Some Global Properties of the Attractive Hubbard Model in the Superconducting Phase: T-Matrix Approximation in 2D

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We have applied the Fast Fourier transform (FFT), which allows to compute efficiently convolution
sums, to solve the set of self-consistent T-matrix equations to get the Green function of the two
dimensional attractive-U Hubbard model below \( T_c \), extending previous calculations of the same
authors. Using a constant order parameter \( \Delta(T) \), we calculated \( T_c \) as a function of electron density
and interaction strength \( U \). These global results deviate from the BCS behavior remarkably.

74.20Mn, 74.25.-q, 74.72.-h

Although the Hubbard model is the most simple model to describe correlated electron behavior in a solid, the
classical treatment is far from trivial. Many attempts have been made to understand the phase diagram. A
fully understood Hubbard model might form the basis of understanding correlated electron systems as much as the
Ising model did for understanding critical phenomena in magnetism. The attractive-U Hubbard model might play
an important role in understanding high-temperature superconductivity and has been attracting much attention in
the past few years. We have implemented the T-matrix approximation which goes beyond the usual mean-field
approximation and becomes exact in the dilute limit, i.e. where only two-particle interactions take place.

We consider the attractive-U Hubbard model in two dimensions on a square lattice (lattice constant \( a \))

\[
H = \sum_{\mathbf{k}, \sigma} \xi_{\mathbf{k}} c_{\mathbf{k} \sigma}^\dagger c_{\mathbf{k} \sigma} + U \sum_{\mathbf{k}, \mathbf{k}' \downarrow, \mathbf{q} \uparrow} c_{\mathbf{k}+\mathbf{q} \uparrow}^\dagger c_{\mathbf{k}'-\mathbf{q} \downarrow} c_{\mathbf{k} \downarrow} c_{\mathbf{k}' \uparrow} \tag{1}
\]

with band energy \( \xi_{\mathbf{k}} = -2t(\cos k_x a + \cos k_y a) \) and on-site attraction \( U < 0, \xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu \), \( \mu \) is the chemical potential, and \( t \), the hopping of electrons between nearest neighbour sites, determines the energy unit. The creation (annihilation) operators for an electron with momentum \( \mathbf{k} \) and spin \( \sigma \) are denoted by \( c_{\mathbf{k} \sigma}^\dagger \) \( (c_{\mathbf{k} \sigma}) \).

The T-matrix (effective interaction) is the sum of particle–particle ladder diagrams with the smallest number of
closed fermion loops. In the low-density limit, these are the dominating terms of the perturbation expansion in terms
of the interaction \( U \). For the Hubbard model, where we have only on-site interactions, the T-matrix approximation
leads to a set of self-consistent equations for the one-particle Green function \( G(\mathbf{k}, i\omega_n) \) in the normal phase

\[
G(\mathbf{k}, i\omega_n) = [i\omega_n - \xi_{\mathbf{k}} + \Sigma(\mathbf{k}, i\omega_n)]^{-1}, \tag{2}
\]

where the diagonal self-energy term

\[
\Sigma(\mathbf{k}, i\omega_n) = \frac{1}{\beta N} \sum_{\mathbf{q}, \mathbf{m}} T(\mathbf{q}, i\epsilon_m) G(\mathbf{q}, -\mathbf{k}, i\epsilon_m - i\omega_n), \tag{3}
\]

depends on the T-matrix

\[
T(\mathbf{q}, i\epsilon_n) = \frac{-U}{1 + U\chi(\mathbf{q}, i\epsilon_n)}, \tag{4}
\]
which is a simple function of the independent pair–susceptibility

\[
\chi(q, i\epsilon_n) = \frac{1}{\beta N} \sum_{k,m} G(k, i\omega_m)G(q-k, i\epsilon_n - i\omega_m).
\] (5)

Here, \(\omega_n = (2n+1)\frac{\pi}{2}\) and \(\epsilon_n = 2n\frac{\pi}{2}\) are the fermionic and bosonic Matsubara frequencies, \(N = N_xN_y\) where \(N_x\) and \(N_y\) are the grid dimensions in \(k\)-space and \(\beta \equiv 1/T\) is the inverse temperature. We fix the chemical potential by the electron density (one spin direction):

\[
n(\beta, \mu) = \frac{1}{\beta N} \lim_{\eta \to 0^+} \sum_{k,n} G(k, i\omega_n)e^{i\omega_n\eta}.
\] (6)

To go below \(T_c\), we introduce a constant order parameter \(\Delta = |\Delta|\) into the Green function following the usual \(2 \times 2\) Nambu matrix formalism and get for the diagonal part the expression (* means complex conjugate)

\[
G(k, i\omega_n) = \frac{\Gamma^*(k, i\omega_n)}{|\Gamma(k, i\omega_n)|^2 + |\Delta|^2}
\] (7)

where

\[
\Gamma(k, i\omega_n) = i\omega_n - \xi_k + \Sigma(k, i\omega_n).
\] (8)

