}_{\vec{k}\sigma}\Big|_{bare}\,\delta n_{\vec{k}\sigma}$$
$$+ \frac{1}{2N(0)}\left[F_0^s(\delta n_\uparrow + \delta n_\downarrow)^2 + F_0^a(\delta n_\uparrow - \delta n_\downarrow)^2\right] \tag{119}$$

This yields a quasi particle description, i.e. an effective mass m^* and two Landau parameters [39,23]

$$\frac{m^*}{m} = \frac{1}{1-\bar{U}^2} \tag{120}$$

$$F_0^a = -p\left[1 - \frac{1}{(1+\bar{U})^2}\right] \tag{121}$$

$$F_0^s = p\left[\frac{1}{(1-\bar{U})^2} - 1\right] \tag{122}$$

where $p = 2|\bar{\epsilon}_0|\,N(0) \simeq 1$. For $\bar{U} \to 1$ the effective mass and F_0^s are seen to diverge, ($K \to 0$) while F_0^a saturates at a small negative value.

As discussed by Anderson and Brinkman [40] and Vollhardt [23] the results for the effective mass, the spin susceptibility χ_s and the compressibility K closely resemble the experimentally measure behavior of the quantitative gas normal liquid ^{3}He at very low T.[41,42]

Hence in the case of ^{3}He, where the effective mass is considerably enhanced over its bare value ($2.76 < m^*/m < 5.76$), the dimensionless interaction parameter is always close to unity, i.e. ^{3}He is always close to the localization transition ("almost-localized" Fermi liquid). Eliminating the interaction parameter $\bar{U}$ in favor of the

pressure-dependent effective mass (120), allows one to calculate the pressure dependence of F_0^a and F_0^s [23]. One finds that, for increasing pressure, F_0^a approaches the pressure-independent value $F_0^a \simeq -\frac{3}{4}$, while F_0^s grows strongly. In particular, the pressure independence of F_0^a implies that the pressure dependence of the spin susceptibility χ_s, (58), comes almost entirely from that of the effective mass m*. Hence the "Wilson ratio"

$$\frac{\chi_s}{\chi_{s,\text{Pauli}}} \Big/ \frac{m^*}{m} = \frac{1}{1+F_0^a} \simeq 4 \tag{123}$$

is also essentially pressure independent. This shows that the strong enhancement of the spin susceptibility over its Fermi-gas value is not due to an incipient ferromagnetic transition ($F_0^a \to -1$) as anticipated by paramagnon theory [43]. The results for F_0^a and F_0^s are borne out by experiment [41,42], qualitatively so in the case of F_0^s (i.e. the compressibiltiy), but even quantitatively for F_0^a (i.e. the spin susceptibility). It tells us that the simple lattice Hamiltonian (65) already describes essential features of the interaction within liquid ^{3}He correctly. In this sense static properties of ^{3}He may be understood to be largely determined by the tendency of the hard cores of the particles to keep well separated, i.e. by an incipient localization of the particles. On the other hand, using a generalized lattice gas model which also allows for less

than half filling and for a compressible lattice, Vollhardt, Wölfle and Anderson [44] have shown, that these properties also obtain <u>without</u> the (some arbitrary) transition itself.

An extension of the lattice-gas model for ^{3}He to finite temperatures was discussed by Seiler et al. [45]. Within the model three different temperature regimes may be distinguished: (i) for $T \ll T_F^*$ the system is a Fermi liquid, (ii) for $T_F^* \lesssim T \lesssim U$ it shows classical behavior, but is still strongly correlated, while (iii) for $T \gg U$ the system behaves free-particle-like. In the second temperature regime the entropy of the almost-localized fermions is bounded by $R\,\ell n2/^3$He atom, because in this temperature range essentially only singly occupied lattice sites exist. Within this framework the crossover from Fermi liquid to classical behavior at $T \sim T_F^*$ has been described, which otherwise is outside the scope of Fermi-liquid theory [13] itself. A good qualitative agreement with the measured specific heat, spin susceptibility, and thermal expansion coefficient is obtained. In particular, it is found that the anomalous behavior of the specific heat, i.e. the sharp kink at about 100 mK and the plateau-like structure above this temperature [42] is caused by the bound of $R\ell n2$ on the entropy.-

Exact Results for the Gutzwiller wave function

Only most recently has it become possible to evaluate expectation values of operators in terms of the Gutzwiller wave function (GWF) without making further approximations [46,47]. Sofar an exact evaluation has been performed in $d = 1$ and $d = \infty$ space dimensions. In particular, in infinite dimensions the results of the Gutzwiller approximation are seen to be the exact results for the GWF. In $d = 1$ it is found that the spin correlation function for $n = 1$ and $U = \infty$ is in excellent agreement with all known rigorous results. It is most interesting to note, that in this limit of no doubly occupied sites (i.e. $g = 0$), the GWF is the exact wave function of a new class of spin $-\frac{1}{2}$ Heisenberg Hamiltonians with long range (i.e. $1/r^2$) interaction [48]. This makes the GWF even more interesting (see part III of these lectures on high-T_c superconductivity).

Heavy Fermion Systems

A rather new class of strongly correlated Fermi systems characterized by a strong short-range repulsion, is that of the socalled "heavy fermion systems" (HFS), which have very unusual properties [4,49,50] . These materials are characterized by a very high effective mass m^*, a strongly enhanced spin susceptibility χ_s , and a Wilson ration $R \sim \chi_s/m^*$ which is not much different from that of a

noninteracting system. These properties of heavy-fermion systems are generally believed to be due to the almost-localized f - electrons of the rare-earth (Ce,Pr,...) or actinide (U,Np,Pn...) components in the heavy-fermion compounds, which experience a strong intra-atomic repulsion and which may hybridize with the spd - conduction electrons.Examples are $CeCu_2Si_2$, UBe_{13}, UPt_3, U_2Zn_{17}. At high T the f-electrons are known to be localized, while for $T \to 0$ the atomic moments of the f-shells normally order magnetically. However, strangely enough, in the HFS the f-electrons seem to become <u>mobil</u> for $T \to 0$ since γ , the prefactor of the linear term in the specific heat (13), (50), and hence m*/m, is strongly enhanced (therefore the name HFS).(It may even come to superconductivity in the abovementioned materials). This means that a large electronic entropy (i.e. degrees of freedom) appear already at low T. This is very similar to ^3He. For example, in the case of UPt_3 one finds [51]

$$\frac{m^*}{m} \simeq 150$$

$$C_v = \gamma T + \gamma' T^3 \ln T$$

$$F_0^a \simeq -(0.5 - 0.9) \quad , \text{ i.e. small, negative}$$

$$\chi_s / m^* \sim 2\text{-}4 \quad , \quad \text{not strongly adhanced}$$

$$F_0^s \sim \frac{m^*}{m} \quad , \quad \text{large}$$

A microscopic approach to HFS which wants to explain these features, has to include that, (i) the distance of the U-atoms is about 4Å, so that there is no atomic overlap of the wave functions, (ii) there is a strong interatomic Coulomb-repulsion between the f-electrons and (iii) that there is hybridization of the f-electrons with the spd-bands. Another important experimental observation [49,50] is that for decreasing T the resistivity $\rho(T)$ first increases (logarithmically and then sharply drops below some temperature T_0) to a T^2-behavior known from Fermi liquid theory (Fig. 15).

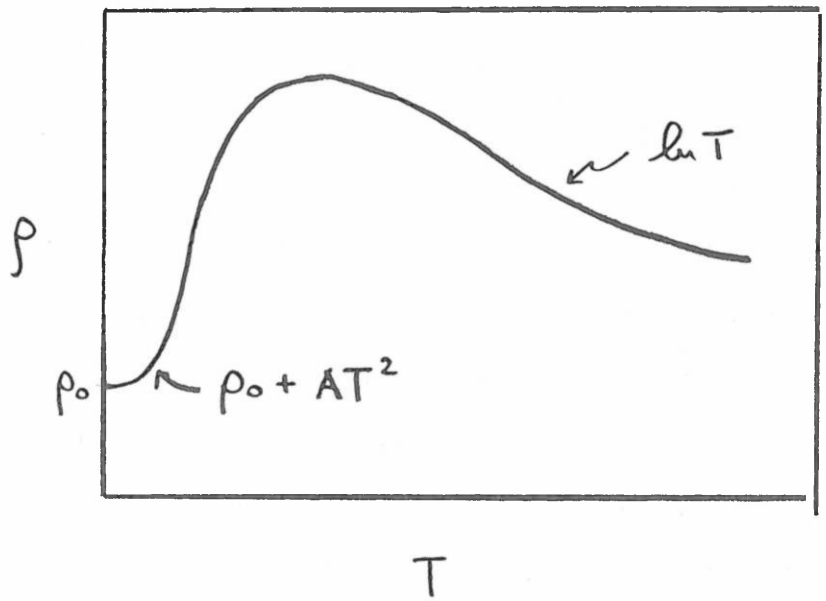

Fig. 15

As a model for this kind of physical behavior one considers the "periodic Anderson model" (PAM), i.e. a generalization of the original Anderson model [52] of a single magnetic "impurity" in a sea of conduction

electrons, to a full <u>lattice</u> of such magnetic moments (i.e. the f-electrons). It is commonly written as

$$\begin{aligned}\hat{H}_{PAM} = & \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} \hat{a}^{+}_{\vec{k}\sigma} \hat{a}_{\vec{k}\sigma} \\ & + E_F \sum_{i,\sigma,\ell} \hat{n}^{f}_{i,\sigma,\ell} + U \sum_{i,\ell} \hat{n}^{f}_{i\uparrow,\ell} \hat{n}^{f}_{i\downarrow,\ell} \\ & + \sum_{\vec{k}\sigma,\ell} V_{\vec{k},\ell} \left[\hat{a}^{+}_{k\sigma} \hat{f}_{\vec{k}\sigma,\ell} + \hat{f}^{+}_{\vec{k}\sigma,\ell} \hat{a}_{\vec{k}\sigma} \right]\end{aligned} \tag{124}$$

where $\hat{a}^{+}_{k\sigma}, \hat{a}_{\vec{k}\sigma}$ are the operators for the conduction electrons, with momentum $\vec{k}$ and spin σ ; $\hat{f}^{+}_{\vec{k}\sigma,\ell}, \hat{f}_{\vec{k}\sigma,\ell}$ are those for the f-electrons with ℓ as the index for the orbital degeneracy, and $\hat{n}^{f}_{i\sigma,\ell} = \hat{f}^{+}_{i\sigma,\ell} \hat{f}_{i\sigma,\ell}$ are the density operators for f-electrons on <u>site</u> i. The first term on the r.h.s. of (123) describes the kinetic energy of the conduction electrons, the second defines the energy of the f-electrons, the third is a Hubbard-term for the f-electrons where one usually assumes $U=\infty$ (no double occupancy) and the fourth term describes the hybridization, i.e. the quantum mechanical mixing between a- and f-electrons. For $V_{\vec{k},\ell}=0$ the orbital degeneracy allows for different ground states, i.e. different f-configurations. Hence it will be the hybridzation, although small in magnitude, which will eventually decide on the ground state. A subtle effect!

