Crossover from BCS superconductivity to BEC of pairs: The role of the lifetime of the pairs.

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The understanding of an electron gas with short coherence length pairs formed by an attractive interaction is believed to be one of the major keys to our theoretical knowledge of the high-\(T_c\)-superconductors. Mainly the deviations of the cuprates from usual metallic Fermi liquid behaviour already in the normal state like e.g. a linear resistivity or the observation of a pseudo gap can result from electron–electron correlations.

We therefore investigate the negative U Hubbard model in two dimensions at low densities using the T-matrix approximation. In the non selfconsistent formulation of the theory the system always shows an instability towards Bose condensation of pairs into an infinite lifetime two–particle bound state. If the calculations are performed selfconsistently pair–pair scattering is included which causes the pairs to have finite lifetime. The physics of these finite lifetime pairs is discussed.

Keywords: negative-U Hubbard model, two-particle bound states, pseudogap, non Fermi-liquid properties

I. INTRODUCTION:

More than a decade ago the high-\(T_c\) superconductors have been discovered. Even if many features of these materials like e.g. the mainly two dimensional transport in the hole doped CuO\(_2\) planes are understood the microscopic mechanisms and models which lead to a wider understanding still need to be investigated.

Already in the normal state above \(T_c\) there are two important issues which need to be explained. The first one (I) is the linear resistivity. In a normal metal the low-temperature dependence of the resistivity is governed by either impurity scattering which gives a constant term or by a Bloch-phonon contribution (\(\sim T^2\)) or in very clean Fermi liquids by the Landau electron–electron scattering of electrons at the Fermi surface (\(\sim T^4\)). Only at high temperatures above the Debye temperature which is of the order of 300-400 K normal metals show a linear resistivity due to phonon contributions.

In the high-\(T_c\)'s however the optimal doped samples show a linear resistivity over the full temperature range, already well below the Debye temperature [1].

The second feature (II) in the normal state which needs to be explained is the occurrence of a pseudo gap. It has been found in many experiments (first in NMR [2]) and also with other methods e.g. tunneling experiments [3]. This pseudo gap is found in the underdoped materials where already at temperatures above the superconducting transition temperature \(T_c\) a gap opens at the Fermi surface.

Also in the superconducting state there is besides the high transition temperature another special feature of the cuprates. This is the short coherence length of the pairs. Usual weak coupling BCS superconductors have coherence lengths \(\xi\) of several hundred lattice constants (\(\sim 1000 \text{ Å}\)) which go together with high quasiparticle densities. Therefore many Cooper pairs (\(\sim 10^6\)) overlap and the two essential conditions for superconductivity, pairing and phase–coherence, occur simultaneously at the same temperature, the mean–field (BCS) \(T_c\).

In the high-\(T_c\) superconductors however the coherence length is very small (\(\xi \approx 10 \text{ Å}\)) of the order of only 3-4 lattice constants. Further the quasiparticle densities are very low since the materials are close to an antiferromagnetic insulator to metal transition. Therefore the pairs barely overlap and might even be treated as spatially well separated pairs. This is believed to be the reason [4] why pairing (opening of a pseudo gap?) and phase coherence (\(T_c\)) might occur at different temperatures.

All these features above motivate the study of a model system which allows to investigate the transition between usual BCS superconductivity to a situation were tightly bound pairs occur. The simplest model system which can describe this is the Hubbard model with an attractive interaction between the electrons.

II. MODEL:

The negative U Hubbard model is:

\[
H = t \sum_{<i,j>} c_i^\dagger c_j + U \sum_i n_i n_j
\]

where the kinetic energy is given by the transfer term \(t\) and the Hubbard attraction \(U\) is chosen to be negative. In the weak coupling case in three dimensions the Fourie
transform of eq. (4) describes just the starting Hamiltonian for the BCS theory.

In the zero density and strong coupling (atomic) limit ($n/U = 0$) the Hamiltonian is solved by local pairs of electrons whose energy is lowered by the attractive energy $U$. Such pairs of electrons can be considered as Bosons.

In the intermediate coupling regime ($|U| \approx$ bandwidth $W$) and for low densities $n$ short coherence length pairs which barely overlap can be described. This is the parameter regime we are interested in in the current work.

