Self-consistent T-matrix approximation to the negative-U Hubbard model: numerical results

1992 J. Phys.: Condens. Matter 4 8565

(http://iopscience.iop.org/0953-8984/4/44/017)

J. Phys.: Condens. Matter 4 (1992) 8565–8572. Printed in the UK

Self-consistent T-matrix approximation to the negative-U Hubbard model: numerical results

R Frésard, B Glaser† and P Wölfle

Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, Physikhochhaus, 7500 Karlsruhe, Federal Republic of Germany

Received 2 July 1992

Abstract. We consider the negative-U Hubbard model on a square lattice in the self-consistent T-matrix approximation. We investigate the influence of the Fermi sea on the bound states which always occur in two spatial dimensions in the presence of an attractive interaction. As long as the binding energy is smaller than the Fermi energy, these bound states are found to be broadened sufficiently that Fermi liquid behaviour is restored. Only in the limit of large binding energy does one expect coexisting stable Bose pairs and dissociated fermions leading to a breakdown of Fermi liquid theory.

1. Introduction

Recently it has been suggested that the normal state of high-T_c superconductors may not be a Landau Fermi liquid [1, 2]. The theoretical arguments given in favour of non-Fermi liquid behaviour are based on an effective one-band Hubbard Hamiltonian for electrons on a two-dimensional square lattice [1, 3]. Little is still known about the properties of this model for strong repulsion near half-filling, despite intense efforts. Chances might be better for obtaining results in the low-density regime. There one expects to have a small parameter, the ratio of scattering length to the average interparticle distance, which should allow one to identify the important processes and to collect the corresponding contributions in renormalized perturbation theory [4].

Degenerate two-dimensional Fermi systems have been studied by several authors [5, 6, 7], the result found being that although the relaxation rate for quasiparticle scattering is enhanced by a factor depending logarithmically on energy, $1/\tau \sim \omega^2 \ln|\omega|$, Fermi liquid behaviour is not destroyed. More recently, there have been suggestions that the appearance of bound states for attractive interaction may lead to a kind of Bose condensation of bound pairs of electrons, coexisting with dissociated pairs, i.e. single unpaired electrons, which would obviously lead to non-Fermi liquid behaviour [8]. This idea is based on the fact that in two dimensions an arbitrarily weak attraction between electrons leads to the formation of a bound state, in contrast to the case of three dimensions. The open question is, however, under which circumstances and to what extent these bound pairs are broken up in the many-body system by the interaction between pairs and with single electrons. In the limit that the binding

† Present address: Debis Systemhaus, Maintenance Services GmbH, D-7022 Leinfelden-Echterdinger, Federal Republic of Germany.

0953-8984/92/448565+08$07.50

energy, E_b, is much greater than the Fermi energy, E_F, it is reasonable to expect stable pairs, mixed with a negligibly small fraction of dissociated electrons. In the opposite limit, however, which is the case of interest here, it is not at all clear whether bound pairs can exist for any length of time exceeding, e.g. the quasiparticle relaxation time. On the contrary, it is to be expected that interactions of the bound pairs with the medium will broaden the bound-state energy level to the extent that it will merge with the continuum. The instability of the Fermi sea with respect to condensation of pairs into a bound state split off from the lower edge of the pair continuum, hypothesized by Schmitt-Rink *et al* [8], would be absent in this case.

The formation of Cooper pairs and the crossover to tightly bound pairs as the pair binding is increased has been discussed for a continuum model in the low-density limit and within a variational scheme for all densities in [10, 9]. For repulsive interaction the structure of the two-particle vertex was investigated in the low-density limit and a pole was discovered, which, however, does not destroy the Fermi liquid properties. One should expect that an extrapolation of the results of [10, 9] into the crossover region will be subject to precisely the corrections calculated in the present work.

In order to study the question of the possible instability of the Fermi sea with respect to condensation of pairs we calculate the lifetime of the bound pairs in the simplest possible conserving approximation, the self-consistent T-matrix scheme.