In the case of a <u>single</u> f-electron ("impurity") as in the original Anderson model [52], the "Kondo effect" is known to occur: For $T \gg T_K$ (T_k = Kondo Temperature) the f-electron has a magnetic moment, which for $T \ll T_K$ is screened by the conduction electrons. A Fermi liquid theory of this effect has been constructed by Nozieres [53] and the exact solution has been found later [54].

The situation, where there is a <u>periodic</u> lattice of f-electrons (PAM), is even more complicated. On the other hand, the periodicity is now expected to introduce a simplifying feature: it may lead to Bloch-states, which allow for <u>coherence</u>. This seems to explain the sharp drop of to a much lower T = 0 value (essentially that given by the impurity concentration) with a T^2-correction as in Landau theory. For more details of this problem, where Gutzwiller-type variational approaches have also been applied [55,56], but where a generally accepted theory does not yet exist , see ref. 4. The discovery of high-T_c superconductivity, and the subsequent boom in research in this field, has brought the investigation of HFS to a sudden stop, although similar problems seem to be involved.

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III. Pair Correlations in Interacting Fermi Systems

The concept of pair correlations in interacting Fermi systems was first introduced in 1957 by Bardeen, Cooper and Schrieffer (BCS) [1] to provide a microscopic understanding of superconductivity. This phenomenon had resisted theoretical explanation for more than 40 years. According to modern interpretation the salient feature of this theory is the concept of spontaneously broken gauge symmetry, or in more elementary language, the fact that the pair correlated state is decribed by a complex rather than a real valued order parameter. This fact is related to the appearance of a gap in the single particle excitation spectrum.

We note, that the broken symmetry and the existence of a gap implies that the superconducting state is not in one-to-one correspondence with the non-interacting ground state. Hence the superconductor is not a "normal Fermi liquid" discussed in part II and thus does not have a finite discontinuity of the momentum distribution at $k = k_F$. Indeed the effects of the interaction leading to the superconducting state cannot be obtained in perturbation theory (see below).

We first want to discuss the so-called weak coupling theory of pair correlations in Fermi systems. As the interaction giving rise to pair correlations becomes weaker, we should expect both the transition temperature T_c to the pair correlated state to decrease and the characteristic length ξ_0 of pair correlations to increase. The small parameter of weak coupling theory is the ratio T_c/T_F or equivalently $1/k_F\xi_0$). In the usual superconductors this is about 10^{-4} - 10^{-3} such that weak coupling theory is a very good starting point, but in the "heavy fermion superconductors" where T_F is much reduced due to the large effective mass m*, this ratio is much larger (10^{-2}-10^{-1}) making the application of weak coupling results quite dubious. For liquid ^{3}He $T_c/T_F \simeq 10^{-3}$; nevertheless weak coupling theory is unfortunately not quite as good as one should expect.

Cooper instability

Following the discussion in ref. [3], let us first consider a simple model problem introduced by Cooper [2] in the pre-stages of BCS-pairing theory. Consider a system of N noninteracting identical fermions of mass m and spin 1/2 in the ground state (the "Fermi sea"). If we add two more particles, the ground state of the N+2 particle system is

of course obtained by putting the two particles in the lowest available states at the Fermi energy. However, what happens if we now switch on an attractive interaction $V(\vec{r}_1-\vec{r}_2)$ just between the two added particles?

Quite generally the wavefunction of our model system is given by the antisymmetrized product of a correlated pair wavefunction $\Phi(\vec{r}_1,\vec{r}_2;\alpha,\beta)$ and an N-particle Slater determinant describing the Fermi sea. The pair wavefunction in turn is a product of the center of mass plane wave, the wavefunction describing the relative motion $\psi(\vec{r}_1-\vec{r}_2)$, and the spin functions $\chi(\alpha,\beta)$

$$\Phi(\vec{r}_1,\vec{r}_2;\alpha,\beta) = e^{\frac{i}{2}\vec{P}\cdot(\vec{r}_1+\vec{r}_2)}\,\psi(\vec{r}_1-\vec{r}_2)\,\chi(\alpha,\beta) \qquad (1)$$

Since the particles are identical by assumption, the pair wavefunction must be antisymmetric upon interchanging particles 1 and 2, implying that either $\psi(\vec{r})$ is odd and $\chi(\alpha,\beta)$ is even (spin triplet state) or vice versa (singlet state).

The important effect of the particles in the Fermi sea is to block the single particle states below the Fermi energy. This is most simply taken into account by working

in the momentum representation. Defining Fourier components by

$$\psi(\vec{r}) = \frac{1}{V}\sum_{\vec{k}} \psi_{\vec{k}}\, e^{i\vec{k}\cdot\vec{r}} = \frac{1}{(2\pi)^3}\int d^3k\, \psi_{\vec{k}}\, e^{i\vec{k}\cdot\vec{r}} \tag{2a}$$

$$V_{\vec{k}} = \int d^3r\, V(\vec{r})\, e^{-i\vec{k}\cdot\vec{r}} \tag{2b}$$

the pair Schrödinger equation takes the form

$$\left(\xi_{\vec{k}+\vec{P}/2} + \xi_{\vec{k}-\vec{P}/2} - E\right)\psi_{\vec{k}} = -\frac{1}{(2\pi)^3}\int_{|\vec{k}'|>k_F} d^3k'\, V_{\vec{k}-\vec{k}'}\, \psi_{\vec{k}'} \tag{3}$$

Here the blocking effect must be taken into account in the sum over intermediate states $\vec{k}'$. For the following it is useful to measure single particle energies from the Fermi level, defining the quasiparticle energy

$$\xi_{\vec{k}} = \frac{\hbar^2 k^2}{2m} - \mu \tag{4}$$

where μ is the chemical potential (equal to the Fermi energy E_F at zero temperature).

It is clear from (3) that the lowest energy E is obtained when the two particles have equal and oppositely directed momenta. We put $\vec{P} = 0$ in the following, because

finite $\vec{P}$ corresponds to a trivial center-of-mass motion of the pair with momentum $\hbar\vec{P}$.

Equation (3) may be separated into angular momentum components due to the assumed spherical symmetry of the interaction potential. By expanding $V_{\vec{k}-\vec{k}'}$, and $\psi_{\vec{k}}$ in terms of Legendre polynomials $P_\ell(\hat{k}\cdot\hat{k}')$ and spherical harmonics $Y_{\ell m}(\hat{k})$ one has

$$V_{\vec{k}-\vec{k}'} = \sum_{\ell=0}^{\infty} (2\ell+1)\, V_\ell(k,k')\, P_\ell(\hat{k}\cdot\hat{k}') \tag{5a}$$

$$\psi_{\vec{k}} = \sum_{\ell,m} a_{\ell,m}\, \psi_\ell(k)\, Y_{\ell m}(\hat{k}) \tag{5b}$$

In order to allow for an explicit analytic solution of (3) we now introduce a further simplifying feature caused specifically by the nature of the <u>electron-phonon</u> interaction. The latter is of central important for the origin of conventional superconductivity since it leads to an effective <u>attraction</u> between electrons, in spite of the omnipresent repulsive electron-electron interaction. For this we note that in the case of a metal there is not only the usual screening of the Coulomb interaction in the electron gas, but also screening due to the <u>ions</u>. Hence the bare Coulomb potential is changed to

$$V^0_{\vec{k}-\vec{k}'} = \frac{4\pi e^2}{q^2} \longrightarrow V_{\vec{k}-\vec{k}'} = V^0_{\vec{k}-\vec{k}'} \cdot \frac{q^2}{q^2+k_0^2} \cdot \left[1 + \frac{\omega^2(q)}{\omega^2-\omega^2(q)}\right]$$

$$\text{with} \quad \vec{q} = \vec{k}-\vec{k}', \quad \omega = \frac{1}{\hbar}\left(\epsilon_{\vec{k}} - \epsilon_{\vec{k}'}\right) \qquad (6)$$

The contribution $\omega^2(q)/[\omega^2 - \omega^2(q)]$ in (6) due to the screening of the ions is shown in Fig. 1. For $\hbar|\omega| \gg \hbar\omega(q) \simeq \hbar\omega_D$,

