The electron gas with a strong pairing interaction: Three particle correlations and the Thouless instability

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We derive simplified Faddeev type equations for the three particle T-matrix which are valid in the Hubbard model where only electrons with opposite spins interact. Using the approximation of dynamical mean field theory these equations are partially solved numerically for the attractive Hubbard model. It is shown that the three particle T-matrix contains a term vanishing \( \sim T^2 \) at the Thouless (or BCS) instability where the two–particle T-matrix diverges. Based on the three particle term we further derive the low density – strong coupling extension for the two-particle vertex function. We therefore understand our equations as a step towards a systematic low density expansion from the weak coupling BCS theory towards the stronger coupling limit.

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I. INTRODUCTION

One of the key questions which remains in the understanding of the unusual superconductors, like the high-\( T_c \)-materials, some heavy Fermion compounds or organic superconductors is connected with the unusual short coherence length of the Cooper pairs. Even without having clarity on the microscopic pairing mechanism and on the evolution of a superconducting phase by e.g. doping an antiferromagnetic insulator with holes, this short ranged pair formation points towards an effective strong electron–electron interaction. It is therefore essential to get a deeper understanding especially of the thermodynamic properties and of finite temperature quantities of the electron gas with a strong attractive interaction.

From the theoretical understanding the electron gas with an attractive interaction has – besides the atomic one – only two well understood limits.

The first one is the weak coupling three dimensional (3D) case. In this case no two–particle bound state has the ability to empty the one–particle continuum and the BCS instability can occur for pairs with zero total momentum at the Fermi surface. BCS–superconductivity of weakly bound pairs with large coherence lengths occurs. These pairs simultaneously establish pair formation and phase coherence of the BCS wave-function.

The second limit which is well understood is the two–particle problem which gives the zero density limit. Solving the two–particle problem in one and two dimensions leads for any strength of the attractive interaction to the formation of a bound state. Since a pair of electrons can be regarded as a boson, the trapping of a pair in the bound state can be understood as a “\( T=0 \) condensation” of a boson into the bound state. Solving the two–particle problem in three and more dimensions leads to a clear criterion to distinguish between the weak and strong coupling limits. In 3D there exists a critical strength of the attractive interaction below which no bound state occurs. This marks the weak coupling regime where at finite densities the BCS instability will occur. Above the critical coupling strength the pair of electrons condenses into the bound state.

The simplest model Hamiltonian where the crossover from the weak coupling regime towards the stronger coupling limit can be investigated is the Hubbard model with a non retarded, attractive, on-site interaction, even though it only shows pairing in the s-wave channel. A more complicated correlation including next neighbor terms can be included later on where superconducting order parameters can occur which have non spherical symmetries. Before extending the Hamiltonian we want to understand the crossover for a simple on-site correlation.

An approach has been widely used to which we refer in agreement with many other authors as T-matrix approach. It accounts for both of the limits discussed above. It exactly solves the two electron problem in the center of mass system and therefore gets exact in any dimension and for any strength of the interaction at zero density. The non–self-consistent T-matrix in the 3D weak coupling case leads to the same equations to determine \( T_c \) as the BCS theory. The formation of a BCS wave-function can be understood as a macroscopic occupation of a bosonic bound state at the Fermi energy by non-interacting pairs. The BCS gap-parameter is then proportional to the density of pairs in the condensate wave function. The most problematic part in applying the T-matrix to finite densities and to the stronger coupling limit is that it neglects pair–pair interactions completely in the non–self-consistent formulation of the theory.

Overall, a self-consistent treatment of the two–particle T-matrix seems to compare well with quantum Monte Carlo results. However, certain features, like e.g. a pseudogap, are either not reported at all from a self-consistent treatment of the T-matrix or are not seen in the integrated density of states but only in the k-dependent spectral functions at extreme parameter ranges. Therefore, it is not too surprising that there is a discussion in the literature on which degree of self-consistency is the right one, which is also motivated by the correct emerging of a superconducting phase at low temperatures. Using any degree of self-consistency accounts in some way for pair–pair interactions. This is however...
occurring in a nonsystematic way, since a small parameter is missing.

In this work we want to tackle the question whether there is a systematic way of extending the T-matrix towards the stronger coupling and finite density regime while keeping the complete dynamics of the equations. As a first step towards this goal we investigate the three particle channel. In the three particle channel the three body problem is usually decomposed into two-body fragmentation channels, which define a set of Lippmann–Schwinger equations. In general, there are three possible two-body fragmentation channels, i.e. three ways of combining two out of three particles to interact via a two-body force, and a three body interaction. However, for the attractive Hubbard model, only two two-body fragmentation channels are left since electrons with identical spin do not interact and an explicit three body interaction is not present. Faddeev spin do not interact and an explicit three body interaction channels are left since electrons with identical spin do not interact and an explicit three body interaction is not present. Faddeev derived a set of coupled equations for the wave functions in momentum space, which include the known solution of the two–particle problem: the two–particle T-matrix. An equivalent formulation was obtained for the transition amplitudes in the three body scattering problem. In this work we follow the same spirit and calculate the three particle T-matrix as an infinite sum over all possible combinations of two–particle T-matrices. Since we are interested in a dynamic instability, we preserve the complete dynamics of the equations in contrast to earlier treatments found in the literature where one was mainly interested in ground state properties.

In order to be able to do an explicit calculation we use k-averaged quantities. Doing so, we arrive at equations which on one hand become exact in any dimension in the strong coupling limit since in the strong coupling limit all dispersion disappears. On the other hand our equations meet the dynamical mean–field theory, which gets exact at infinite dimensions for any coupling strength since the problem can be mapped in infinite dimensions onto a local impurity problem because all correlations become local. The two–particle T-matrix has been studied in the absence of k-dispersion and it has been shown that the essential physics of the Thouless instability remains intact. There is however one important difference between the limit of infinite dimensions and the strong coupling case. In infinite dimensions one clearly has to distinguish between zero momentum and momenta which are non zero. In the strong coupling limit the k-dispersion vanishes. Therefore it is not necessary to treat k=0 separately.