2. Self-consistent T-matrix approximation

We consider the Hubbard model for electrons on a square lattice with attractive interaction U

$$H = \sum_{\boldsymbol{k},\sigma} \epsilon_{\boldsymbol{k}} c^{+}_{\boldsymbol{k},\sigma} c_{\boldsymbol{k},\sigma} + U \sum_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q}} c^{+}_{\boldsymbol{k}+\boldsymbol{q}\uparrow} c^{+}_{-\boldsymbol{k}\downarrow} c_{-\boldsymbol{k}'\downarrow} c_{\boldsymbol{k}'+\boldsymbol{q}\uparrow} \tag{1}$$

where $\epsilon_{\boldsymbol{k}} = -2t(\cos k_x + \cos k_y)$.

In the low-density limit, the dominating terms in the perturbation expansion in terms of the interaction U are those with the smallest number of closed fermion loops, i.e. the particle–particle ladder diagrams. The latter diagrams are summed up to give the T-matrix. In the case of only on-site interactions, as in the Hubbard model, the T-matrix is found as a geometric series

$$T(\boldsymbol{q}, \mathrm{i}\epsilon_n) = -U/[1 + U\chi(\boldsymbol{q}, \mathrm{i}\epsilon_n)] \tag{2}$$

where $\chi(\boldsymbol{q}, \mathrm{i}\epsilon_n)$ is the pair susceptibility

$$\chi(\boldsymbol{q}, \mathrm{i}\epsilon_n) = T \sum_{\boldsymbol{k},m} G(\boldsymbol{k}, \mathrm{i}\omega_m) G(\boldsymbol{q}-\boldsymbol{k}, \mathrm{i}\epsilon_n - \mathrm{i}\omega_m). \tag{3}$$

The single-particle Green's functions G are given in terms of the self-energy, Σ, as

$$G(\boldsymbol{k}, \mathrm{i}\omega_n) = 1/[\mathrm{i}\omega_n - \epsilon_{\boldsymbol{k}} + \mu - \Sigma(\boldsymbol{k}, \mathrm{i}\omega_n)]. \tag{4}$$

The self-energy expression

$$\Sigma(\boldsymbol{k}, \mathrm{i}\omega_n) = -T \sum_{\boldsymbol{q},m} T(\boldsymbol{q}, \mathrm{i}\epsilon_m) G(\boldsymbol{q}-\boldsymbol{k}, \mathrm{i}\epsilon_m - \mathrm{i}\omega_n) \tag{5}$$

closes the system of equations. The above approximation is conserving.

3. Results

We solve the system of equations (2)–(5) on a 21×21 lattice and for 500 Matsubara frequencies, and then perform the analytical continuation [11]. In the following we discuss the solution of these equations for $U/t = -2.5$, in which case the binding energy of a zero-momentum pair in the absence of the Fermi sea is $E_b/t = 0.65$. In figure 1, we show the imaginary part of the particle–particle T-matrix for $U/t = -2.5$, for several momenta and densities as a function of the energy. One can see how the bound state develops at the lower band edge of the spectrum when q is larger than $2k_F$ (i.e., $q = (3/5, 3/5)\pi$ and larger for $n = 0.32$ in figure 1(*a*), E_F/t being 1). This bound state is seen to be increasingly sharp as q approaches the zone boundary, as the available phase space for the scattering of bound pairs becomes more and more restricted. Nevertheless, the bound state does not split off the continuum spectrum, and the lifetime always remains finite as no gap opens in the two-particle excitation spectrum. This is in contrast to the non-self-consistent calculation, where a bound state appears separated from the continuum scattering states and is thus seen to be stable.