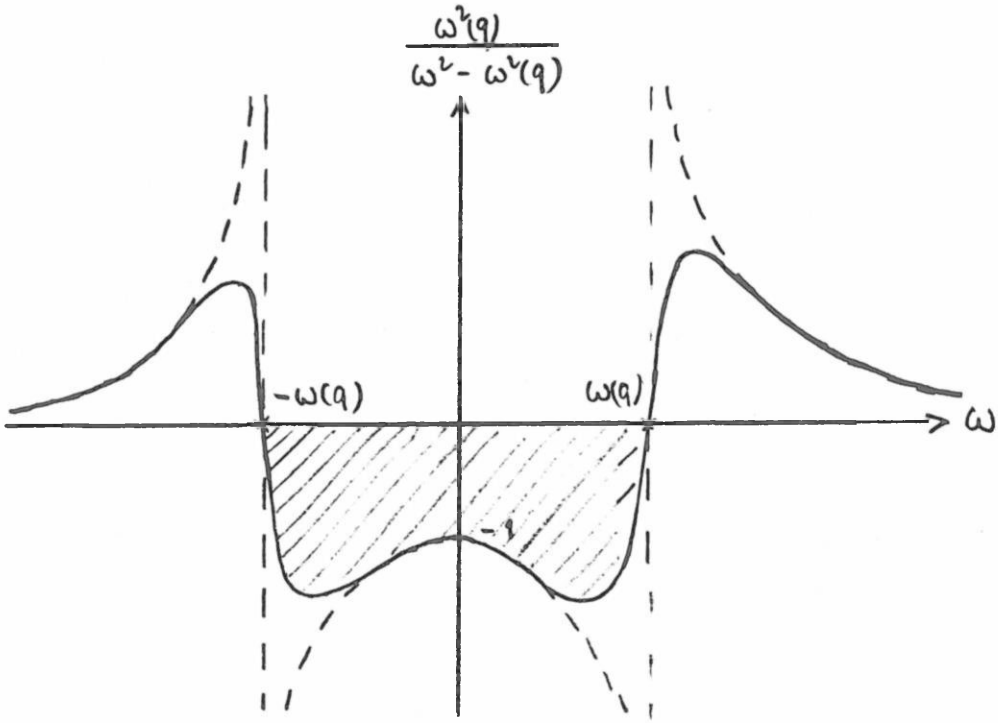


Fig. 1

where ω_D is the Debye-frequency, the corrections of the effective interaction due to the lattice (i.e. phonons) is neglegible. Since $\hbar\omega_D \simeq 10^{-3}E_F$, only electrons in a thin shell of width $\hbar\omega_D$ around the Fermi surface will be affected, i.e. will "feel" this electron-phonon

interaction. In particular, for $\hbar|\omega| \lesssim \hbar\omega_D$, the phonon contribution to (6) leads to a minus-sign, i.e. to an <u>attractive</u> interaction! Hence $V_{\vec{k}-\vec{k}'}$ may be approximated by a step-like model-interaction by putting $V_\ell(k,k')$ equal to a constant within a thin shell around the Fermi surface and zero elsewhere,

$$V_\ell(k,k') = \begin{cases} V \ , \ \text{for} \ |\xi_{\vec{k}}|, |\xi_{\vec{k}'}| \leq \epsilon_c \ll E_F \\ \\ 0 \ , \ \text{otherwise.} \end{cases} \tag{7}$$

Equation (3) then reduces to the separable integral equation

$$(2\xi_{\vec{k}} - E)\,\psi_\ell(k) = -\tfrac{1}{2} V_\ell \, N(0) \int_0^{\epsilon_c} d\xi_{k'}\, \psi_\ell(k') \tag{8}$$

where the density of states N(0) has been taken out of the integral, $N(\xi)$ being a slowly varying function on the scale of ϵ_c.

By inspection of (8) one can see immediately that for attractive interaction ($V_\ell < 0$) the energy eigenvalue E is necesarily negative. So, in the presence of the Fermi sea, the two test particles form a bound state for <u>arbitrarily</u> weak attractive interaction. The bound state is formed with relative orbital angular momentum L

corresponding to the strongest attractive interaction parameter V_L. The correlated pair is called "Cooper pair".

Cooper's problem is in marked contrast to the two particle problem without blocking effect, where a bound state is formed only if the potential is sufficiently attractive. An accurate necessary condition for the existence of a bound state is

$$\int d^3r \; |V(\vec{r})|^{3/2} > \frac{\pi^2}{4}\left(\frac{3\hbar^2}{2m}\right)^{3/2} \tag{9}$$

and the lowest bound state is always an s-state.

In the so-called "weak-coupling" limit, i.e. for $N(0)V_L \ll 1$, the solution of (8) is given by

$$E = -2\epsilon_c \, e^{-\frac{4}{N(0)|V_L|}} \quad , \quad V_L = \min_{\ell}\{V_\ell\} < 0 \tag{10a}$$

$$\psi_{\vec{k}} = \sum_m a_{Lm} \frac{\theta(\epsilon_c - |\xi_{\vec{k}}|)}{2\xi_{\vec{k}} - E} Y_{Lm}(\hat{k}) \tag{10b}$$

where $\theta(x)$ is the unit step function.

The wave function of the pair in position space, obtained by Fourier inverting (10b), is found as

$$\psi(\vec{r}) = \sum_{m} a_{Lm} \, Y_{Lm}(\hat{r}) \, \psi_L(r) \tag{11a}$$

where

$$\psi_L(r) = \frac{1}{2} \int_0^{\epsilon_c} d\xi_k \, \frac{N(0)}{2\xi_k - |E|} \, j_L(kr) \tag{11b}$$

The spherical Bessel functions $j_L(x)$ vanish as x^L for $x \to 0$, possess a first maximum at $x \simeq L$ and approach the asymptotic behaviour $\sin(x - L\pi/2)/x$ for $x \gg 1$. However, the k-components of the wave-function with $\xi_k < |E|$ interfere destructively, causing the wave function to vanish more rapidly than $1/r$ for $r > \hbar v_F/|E|$. Thus, the extension of the pair wave function, the so-called "correlation length" or "coherence length", is given by $\xi_0 \simeq \hbar v_F/|E|$.

A schematic picture of $\psi_1(r)$, the wave function for L= 1, is shown in Fig. 2.

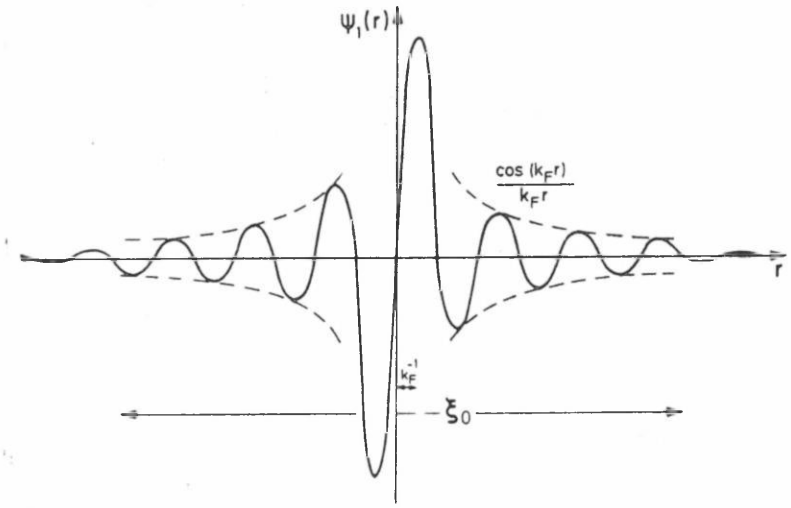


Fig. 2

The BCS Variational Wave Function

If the formation of a bound pair is energetically advantageous in Cooper's problem, one is to expect that if all particles interact with each other, the formation of correlated pairs of particles with momenta $(\hbar\vec{k}, -\hbar\vec{k})$ is still profitable. This expectation led Bardeen, Cooper and Schrieffer [1] to postulate a correlated wave function for electrons in superconductors, which is a properly antisymmetrized product of pair wave functions. In its simplest form, i.e. for pairing with total spin s = 0 it is given by

$$|\psi_{BCS}\rangle = \prod_{\vec{k}} \left[u_{\vec{k}} + v_{\vec{k}}\, \hat{a}^{+}_{\vec{k}\uparrow}\, \hat{a}_{-\vec{k}\downarrow} \right] |0\rangle \tag{12}$$

where $|0\rangle$ is the vacuum. Here $u_{\vec{k}}$($= u_{-\vec{k}}$) and $v_{\vec{k}}$ ($=v_{-\vec{k}}$) are variational parameters (in general complex) with

$$|u_{\vec{k}}|^2 + |v_{\vec{k}}|^2 = 1 \tag{13}$$

The operator in (12) acting on $|0\rangle$ creates pairs of (quasi)particles in a one-particle state $(\vec{k}\uparrow, -\vec{k}\downarrow)$. Hence $v_{\vec{k}}(u_{\vec{k}})$ is the probability amplitude for a pair state being occupied (unoccupied).

The normal state $|\psi_0\rangle$ is obtained from (12) by

$$\begin{aligned} u_{\vec{k}} &= 0, \quad v_{\vec{k}} = e^{i\phi_{\vec{k}}} && \text{for } |\vec{k}| < k_F \\ u_{\vec{k}} &= e^{i\phi_{\vec{k}}}, \quad v_{\vec{k}} = 0 && \text{for } |\vec{k}| > k_F \end{aligned} \tag{14}$$

such that

$$|\psi_0\rangle = \prod_{|\vec{k}|<k_F} \hat{a}^{+}_{\vec{k}\uparrow}\, \hat{a}^{+}_{-\vec{k}\downarrow}\, |0\rangle \tag{15a}$$

$$\stackrel{!}{=} \prod_{|\vec{k}|<k_F} \hat{a}^{+}_{\vec{k}\uparrow}\, \hat{a}^{+}_{\vec{k}\downarrow}\, |0\rangle \tag{15b}$$

Eq. (15) is just the usual Slater determinant.

The $u_{\vec{k}}$, $v_{\vec{k}}$ in (12) may either be determined by straightforward minimization of the energy expectation value in terms of $|\psi_{BCS}\rangle$ or by direct diagonalization of the BCS-Hamiltonian (see below).

We note, that $|\psi_{BCS}\rangle$ in (12) is a superposition of wave functions with 0,2,4,...N particles. This implies the following degeneracy: if $\{u_{\vec{k}}, v_{\vec{k}}\}$ characterizes the ground state $|\psi_{BCS}\rangle$, then states $|\psi_{BCS}(\theta)\rangle$ - characterized by $\{u_{\vec{k}}, e^{i\theta} v_{\vec{k}}\}$- with <u>fixed</u>, real θ are <u>energetically degenerate</u>! This property is referred to as "spontaneously broken gauge symmetry", since the phase factor $e^{i\theta}$ corresponds to a U(1)-symmetry which is <u>broken</u> if θ has a definite value. It implies the existence of a macroscopic spatially independent phase θ, while at the same time the particle number is not conserved (uncertainty relation!). On the other hand, as shown by Anderson [4] the superposition

$$\psi(N) = \int_0^{2\pi} d\theta \; e^{-i\theta \frac{\hat{N}}{2}} \; |\psi_{BCS}(\theta)\rangle \tag{16}$$

with $\hat{N}$ as particle number operator, yields a state with definite particle number.