In the two–body problem the instability in the particle–particle channel is called ‘Thouless instability’. It is given by the equation

\[ 1 + U \chi(K = 0, \Omega = 0) = 0, \]  

(1)

where \( U \) is the attractive on-site interaction and \( \chi(K, \Omega) \) is the susceptibility in the particle–particle channel. We show in this paper that in the three particle channel the equivalent of this equation will be given by a determinant of a matrix which becomes zero at the formation of a three particle bound state. It has been discussed earlier that three particle terms should be included, although they only lead to logarithmic improvement in 2D with respect to a low density expansion. However, a systematic low density expansion should contain the three particle terms as a next step beyond the two–particle T-matrix. In the case of nuclear many body theory the \( \alpha \)-particle as a four particle bound state is of particular low energy and has been discussed by Röpke et al.

The paper is organized as follows: In section II we derive simplified equations for three particles valid in the Hubbard model where electrons with opposite spin do not interact. The three particles scatter in the vicinity of the Fermi surface. In section III we show how in a close analogy to an earlier work of Gorkov et al. the three particle terms can be used to derive a systematic low density –strong coupling extension for the two particle vertex of a pair of electrons with opposite spins. In section IV we apply a k-average and show that the equations reproduce the known results in the two–particle channel. We pay special attention to keeping the number of Matsubara frequencies small which are needed for the calculation. The analytical extensions to correct the sums over Matsubara frequencies are given in appendices. Having established a numerical solution of the two–particle problem which involves only a minimum of Matsubara frequencies, we are able to tackle the three particle instability in section V.

II. THREE PARTICLE INTERACTIONS

All information on the three particle problem is contained in a six–time correlation function

\[ \langle T_\tau [c_{i,\sigma}(\tau_1)c_{j,-\sigma}(\tau_2)c_{k,\sigma}(\tau_3)c_{k',-\sigma}(\tau_4)c_{j',\sigma}(\tau_5)c_{i',\sigma}(\tau_6)] \rangle. \]

(2)

Where the \( c_{i,\sigma}^\dagger, c_{i,\sigma} \) denote creation and annihilation operators of an electron with spin \( \sigma \) on the lattice site \( i \) at imaginary time \( \tau \), respectively. The brackets \( \langle \cdot \rangle \) denote the thermal average and \( T_\tau \) is the time ordering operator. In the first glance it seems to be hopeless to calculate such a correlation function. However time translational invariance in thermal equilibrium and spatial translational invariance on the lattice reduce the number of independent variables to five. Performing all calculations in frequency and momentum space will further allow via the Faddeev equations to solve as well in the ”input” as in the ”output” channel the occurring two–particle problem by integrating over the relative momentum and energy of a pair. We therefore arrive at functions for the three particle channel which depend on three dynamical variables only. It is convenient to chose the total energy and momentum of the triple as one of them.

As already mentioned in the introduction, the three particle terms can be built up by a repeated use of two–
The special simplification in the case of the attractive Hubbard model with only a non retarded, on-site attraction, \( U < 0 \), is given by the fact that first there is no direct three particle interaction and second that the correlation \( U \) is only effective between two charge carriers of different spin which are on the same lattice site. Therefore there is only one nontrivial three particle channel where two charge carriers carry a spin \( \sigma \) and the third one has opposite spin \( -\sigma \). In the following, we use a convenient short hand notation for the combination of summations over Matsubara frequencies and \( k \)-space summations.

\[
\frac{1}{\beta} \sum f(\omega_1) = \frac{1}{\beta} \sum_{n} \frac{1}{N} \sum_{k^1} f(i\omega_n^1, k^1)
\]

We use capital Greek letters for Bosonic and small ones for Fermionic Matsubara frequencies. Using this notation, the Green function of the unperturbed system reads

\[
G^{0\sigma}(\omega_1) = \frac{1}{i\omega_n^1 - \epsilon(k^1) + \mu}.
\]

where \( \mu \) is the chemical potential and \( \sigma \) refers to the spin index which is for our system of electrons (or holes) \( \pm 1/2 \).

The susceptibility in the particle–particle channel for a pair of electrons with opposite spin is

\[
\chi(\Omega_h) = \frac{1}{\beta} \sum f(\omega_1) G^{0\sigma}(\omega_1) G^{0\sigma}(\Omega_h - \omega_1)
\]

\[
= \frac{1}{\beta} \sum_n \frac{1}{N} \sum_{k^1} \frac{1}{i\omega_n^1 - \epsilon(k^1) + \mu} \times \frac{1}{\delta \Omega_{m}^h - i\omega_n^1 - \epsilon(K^h - k^1) + \mu}.
\]

The usual two–particle T-matrix results from an infinite geometrical series which results from solving the (in this case trivially solvable) Bethe–Salpeter equation.

\[
\Gamma(\Omega_h) = \frac{U}{1 + U \chi(\Omega_h)}
\]

This is a vertex function which adds all possible interactions in the particle–particle channel to the usual direct Hubbard interaction. It contains the full solution of the two particle problem in the center of mass coordinate system and therefore allows the formation of a two–particle bound state if the denominator \( 1 + \chi(\Omega_h) \) becomes zero. This is occurring first at the chemical potential \( (i\Omega_{n}^h = 0) \) and for zero total momentum of the pair \( K^h = 0 \) and defines the Thouless criterion for the superconducting instability. Note that we use a different notation for the sign of \( \chi(\Omega_h) \) then in a previous work which is now in agreement with the book of e.g. Schrieffer, but is different from the one used e.g. in Ref. 23.