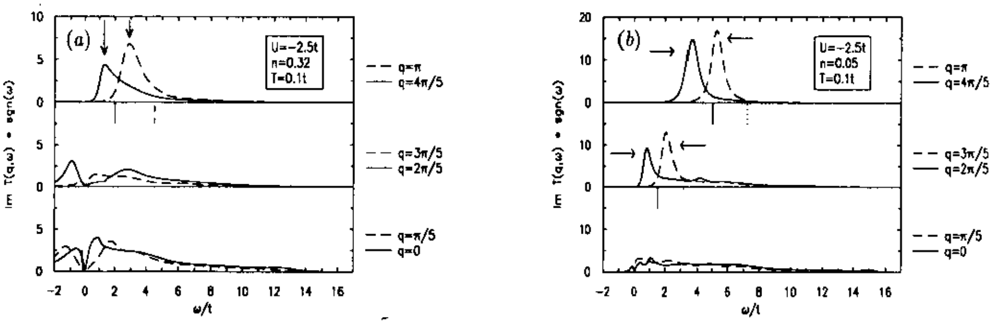

Figure 1. Imaginary part of the particle–particle T-matrix as a function of frequency for several momenta $k = (q, q)$ as labelled in the figure for $U/t = -2.5$, and $T/t = 0.1$ and $n = 0.32$, figure 1(*a*), and $n = 0.05$, figure 1(*b*). The vertical bars indicate the lower edge of the continuum of the scattering states. The arrow shows the position of the bound state.

For lower densities, for instance for $n = 0.05$ where $E_F = 0.15$ and $2k_F$ is very close to 0, the situation is qualitatively different, as shown in figure 1(*b*). Even though the bound state is still forming for $q > 2k_F$ and becomes sharper with increasing q, its location with respect to the continuum states is different. When q is large enough the bound state tends to separate from the continuum and its lifetime becomes much larger. This occurs because the binding energy of the pairs is much larger than the Fermi energy, and because the scattering of a single electron by a pair with large momentum is strongly reduced due to the statistical factors. Moreover, lowering temperature makes the bound state more stable.

In figure 2 we show the single-particle spectral function as a function of frequency for several values of the momentum along the diagonal of the Brillouin zone. For rather large density ($n = 0.32$, figure 2(*a*)), the effect of the interaction is accounted for by a broadening of the peaks and by the appearance of an incoherent background. Even though the particle–particle T-matrix exhibits quite a sharp structure, the influence of the latter on the physical properties is quite weak. Indeed, the low-frequency dependence of Im $\Sigma(k_F, \omega)$ shows that the system behaves as a Fermi liquid. This behaviour is expected to be very strongly affected by lowering the density down to values for which the bound state separates out of the continuum. As an intermediate situation, let us consider $n = 0.05$, figure 2(*b*), where, as a qualitative difference, a satellite band appears below the quasi-particle peak for large momenta. The latter results from the separation of the bound state from the continuum. It is caused by a pole at z in the complex frequency plane in the Green's function which is approaching the quasi-particle pole at z_{qp} as momentum is decreased as displayed in figure 3. For this particular choice of the parameters one gets Re $z <$ Re z_{qp} and Im $z <$ Im z_{qp} with both imaginary parts becoming of the same order of magnitude when the momentum tends to zero. For the latter case one is left with a peak in the spectral function resulting from a mixture of a quasi-particle with an unstable pair. When the lifetime of the pairs will be larger than the one of the quasi-particles, one will obtain a breakdown of the Fermi liquid picture. On lowering density, the latter is gradually replaced by a Bose gas picture showing a Bose–Einstein condensation only for $T \ll E_F \ll E_b$, where E_b is the binding energy. Otherwise, as long as the system does not show an instability either with respect to superconductivity or to charge-density wave, our results indicate that the Fermi liquid picture remains valid.