The BCS-Hamiltonian

A pairing Hamiltonian which contains the bare essentials for Cooper-pairing has the form

$$\hat{H}_{BCS} = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} \hat{n}_{\vec{k}\sigma} + \sum_{\vec{k}\vec{k}'} V_{\vec{k},\vec{k}'} \hat{a}^{+}_{\vec{k}\uparrow} \hat{a}^{+}_{-\vec{k}\downarrow} \hat{a}_{-\vec{k}'\downarrow} \hat{a}_{\vec{k}'\uparrow} \tag{17}$$

The second term in (17) scatters pairs from $(\vec{k}'\uparrow, -\vec{k}'\downarrow)$ to $(\vec{k}\uparrow, -\vec{k}\downarrow)$. The expectation value of $\hat{H}_{BCS} - \mu \hat{N}$ in terms of (12) is given by

$$\langle \hat{H}_{BCS} - \mu \hat{N} \rangle = 2 \sum_{\vec{k}} \xi_{\vec{k}} |v_{\vec{k}}|^2 + \sum_{\vec{k}\vec{k}'} V_{\vec{k}\vec{k}'} u_{\vec{k}} v^*_{\vec{k}} u^*_{\vec{k}'} v_{\vec{k}'} \tag{18}$$

which may now easily be minimized w.r.t. $u_{\vec{k}}$, $v_{\vec{k}}$ [6]. However, this method does not yield <u>excited</u> states easily. Therefore we prefer the solution of (17) by a canonical transformation.

The phase-coherent superposition of states with $(\vec{k}\uparrow, -\vec{k}\downarrow)$ implies that

$$\langle \hat{a}_{\vec{k}\uparrow} \hat{a}_{-\vec{k}\downarrow} \rangle \neq 0 \tag{19}$$

in contrast to the normal case. Introducing the T = 0 expectation values

$$\langle \hat{a}^{\dagger}_{\vec{k}\sigma} \hat{a}_{\vec{k}\sigma} \rangle = n_{\vec{k}} \quad (= |v_{\vec{k}}|^2) \tag{20a}$$

$$\langle \hat{a}_{-\vec{k}\downarrow} \hat{a}_{\vec{k}\uparrow} \rangle \equiv F_{\vec{k}} \quad (= v_{\vec{k}} u^*_{\vec{k}}) \tag{20b}$$

with $F_{\vec{k}}$ as the "anomalous expectation value" or "pair amplitude", we now treat $\hat{H}_{BCS} - \mu \hat{N}$ in a mean field approximation, by factorizing the 4-fermion interaction term in (17) into 2-fermion terms, just as in the case of the Hubbard-model (see eq.(83) in part II). Thereby we assume that a given pair feels the other pairs only via a "mean field". Since we are only interested in the difference in energy relative to the usual Hartree-Fock approximation we only concentrate on the <u>anomalous</u> expectation values $F_{\vec{k}}$, $F^*_{\vec{k}}$ by subtracting the <u>normal</u> contributions $n_{\vec{k}}$ etc. Hence

$$(\hat{H}_{BCS} - \mu \hat{N})\Big|_{\substack{\text{mean} \\ \text{field, anom.}}} \equiv \hat{H}_{MF} \tag{21}$$

$$= \sum_{\vec{k}\sigma} \xi_{\vec{k}} \hat{a}^{\dagger}_{\vec{k}\sigma} \hat{a}_{\vec{k}\sigma} + \sum_{\vec{k}} \left[\Delta^*_{\vec{k}} \hat{a}_{-\vec{k}\uparrow} \hat{a}_{\vec{k}\downarrow} + \hat{a}^{\dagger}_{\vec{k}\downarrow} \hat{a}^{\dagger}_{-\vec{k}\uparrow} \Delta_{\vec{k}} \right]$$

where

$$\Delta_{\vec{k}} = \sum_{\vec{k}'} V_{\vec{k}\vec{k}'} F_{\vec{k}'} \tag{22}$$

The resulting mean field Hamiltonian $\hat{H}_{MF}$ is bilinear and may be diagonalized by a canonical transformation, which eliminates the "off-diagonal" terms $\hat{a}_{-\vec{k}\uparrow}\hat{a}_{\vec{k}\downarrow}$ and $\hat{a}^{\dagger}_{\vec{k}\uparrow}\hat{a}^{\dagger}_{-\vec{k}\downarrow}$. This is achieved by the operators [7]

$$\hat{b}_{\vec{k}\sigma} \equiv u_{\vec{k}}\,\hat{a}_{\vec{k}\sigma} - \sigma v_{\vec{k}}\,\hat{a}^{\dagger}_{-\vec{k},-\sigma} \tag{23}$$

which obey Fermi anti-commutation relations. Replacing the $\hat{a}_{\vec{k}\sigma}$-operators in (21) by $\hat{b}_{\vec{k}\sigma}$ etc, and demanding that the coefficient of $\hat{b}^{\dagger}_{\vec{k}\sigma}\hat{b}^{\dagger}_{-\vec{k}\sigma}$ vanishes, leads to the condition

$$2\xi_{\vec{k}}\,u_{\vec{k}}v_{\vec{k}} = \Delta_{\vec{k}}u_{\vec{k}}^2 - \Delta^*_{\vec{k}}v_{\vec{k}}^2 \tag{24}$$

and hence, with (13),

$$u_{\vec{k}}^2 = \frac{1}{2}\left[1 + \frac{\xi_{\vec{k}}}{E_{\vec{k}}}\right] \tag{25a}$$

$$v_{\vec{k}}^2 = \frac{1}{2}\left[1 - \frac{\xi_{\vec{k}}}{E_{\vec{k}}}\right] \tag{25b}$$

where

$$E_{\vec{k}} = \sqrt{\xi_{\vec{k}}^2 + |\Delta_k|^2} \tag{26}$$

Now, $\hat{H}_{MF}$, (21), takes the form

$$\hat{H}_{MF} = \sum_{\vec{k}} \left\{ |\Delta_{\vec{k}}|^2 \left[\frac{1}{2E_{\vec{k}}} - \frac{1}{E_{\vec{k}} + \xi_{\vec{k}}} \right] + E_{\vec{k}} \sum_{\sigma} \hat{b}^{+}_{\vec{k}\sigma} \hat{b}_{\vec{k}\sigma} \right\} \tag{27}$$

Since $\hat{b}^{+}_{\vec{k}\sigma} \hat{b}_{\vec{k}\sigma}$ is a positive operator, the ground state $|\psi\rangle$ is characterized by

$$\hat{b}_{\vec{k}\sigma} |\psi\rangle = 0 \tag{28}$$

i.e. excited states are obtained by letting $\hat{b}^{+}_{\vec{k}\sigma}$ operate on $|\psi\rangle$. Hence

$$|\psi, \vec{k}\alpha\rangle \equiv \hat{b}^{+}_{\vec{k}\alpha} |\psi\rangle \tag{29}$$

is a one-particle excitation, called "Bogoliubov quasiparticle" (BQP). It is an eigenstate of the momentum with eigenvalue $\hbar\vec{k}$. The one-particle excitation energy is given by

$$E_{\vec{k}} = \sqrt{\xi_{\vec{k}}^2 + |\Delta_{\vec{k}}|^2} \tag{30}$$

showing that the spectrum has an <u>energy gap</u> $\Delta_{\vec{k}}$ (see Fig.3), which in general may depend on the direction of $\vec{k}$.

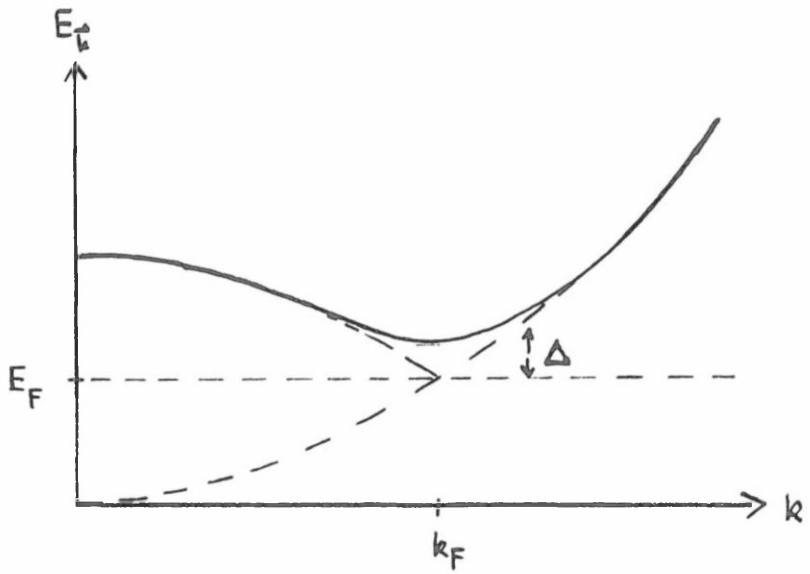


Fig. 3

<u>The gap equation at finite temperatures</u>

The expectation values at <u>finite</u> temperatues are obtained from

$$\langle \hat{O} \rangle = \frac{Tr\left[\hat{O}\, e^{-\beta \hat{H}_{MF}}\right]}{Tr\, e^{-\beta \hat{H}_{MF}}} \tag{31}$$

Now F_k , (20b),(and thereby Δ_k) become T-dependent.