For later use we define the functions

\[
\Gamma^{(i)}(\Omega_h) := \frac{(-U)^{i}}{1 + U \chi(\Omega_h)}.
\]

with \( l \in \{0, 1, 2\} \). Here \( \Gamma^{(0)}(\Omega_h) \) is a two–particle propagator and \( \Gamma^{(2)}(\Omega_h) \) is the above defined vertex \( \Gamma \) without the single interaction between the particles. The definition of the different \( \Gamma^{(i)}(\Omega_h) \) will be needed later on to be able e.g. to treat the contribution of the Hartree term separately.

Following the ideas of Faddeev, the three particle terms can be broken up into a two–particle problem plus an additional particle. Therefore, we define the following functions.

\[
F_1(\omega_1, \omega_2, \omega_3) := -G^{0\sigma}(\omega_1) G^{0\sigma}(\omega_2) \Gamma(\omega_2 + \omega_3)
\]

This function is illustrated in Fig. 3a. It contains all possible repeated correlations between particle (2) and (3) and contains the propagator for particle (1) which does not interact with any of the other two particles. \( F \) is already a part of a fully interacting six-time correlation function. However the time and spatial translational invariance together with solving the two particle problem in it’s center of mass system has in frequency and momentum space reduced the function to an expression which contains only three independent dynamical variables.

The second function which we define is:

\[
F_3(\omega_3, \omega_2', \omega_1) := -G^{0\sigma}(\omega_3') G^{0\sigma}(\omega_2') \Gamma(\omega_1 + \omega_2')
\]

This function is shown in Fig. 3b. The functions \( F_1 \) and \( F_3 \) represent the only possible two–body fragmentation channels which are present in the attractive Hubbard model. A repeated application of \( F_3 \) and \( F_1 \) turns the frequency \( \omega_2' \) into an internal frequency over which a summation has to be performed. A diagrammatic illustration of this term is shown in Fig. 3.

\[
\frac{1}{\beta} \sum_{2'} F_3(\omega_3, \omega_2', \omega_1) F_1(\omega_1, \omega_2, \omega_3') \delta_{\omega_2 + \omega_3', \omega_2'}
\]

The delta function stems from energy and momentum conservation for a pair. It is more convenient to introduce a new variable. This is the total energy (and momentum) of all three particles \( \omega_g = \omega_1 + \omega_2 + \omega_3 \) since it is a conserved quantity for the three particle scattering events. In this way we define

\[
M^{(1)}(\omega_g, \omega_3, \omega_3') := \frac{1}{\beta} \sum_{2'} F_3(\omega_3, \omega_2', \omega_g - \omega_2' - \omega_3') \times F_1(\omega_1, \omega_2 - \omega_3, \omega_3')
\]

Note that all the Pauli blocking factors which are of importance for the discussion of three body interactions in nuclear matter are included in the summation over Matsubara frequencies due to the analytic properties of thermal Green functions.
We can now successively construct all possible interactions among three particles by applying alternate scattering in the only possible two-body fragmentation channels by a repeated application of \( M^{(1)} \). For example applying \( M^{(1)} \) twice gives one additional internal frequency (and momentum) and therefore yields an additional summation.

\[
M^{(2)}(\omega_g, \omega_3, \omega_y) := \frac{1}{\beta} \sum_{\nu'} M^{(1)}(\omega_g, \omega_3, \omega_{3\nu'}) M^{(1)}(\omega_g, \omega_{3\nu'}, \omega_y) =: M^{(1)} \otimes M^{(1)}
\]

(12)

This defines a formal product for the alternate interaction. In appendix \( \text{A} \) we show that this formal product can also be written by introducing a metric. This product can be repeated several times:

\[
M^{(n)}(\omega_g, \omega_3, \omega_{3\nu}) = \frac{1}{\beta^{(n-1)}} \sum_{\nu''} M^{(1)}(\omega_g, \omega_3, \omega_{3\nu''}) \times M^{(1)}(\omega_g, \omega_{3\nu''}, \omega_{3\nu'}) \cdots M^{(1)}(\omega_g, \omega_{3\nu}, \omega_y) = M^{(1)} \otimes M^{(1)} \otimes \ldots \otimes M^{(1)}
\]

(13)

In the same spirit one can define a neutral element for the product defined in Eq. (\text{13}).

\[
M^{(n)} \otimes E = M^{(n)}
\]

(14)

which leads to:

\[
E = \beta \delta_{\omega_{3\nu}, \omega_{3\nu'}} = \beta \delta_{\omega_3(\nu), \omega_3(\nu')} N \delta_{k_{3\nu}, k_{3\nu'}}
\]

(15)

It can be seen immediately that the function \( E \) fulfills all properties of a neutral element with respect to the product defined in Eq. (\text{12}).

\[
M^{(n)} \otimes E = \frac{1}{\beta} \sum_{\nu''} M^{(n)}(\omega_g, \omega_3, \omega_{3\nu''}) \delta_{\omega_{3\nu''}, \omega_{3\nu'}} = M^{(n)}(\omega_g, \omega_3, \omega_y)
\]

(16)

We are now able to express all possible interactions which can occur between three particles in the attractive Hubbard model. This is given by the infinite sum over all the three body interaction terms \( M^{(n)} \). It yields a geometrical series which has to be calculated.

\[
M^{\text{tot}}(\omega_g, \omega_3, \omega_y) = \sum_{n=0}^{\infty} M^{(n)}(\omega_g, \omega_3, \omega_y) = \beta \delta_{\omega_3, \omega_y} + M^{(1)}(\omega_g, \omega_3, \omega_y) + \frac{1}{\beta} \sum_{\nu'} M^{(1)}(\omega_g, \omega_3, \omega_{3\nu'}) M^{(1)}(\omega_g, \omega_{3\nu'}, \omega_y) + \ldots
\]

(17)

which can be formally written as:

\[
M^{\text{tot}}(\omega_g, \omega_3, \omega_y) = \left[ \beta \delta_{\omega_3, \omega_y} - M^{(1)}(\omega_g, \omega_3, \omega_y) \right]^{-1}
\]

(18)

The inversion has to be such that

\[
M^{\text{tot}} \otimes \left[ E - M^{(1)} \right] = E.
\]

