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LETTER TO THE EDITOR

Some global properties of the attractive Hubbard model in the superconducting phase: the T-matrix approximation in two dimensions

S Schafroth†, J J Rodríguez-Núñez‡ and H Beck§

† Physik-Institut der Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland
‡ Universidad Federal Fluminense, Instituto de Física, Avenida Litorânea S/N, Boa Viagem, 24210-340 Niterói, Brazil
§ Université de Neuchâtel, Institut de Physique, Rue A L Breguet 1, CH-2000 Neuchâtel, Switzerland

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Abstract. We have applied the fast Fourier transform, which allows one 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 by the same authors. Using a constant order parameter $\Delta(T)$, we calculated T_c as a function of the electron density and interaction strength U. These global results deviate from the BCS behaviour remarkably.

Although the Hubbard model [1] is the simplest model for describing correlated electron behaviour in a solid, the mathematical 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 an understanding of correlated electron systems, much as the Ising model did for the understanding of critical phenomena in magnetism. The attractive-U Hubbard model might play an important role in the understanding of 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 [2].

We consider the attractive-U Hubbard model in two dimensions on a square lattice (lattice constant a) [3]:

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

with band energy $\epsilon_{\boldsymbol{k}} = -2t(\cos k_x a + \cos k_y a)$ and on-site attraction $U < 0$, where $\xi_{\boldsymbol{k}} = \epsilon_{\boldsymbol{k}} - \mu$, μ 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 $\boldsymbol{k}$ and spin σ are denoted by $c^{\dagger}_{\boldsymbol{k}\sigma}$ ($c_{\boldsymbol{k}\sigma}$).

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 [4] in the normal phase:

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

where the diagonal self-energy term

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

depends on the T-matrix

$$T(\boldsymbol{q}, \mathrm{i}\epsilon_n) = \frac{-U}{1 + U\chi(\boldsymbol{q}, \mathrm{i}\epsilon_n)} \tag{4}$$

which is a simple function of the independent pair susceptibility

$$\chi(\boldsymbol{q}, \mathrm{i}\epsilon_n) = \frac{1}{\beta N} \sum_{\boldsymbol{k},m} G(\boldsymbol{k}, \mathrm{i}\omega_m) G(\boldsymbol{q} - \boldsymbol{k}, \mathrm{i}\epsilon_n - \mathrm{i}\omega_m). \tag{5}$$

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

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

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

$$G(\boldsymbol{k}, \mathrm{i}\omega_n) = \frac{\Gamma^*(\boldsymbol{k}, \mathrm{i}\omega_n)}{|\Gamma(\boldsymbol{k}, \mathrm{i}\omega_n)|^2 + |\Delta|^2} \tag{7}$$

where

$$\Gamma(\boldsymbol{k}, \mathrm{i}\omega_n) = \mathrm{i}\omega_n - \xi_{\boldsymbol{k}} + \Sigma(\boldsymbol{k}, \mathrm{i}\omega_n). \tag{8}$$

Equation (7) reduces to the usual BCS Green function when the self-energy term is set to zero (or to the Hartree shift). Δ is our approximation for $\Sigma_{12}(\boldsymbol{k}, \mathrm{i}\omega_n)$, the off-diagonal self-energy. The order parameter $\Delta(T)$ is determined by

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

which closes the set of equations.

To solve the set of equations (3)–(7) and (9) we apply the following scheme.

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

(ii) Calculate $\chi(\boldsymbol{q}, \mathrm{i}\epsilon_m)$, $T(\boldsymbol{q}, \mathrm{i}\epsilon_m)$ and $\Sigma(\boldsymbol{k}, \mathrm{i}\omega_n)$ using equations (5), (4) and (3).

(iii) At this point, we need an improved estimation of μ and Δ. To get a stable iteration scheme, both parameters must be adjusted simultaneously. We do that by searching for a solution (μ, Δ) for equations (6) and (9) using a Newton algorithm. For technical purposes we neglect the dependence on μ and Δ for the self-energy, so as to be able to numerically calculate the partial derivatives needed for the Newton algorithm. Because of that approximation we cannot use the new estimate of (μ, Δ) directly. Instead we move

only a small step, in the μ–Δ plane, from the current point to the new point (about one third of the total distance).