The BQPs are independent fermions

$$\langle \hat{b}^{+}_{\vec{k}\sigma} \hat{b}_{\vec{k}'\sigma'} \rangle = \delta_{\vec{k}\vec{k}'} \delta_{\sigma\sigma'} n_{\vec{k}} \tag{32}$$

where

$$n_{\vec{k}} = \frac{1}{e^{\beta E_{\vec{k}}} + 1} \tag{33}$$

is the Fermi-Dirac distribution, but with the energy dispersion $E_{\vec{k}}$,(30), for BQPs. Using the inverse of (23) one obtains

$$\langle \hat{a}^{+}_{\vec{k}\uparrow} \hat{a}_{\vec{k}\uparrow} \rangle = \frac{1}{2} \left(1 + \frac{\xi_{\vec{k}}}{E_{\vec{k}}}\right) n_{\vec{k}} + \frac{1}{2} \left(1 - \frac{\xi_{\vec{k}}}{E_{\vec{k}}}\right) (1 - n_{\vec{k}}) \tag{34}$$

and for the anomalous expectation value

$$F_{\vec{k}} = - \frac{\Delta_{\vec{k}}}{2E_{\vec{k}}} (1 - 2n_{\vec{k}}) \tag{35}$$

From this the (self consistent) "gap-equation" (22), which describes the T-dependence of $\Delta_{\vec{k}}(T)$ is found as

$$\Delta_{\vec{k}} = - \sum V_{\vec{k}\vec{k}'} \frac{\Delta_{\vec{k}'}}{2E_{\vec{k}'}} \tanh \frac{E_{\vec{k}'}}{2k_B T} \tag{36}$$

The $\vec{k}$-dependence of a gap-function with definite orbital angular momentum L may be decomposed as

$$\Delta_{\vec{k}}^{(L)} = \sum_{m=-L}^{L} a_m Y_{Lm}(\Omega_k) \tag{37}$$

For conventional superconductivity the pair interaction for L = 0 is strongest:

$$\Delta_{\vec{k}}^{(L=0)} = \Delta \tag{38}$$

Using (7) with $\epsilon_c = \hbar\omega_D$, the gap equation takes the form

$$\frac{1}{\lambda} = \int_0^{\hbar\omega_D} d\xi_k \, \frac{\tanh \frac{E_k}{2k_BT}}{E_k} \tag{39}$$

where $\lambda \equiv \frac{1}{2}|V_0|\, N(0)$ is the coupling constant. Eq. (39) yields the critical temperature T_c , where Δ vanishes, as

$$T_c = c_0 \frac{\hbar\omega_D}{k_B} e^{-1/\lambda} \tag{40}$$

with $c_0 = 2e^{\gamma}/\pi \simeq 1.13$ and the T = 0 gap as

$$\Delta(0) = 2\hbar\omega_D e^{-1/\lambda} \tag{41}$$

The ratio

$$\vec{S}_{\alpha\beta,\alpha'\beta'} = \vec{\sigma}_{\alpha\alpha'}\,\delta_{\beta\beta'} + \delta_{\alpha\alpha'}\,\vec{\sigma}_{\beta\beta'} \tag{48}$$

The square of the energy gap in terms of $\vec{\Delta}(\vec{k})$ (i.e. the eigenvalue of $\underline{\Delta}_{\vec{k}}\,\underline{\Delta}^{\dagger}_{\vec{k}}$) is given by

$$|\Delta_{\vec{k}}|^2_{\pm} = \vec{\Delta}(\vec{k})\cdot\vec{\Delta}^*(\vec{k}) \pm \sqrt{-\left[\vec{\Delta}(\vec{k})\times\vec{\Delta}^*(\vec{k})\right]^2} \tag{49}$$

The quantity $\langle\vec{\Delta}\times\vec{\Delta}^*\rangle$ represents a kind of "spin angular momentum" of the Cooper pair, at least locally on the Fermi surface. A state with $\langle\vec{\Delta}\times\vec{\Delta}^*\rangle \neq 0$ is therefore <u>magnetic</u>. States with the much simpler structure $\underline{\Delta}\,\underline{\Delta}^{\dagger} \propto \underline{1}$ (and hence $\langle\vec{\Delta}\times\vec{\Delta}^*\rangle = 0$) are called "unitary" states.

Superfluid ^{3}He

Immediately after BCS-theory had been established, it became clear that the same kind of instability, i.e. Cooper pairing, should in principle also be possible in liquid ^{3}He. Clearly, in this case the strong hard core repulsion would demand pairing with $L > 0$, such that at zero relative distance the Cooper pair wave function is made to vanish (see Fig. 2). This immediately implies an anisotropic pair wave function, with either S = 0 (singlet state) and L=2,4,... or with S = 1 (triplet state) with L = 1,3,.... It took a long, intensive experimental search into the milli-Kelvin regime until Osheroff, Richardson and Lee [8] discovered the superfluidity of ^{3}He on Christmas of 1971 at, T_c = 2.6mK (for experimental reviews, see refs. 9,10). In fact, three different phases were found: the A and B-phases in zero external magnetic field, and the A_1-phase in a finite field. The phase diagram is shown in Fig. 4 on a logarithmic temperature scale. In Fig. 5 the magnetic field is also included.

Today we know that in superfluid ^{3}He Cooper-pairs (CP) form in a relative S = 1, L = 1 (triplet, p-wave) state. In contrast to conventional superconductivity (S=0, L = 0) with a pair wave function

$$|\psi_{s.c.}\rangle = |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \tag{50}$$

this wave function now has <u>three</u> substates w.r.t. spin

$$|\psi_{triplet}\rangle = \psi_{\uparrow\uparrow}(\vec{k})\,|\uparrow\uparrow\rangle + \psi_{\uparrow\downarrow}(\vec{k})\,|\uparrow\downarrow + \downarrow\uparrow\rangle + \psi_{\downarrow\downarrow}(\vec{k})\,|\downarrow\downarrow\rangle \tag{51}$$

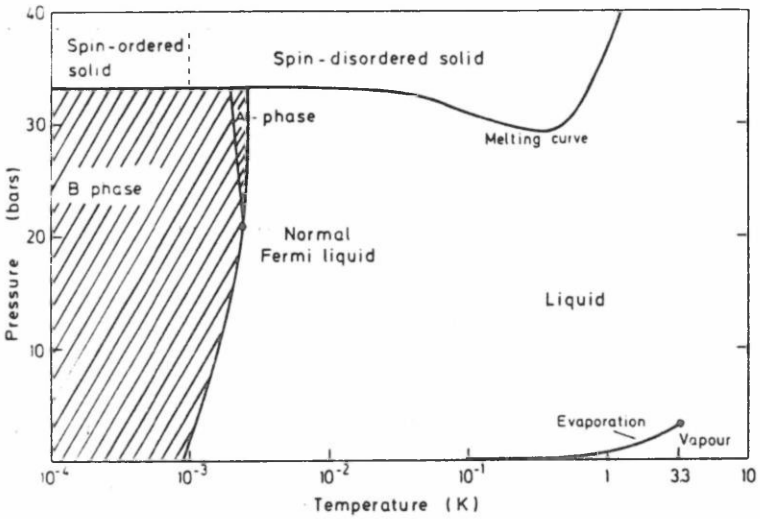


Fig. 4

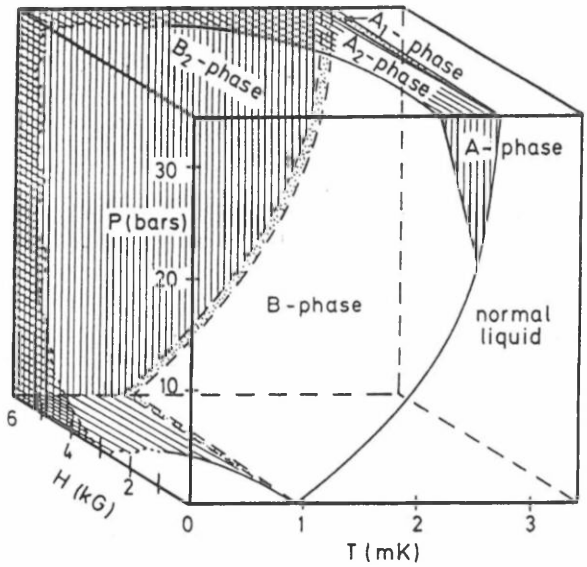


Fig. 5

Because of L = 1 there will also be three substates w.r.t. to orbital space, as expressed in the $\vec{k}$-dependent amplitudes $\psi_{\uparrow\uparrow}(\vec{k})$ etc. Hence the pair wave function involves 3 x 3 = 9 substates, expressible by 9 complex parameters. In particular, the anisotropy of the CPs will now lead to macroscopic ordering not only of the overall phase, but also of the quantization axes ("preferred directions") in spin- and orbit-space (for theoretical reviews, see refs. 3,11 and ref. 6).

The order parameter itself now has the form as in (46) with

$$\vec{\Delta}_\mu(\vec{k}) = \sqrt{3}\,\Delta \sum_{j=1}^{3} A_{\mu j}\,\hat{k}_j \tag{52}$$

because of L = 1. The complex 3 x 3 matrix $A_{\mu j}\,(\equiv \mathbb{A})$ is a "bi-vector" in spin and orbit space.

Equivalently, $\vec{\Delta}_\mu(\vec{k})$ can be represented by a linear combination of L = 1 angular momentum eigenstates $Y_{1m}(\hat{k})$, m = 0, ±1.

Pairing-interaction in superfluid ^{3}He

The origin for pairing in liquid ^{3}He is much more complicated than in a superconductor, since now the attraction must arise within the one-component system itself. The van-der-Waals attraction is a possible candidate but leads to unrealistically small T_c. Besides that, since T_c << 100mK, the description has to involve the quasi-particle picture. This problem has, in fact, not yet been solved satisfactorially! One simple (but incomplete) mechanism for attraction involves the exchange of spin fluctuations. Since $\chi_s^{^3He} \gg \chi_s^0$, a given spin will easily polarize its surrounding medium, generating a local molecular field. A second spin, when coming by, will see this polarization and be attracted (repelled) if its spin is parallel (anti-parallel). This "explains" the existence of an additional spin-dependent, effective interaction

between the nuclear spins of two ^{3}He-atoms, which favors triplet- pairing.

A quantitative formulation of this mechanism within the QP-picture, which makes use of the QP-interaction as a molecular field, yields [3]

$$V^{eff}_{\vec{k}\vec{k}'} = -(f_0^a)^2 \; \mathrm{Re}\; \chi_s(\vec{q},\omega)\; \vec{\sigma}\cdot\vec{\sigma}' \tag{53}$$

where $\chi_s(\vec{q},\omega)$ is the dynamic spin susceptibility and f_0^a is the $\ell = 0$ part of the spin dependent QP-interaction. This acts in addition to the <u>direct</u> spin-dependent QP-interaction (see eq. (40), part II)

$$V^{direct}_{kk'} = f_0^a \; \vec{\sigma}\cdot\vec{\sigma}' \tag{54}$$

which is also attractive since in ^{3}He $f_0^a < 0$. Note that the attraction in (53) is <u>independent</u> of the sign of f_0^a ! In fact, other molecular fields $f_\ell^{s,a}$ than f_0^a will equally lead to such an attraction but, most likely, are of less importance [3].