Equation (8) reduces to the usual BCS Green function when the self-energy term is set to zero (or to the Hartree shift). \(\Delta\) is our approximation for \(\Sigma_{12}(k, i\omega_n)\), the off-diagonal self-energy. The order parameter \(\Delta(T)\) is determined by

\[
\frac{1}{U} = \frac{1}{\beta N} \sum_{k,n} \frac{1}{|\Gamma(k, i\omega_n)|^2 + |\Delta|^2}
\] (9)

which closes the set of equations.

To solve the set of equations (3), (4), (5), (6), (7) and (9) we apply the following scheme:

1. Start by calculating \(G_0(k, i\omega_n)\), i.e. the Green function for the free system (\(\Sigma = 0\)). A suitable initial value for \(\mu\) and \(\Delta\) must be given (\(\mu = -3.5\) and \(\Delta = 0.5\) are reasonable values for \(T = 0.1, U = -4\) and \(n = 0.1\)).

2. Calculate \(\chi(q, i\epsilon_m), T(q, i\epsilon_m)\) and \(\Sigma(k, i\omega_n)\) using equations (3), (4) and (5).

3. At this point, we need an improved estimation of \(\mu\) and \(\Delta\). To get a stable iteration scheme, both parameters must be adjusted simultaneously. We do that by searching a solution \((\mu, \Delta)\) for equations (3) and (4) using a Newton algorithm. For technical purposes we neglect the dependence on \(\mu\) and \(\Delta\) for the self–energy to be able to numerically calculate the partial derivatives needed for the Newton algorithm. Because of that approximation we cannot take the new estimate of \((\mu, \Delta)\) directly. Instead we go only a small step, in the \(\mu - \Delta\) plane, from the current point to the new point (about one third of the total distance).

4. Calculate an improved Green function using the new parameters \(\mu\) and \(\Delta\).

5. Repeat steps 2 to 4 until the electron density has reached its desired value within a given tolerance.

In order to obtain results which are independent of finite size, one should use at least some \(10^3\) Matsubara frequencies and a grid of \(30 \times 30\) lattice points. The above scheme works in principle but a closer look at the equations for \(\chi\) and \(\Sigma\) shows that the straightforward implementation of these equations does not work in practice. This is due to the 4-fold loops which would occur in the computer program. Suppose we use 2000 Matsubara frequencies and a \(30 \times 30\) grid. Then we have to carry out for every grid point and every frequency the double sum over all frequencies and all grid points. This are of the order \((30^2 \times 2000)^2 = 3.24 \times 10^{12}\) complex operations. Even one of the fastest super–computers would need one to several hours to make one iteration step.

Since the frequency and momentum summations are convolutions, we evaluate them using the fast Fourier transform. The transforms \(k \rightarrow x\) and \(x \leftarrow x\) are the usual ones and we do not elaborate them any further. The transforms from \(\tau \rightarrow i\omega\) and \(\tau \leftarrow i\omega\) are described in more detail. In the following, the notation
\[ \mathcal{FRT}_M[F(x_j)]_n = \frac{1}{\sqrt{M}} \sum_{j=0}^{M-1} e^{-2\pi i \frac{j n}{M}} F(x_j) \]  

(10)

and

\[ \mathcal{FRT}_M^{-1}[F(x_n)]_j = \frac{1}{\sqrt{M}} \sum_{n=0}^{M-1} e^{2\pi i \frac{j n}{M}} F(x_n) \]  

(11)

is used. The Matsubara frequencies are slightly redefined to be more suitable (having non–zero indices) for numerical work and read:

\[ \omega_n = (2n + 1 - M) \frac{\pi}{\beta}, \quad \epsilon_n = (2n - M) \frac{\pi}{\beta}. \]  

(12)

We discretize the integral

\[ G(i\omega_n) = \int_0^\beta d\tau e^{i\omega_n \tau} G(\tau) \]  

(13)

by writing \( \tau_j = j\Delta\tau, \quad j = 0 \ldots M - 1 \) where \( \Delta\tau = \frac{\beta}{M} \) and \( M \) is the number of Matsubara frequencies used. We obtain

\[ G(i\omega_n) = \frac{\beta}{\sqrt{M}} \mathcal{FRT}_M^{-1}[e^{i\pi j(\frac{1}{M} - 1)}G(\tau_j)]_n. \]  

(14)