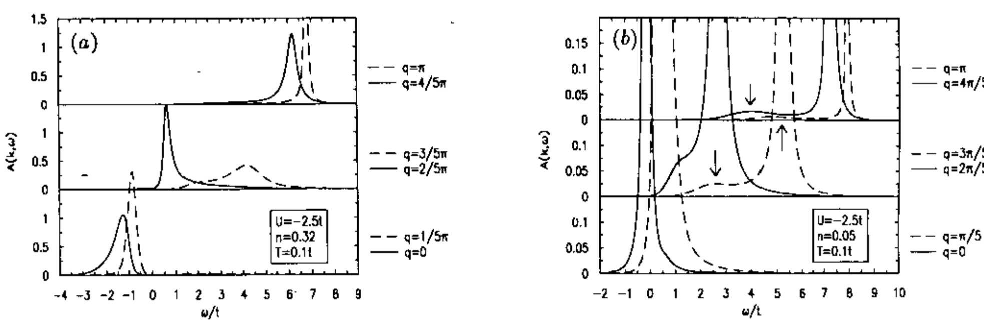

Figure 2. Imaginary part of the one-electron Green's function as a function of frequency for several momenta $\boldsymbol{k} = (q, q)$ as labelled in the figure for $U/t = -2.5$, $T/t = 0.1$ and (*a*) $n = 0.32$, (*b*) $n = 0.05$. The arrow indicates a satellite peak.

In figure 3 we display the most important poles of the single-particle Green's function at k_F in the complex frequency plane for two densities. The latter two are chosen such that one Fermi wave-vector matches one point of our discretization in $\boldsymbol{k}$-space. For both densities a quasi-particle builds up and its lifetime is longest as compared with all other 'particles'. On top of this quasi-particle pole, another pole resulting from the bound state in the particle–particle T-matrix is approaching the real frequency axis when the density decreases. As seen in figure 3, the location of the latter is very strongly density-dependent and it is obvious that its influence on the physical properties is very weak unless the density and the temperature are strongly reduced, in such a way that it will become closer to the real axis than the quasi-particle pole. Moreover the strength of this pole is very small, compared to that of the quasi-particle, and only an increase in the interaction leads to an increase in its strength.

In figure 4, we display the imaginary part of the self-energy on the Fermi surface as function of frequency for several temperatures and a rather large density ($n = 0.32$).

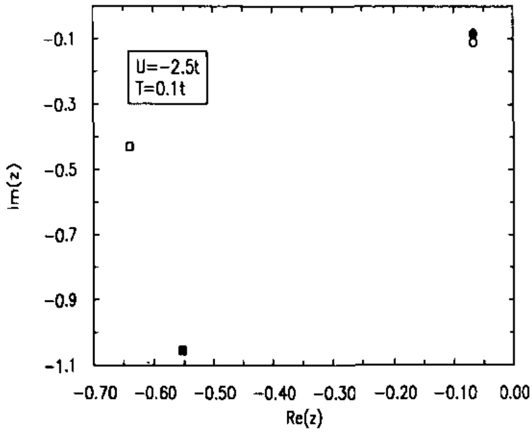

Figure 3. Poles of the one-particle Green's function at k_F in the complex frequency plane. Quasi-particle (bound particle) pole for: empty circle (square)—$n = 0.05$, full symbols—$n = 0.09$.

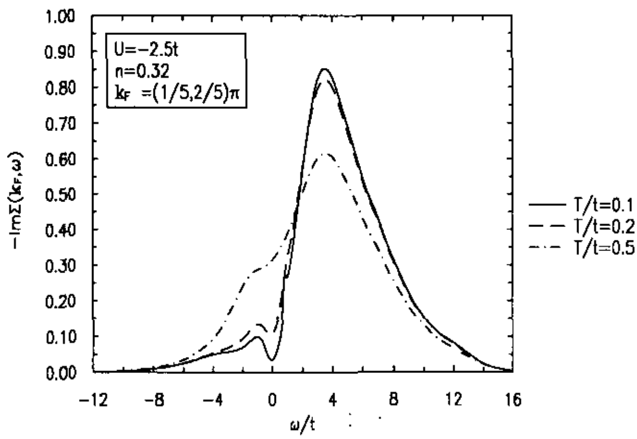

Figure 4. Imaginary part of the self-energy for a wavevector lying on the Fermi surface as function of frequency for several temperatures at $U/t = -2.5$.