III. T-MATRIX:

An approximation which allows to access the low density regime and which also describes pair formation is the T-matrix approximation. It is often also called ladder-approximation or Brückner-Hartree-Fock theory. In this theory the infinite sum over all scattering events between two electrons enters in the vertex function $\tilde{\Gamma}$.

$$\tilde{\Gamma}(\mathbf{K}, i\Omega_n) = \frac{U}{1 - U \chi(\mathbf{K}, i\Omega_n)}$$

(2)

With $\mathbf{K}$ being the total momentum of a pair and $\Omega_n$ Bosonic Matsubara frequencies. The susceptibility $\chi(\mathbf{K}, i\Omega_n)$ is given by the product of two one-particle Green’s functions $G(\mathbf{k}, i\omega_m)$.

$$\chi(\mathbf{K}, i\Omega_n) = \frac{-1}{N \beta} \sum_{m, \mathbf{k}} G(\mathbf{K} - \mathbf{k}, i\Omega_n - i\omega_m)G(\mathbf{k}, i\omega_m)$$

(3)

Spin indices are left out since only singlet pairs can be formed with an on-site attraction.

A. Thouless-criterion:

The physics which is described with the T-matrix approximation depends crucially on the appearance of a two particle bound state which is given by a zero of the denominator of eq. (2) reaches the chemical potential first at $\mathbf{K} = 0$ and is called the Thouless instability $\chi$.

$$\chi(\mathbf{K} = 0, i\Omega_n) = \frac{1}{U}$$

(4)

Here we have to distinguish between two different cases: In the first one (I) the chemical potential is in the one particle continuum. One has a Fermi surface. This happens in the weak coupling 3D case when a BCS instability is formed at the Fermi surface. The Thouless instability occurs when the system is cooled down towards $T_c$. Eq. (3) is (if $\chi = \chi^0$ is build up from noninteracting one-particle Green’s functions $G^0$) identical to the equation which determines $T_c$ in the BCS theory.

In the second case (II) the chemical potential is below the one-particle continuum. When considering $\chi^0$ this can always lead to a bound state at $\mathbf{K} = 0$ in 1D and 2D. In 3D this condition only leads to a bound state below the one-particle continuum if $|U| > U_{crit}$. Such a bound state can be populated by pairs of electrons which obey Bose statistics and therefore Bose condensation can occur. A Fermi surface will be lost at low temperatures. The $\mathbf{K}$-dispersion of such a bound state is shown in fig. (a).

B. The selfenergy:

The vertex function can now be used to build up a full Green’s function and different degrees of selfconsistency are possible. In this work we only want to focus on two ways to close the equations.

1. Non selfconsistent calculation

The first one is the non-selfconsistent calculation (see fig. (b)):

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FIG. 1. Diagram for the single-particle Green’s function (solid line) in the non self-consistent approximation. The thin solid lines represent the non-interacting Green’s function, the thick lines fully interacting Green’s functions and the wavy lines represent the interaction $U$.

$$G(\mathbf{k}, i\omega_n) = (G^0(\mathbf{k}, i\omega_n))^{-1} - \Sigma^0(\mathbf{k}, i\omega_n))^{-1}$$

(5)

were the selfenergy $\Sigma^0(\mathbf{k}, i\omega_n)$ is build up from the vertex function:

$$\Sigma^0(\mathbf{k}, i\omega_n) = \frac{1}{N \beta} \sum_{m, \mathbf{q}} \Gamma^0(\mathbf{k} + \mathbf{q}, i\omega_m + i\omega_n)G^0(\mathbf{q}, i\omega_m)$$

(6)

The system now consists of pairs of electrons which can only thermally be excited and can at finite temperatures be described as a mixture of Bosons (pairs) and Fermions. At zero temperature Bose condensation of the pairs into the two-particle bound state always occurs. This has been shown by Schmitt-Rink et al. [5] was a version of the T-matrix theory was applied which was not even conserving on a one-particle level.
2. selfconsistent calculation

The second possibility we want to discuss here is the fully selfconsistent version of the T-matrix. Other degrees of selfconsistency have been discussed e.g. by Janko et al. [7]. Why we concentrate our discussion on the fully selfconsistent T-matrix calculation will be investigated elsewhere [8].

\[ G(k, i\omega_n) = \left( G^0(k, i\omega_n) - \Sigma(k, i\omega_n) \right)^{-1} \]  

\[ \Sigma(k, i\omega_n) = \frac{1}{N\beta} \sum_{m,q} \Gamma(k + q, i\omega_m + i\omega_n)G(q, i\omega_m) \]  

In the zero density limit \( \langle n/U = 0 \rangle \) eqs. (5) and (7) are identical. However at finite densities a different physical scenario is now included in eq. (6). In this way the pairs can already at zero temperature have finite lifetime, they therefore deviate from Bose statistics and therefore the Bose condensation is strongly hindered (see fig. 3).