(19)

If on decreasing temperature the function \( E - M^{(1)} \) ceases to be invertible this defines an instability in the three particle channel. Such an instability marks the appearance of a three particle bound state. In section \( \text{V} \) we show that in dynamical mean–field theory, which means in the absence of \( k \)-dependence where \( \omega_h \rightarrow i\omega_h \), the condition for the instability can be expressed as

\[
\text{det}[E_{k\text{-aver}} - M^{(1)}(k_{k\text{-aver}})] = 0.
\]

(20)

This determinant has to be calculated for an infinite number of infinite dimensional arrays. However, restricting the number of Matsubara frequencies to a finite number allows to calculate the condition for an instability in the three particle channel. This is the three particle equivalent of the Thouless instability (\text{6}) which occurs for scattering of two particles. We like to mention that a general formulation for an arbitrary interaction has been given by Ethofer and Schuck and their equations in the p-p-p-channel contain the complete dynamics as our present work does. Due to the particular simple interaction of the Hubbard model, our equations obtain the much simpler form given in this article.

In nuclear physics it is often convenient to use simplified formulas for the three–particle T-matrix which depend only on one dynamical variable \( z \) instead of an expression which depends on three dynamical variables \( (\omega_g, \omega_3, \omega_y) \). The reason for this is that usually only the dependence on the center of mass \( (z \leftrightarrow \omega_g) \) is considered. Such equations are recovered when all internal initial times are set to zero when therefore all internal dynamics of the triple is neglected:

\[
M(\omega_g, k_3, k_y) = \lim_{n \to \infty} \sum_{\nu'} N \delta_{k_3(\nu'), k_y(\nu')} M(\omega_g, \omega_3, \omega_y)
\]

(21)

In section \( \text{IV} \) we restrict ourself to an approximation which, as we will show, preserves the main physics and mathematics of the two particle Thouless instability together with the complete dynamics of the equations. Afterwards, we are going to show how the physics is altered due to an inclusion of the three particle terms.

III. SYSTEMATIC LOW DENSITY – STRONG COUPLING EXTENSION OF THE TWO PARTICLE T-MATRIX

In this section we show how the three particle T-matrix can be incorporated to derive a low density strong coupling extension of the equations in the particle–particle...
channel which lead to the BCS instability. For a continuous system with a non retarded interaction it has been shown by Gorkov and Melik-Barkhudarov\cite{2} that a term which is first order in low density (\(\sim k_F a\)) can be used to obtain a low density correction for the two particle instability. The equations of\cite{2} contain however only a correction which is of second order perturbation theory in the interaction. The term which was considered in\cite{2} is illustrated in Fig. 3. In the Hubbard model this correction is exactly zero since a direct interaction between particles with the same spin is not present. To calculate the next low density correction for the attractive Hubbard model the first non trivial term is of third order in the interaction \(U\) (the term of second order will only lead to a Hartree shift). It is illustrated in Fig. 4.

\[
U^{0}_{\text{eff}}(\Omega, \mu, T) \chi(\Omega) = U \chi(\Omega) + \\
- \frac{U^3}{\beta^3} \sum_{2,3,4} G^0(\Omega - \omega_2)G^0(\omega_2)G^0(\omega_3)G^0(\Omega - \omega_2) \\
\Gamma(\omega_3 + \omega_2)G^0(\omega_2 + \omega_3 - \omega_4)G^0(\omega_4) \tag{22}
\]

The infinite sum over all the terms up to infinite order of the interaction \(U\) involves the three particle T-matrix \(M^{\text{tot}}(\omega_g, \omega_3, \omega_4)\) and is shown in Fig. 3. To obtain this we define the function:

\[
H(\Omega - \omega_3, \omega_3, \omega_4) = \frac{U}{\beta} \sum_{2} G^0(\omega_2)G^0(\Omega - \omega_2) \\
\Gamma(\omega_3 + \omega_2)G^0(\omega_2 + \omega_3 - \omega_4)G^0(\omega_4) \tag{23}
\]

which can be obtained by replacing one T-matrix in the derivation of Eq. (14) by the bare interaction \(U\). Therefore one can obtain the effective two particle interaction by calculating the product \(H \otimes M^{\text{tot}}\):

\[
U_{\text{eff}}(\Omega, \mu, T) \chi(\Omega) = U \chi(\Omega) + \\
+ \frac{2}{\beta} \sum_{\omega_3} \left[ H \otimes M^{\text{tot}} \right] (\Omega + \omega_3, \omega_3, \omega_3) \\
- \frac{2U^2}{\beta} \sum_{2} G^0(\Omega - \omega_2)G^0(\omega_2)G^0(\omega_2) \frac{1}{\beta} \sum_{3} G^0(\omega_3) \tag{24}
\]

where the last term is the term of second order which contains the Hartree term. It has to be subtracted in order to obtain a consistent inclusion of the Hartree term. The summation over \(\omega_3\) closes all the possible three particle terms with a hole line making Eq. (24) a low density strong coupling correction. The factor of 2 stems from the two possible realizations of the three particle correction which are \(\uparrow \downarrow \uparrow\) and \(\downarrow \uparrow \uparrow\) as combinations for the spins of the triple. The product is given as:

\[
\left[ H \otimes M^{\text{tot}} \right] (\omega_g, \omega_3, \omega_4) = \frac{1}{\beta} \sum_{4} H(\omega_g, \omega_3, \omega_4)M^{\text{tot}}(\omega_g, \omega_4, \omega_3) \tag{25}
\]

Equation (24) leads to the low density – strong coupling extension of the two particle instability when inserted into the Thouless criterion:

\[
1 + U_{\text{eff}}(\Omega = 0, T, \mu) \chi(\Omega = 0) = 0 \tag{26}
\]

The correction due to the three particle terms vanishes in the zero density limit. In the limit of vanishing density the summation over \(1/\beta \sum_{\omega_3}' \left[ H \otimes M^{\text{tot}} \right] \) gives zero and Eq. (26) gets identical with the instability of the two particle T-matrix. The correction due to the product \([H \otimes M^{\text{tot}}]\) vanishes also at high temperatures since all pair propagators go to zero at infinite temperature

\[
\lim_{\beta \rightarrow 0} \chi(\Omega) = 0 \tag{27}
\]

Eq. (26) gets further exact in the weak coupling regime where it reduces for all densities to the Thouless or BCS condition for a two particle instability since the lowest order correction to \(U\) is of third order in perturbation theory.