<u>The free energy</u>

Close to T_c, where $\Delta_{\vec{k}}(T) \ll k_B T_c$, the free energy may be expressed in powers of the order parameter (OP), giving rise to a "Ginzburg-Landau functional". While for a usual superconductor this simply yields

$$F = \alpha \Delta\Delta^* + \tfrac{1}{2}\beta(\Delta\Delta^*)^2 \tag{55}$$

the functional for an OP with the structure of (52) has to be constructed by contracting all indices in the general second- and fourth-order term

$$\begin{aligned} F = \alpha \Delta^2 \mathrm{Tr}(AA^\dagger) + \tfrac{1}{2}\Delta^4 \Big\{ & \beta_1 |\mathrm{Tr}\, A\tilde{A}|^2 \\ & + \beta_2 [\mathrm{Tr}(AA^\dagger)]^2 + \beta_3 \mathrm{Tr}[(A\tilde{A})(A\tilde{A})^*] \\ & + \beta_4 \mathrm{Tr}[(AA^\dagger)^2] + \beta_5 \mathrm{Tr}[(AA^\dagger)(AA^\dagger)^*] \Big\} \end{aligned} \tag{56}$$

There are now <u>five</u> fourth order terms. The coefficients α, β_i depend explicitly on pressure. In weak coupling approximation one obtains $\beta_2 = \beta_3 = \beta_4 = -\beta_5 = -2\beta_1$. The calculation of "strong coupling corrections" to the β_i is difficult [12].

The energy functional (56) involves 18 parameters. Its minimization leads to a highly complicated problem. Although the most important minima (corresponding to the measured phases) are known [13,14], it has not yet been solved in full generality. In this situation symmetry investigations of the free energy (56) prove to be a very powerful method [15,16]. They make use of the symmetry group

$$G = SO(3)_{\vec{S}} \times SO(3)_{\vec{L}} \times U(1)_{\Phi}$$

under which the free energy (56) is invariant. By a classification of the subgroups of (57), possible phases with a remaining symmetry $H \in G$ are found, which indeed correspond to the known A,B etc. phases. This then also establishes the <u>broken</u> symmetries R = G/H of the respective phases.

<u>B-phase</u>

According to weak coupling theory the B-phase should be the stable phase at <u>all</u> temperatures [17]. Its order parameters structure is

$$A_{\mu j} = \frac{1}{\sqrt{3}} \delta_{\mu j} \tag{57a}$$

i.e.

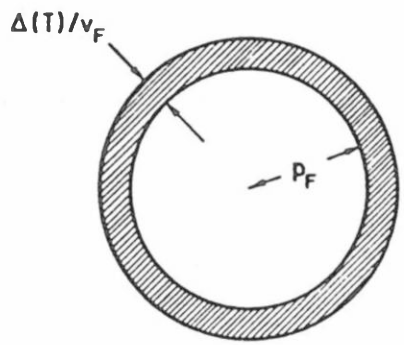
$$\vec{\Delta}_{\mu} = \Delta \hat{k}_{\mu} \tag{57b}$$

In fact, more generally it reads

$$A_{\mu j} = \frac{1}{\sqrt{3}} R_{\mu j} (\hat{n}, \theta) \tag{58}$$

where $R_{\mu j}$ is a rotation matrix describing a relative rotation between spin- and orbital space, parametrized by a

rotation axis $\hat{n}$ and a rotation angle θ . The energy gap is found to be <u>isotropic</u> (Fig. 6)



^{3}He - B

Fig. 6

$$\Delta_B(\hat{k}) = \Delta \tag{59}$$

just as in superconductivity, <u>in spite of the intrinsic anisotropy of the CP</u>! Hence the B-phase is also called "(pseudo)- isotropic" phase; it has many features in common with usual superconductivity. The anisotropy shows up for example in dynamic properties. The B-phase contains all three spin states in (51) in equal proportion. A magnetic field will not feel the $|\uparrow\downarrow + \downarrow\uparrow\rangle$ component, and hence its spin susceptibility at T = 0 is given by its

normal state value minus one third of the superfluid component.

The specific heat at low T is that of a superconductor

$$C_v \propto e^{-\frac{\Delta}{k_B T}} \tag{60}$$

owing to the isotropic gap, across which excitations have to be lifted.

A-phase

The existence of this second phase [18], which is stable only above pressures of ~20 bar, contradicts weak coupling theory. An explanation of its stability has to rely on strong coupling corrections. Indeed, spin fluctuation effects (which become more important at higher pressures) have been shown to play an important role in its stabilization [19]. The A-phase is a socalled "equal spin pairing" state, since pairing in this phase only involves the two components $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ in (51). This leads to a strong anisotropy of the OP matrix

$$A_{\mu j} = \frac{1}{\sqrt{2}} \hat{d}_\mu \, (\hat{m} + i\hat{n})_j \tag{61}$$

where $\hat{d}$ is a unit vector in spin space and $\hat{m} \perp \hat{n}$ are unit vectors in orbital space. Consequently, the OP vector is of the form

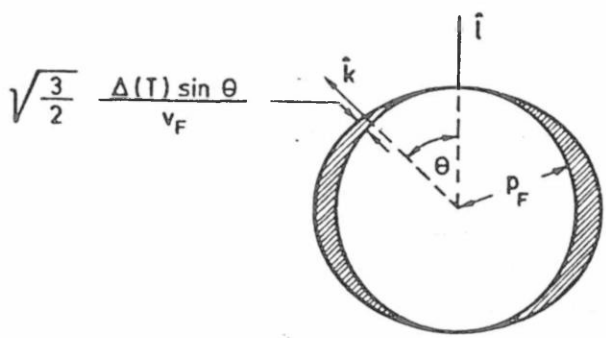
$$\vec{\Delta}_\mu(\hat{k}) \propto \hat{d}_\mu (\hat{k}_x + i\hat{k}_y); \quad \propto Y_{1,-1}(\hat{k}) \tag{62}$$

and the energy gap itself reads

$$\Delta(\hat{k}) = \Delta_0 \sqrt{1-(\hat{k}\cdot\hat{\ell})^2} \tag{63a}$$

$$= \Delta_0 \, |\sin \theta_{\hat{k}}| \tag{63b}$$

where $\Delta_0 = \sqrt{3/2}\ \Delta$ and $\hat{\ell} = \hat{m} \times \hat{n}$ is the orbital angular momentum of the CP; here $\theta_{\hat{k}}$ is the angle between $\hat{\ell}$ and $\hat{k}$, the direction on the Fermi surface as shown in Fig. 7.



^{3}He - A

Fig. 7

We see that the energy gap now has zero points ("nodes"). This leads to very profound consequences: In particular, even in the limit $T \rightarrow 0$ excitation of quasiparticles may now take place (see Fig. 8). Hence, even well below E there is a finite density of states as shown in Fig. 9,

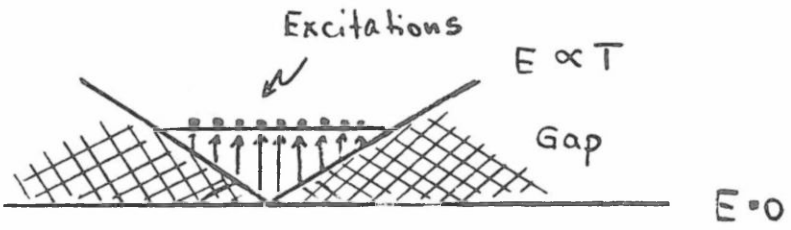


Fig. 8

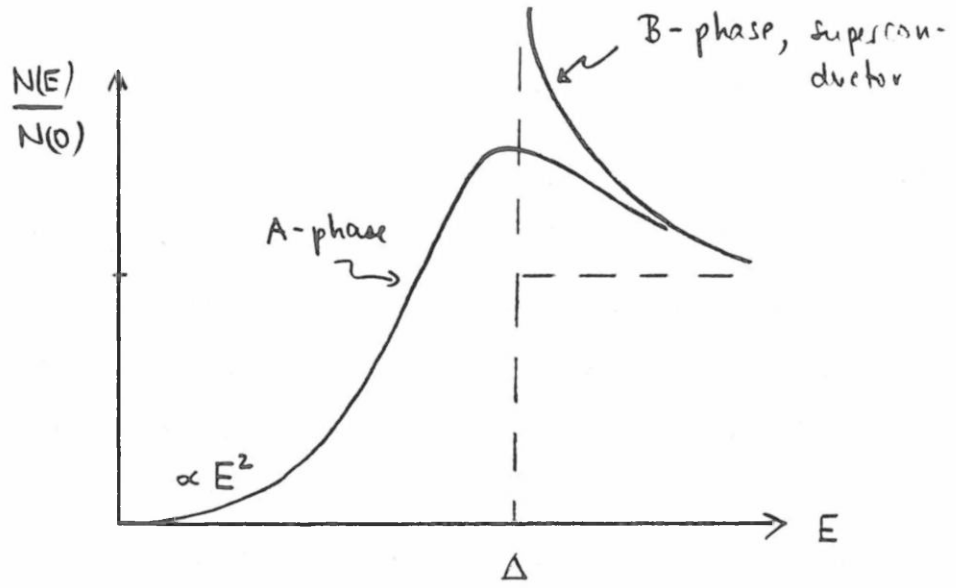


Fig. 9

with $N(E) \propto E^2$ for $E \to 0$. As a consequence the low-T behavior of c_v goes as

$$C_v \propto C_v\big|_{normal} \times \left(\frac{T}{\Delta_0}\right)^2 \tag{64a}$$

$$\propto \frac{T^3}{\Delta_0^2 T_F} \tag{64b}$$

i.e. has a power-law behavior. The T^2-dependence in (64a), which acts in addition to the normal linear T-dependence of the normal system, is precisely due to the E^2-dependence of N(E).

Macroscopic Quantum Coherence in the A-phase

In any superfluid (be it isotropic or anisotropic) the phase of the OP is a macroscopic variable. In addition, the intrinsic anisotropy of the CP-wave function in superfluid ^{3}He with S = 1, L = 1, which leads to the

existence of quantization axes in spin- and orbit space, also implies macroscopically defined preferred <u>directions</u>.