\[ \Gamma(K, i\Omega_n) = \hat{\Gamma}(K, i\Omega_n) - U = \frac{U^2 \chi(K, i\Omega_n)}{1 - U \chi(K, i\Omega_n)} \]  

We approximate the functions \( G(k, i\omega_n), \chi(K, i\Omega_n), \Gamma(K, i\Omega_n) \) and \( \Sigma(k, i\omega_n) \) by a series of delta functions along the real axis e.g.:

\[ G(k, i\omega_n) = \sum_j a_j^k \delta(i\omega_n - b_j) \]  

In order to solve the system of selfconsistency equations we use a spectral representation for all correlation functions. The vertex function is turned into an analytic function \( \Gamma(K, i\Omega_n) \) by subtracting the Hubbard energy \( U \) which is identical to subtracting the Hartree term from the self energy.
is achieved. The details of the method, especially how to choose the frequency points $b_j$ are explained in appendix A.

IV. RESULTS

We have solved the equations on a 2D system, a finite lattice with periodic boundary conditions. The results we present in the following were obtained on a 12x12 lattice. The attractive interaction was chosen to be equal to the bandwidth $U = -8t$. At finite densities we find completely different physics if we compare the selfconsistent and the non-selfconsistent calculations. In fig. 3 we have plotted the chemical potential as a function of temperature. Note that the Hartree term is still ignored. In the non–selfconsistent calculation the chemical potential always ends up in the two–particle bound state, roughly $\mu = -\frac{1}{2}\sqrt{U^2 + \Delta^2}$ (with $\Delta$ the bandwidth) below the middle of the unperturbed band. If we solve the T-matrix self-consistently we get the chemical potential back into the one-particle continuum, we regain a Fermi–like surface but we never reach a superconducting instability. Note that the Thouless criterion in fig. 3 refers only to the superconducting instability of a non selfconsistent calculation. We further get quasiparticle peaks at $K = (\pi, \pi)$ in the one–particle density of states whereas the non–selfconsistent calculation shows (at low enough temperatures) a gap at the chemical potential which is often interpreted as the origin of the pseudo–gap. For a large temperature range we further find a linear dependence of the quasiparticle scattering rate with temperature which may explain the linear resistivity.

In the current work we want to focus on two–particle properties. In the non–selfconsistent version of the T-matrix a two–particle bound state is present. At $K = (\pi, \pi)$ it evolves into which is called the $\eta$-mode. This is shown in fig. 3 (a).

In order to answer the question how remnants of the two–particle bound state show up in the selfconsistent calculation we have plotted fig. 3 (b). In this figure we show that the only remnant of the bound state is a weakly dispersive, strongly lifetime broadened resonance in the two–particle correlation function directly above the chemical potential. It is remarkable that also when Boson–Fermion models are discussed the Bosonic energy level is mostly put directly above the chemical potential. Also the $\eta$–mode only partially survives the selfconsistent calculation. Even at $K = (\pi, \pi)$ the two–particle resonance is strongly lifetime broadened and lies now less than $U$ below the middle of the unperturbed band (here zero). At zero density however we regain the $\eta$–mode and the two solutions for the selfconsistent and non–selfconsistent calculation fall together.

FIG. 4. Schematic of the dispersion of the two-particle bound state below the non-interacting continuum of the susceptibility $\chi(K, \Omega)$ (shaded region) as it arises in a non selfconsistent formulation (a). At low enough temperatures the chemical potential ends always at the $K = 0$ two–particle bound state. Below (b) we have plotted the same picture as it arises from a selfconsistent calculation done for the density $n=0.4$, temperature $k_B T=0.16[t]$ and interaction $U = -8t$ on a 12x12 lattice. The two particle bound state is disappeared and only a strong weakly dispersive two–particle resonance directly above the chemical potential (dashed line) is present.
n=0 were the selfconsistent and the non–selfconsistent lifetime of the pairs increases until it reaches infinity at n=0 infinity were also the η-mode will be recovered. Although similar tendencies have been found earlier by other authors [12–14] we are able to work out many de-

lations strongly alters the physics which is described by this theory. Due to selfconsistency the pairs can interact with each other which causes them to have finite lifetime. These finite lifetime pairs can no longer Bose condensate and therefore Fermi-liquid-like properties are regained. These finite lifetime pairs can no longer Bose condensate and therefore Fermi-liquid-like properties are regained. This means the spectral representation of G(k, iωn) is approximated by a series of δ functions. In this work the frequencies b_j were kept fixed throughout the whole calculation (opposite to our previous work [15]). In order to access low temperatures and work with a finite number of frequencies we sampled the frequency points with a tanh function. In this way we make sure that at the chemical potential two frequency points are always closer to each other then k_BT.