(iv) Calculate an improved Green function using the new parameters μ and Δ.

(v) Repeat steps (ii) to (iv) until the electron density has reached its desired value within a given tolerance.

In order to obtain results which are independent of the finite size, one should use at least some 10^3 Matsubara frequencies and a grid of 30×30 lattice points. The above scheme works in principle, but a closer look at the equations for χ and Σ shows that the straightforward implementation of these equations does not work in practice. This is due to the fourfold loops which would occur in the computer program. Suppose we use 2000 Matsubara frequencies and a 30×30 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 leads to of the order of $(30^2 \times 2000)^2 = 3.24 \times 10^{12}$ complex operations. Even one of the fastest supercomputers 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 (FFT). The transforms $\boldsymbol{k} \to \boldsymbol{x}$ and $\boldsymbol{x} \to \boldsymbol{k}$ are the usual ones and we do not elaborate on them any further. The transforms from $\tau \to \mathrm{i}\omega$ and $\mathrm{i}\omega \to \tau$ are described in more detail. In the following, the notation

$$\mathcal{FFT}_M[F(x_j)]_n = \frac{1}{\sqrt{M}} \sum_{j=0}^{M-1} \mathrm{e}^{-2\pi \mathrm{i} jn/M} F(x_j) \tag{10}$$

and

$$\mathcal{FFT}_M^{-1}[F(x_n)]_j = \frac{1}{\sqrt{M}} \sum_{n=0}^{M-1} \mathrm{e}^{2\pi \mathrm{i} nj/M} F(x_n) \tag{11}$$

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

$$\omega_n = (2n + 1 - M)\frac{\pi}{\beta} \qquad \epsilon_n = (2n - M)\frac{\pi}{\beta}. \tag{12}$$

We discretize the integral

$$G(\mathrm{i}\omega_n) = \int_0^\beta \mathrm{d}\tau \ \mathrm{e}^{\mathrm{i}\omega_n \tau} G(\tau) \tag{13}$$

by writing $\tau_j = j\,\Delta\tau, \ \ j = 0, \ldots, M-1$, where $\Delta\tau = \beta/M$ and M is the number of Matsubara frequencies used. We obtain

$$G(\mathrm{i}\omega_n) = \frac{\beta}{\sqrt{M}} \mathcal{FFT}_M^{-1}[\mathrm{e}^{\mathrm{i}\pi j(1/M-1)} G(\tau_j)]_n. \tag{14}$$

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

$$X(\mathrm{i}\epsilon_n) = \frac{\beta}{\sqrt{M}} \mathcal{FFT}_M^{-1}[\mathrm{e}^{-\mathrm{i}\pi j} X(\tau_j)]_n \tag{15}$$

where X is either χ or Σ. We can now rewrite equations (5) and (3) to read

$$\chi(\mathrm{i}\epsilon_n) = \frac{\beta}{\sqrt{M}} \mathcal{FFT}_M^{-1}[\mathrm{e}^{-\mathrm{i}\pi j} G^2(\tau_j)]_n \tag{16}$$

and

$$\Sigma(\mathrm{i}\omega_n) = -\frac{\beta}{\sqrt{M}} \mathcal{FFT}_M^{-1}[\mathrm{e}^{\mathrm{i}\pi j(1/M-1)} T(\tau_j) G(-\tau_j)]_n. \tag{17}$$

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

We also need to calculate the electron density, but evaluating (6) numerically is not possible. To remove the limit $\eta \to 0^+$, we make use of the definition of the Green function:

$$G(\tau) = \langle c^\dagger(\tau)c(0)\rangle \qquad \tau > 0 \tag{18}$$

and

$$G(-\tau) = \langle c(0)c^\dagger(-\tau)\rangle = -1 + \langle c^\dagger(-\tau)c(0)\rangle \qquad \tau > 0. \tag{19}$$