In the superfluid A-phase, the structure of the order parameter in (62) shows that macroscopic ordering takes place both in spin space (expressed by a direction $\hat{d} \perp \vec{S}$) and, independently, in orbital space, where the preferred direction is given by $\hat{\ell}$, the direction of the orbital angular momentum of the CPs. Therefore ^{3}He-A may be called a "superfluid, magnetic, liquid crystal" since it simultaneously combines the features of a superfluid, a magnetically ordered system and a liquid crystal.

The preferred directions form macroscopically defined "textures". The actual direction of these textures may be externally oriented:

(i) the $\hat{\ell}$ -vector has to stand perpendicular to any surface, so that the CP does not "bump" into the wall, which would make it break up. It may also be influenced by external electric fields, supercurrents etc.

(ii) the $\hat{d}$-vector has to stand perpendicular to an external magnetic field.

The Dipolar Interaction

The directions $\hat{d}$ and $\hat{\ell}$ are not independent. The tiny dipole-dipole interaction of the ^{3}He-nuclei leads to an (anisotropic) spin-orbit coupling between the two partners of a CP, which prefers $\vec{S} \perp \hat{\ell}$ ("end-to-end" configuration) and thus $\hat{d} \parallel \hat{\ell}$. Hence there is a term in the free energy

$$E_{dipole} \propto - g_D \int d\vec{r}\, (\hat{d}\cdot\hat{\ell})^2 \tag{65}$$

where $g_D \propto \lambda_D \Delta_0^2$ is the coupling constant with

$$\lambda_D \sim \frac{(\gamma\hbar)^2}{a^3} \simeq 10^{-7}\,[K] \tag{66}$$

Why is it important at all at temperatures 2×10^{-3}K? The answer is subtle [3]: although $\hat{d}$ and $\hat{\ell}$ are macroscopically ordered, their <u>relative</u> orientation is undetermined by the interactions which lead to the superfluid state and which are all spin-orbit symmetric. In this situation any residual interaction which is spin-orbit <u>unsymmetric</u> (such as the dipolar interaction), as small as it may be, leads to a relative orientation of $\hat{d}$ and $\hat{\ell}$.

This coupling has many drastic consequences, of which we only mention three.

1) The energy in (65) is the same for $\hat{d} \parallel \hat{\ell}$ and $\hat{d} \parallel -\hat{\ell}$. This degeneracy allows for topologically stable "domain walls" between regions with $\hat{d} \parallel \hat{\ell}$ and $\hat{d} \parallel -\hat{\ell}$, just as in a ferromagnet [20];

2) The dipolar coupling makes its appearence in NMR experiments, since it contributes an additional term $\vec{R}_D$ ("dipolar torque") to the usual equation for the spin dynamics [3,21]

$$\frac{d\vec{S}}{dt} = \gamma \vec{S} \times \vec{H} + \vec{R}_D(\lambda_D) \tag{67}$$

In particular this implies the existence of <u>longitudinal</u> NMR, since a change $\Delta\vec{H}$ in the direction of an external static magnetic field $\vec{H}$ will lead to a change in $\vec{S}$ and will thereby drive $\hat{d}$ away from $\hat{\ell}$. Since $\hat{d}$ is coupled to $\hat{\ell}$, the dipolar interaction acts as a <u>restoring</u> force and leads to a longitudinal resonance frequency

$$\Omega_L = \sqrt{\omega_L^2 + \Omega_0^2(T)} \tag{68}$$

(i.e. to a frequency shift $\Omega_L - \omega_L > 0$) where $\omega_L = \gamma H$, and Ω_0/γ is equivalent to a local magnetic field of $\sim$ 30 Gauss (in a liquid!!).

3) A sound wave may induce internal oscillations of the CP-structure, and couples to the direction of $\hat{\ell}$ [22]. This leads to sound attenuation. Because of the dipolar

coupling of $\hat{\ell}$ to $\hat{d}$, a change of a small (i.e. ~30 Gauss) external magnetic field (which is sufficient to orient the nuclear spins, i.e. $\hat{d}$) will thereby change the sound attenuation, i.e. as non-magnetic property.

Heavy Fermion Superconductors

The experimental discovery of superconductivity in some of the heavy fermion systems ($CeCu_2Si_2$, UPt_3, UB_{13}) was a great surprise (for reviews, see ref. 23-25). After all, it seemed to involve the (almost) localized f-electrons, although superconductivity needs "mobile" electrons. Furthermore, the magnetic moments on the Ce/U-atoms can be expected to suppress s-wave, singlet pairing. Indeed the measurements of the specific heat, relaxation time T_1, heat conduction, sound attenuation and penetration depth were found to be quite different to "usual" BCS superconductors. In particular, the low-T properties seemed to obey a power-law behavior in T, rather than exponential behavior typical for the latter systems. However, direct comparison is dubious, since $T_F^* \simeq 10^{-3} T_F$ in these systems can be rather low, such that $\hbar\omega_D / k_B T_F^* \sim 1$. This makes conventional pairing theory ($\hbar\omega_D / E_F \ll 1$) invalid. The natural questions are then (i) what the nature of the attractive interaction is, and (ii) what kind of pairing is involved.

In this situation superfluid ^3He had a great influence, owing to its well established power-law dependences. For example, it was suggested that UBe_{13} was similar to the A-phase [26] ("triplet"-pairing), and that the powerlaw dependence of c_V enabled one to discern whether the order parameter of the superconducting state had point nodes ($c_V \propto T^3$) or lines of nodes ($c_V \propto T^2$).

The main problem is that the strong spin-orbit coupling ($\propto Z^4$) makes a classification of "singlet" vs. "triplet" questionable. In fact, for crystal structures with inversion symmetry there are only four degenerate states

$$|\vec{k}\rangle, \quad P|\vec{k}\rangle, \quad T|\vec{k}\rangle, \quad PT|\vec{k}\rangle \tag{69}$$

where P = Parity, T = time inversion. So CP-amplitudes can only be distinguished w.r.t. <u>even</u> or <u>odd</u> parity [27]. In spite of a lot of experimental and theoretical work on this problem [23-25] no clear decisive conclusion about the pairing interaction and the nature of pairing has been reached yet.

<u>Theoretical Approach to High-T_C Superconductivity</u>

The intensity of the theoretical and experimental activity in the investigation of high-T_C superconductivity, following Bednorz and Müller's [28] seminal work, is

unparalleled in the history of condensed matter physics. This discovery of superconductivity at temperatures more than three times as high as previously known came as a total surprise to anybody in the field [29].

The new superconductors are all based on doped La_2CuO_4 ("copper-oxides"). There are essentially two classes of materials: (i) $La_{2-x}M_xCuO_{4-y}$, where M = Sr, Ba, Ca,..., with $T_c \simeq$ 40K and (ii) $RE_1Ba_2Cu_3O_{7-y}$, where RE = Y,La,Eu,..., with $T_c \simeq$ 90K. They have a layered perovskite structure, where the Cu-O_2 layers are only weakly linked.

Band structure calculations suggest a Cu^{2+} valence which is in an $S = \frac{1}{2}$ state (without orbital degeneracy). This Cu^{2+} state is strongly hybridized with the adjacent p-levels of the oxygen. In essence this leads to a single half-filled band of $S = \frac{1}{2}$ spins on the Cu-sites with a moderately strong on-site repulsion. Because of the square-lattice structure of the Cu-atoms in the xy-plane, the kinetic energy may be assumed to be given by next neighbor overlap with a tight-binding dispersion

$$\epsilon_{\underline{k}} = 2t \left(\cos k_x a + \cos k_y a \right) \tag{70}$$

In view of the necessity of doping to produce superconductivity in the copper-oxides (the superconductivity always occurs in the vicinity of a metal-insulator transition), the underlying theoretical model

seems to be the nearly half-filled Hubbard-model [30], perhaps extended to contain next-neighbor interaction as well [31]. So we again encounter this simple quantum mechanical model - the simplest of all models to describe correlations among fermions.

The Hubbard Model at large U

In order to study the Hubbard-Hamiltonian (eq. (65) in part II) at large U/t, it is convenient to derive an effective Hamiltonian, which is correct up to order t^2/U [32]. In the nearly half-filled band case ($\delta \equiv 1-n \ll 1$) and to leading order in t/U, there are only two contributions to the energy: (i) the hopping term, which is provided by the motion of holes, i.e. is of order ($-\delta t$) and hence vanishes for $\delta = 0$, and (ii) virtual hopping, associated with the build-up and subsequent decay of a doubly occupied site and a hole, starting from two single next neighbor spins with opposite directions. This energy is proportional to the full density n. Note, that a real process of the formation of doubly occupied site is suppressed since it would contribute an energy U.