On the example of the susceptibility we want to show how we can calculate the spectral representation of a product function from the one-particle Green’s functions:

\[ \chi(K, i\Omega_n) = -\frac{1}{N\beta} \sum_{m,k} G(K-k, i\Omega_n-i\omega_m)G(k, i\omega_m) \]

When inserting the spectral representation for G(k, iωn) we get:

\[ \chi(K, i\Omega_n) = -\sum_k \sum_{j,l} \frac{1}{\beta} \sum_m a_{j,K-k}^k a_{l,k}^k \frac{1}{i\Omega_n-b_j} \frac{1}{i\omega_m-b_l} \]

\[ = \sum_k \sum_{j,l} \frac{a_{j,K-k}^k a_{l,k}^k}{i\Omega_n-b_j-b_l} \left( \frac{1}{1+e^{-\beta b_j}} - \frac{1}{1+e^{-\beta b_l}} \right) \]

\[ = \frac{1}{2} \sum_k \sum_{j,l} \frac{a_{j,K-k}^k a_{l,k}^k}{i\Omega_n-b_j-b_l} \left( \tanh \left( \frac{\beta b_j}{2} \right) + \tanh \left( \frac{\beta b_l}{2} \right) \right) \]

VI. ACKNOWLEDGEMENT

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APPENDIX A: SELFCONSISTENT PROCEDURE

In order to solve the selfconsistent equations we apply a method which enables us to work entirely along the real frequency axis. We do an Ansatz for the correlation functions (here e.g. G(K, iωn)) of the following form:

\[ G(k, i\omega_n) = \sum_j \frac{\delta_{ij}}{i\omega_n-b_j} \]

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FIG. 5. Lifetime of the pair for the selfconsistent calculation above with the same parameters as in figs. 3 and 4. We have compared two different densities. With decreasing density the lifetime of the pairs strongly increases until it reaches infinity at n=0 infinity were also the η-mode will be recovered.

To quantify how strongly the pairs are lifetime-broadened we have plotted in fig. 3 the dispersion of the pair lifetime which is at a first approximation given by:

\[ \tau = \frac{1}{U^2} \chi''(\Omega_0) \]

were \( \Omega_0 \) is the frequency at which the two–particle resonance occurs. The positions of the poles and the imaginary part of the susceptibility at that points were extracted from our numerical results. At K = (0, 0) the pairs live longest. With decreasing particle number the lifetime of the pairs increases until it reaches infinity at n=0 were the selfconsistent and the non-selfconsistent solutions fall together.

V. CONCLUSION

We have shown in this work that a selfconsistent inclusion of pair–pair scattering into the T-matrix calculation strongly alters the physics which is described by this theory. Due to selfconsistency the pairs can interact with each other which causes them to have finite lifetime. This finite lifetime pairs can no longer Bose condensate and therefore Fermi-liquid-like properties are regained. Although similar tendencies have been found earlier by other authors [12–14] we are able to work out many details and to reach very small temperatures. This is due to the fact that we use a semi-analytical method were all frequency integrations are done analytically and only the k-space summation has to be done numerically. Since we find the same results for finite lattices and for the continuum in infinite dimensions [15] we do not believe that our results in general are sensitive to finite size effects.

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We now have determined $\chi(K, i\Omega_n)$ on $N(N + 1)/2$ frequency points. These have to be sorted numerically and distributed onto the nearest frequency points $b_j$. In order to calculate $\Gamma(K, i\Omega_n)$ from $\chi(K, i\Omega_n)$ we have to apply a numerical broadening which must again be smallest at the chemical potential. In this way we get a complex function $\chi(K, i\Omega_n)$ from which we calculate the complex function $\Gamma(K, i\Omega_n)$. From the imaginary part of $\Gamma(K, i\Omega_n)$ we calculate the amplitudes for the spectral representation for $\Gamma(K, i\Omega_n)$. Finally we get:

$$\Gamma(K, i\Omega_n) = \sum_{j}^{N} \frac{g_j^K}{i\Omega_n - b_j}$$

(15)

A similar set of equations has to be solved for $\Sigma(k, i\omega_n)$ and $G(k, i\omega_n)$. In this way the selfconsistency is closed. We defined our solution to be selfconsistent if the mean–square deviation of all the amplitudes $a_k^b$ between two consecutive selfconsistency steps was below a certain threshold.

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