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

$$n = \frac{1}{2}[G(0^+) + G(0^-)] + \frac{1}{2} = G(0) + \frac{1}{2}. \tag{20}$$

Therefore, the electron density now reads

$$n(\beta, \mu) = \frac{1}{2} + \frac{1}{\beta N}\sum_{\boldsymbol{k},n} G(\boldsymbol{k}, \mathrm{i}\omega_n). \tag{21}$$

This is an expression which can be evaluated easily. A similar correction for $G(\tau = 0)$ must be applied in equations (16) and (17). Our equation (21) generalizes equation (3.1.2) of Mahan [5].

We have compared $n(\beta, \mu)$ for the cases where $\Sigma = 0$ and $\Sigma = nU/2$ (the Hartree shift) with the exact results and concluded that a grid of 32×32 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 the 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 (an M-point Padé approximant) to the calculated values [6]. The dynamical properties of the attractive Hubbard model in the superconducting phase are discussed in reference [7]. 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:

$$C_M(z) = \cfrac{a_1}{1 + \cfrac{a_2(z - z_1)}{1 + \cdots + \cfrac{a_M(z - z_{M-1})}{1 + \cdots}}} \tag{22}$$

where the coefficients a_i are to be determined so that

$$C_M(z_i) = u_i \qquad i = 1, 2, \ldots, M \tag{23}$$

which is fulfilled when the a_i are given by the recursion

$$a_i = g_i(z_i) \qquad g_1(z_i) = u_i \qquad i = 1, 2, \ldots, M \tag{24}$$

and

$$g_p(z) = \frac{g_{p-1}(z_{p-1}) - g_{p-1}(z)}{(z - z_{p-1})g_{p-1}(z)} \qquad p \geqslant 2. \tag{25}$$

Once the coefficients a_i are determined for a particular function, the function values at a real frequency ω can be obtained by setting $z = \omega + \mathrm{i}\delta$ in (22), where δ is used to remove unphysical peak structures due to finite-size effects. The choice $\delta = 0.1$–0.2 is appropriate for our calculations. In reality, the choice of δ is dictated by the precision with which the self-consistency in the Matsubara frequencies is achieved. This point has been discussed by Georges *et al* [8]. In this letter we limit the discussion of the results to the regime where $T < T_c$, since results for $T > T_c$ are reported elsewhere [9].

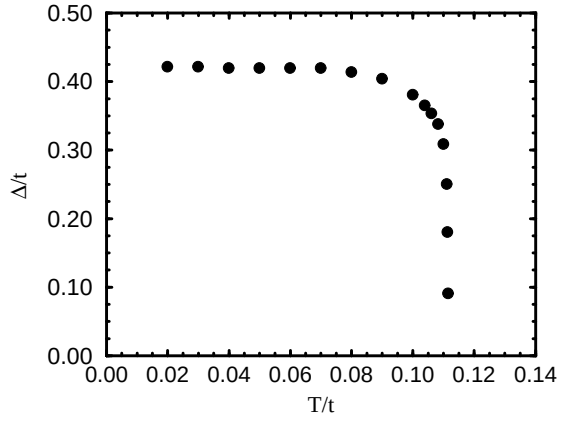

Figure 1. The order parameter Δ versus temperature for the density $n = 0.1$ and interaction strength $U = -4t$.

Figure 1 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 $\boldsymbol{k}$-space and 1024 Matsubara frequencies. The order parameter shows a very sharp drop to zero (compared with BCS behaviour) which indicates the strong influence of fluctuations for all temperatures. $\Delta(T = 0)$ is nearly twice as large as the corresponding Δ_{BCS} whereas the critical temperature is much lower than T_c^{BCS}—by more than a factor of 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, which is opposite to the case considered by Martín-Rodero and Flores [10] who find the BCS universal ratio in the 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 2. 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 [11]. It is therefore anticipated that the critical temperature near half-filling will be reduced even in the weak- and intermediate-coupling regimes. The absence of this property in our results can be attributed to the neglect of the particle–hole channel (charge fluctuations) in the T-matrix. Thus, we should restrict ourselves to low densities where the T-matrix approach is indeed