The kinetic part of the Hubbard-Hamiltonian (II 65b) for next-neighbor hopping ($t_{ij} \equiv -t$) may be rewritten as

$$\hat{H}_0 = \hat{T}_H + \hat{T}_D + \hat{T}_{mix} \tag{71}$$

where

$$\hat{T}_H = -t \sum_{\langle ij \rangle} \sum_{\sigma} (1-\hat{n}_{i,-\sigma})\, \hat{c}^{\dagger}_{i\sigma}\, \hat{c}_{j\sigma}\, (1-\hat{n}_{j,-\sigma}) \tag{72a}$$

$$\hat{T}_D = -t \sum_{\langle ij \rangle} \sum_{\sigma} \hat{n}_{i,-\sigma}\, \hat{c}^{\dagger}_{i\sigma}\, \hat{c}_{j\sigma}\, \hat{n}_{j,-\sigma} \tag{72b}$$

$$\hat{T}_{mix} = -t \sum_{\langle ij \rangle} \sum_{\sigma} \Big[\hat{n}_{i,-\sigma}\, \hat{c}^{\dagger}_{i\sigma}\, \hat{c}_{j\sigma}\, (1-\hat{n}_{j,-\sigma}) + (1-\hat{n}_{i,-\sigma})\, \hat{c}^{\dagger}_{i\sigma}\, \hat{c}_{j\sigma}\, \hat{n}_{j,-\sigma} \Big] \tag{72c}$$

Here $\hat{T}_H$ and $\hat{T}_D$ describe the hopping of holes and doubly occupied sites, respectively. Hence they do not change the number of doubly occupied sites, while $\hat{T}_{mix}$ does. To eliminate $\hat{T}_{mix}$ to lowest order in t/U, i.e. to avoid mixing of the "lower" and the "upper" Hubbard bands, a unitary transformation $\hat{S}$ is applied to $\hat{H} = \hat{H}_0 + \hat{H}_1$ (II,65)

$$\hat{H}_{eff} = e^{i\hat{S}}\, \hat{H}\, e^{-i\hat{S}} = \hat{H} + i\,[\hat{S}, \hat{H}] + \cdots \tag{73}$$

with the condition

$$i\,[\hat{S}, \hat{T}_H + \hat{T}_D + \hat{H}_1] = -\hat{T}_{mix} \tag{74}$$

In the case of no doubly occupied sites one finds,

$$\hat{H}_{eff} = \hat{T}_H + i\,[\hat{S}, \hat{T}_{mix}] \tag{75a}$$

$$= \hat{T}_H + \frac{4t^2}{U} \sum_{\langle ij \rangle} \left(\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} \right) \tag{75b}$$

where all terms of order t^3/U^2, $\delta \cdot t^2/U$, $\delta^2 t$ have been neglected and the μ-th component of the spin vector $\vec{S}_i$ at site i is defined as

$$(\vec{S}_i)_\mu \equiv \hat{c}_i^\dagger \vec{\sigma}_\mu \hat{c}_i \tag{76}$$

Here

$$\hat{c}_i^\dagger \equiv \begin{pmatrix} \hat{c}_{i\uparrow}^\dagger \\ \hat{c}_{i\downarrow}^\dagger \end{pmatrix} \tag{77a}$$

and

$$\vec{\sigma} = \frac{1}{2}\vec{\tau} \tag{77b}$$

is given in terms of the Pauli matrices $\vec{\tau} = (\tau_x, \tau_y, \tau_z)$. For the exactly half-filled band $(\delta = 0)$ one has $\hat{T}_{\hat{H}}\big|_{\delta=0} = 0$ and hence

$$\hat{H}_{eff} = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j \tag{78}$$

up to a constant; here $J = 4t^2/U$. So the Hubbard Hamiltonian is seen to transform into that for the anti-ferromagnetic Heisenberg model with coupling $J = 4t^2/U$. This old [33] and wellknown result may be used to deduce the next and next-next neighbor spin-correlation function

for the Hubbard model in the limit n = 1, $U \to \infty$ from the results for the anti-ferromagnetic Heisenberg chain [34,35]. If terms of order $8t^2/U$ are included, $\hat{H}_{eff}$ reads [36]

$$\hat{H}_{eff} = \hat{T}_H + \frac{4t^2}{U} \sum_{\langle ij \rangle} \left[\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} \hat{n}_i \hat{n}_j \right] + \hat{H}^{(3)}_{eff} \tag{79}$$

where $\hat{n}_i = \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}$ and

$$\hat{H}^{(3)}_{eff} = \sum_i \sum_{j \neq j'} \sum_\sigma \left[\hat{c}^\dagger_{i+j,\sigma} \hat{n}_{i,-\sigma} \hat{c}_{i+j',\sigma} + \hat{c}^\dagger_{i+j,-\sigma} \hat{c}^\dagger_{i,\sigma} \hat{c}_{i,-\sigma} \hat{c}_{i+j',\sigma} \right] \tag{80}$$

(with j, j' as next neighbor sites to i) describes 3-site processes, in addition to the 2-site contributions from $\sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$.

The effective Hamiltonians (75b), (79) are particularly suited for systematic, controlled numerical investigations in the large-U limit of the Hubbard Hamiltonian [32,26,37]. This is best done in terms of variational wave functions, such as the original Gutzwiller wave function $|\psi_G\rangle$ (II 107) [32] or improvements [37] of $|\psi_G\rangle$, where as a starting wave function the anti-ferromagnetic Hartree-Fock wave function $|\psi_{AF}\rangle$, (II 93), is used. Another such wave function will be discussed below.

A somewhat different kind of approach to the Hubbard Hamiltonian for U/t >>1 is that of introducing auxiliary

Bose fields (which are supposed to keep track of the single occupancy of lattice sites) and then treating the rewritten Hamiltonian in a mean field approximation as in the BCS-case [31,38].

The Resonating-Valence-Band (RVB)-State

The RVB-state [30] was suggested by Anderson [39] in 1973 as a possible ground state of the antiferromagnetic spin-$\frac{1}{2}$ Heisenberg Hamiltonian, (78), when applied to a two-dimensional, triangular lattice. On a triangular lattice anti-ferromagnetic coupling necessarily leads to frustration and hence a Néel-type state cannot be formed. In essence, the RVB state consists of a "liquid" of nearest neighbor singlet pairs which are allowed to move (i.e. "fluctuate", "resonate") as shown in Fig. 10.

Fig. 10

All sites are occupied and hence the RVB-state is an insulating state.

The RVB-state is expected to be a possible ground-state not only for the 2-dimensional triangular lattice but also for a square lattice if, for example, a suitable next-nearest neighbor interaction leads to frustration.

That a superposition of singlet pairs $\frac{1}{\sqrt{2}}|\uparrow\downarrow-\downarrow\uparrow\rangle$ leads to a better ground state energy for (78) than a pure Néel-state(and hence is closer in nature to the exact Bethe-solution [34]), was already realized by Hulthen [34]. Indeed, while the latter leads to an energy

$$E_{Néel} = N \times \left(-\frac{1}{4}J\right) = -\frac{1}{4}NJ \tag{81a}$$

where N is the number of particles, the former yields

$$E_{sing} = \frac{N}{2} \times \left(-\frac{3}{4}J\right) = -\frac{3}{8}NJ \tag{81b}$$

since for a singlet

$$0 = \vec{S}^2 = (\vec{S}_1 + \vec{S}_2)^2 = 2 \times \frac{3}{4} + 2\,\vec{S}_1 \cdot \vec{S}_2 \tag{82}$$

and hence $\vec{S}_1 \cdot \vec{S}_2 = -\frac{3}{4}$.

More precisely, the RVB state is determined by singlets

$$\hat{b}^{+}_{ij} = \frac{1}{\sqrt{2}} \left(\hat{c}^{+}_{i\uparrow} \hat{c}^{+}_{j\downarrow} - \hat{c}^{+}_{i\downarrow} \hat{c}^{+}_{j\uparrow} \right) \tag{83a}$$

which are superimposed

$$\hat{b}^{+} = \frac{1}{\sqrt{N}} \sum_{\langle ij \rangle} \hat{b}^{+}_{ij} \tag{83b}$$

However, if $\hat{b}^{+}$ is now applied to the vacuum state N/2 times to build up an N-particle state, many doubly occupied sites will be created which are energetically unfavorable and hence have to be projected out by the Gutzwiller projection operator

$$\hat{P}_{D} = \lim_{\langle \hat{D} \rangle \to 0} g^{\hat{D}} = \prod_{i} \left[1 - \hat{D}_{i} \right] \tag{84}$$

So the RVB -state has the form

$$|\psi_{RVB}\rangle = \hat{P}_{D} \left(\hat{b}^{+} \right)^{N/2} |0\rangle \tag{85}$$

In Fourier representation

$$\hat{b}^{+} = \sum_{\vec{k}} a(\vec{k}) \, \hat{c}^{+}_{\vec{k}\uparrow} \hat{c}^{+}_{-\vec{k}\downarrow} \tag{86a}$$

where for a simple cubic lattice

$$a(\vec{k}) = 2 \sum_{j} \cos k_{j} \tag{86b}$$

Clearly, $|\psi_{RVB}\rangle$ is a special form of the BCS-wave function (12), namely that with N/2 pairs

$$|\psi_{RVB}\rangle = \hat{P}_{\hat{S}}\, \hat{P}_{N/2} \prod_{\vec{k}} \left[u_k + v_k\, \hat{c}^{\dagger}_{k\uparrow}\, \hat{c}^{\dagger}_{-k\downarrow} \right] |0\rangle \tag{87}$$

where $a(\vec{k}) = v_{\vec{k}} / u_{\vec{k}}$ and $\hat{P}_{N/2}$ projects on the subspace with N/2 pairs. The spin-singlets may be viewed as "pre-existing Cooper-pairs" [30,38].

To allow for superconductivity in this half-filled, insulating state of pre-existing Cooper pairs, it is essential to introduce holes into the lattice (e.g. by doping) which will make the system a metal.

To test this picture one may apply mean field theories to $\hat{H}_{eff}$, (79), as done in refs. 31,38, or use $|\psi_{RVB}\rangle$, (85), (86), by parametrizing $a(\vec{k})$ so that $|\psi_{RVB}\rangle$ has a particular symmetry. For example, one may use [36] a "BCS-type" form

$$a(\vec{k}) = \frac{\Delta(\vec{k})}{\xi_{\vec{k}} + \sqrt{\xi_{\vec{k}}^2 + \Delta^2(\vec{k})}} \tag{88}$$

with $\xi_{\vec{k}} = \epsilon_{\vec{k}} - \mu$ and where $\Delta(\vec{k})$ is <u>variational</u> parameter, which may be chosen as

$$\Delta(\vec{k}) = \Delta \qquad \text{("s-wave")} \tag{89a}$$

$$= \Delta\left(\cos k_x a - \cos k_y a\right) \qquad \text{("d-wave")} \tag{89b}$$

$$= \Delta \left(\cos k_x a + \cos k_y a \right) - \mu \qquad \text{("extended s-wave")} \qquad (89c)$$

Note, that for a half-filled band (δ = 0) the form (89c), where $\Delta(\vec{k}) \propto \xi_{\vec{k}}$, is equivalent to the original Gutzwiller wave function (II, 107). It is found [36] that for δ = 0 the d-wave RVB-state and the anti-ferromagnetically ordered state have about the same energy. However, for $\delta \simeq 0.1$ d-wave superconductivity is favored.

These findings about a possible mechanism of high-T_C superconductivity, just as all the others (and there are <u>many!</u>) can only be viewed as preliminary. In fact, there are still more open questions than answers. But, after all, this keeps things exciting ...

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