The phase factor \( e^{i\pi j(\frac{1}{M} - 1)} \) arises because of the fermionic frequencies \( \omega_n \) and the shift in the definition of \( \omega_n \). Similarly one can define the transforms for the bosonic frequencies as

\[ X(i\epsilon_n) = \frac{\beta}{\sqrt{M}} \mathcal{FRT}_M^{-1}[e^{-i\pi j}X(\tau_j)]_n, \]  

(15)

where \( X \) is either \( \chi \) or \( \Sigma \). We can now rewrite equations (13) and (14) to read:

\[ \chi(i\epsilon_n) = \frac{\beta}{\sqrt{M}} \mathcal{FRT}_M^{-1}[e^{-i\pi j}G^2(\tau_j)]_n \]  

(16)

and

\[ \Sigma(i\omega_n) = -\frac{\beta}{\sqrt{M}} \mathcal{FRT}_M^{-1}[e^{i\pi j(\frac{1}{M} - 1)}T(\tau_j)G(-\tau_j)]_n. \]  

(17)

These expressions are also well suited for parallel machines since the 3D–FFT (two space and one imaginary time dimension) can be decomposed into parallel processes.

We also need to calculate the electron density, but evaluating (18) numerically is not possible. To remove the limit \( \eta \to 0^+ \), we make use of the definition of the Green function

\[ G(\tau) = \langle c(\tau) c(0) \rangle, \quad \tau > 0 \]  

(18)

and

\[ G(-\tau) = \langle c(0) c(\tau) \rangle = -1 + \langle c(\tau) c(0) \rangle, \quad \tau > 0. \]  

(19)

Taking the sum \( G(\tau) + G(-\tau) \) and letting \( \tau \to 0^+ \) we get

\[ n = \frac{1}{2} [G(0^+) + G(0^-)] + \frac{1}{2} = G(0) + \frac{1}{2}. \]  

(20)

Therefore, the electron density now reads

\[ n(\beta, \mu) = \frac{1}{2} + \frac{1}{\beta N} \sum_{k, n} G(k, i\omega_n), \]  

(21)
an expression which can be evaluated easily. A similar correction for \(G(\tau = 0)\) must be applied in equations (16) and (17). Our Eq. (21) generalizes Eq. (3.1.2) of Mahan.

We have compared \(n(\beta, \mu)\) for the cases \(\Sigma = 0\) and \(\Sigma = nU/2\) (the Hartree shift) with the exact results and concluded that a grid of \(32 \times 32\) lattice sites and 2048 frequencies is a lower limit for \(U = -4\) and temperatures down to \(T = 0.1\). For larger \(|U|\) and/or lower temperatures one should increase the number of frequencies.

So far we have evaluated the Green function at the Matsubara points. Normally, we are really interested in the Fourier transform of the retarded real-time Green function which is a function of real frequency. In principle, we get this function by analytic continuation of the complex frequency Green function from the Matsubara points to the real axis. Since the resulting integral equations would be more complicated (involving integrals over Fermi and Bose distribution functions) than the discrete frequency summations, we first calculate the Green function at the Matsubara points as described in the preceding section. Then we continue to the real frequency axis by fitting a rational function (M-point Padé approximant) to the calculated values. The dynamical properties of the attractive Hubbard model in the superconducting phase is discussed in Ref. Here, we concentrate on the global properties of the attractive Hubbard model.

The algorithm works as follows: Given a function \(f(z_i) = u_i\) with values \(u_i\) at \(M\) complex points \(z_i, i = 1, 2, \ldots, M\), the Padé approximant is defined as a ratio of two polynomials which can be written as a continued fraction

\[
C_M(z) = \frac{a_1}{1 + \frac{a_2(z - z_1)}{1 + \frac{a_3(z - z_2)}{1 + \cdots}}}
\]

where the coefficients \(a_i\) are to be determined so that

\[
C_M(z_i) = u_i, \quad i = 1, 2, \ldots, M
\]

which is fulfilled when the \(a_i\) are given by the recursion

\[
a_i = g_i(z_i), \quad g_i(z_i) = u_i, \quad i = 1, 2, \ldots, M
\]

and

\[
g_p(z) = \frac{g_{p-1}(z_p) - g_{p-1}(z)}{(z - z_{p-1})g_{p-1}(z)}, \quad p \geq 2.
\]

Once the coefficients \(a_i\) are determined for a particular function, the function values at a real frequency \(\omega\) can be obtained by setting \(z = \omega + i\delta\) in (22), where \(\delta\) is used to remove unphysical peak structures due to finite size effects. The choice \(\delta = 0.1 \ldots 0.2\) is appropriate for our calculations. In reality, the choice of \(\delta\) is given by the precision with which the self-consistency in the Matsubara frequencies is done. This point has been discussed by Georges et al. In this paper we limit the discussion of the results to the regime \(T < T_c\), since results for \(T > T_c\) are reported elsewhere.