A numerical solution of Eq. (24) for the limit of vanishing \(k\)-dispersion is in progress and will be published elsewhere.\cite{3} It is also possible to solve Eq. (24) in a self-consistent way where selfconsistency has to be achieved for the function \(U_{\text{eff}}(\Omega, \mu, T)\). This might enlarge the applicability of Eq. (24) even beyond the low density regime. We further like to mention that the frequency and momentum dependence of \(U_{\text{eff}}(\Omega, \mu, T)\) in Eq. (24) does not lead to a retarded interaction since the variable \(\Omega\) refers to the total momentum and total energy of a pair who’s interaction is being treated.

\section{Solution of the Two–Particle Problem}

We need a reliable solution of the two particle problem, if we want to solve the three–particle problem since the two–particle T-matrix enters into the Faddeev equations. We will solve the three particle problem only in a \(k\)-averaged approximation, therefore we show in this section that (i) we are able to reproduce the known results of the two–particle T-matrix using a \(k\)-average and (ii) we demonstrate that we are able to solve this equations using a minimum of Matsubara frequencies which is the essential basis to calculate in Sec. 3 quantities for the three particle problem.

In the noninteracting limit \(U = 0\) the free \(k\)-averaged Green function is

\[
G^0(i\omega_n) = \int_{-\infty}^{\infty} \frac{D(\epsilon)}{i\omega_n - \epsilon + \mu} d\epsilon. \tag{28}
\]

\(D\) is the noninteracting global density of states. Since we are heading towards a systematic low-density expansion we are mainly interested in low band fillings. Therefore we approximate the density of states \(D\) by a rectangular shaped one, which shows the correct analytical behavior for a 2D system at the lower and upper band edge.

\[
D(\epsilon) = \frac{1}{W} [\Theta(\epsilon + W/2) - \Theta(\epsilon - W/2)] \tag{29}
\]
W is the bandwidth. This density of states results in
\[
G^0(i\omega_n) = \frac{1}{W} [\ln(i\omega_n + W/2 + \mu) - \ln(i\omega_n - W/2 + \mu)].
\] (30)

The k-averaged pair susceptibility can be calculated from the k-averaged Green functions.
\[
\chi(i\Omega_n) = \frac{1}{N} \sum_K \chi(K, i\Omega_n)
\]
\[
= \frac{1}{\beta N^2} \sum_{K, k, m} G^0(k, i\omega_m)G^0(K - k, i\Omega_n - i\omega_m)
\]
\[
= \frac{1}{\beta} \sum_m G^0(i\omega_m)G^0(i\Omega_n - i\omega_m)
\] (31)

The analytical correction for calculating \(\chi\) is shown in appendix B.2. We approximate the k-averaged vertex
\[
\Gamma(i\Omega_n) = \frac{U^2 \chi(i\Omega_n)}{1 + U \chi(i\Omega_n)}
\] (32)

\(\Gamma^{(2)}(i\Omega_n)\) is used (see Eq. (B3)) which contains the infinite sum of all possible interactions within the pair except the single interaction. The single interaction \(U\) only leads to a Hartree term when inserted into the selfenergy. The Hartree term shall be considered separately. The full interacting Green function is
\[
G(i\omega_n) = [G^0(i\omega_n)^{-1} - \Sigma^0(i\omega_n)]^{-1}
\] (33)

with the self-energy
\[
\Sigma^0(i\omega_n) = \frac{1}{\beta} \sum_{m=-\infty}^{\infty} \Gamma^{(2)}(i\omega_n + i\omega_m)G^0(i\omega_m).
\] (34)

1. Particle number \(n\)

Since we need the two particle terms in the three particle T-matrix we demonstrate in the following that we are able to obtain the main results of the two particle T-matrix calculation by applying the k-average. We put special emphasis on keeping the number of Matsubara frequencies small.

The expectation value of the particle number with a certain spin \(\sigma\) is calculated from the single particle Green function.
\[
\langle n_{\sigma}\rangle(\beta, \mu) = \lim_{\eta \to 0} \frac{1}{\beta} \sum_{l=-\infty}^{\infty} G(i\omega_l) e^{i\omega_l \eta}
\]
\[
= \frac{2}{\beta} \sum_{l=0}^{\infty} \text{Re} G(i\omega_l) + \frac{1}{2}
\] (35)

The total particle number \(n\) is the sum over the two spins.
\[
\langle n \rangle = 2\langle n_{\uparrow} \rangle + 2\langle n_{\downarrow} \rangle = 2\langle n_{\sigma} \rangle
\] (36)

To obtain Fig. VII we have solved Eqs. (30) - (34) non-self-consistently. We have plotted the lines of constant densities \(\langle n_{\sigma} \rangle = \langle n \rangle / 2\) in the plane of the thermodynamic parameters, the chemical potential without the Hartree contribution \(\tilde{\mu} = \mu - U \langle n \rangle / 2\) and the temperature \(T\). We were able to use only a maximum number of \(N_{\text{max}} = 60\) Matsubara frequencies by applying the analytical corrections which are shown in appendix B. Using these \(N_{\text{max}}\) Matsubara frequencies we reach temperatures which are as low as \(k_B T = 0.01 W / 2\). One has to assure that the range which is covered by the \(N_{\text{max}}\) Matsubara frequencies is larger than the bandwidth of the system
\[
2 (2N_{\text{max}} + 1) \pi > \frac{W}{\beta}
\] (37)

In this way less than one hour computer time on a Pen- tium II with 450 MHz was needed to obtain figure VII. All lines of constant density collapse into the bound state level on lowering the temperature. A result which has been first obtained by Schmitt-Rink et al. who used a non conserving approach. In our approach the particle number is conserved and reaches 1 at the Thouless instability.