For the highest temperature, $T/t = 0.5$, i.e. for a temperature which is close to the binding energy of the $q = 0$ pair which is 0.65, Im Σ only exhibits a very smooth structure in the vicinity of zero frequency. Even though the electrons can form bound pairs with a large total momentum, the system is clearly well described in a quasi-particle picture as there are no well-defined pairs in the Fermi sea. Lowering the temperature down to $T/t = 0.2$, and even down to 0.1, does not stabilize the pairs to the extent that their lifetime will be larger than that of the quasi-particle. We rather see how the Fermi liquid behaviour of $\mathrm{Im}\,\Sigma$ sets in as temperature decreases.

In figure 5, we plot density versus chemical potential for $U/t = -2.5$ as obtained from

$$n(T, \mu) = T \sum_{\boldsymbol{k},n,\sigma} G(\boldsymbol{k}, \mathrm{i}\omega_n). \tag{6}$$

Even at temperatures which are smaller than the binding energy, but larger than the superconducting T_c [12], the density is seen to be only very weakly affected at the lower band edge of the free system by the interaction, as displayed in the inset. The difference gradually sets in when chemical potential increases and the $n(\mu)$ relation is dominated by the Fermi statistics of the non-interacting limit corrected by the Hartree term (i.e. by replacing G by G_0 in (3) and (5) and evaluating (6) [13]) over a very wide range of densities. The self-consistent scheme clearly does not lead to dramatic changes.

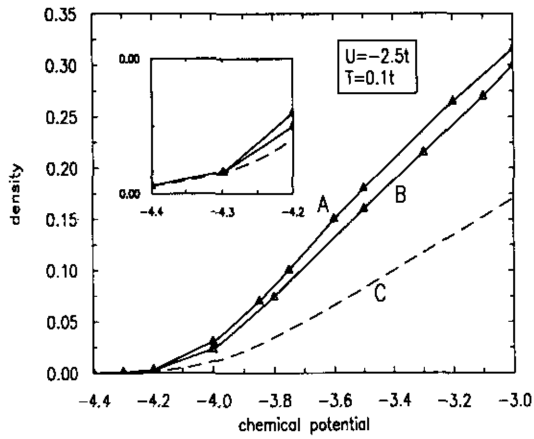

Figure 5. Density versus chemical potential for the self-consistent calculation (A) and the non-self-consistent one (B) for $U/t = -2.5$, and in the non-interacting limit (C) for $T/t = 0.1$.

In figure 6, we display the two-particle excitation spectrum for two different densities. It consists of two bands: (i) the two-particle band as obtained from the two-particle propagator and (ii), for $q > 2k_F$, the bound-state band. The two-particle propagator exhibits a pole, or more precisely several poles as discussed in detail in the continuum limit in [10], in the complex energy plane for any momentum. However, the lifetime of such a state is very short when it is lying at or in the vicinity of the Fermi sea. When the Fermi energy is larger than the binding energy, for instance $n = 0.18$, figure 6(*a*), the presence of the Fermi sea on the bound state is even stronger: it is allowed to exist only for $q > 2k_F$. Otherwise two electrons do not gain any energy in forming a pair having a total momentum smaller than $2k_F$. When $E_b \gg E_F$, figure 6(*b*), the bound states are seen to have a much larger lifetime and do exist for most of the k-states. Even though they are not totally separated from the scattering states, they are stable enough to create a satellite band, which we find in the spectral function. However, they are not stable enough to cause a Bose–Einstein condensation of the pairs. This is the situation which will prevail in most of the phase diagram for temperatures larger than T_c. In particular, we were able to determine the superconducting T_c by using Thouless's criterion [14] for several densities without encountering a Bose–Einstein condensation of the local pairs. The latter is thus restricted to very low densities and temperatures, which are out of the scope of current computer performances.