Figure 3 shows the temperature dependence of the order parameter for \(n = 0.1\) and \(U = -4t\). The system size is 32 by 32 grid points in \(k\)-space and 1024 Matsubara frequencies. The order parameter shows a very sharp drop to zero (compared with BCS behavior) which indicates the strong influence of fluctuations for all temperatures. \(\Delta(T = 0)\) is nearly twice as large as the corresponding \(\Delta_{BCS}\) whereas the critical temperature is much lower then \(T_c^{BCS}\) by more than a factor three. For example, \(\Delta(0)/T_c \approx 3.86\), which is more than twice the BCS ratio \((\approx 1.76)\). This implies that we are not in the weak coupling limit, opposite to the case of Martín-Rodero and Flores who find the BCS universal ratio in second order of perturbation for the continuous Hubbard model. The value of \(\Delta(T) = 0\) defines the critical temperature, \(T_c\). In order to calculate \(T_c\) we have drawn a straight line close to the sharp drop of the order parameter. Near the critical temperature we had some convergence problems. However, the evaluation of \(T_c\) is precise because it is calculated as described previously.

The density dependence of \(T_c\) is plotted in Figure 3. It is well known, that in the strong coupling limit the attractive–U Hubbard model close to half-filling can be mapped to a Heisenberg model which shows no Kosterlitz–Thouless transition. It is therefore expected, that the critical temperature near half-filling is reduced even in the weak– and intermediate–coupling regime. The lack of this property in our results can be attributed to the neglect of the particle–hole channel (charge fluctuations) in the T–matrix. Then, we should restrict ourselves to low densities where the T–matrix approach is indeed valid. To treat higher densities, we should implement, for example, the FLEXC approach which we are pursuing at this moment for the attractive Hubbard model. Here, we mention that the T–matrix and FLEXC approaches are conserving in the Kadanoff-Baym sense. Denteneer et al. obtained the critical temperature by calculating the helicity modulus associated with a wavelike distortion (\(\Delta_j = |\Delta(exp(2i\mathbf{qr}_j))|\)) of the order parameter in the BCS approximation as a function of temperature and subsequent comparison with the
Kosterlitz–Thouless relation between critical temperature and helicity modulus. But they miss the logarithmic drop to zero when approaching half-filling.

Figure 3 shows the critical temperature as a function of interaction strength. In contrast to the BCS behavior (which shows an exponential increase of $T_c$ small $|U|$ and goes linear in $|U|$ for larger values), the increase of $T_c$ is reduced drastically. The expected decrease of $T_c$ for large $|U|$ can not be observed for the values of $U$ treated here. The expectation is based on the fact, that for strong attraction and near to half-filling the model can be mapped onto a pseudo–spin model with effective interaction constant $J = 4\pi^2/|U|$, resulting in a $T_c$ decreasing with increasing $|U|$. The behavior we observe for $T_c/t$ vs $U/t$ is similar to the one obtained by Nozières and Schmitt-Rink using the Thouless’ criteria in the normal phase. Most likely we have to include additional fluctuations in the off-diagonal self-energy. Contrary to the normal state calculations where, for $\rho = 0.1$, we could not obtain convergence for $|U| > 4.0$, now in the superconducting phase the program is stable for large values of $|U|$.

In conclusion, we have calculated the critical temperature of the negative–U Hubbard model within the T–matrix approximation. The expected smooth cross-over from BCS to Bose–condensation can not be fully observed in the parameter space studied in this paper. Although the exponential-to-linear increase of $T_c^{BCS}$ with growing $|U|$ is reduced drastically, an optimal critical temperature has not been found. Perhaps we should fully go beyond BCS in the off-diagonal self-energy, as it has been done by Shafroth and Rodríguez-Núñez. In this work, the authors have studied the dynamical properties of the attractive Hubbard model in presence of double fluctuations. As previously discussed, we have obtained that $\Delta/T_c$ is more than twice the BCS value. To get $T_c = 0$ at half-filling we must include charge fluctuations. Investigations along these lines is under way. The value $\Delta(0)/T_c \approx 3.86$ and the temperature behavior of $\Delta(T)$ at $U/t = -4.0$, $n = 0.1$ are very different with respect to BCS results. These global results suggest that for $U/t = -4.0$, $n = 0.1$ we are already in the intermediate coupling regime where correlations are important.

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FIG. 1. Order parameter $\Delta$ versus temperature for density $n = 0.1$ and interaction strength $U = -4$.

FIG. 2. Critical temperature $T_c$ versus electron density $n$ ($n = 0.5$ corresponds to half-filling) for an interaction strength $U = -4$. 
FIG. 3. Critical temperature $T_c$ for various interaction strengths $U$ for constant density $n = 0.1$. 