2. Double occupancy

In this section the two particle correlation \(\langle n_{\uparrow} n_{\downarrow} \rangle\) is computed from the two particle propagator \(\Gamma^{(0)}\).
\[
\langle n_{\uparrow} n_{\downarrow} \rangle = \frac{1}{\beta} \sum_{m=-\infty}^{\infty} \Gamma^{(0)}(i\Omega_m)
\] (38)

In Fig. VII we have plotted lines of constant double occupancy \(\langle n_{\uparrow} n_{\downarrow} \rangle\) in the plane of the thermodynamical variables \(\tilde{\mu}, T\). We have chosen the values of \(\langle n_{\uparrow} n_{\downarrow} \rangle\) such that some match the square of \(\langle n \rangle / 2\) in Fig. VII. In the limit of high temperatures or of vanishing interaction \((U \to 0)\) all correlations disappear and \(\langle n_{\uparrow} n_{\downarrow} \rangle = (\langle n \rangle / 2)^2\) To be specific: At high temperatures the line with \(\langle n_{\uparrow} n_{\downarrow} \rangle = 0.04\) will join the line with \(\langle n \rangle = 0.4\) in Fig. VII and the one with \(\langle n_{\uparrow} n_{\downarrow} \rangle = 0.09\) will join the line with \(\langle n \rangle = 0.6\). On lowering the temperature however, correlations become important and \(\langle n_{\uparrow} n_{\downarrow} \rangle\) exceeds the value of \((\langle n \rangle / 2)^2\). Close to the Thouless instability \(\langle n_{\uparrow} n_{\downarrow} \rangle\) even diverges. A diverging value of \(\langle n_{\uparrow} n_{\downarrow} \rangle\) marks an unphysical behavior since a pair of particles cannot be more than completely correlated. Therefore \(\langle n_{\uparrow} n_{\downarrow} \rangle\) should not exceed the value of \(\langle n \rangle / 2\). The behavior in the non-self-consistent T-matrix calculation can be understood since summing over bosonic Matsubara frequencies in Eq. (32) occupies the bound state with a Bose distribution and \(\langle n_{\uparrow} n_{\downarrow} \rangle \to \infty\) marks the macroscopic occupation of the bosonic bound state with non-interacting pairs. A large part of this unphysical behavior is due to the neglect of pair-pair interactions in the
non–self-consistent T-matrix. Self-consistency seems to repair such a behavior but is uncontrolled since a small parameter is missing. In order to achieve a systematic expansion with finally the density as a small parameter we perform a numerical investigation of the three particle terms in the next section to answer the question, whether this unphysical divergence could be canceled by the sum of all three particle scattering processes which contribute to \( \langle n_f n_l \rangle \).

V. THREE PARTICLE CHANNEL

In the k-averaged approximation the three particle terms are obtained by replacing \( \omega_k \rightarrow i \omega_n^k \). Doing so, we obtain

\[
M^{\text{tot}}(i \omega_n^g, i \omega_m, i \omega_{m'}) = \left[ E - M^{(1)}(i \omega_n^g) \right]^{-1}_{m,m'}
\]

(39)

for the three particle ladder \( M^{\text{tot}} \). This means that in the k-averaged approximation \( M^{\text{tot}} \) can be obtained by inverting the right hand side of Eq. (39) and multiplying it with a prefactor of \( \beta^2 \). However, this is an infinite (due to \( \omega_n^g \)) number of inversions of infinite dimensional matrices which has to be performed. Our efforts described in the previous section IV and in appendix B enable us to reduce the number of Matsubara frequencies needed for such an inversion to such a low value that the inversion of Eq. (39) can be performed. In the present work we want to answer the question what is the behavior of the three particle terms at the two–particle instability.

In Fig. 8 we have plotted the logarithm of the determinant

\[
\det \left[ \beta \delta_{m,m'} - M^{(1)}(i \omega_n^g, i \omega_m, i \omega_{m'}) \right]
\]

(40)

for one chosen total Matsubara frequency \( i \omega_n^g = i \pi/\beta \), for an attractive interaction \( U = -2[W/2] \) at a chemical potential \( \tilde{\mu} = -0.5[W/2] \) for which \( T_c \) turns out to be \( T_c \approx 0.33301[W/2] \). On lowering the temperature the determinant diverges at the Thouless instability proportional to \( (T - T_c)^{-2} \). This is plotted in Fig. 8 for 60 and 120 as the maximum number of Matsubara frequencies. In contrast to this, the equivalent of the determinant in the particle–particle channel (see Eq. (11)) goes to zero linearly in \( (T - T_c) \) at the instability. This has two important consequences. The first one is that even with a direct inclusion of the three particle terms the double occupancy will still diverge at the Thouless instability, this is due to the fact that the double occupancy will be calculated as a sum of all two particle terms which diverge at the Thouless instability plus contributions from the three particle terms which vanish at the two–particle instability and have therefore no chance to cancel the diverging two–particle terms. The second consequence is therefore that a correct inclusion of the three particle terms has to go via a renormalization (possibly even in a selfconsistent way) of the two particle instability. The renormalization is caused by a third particle as derived in Eq. (24).

VI. CONCLUSION

In this article we present simplified equations for the three particle terms of the attractive Hubbard model. In particular the fact that in the Hubbard model electrons with identical spin do not interact directly with each other, enables us to simplify the equations considerably. Based on the three particle terms we derive in sec. 11 a low density strong coupling extension of the two particle vertex function (Eq. (24)). A third particle renormalizes the effective interaction in the two particle channel and therefore leads to a density and coupling strength dependent reduction of \( T_c \).