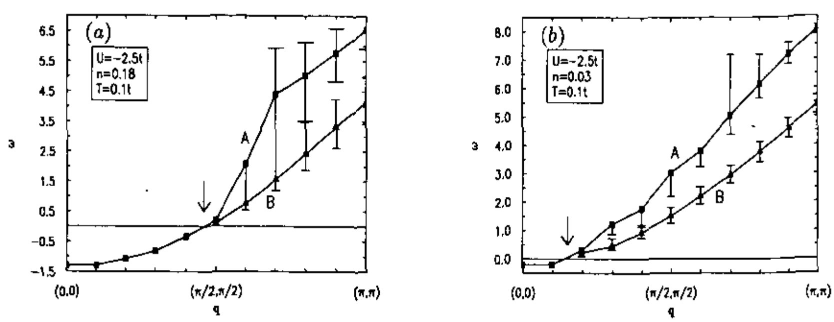

Figure 6. Two-particle excitation spectrum arising from the poles of the two-particle propagator, curve A, and the two-particle T-matrix, curve B. Error bars indicate the width at half-maximum as long as the peaks are well separated. The parameters are $U/t = -2.5$, $T/t = 0.1$ and (*a*) $n = 0.18$, (*b*) $n = 0.03$. The arrow indicates $q = 2k_F$.

In conclusion, we have investigated the negative-U Hubbard model on a square lattice in the framework of the self-consistent T-matrix approximation. Our results show that the presence of the Fermi sea prevents the bound states from having a strong influence on the physical properties, as long as the Fermi energy is larger than the binding energy in the $k = 0$ channel. The system consists of a mixture of bound pairs and unpaired electrons building up quasi-particles, whose lifetime is much larger than that of the pairs.

Acknowledgments

We thank Dr M Dzierzawa and Dr T Kopp for useful discussions. This work has been supported by the Fonds National Suisse de la Recherche Scientifique and by the Deutsche Forschungsgemeinschaft under SFB 195.

References

[1] Anderson P W 1988 *Frontiers and Borderlines in Many-Particle Physics (International Enrico Fermi School of Physics, Course CIV)* ed R A Broglia and J R Schrieffer (Amsterdam: North-Holland)

[2] Varma C M, Littlewood P B, Schmitt-Rink S, Abrahams E and Ruckenstein A E 1989 *Phys. Rev. Lett.* **63** 1996

[3] Anderson P W 1990 *Phys. Rev. Lett.* **64** 1839

[4] Galitskii V M 1958 *Zh. Eksp. Teor. Fiz.* **34** 151 (Engl. Transl. 1958 *Sov. Phys.-JETP* 7 104)

[5] Eagles D M 1969 *Phys. Rev.* **186** 456

[6] Hodges C, Smith H and Wilkins J W 1971 *Phys. Rev.* B **4** 302

[7] Bloom P 1975 *Phys. Rev.* B **12** 125

[8] Schmitt-Rink S, Varma C M and Ruckenstein A E 1989 *Phys. Rev. Lett.* **63** 445

[9] Randeria M, Duan J M, and Shieh L Y 1989 *Phys. Rev. Lett.* **62** 981
Engelbrecht J and Randeria M 1990 *Phys. Rev. Lett.* **65** 1032

[10] Fukuyama H, Hasegawa Y and Narikiyo O 1991 *J. Phys. Soc. Japan* **60** 2013
Narikiyo O 1991 Two-dimensional Hubbard model at low electron density *PhD Thesis* University of Tokyo

[11] Vidberg H J and Serene J W 1977 *J. Low. Temp. Phys.* **29** 179

[12] Scalettar R T, Loh E Y, Gubernatis J E, Moreo A, White S R, Scalapino D J, Sugar R L and Dagotto E 1989 *Phys. Rev. Lett.* **62** 1407

[13] Serene J W 1989 *Phys. Rev.* B **40** 10873
[14] Thouless D J 1960 *Ann. Phys., NY* **10** 5533