In order to solve some of the equations we derived, we applied a k-averaged approximation which becomes formally equivalent to the dynamical mean–field theory where all correlations become local. Using such a k-averaged approximation we are able to actually calculate three particle quantities with its complete dynamics. We investigate the three particle ladder, where the condition for the Thouless instability in the two–particle channel (see Eq. (6)) is now replaced by a determinant of a matrix. This determinant diverges proportional to \( (T - T_c)^{-2} \) as the Thouless instability is reached. In the near future it should be possible to extend the present calculations in three ways. First, the double occupancy as a function of the thermodynamic parameters including all three particle terms should be investigated. Calculating this quantity at low densities should answer the question which degree of self-consistency is the best one if the two–particle T-matrix is evaluated self-consistently. This question is currently discussed in the literature.1,2

Second, at temperatures below the Thouless instability one should continue the determinant (see Eq. (11)) to the real axis with respect to \( i \omega_n^g \) in order to obtain a condition for a three particle bound state which should arise as the determinant vanishes at the real axis. The most important extension is a numerical exploration of Eq. (24) in the space of the thermodynamic variables \( \mu \) and \( T \). This is currently under investigation.

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APPENDIX A: PRODUCT OF THREE PARTICLE INTERACTIONS INVOLVING A METRIC

The formal product defined in Eq. (12) can also be written by introducing a metric tensor

\[ g^{ij} = \beta \delta_{ij} = \beta \delta_{\omega_i, \omega_j} N \delta_{k_i, k_j} \]  

(A1)

where the last term reminds on the definition in Eq. (1). This leads to a co- and contravariant notation for the matrices using the Einstein sum convention.

\[ M^{(1)}(\omega_1, \omega_2, \omega_3) \rightarrow M_{\delta m} \]  

(A2)

The formal product then reads:

\[ M \otimes N = M_{\delta m} N_{\delta n}^\prime = M_{\delta m} \otimes N_{\delta n}^\prime \]  

(A3)

In the derivation presented in sec. II and III we did only use the notation defined in Eq. (12).

APPENDIX B: ANALYTICAL CORRECTIONS

The infinite sums over Matsubara frequencies cannot be evaluated numerically. \( N_{\text{max}} \) denotes the maximum number of Matsubara frequencies that we want to sum over numerically. To preserve the features of the infinite sums, the addends are approximated for large Matsubara frequencies by terms, which can be summed analytically for an infinite number of Matsubara frequencies.

1. The particle number

The real parts of the interacting Green functions in (28) are approximated by the noninteracting Green functions for large Matsubara frequencies (MFs). The noninteracting Green functions exhibit a \( 1/ (i \omega_n + \mu) \)-dependence for large MFs.

\[ G_0(i \omega_n) \quad \omega_n \rightarrow \infty \]  

\[ G_\delta(i \omega_n) \equiv \frac{1}{i \omega_n + \mu} \]  

(B1)

\[ n(\beta, \mu) \approx \frac{2}{\beta} \sum_{l=0}^{N_{\text{max}}} \text{Re} G(i \omega_l) + \frac{2}{\beta} \sum_{l=N_{\text{max}}+1}^{\infty} \text{Re} G_\delta(i \omega_l) + \frac{1}{2} \]  

(B2)

The 1/2 stems from the sum over the imaginary part where a sum over \( \sin(x)/x \) occurs.

2. The pair susceptibility

For the numerical calculation of the pair susceptibility, we look at the infinite sum (31). The two Green functions have to be approximated by \( G_\delta \) for values of \( i \omega_n \) which are far away from the real axis, e.g. for \( n > N_{\text{max}} \) and \( n < -N_{\text{max}} - 1 \).

\[ \chi_\delta(i \Omega_m) = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} G_\delta(i \omega_n) G_\delta(i \Omega_m - i \omega_n) \]  

\[ = \frac{\tanh \frac{\beta \mu}{2}}{i \Omega_m + 2 \mu} \]  

(B3)

\[ \Omega_m - \omega_n = \frac{2 m \pi}{\beta} - \frac{(2 n + 1) \pi}{\beta} = \frac{[2(m - n) - 1] \pi}{\beta} = \omega(m - n - 1) \]  

(B4)

where \( \omega(n) \approx \frac{2 N_{\text{max}}}{\beta} \). Therefore we replace the noninteracting Green functions in (31) by their definitions (28). This results in two integrations over \( \epsilon \) and \( \epsilon' \).

\[ \chi(i \Omega_m) \approx \frac{1}{\beta} \sum_{n=2 N_{\text{max}} - 1}^{2 N_{\text{max}}} \left[ G_h(i \omega_n) G_h(i \omega_{m-n-1}) - G_\delta(i \omega_n) G_\delta(i \Omega_m - i \omega_n) \right] + \chi_\delta(i \Omega_m) \]  

with

\[ G_h(i \omega_l) = \begin{cases} G_0(i \omega_l), & -N_{\text{max}} - 1 \leq l \leq N_{\text{max}} \\ G_\delta(i \omega_l), & \text{otherwise} \end{cases} \]  

(B5)

In subsequent chapters it will be necessary to approximate the pair susceptibility for large Bosonic MFs. Therefore we replace the noninteracting Green functions in (31) by their definitions (28). This results in two integrations over \( \epsilon \) and \( \epsilon' \).

\[ \chi(i \Omega_m) = \frac{1}{\beta W^2} \sum_{n=-\infty}^{\infty} \int \frac{d\epsilon}{W} \int \frac{d\epsilon'}{W} \frac{1}{i \omega_n - \epsilon + \mu} \times \frac{1}{i (\Omega_m - \omega_n) - \epsilon' + \mu} \]  

(B6)

If we interchange the two integrations with the summation over \( m \), carry out the summation, transform the integration coordinates to \( x = \epsilon + \epsilon' \) and \( y = \epsilon - \epsilon' \), we can integrate over \( y \) analytically. The resulting spectral representation of \( \chi \) can be approximated for large Matsubara frequencies by \( \chi_W \).

\[ \tilde{f}_W(\beta, \mu) = \frac{-1}{\beta W} \ln \frac{1 + \cosh[\beta(W/2 - \mu)]}{1 + \cosh[\beta(W/2 + \mu)]} \]  

(B7)

\[ \chi_W(i \Omega_m) = \frac{\tilde{f}_W}{i \Omega_m + 2 \mu} \]  

(B8)

Here \( \tilde{f}_W \) denotes the averaged spectral function for \( \chi \). The function \( \chi_W \) has been used to obtain the results shown in section V1 and V2.
3. The self-energy

Looking at the definition of the self-energy \( \Sigma \) we have to approximate the vertex \( \Gamma^{(2)} \). It can be approximated in first order of \( \frac{1}{\Omega_m} \) for large \( \Omega_m \) by \( U^2 \chi_W \). Hence we calculate the following infinite sum.

\[
\Sigma_W(i\omega_m) = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} U^2 \chi_W(i\omega_m + i\omega_n)G_\delta(i\omega_n)
= U^2 f_W(\beta, \mu) \left[ \frac{1}{i\omega_m + \mu} \right] \tag{B9}
\]

The analytically corrected sum over a finite number of MFs is a term of the form

\[
\Sigma(i\omega_m) \approx \frac{1}{\beta} \sum_{n=2N_{\text{max}}-2}^{2N_{\text{max}}} \left[ G^0(i\omega_n)\Gamma^{(2)}(i\omega_m + i\omega_n) - G_\delta(i\omega_m)U^2 \chi_W(i\omega_m + i\omega_n) \right] + \Sigma_W(i\omega_m) \tag{B10}
\]

It gives the expression of \( \Sigma(i\omega_m) \) which contains the numerically summed expression for the self-energy for Matsubara frequencies close to the real axis and contains the analytical correction for MFs far away from the real axis.

4. The double occupancy

The two particle propagator \( \Gamma^{(0)}(i\Omega_m) \) equals \( \chi_W(i\Omega_m) \) at large \( \Omega_m \). Therefore we utilize

\[
\frac{1}{\beta} \sum_{m=-\infty}^{\infty} \chi_W(i\Omega_m) = \frac{f_W(\beta, \mu)}{1 - e^{-\beta \mu}} \tag{B11}
\]

to correct the sum in Eq. (38) analytically.

5. Three particle ladder segment \( M^{(1)} \)

For the analytical correction of the sum in Eq. (10) again for the case of vanishing k-dispersion we look at the \( \omega_2 \) depending terms. Here the terms of the product in Eq. (10) which do not contain \( \omega_2 \) are not shown.

\[
\frac{1}{\beta} \sum_{n} G_\delta(i\omega_2 + i\omega_3 - i\omega_2') G_\delta(i\omega_2 - i\omega_2') \times G_\delta(i\omega_2') \left[ -U + U^2 \chi_W(i\omega_3 + i\omega_2') \right] \tag{B12}
\]

with

\[
\begin{align*}
    a_0 &= e^{\beta \mu} \\
    a &= e^{\beta \mu} + 1 \\
    b &= e^{\beta \mu} - 1 \\
    \bar{b} &= 3 \mu + i\omega_g \\
    b &= \mu + i\omega_3 \\
    b' &= \mu + i\omega_3 \\
    c &= 2 \mu - i\omega_3 + i\omega_g \\
    c' &= 2 \mu - i\omega_3 + i\omega_g \\
    d &= i\omega_3 + i\omega_3 \\
    o &= \omega_2^2 + \omega_3 \omega_3 - i\omega_3(d - 4\mu) - 4d\mu + 2\mu^2
\end{align*} \tag{B13}
\]

This allows to calculate the three particle function \( M(\omega_2, \omega_3, \omega_2') \) for the case of a neglected k-dispersion. In section III the determinant of \( E - M \) close to the Thouless instability is investigated.

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FIG. 1: The function $F_1(\omega_1, \omega_2, \omega_3')$ is shown diagrammatically in Fig. 1a. The shaded area denotes the T-matrix and represents all the possible interactions between particle 2 and 3. Fig. 1b shows the function $F_2(\omega_3, \omega_2', \omega_1)$. 
FIG. 2: The repeated application of $F_1$ and $F_3$ gives the function $M^{(3)}(\omega_y, \omega_3, \omega_3)$. This is shown as a diagrammatic representation.
FIG. 3: Low density correction which was considered in [3].
The last term does not give any contribution for the attractive
Hubbard model since a direct interaction between particles of
identical spin is not present.
FIG. 4: First non-vanishing term for a systematic low density correction which is of third order in the interaction $U$. 
FIG. 5: Infinite sum over all orders of the interaction $U$ which gives the complete low-density strong coupling extension formulated in Eq. (24) with the exception of the Hartree term which has to be subtracted.
FIG. 6: Lines of fixed particle numbers on the $T$-$\tilde{\mu}$-plane. The attractive interaction $U$ is equal to the bare bandwidth $W$ and $n = 1$ denote half filling. At low temperatures all lines of constant density collapse into the two-particle bound state.

FIG. 7: Lines of fixed $\langle n_\uparrow n_\downarrow \rangle$ on the $T$-$\tilde{\mu}$-plane. At the Thouless instability $\langle n_\uparrow n_\downarrow \rangle$ diverges. The attractive interaction $U$ is equal to the bare bandwidth $W$. 
FIG. 8: The determinant given in eq. [40] diverges at the Thouless instability proportional to $(T - T_c)^{-2}$. This is shown for $\tilde{\mu} = -0.5$ and $T_c \approx 0.37$ for two maximum numbers of Matsubara frequencies $M = 60$ and $M = 120$. The total frequency $i\omega_n$ was chosen at $n = 1$. The attractive interaction $U$ is equal to the bare bandwidth $W$. For a comparison the value of $1 + U \chi$ which goes to zero linearly in $T$, with $(T - T_c)$, is plotted.