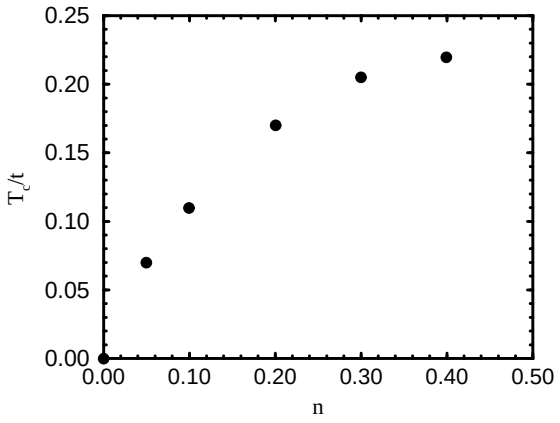

Figure 2. The critical temperature T_c versus electron density n ($n = 0.5$ corresponds to half-filling) for an interaction strength $U = -4t$.

valid. To treat higher densities, we should implement, for example, the FLEXC approach [12] goal 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 [2]. Denteneer *et al* [13] obtained the critical temperature by calculating the helicity modulus associated with a wavelike distortion ($\Delta_j = |\Delta| \exp(2\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}_j)$) of the order parameter in the BCS approximation as a function of temperature and subsequent comparison with the Kosterlitz–Thouless relation between the critical temperature and helicity modulus—but they miss the logarithmic drop to zero when approaching half-filling.

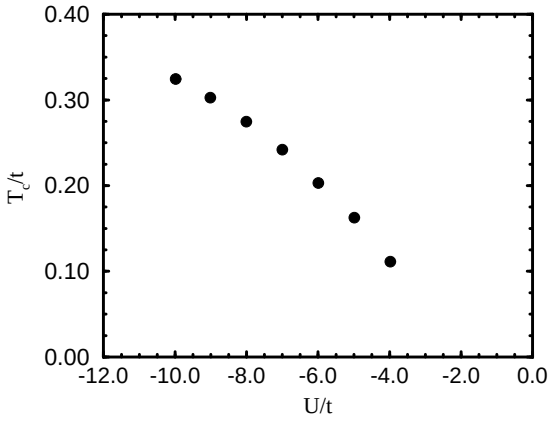

Figure 3. The critical temperature T_c for various interaction strengths U for the constant density $n = 0.1$.

Figure 3 shows the critical temperature as a function of the interaction strength. In contrast to the BCS behaviour (which shows an exponential increase of T_c for small $|U|$ and becomes linear in $|U|$ for larger values), the increase of T_c is reduced drastically. The expected decrease of T_c for large $|U|$ cannot be observed for the values of U treated here.

This 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 the effective interaction constant $J = 4t^2/|U|$, resulting in a T_c decreasing with increasing $|U|$. The behaviour that we observe for T_c/t versus U/t is similar to the one obtained by Nozières and Schmitt-Rink [14] using the Thouless criteria for the normal phase. Most probably we would have to include additional fluctuations in the off-diagonal self-energy [15]. Unlike in the case of the normal-state calculations where, for $\rho = 0.1$, we could not obtain convergence for $|U| > 4.0$, in the superconducting phase the program is stable for large values of $|U|$. Just recently we have found that to get convergence for large $|U|$ and/or small T we have to move in the proper way in the parameter space (μ, ρ). See reference [15].

In conclusion, we have calculated the critical temperature of the negative-U Hubbard model within the T-matrix approximation. The expected smooth crossover from BCS to Bose condensation cannot be fully observed in the parameter space studied in this letter. 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 calculations in the off-diagonal self-energy, as has been done by Schafroth and Rodríguez-Núñez [15]. In this work [15], the authors have studied the dynamical properties of the attractive Hubbard model in presence of *double fluctuations*. As previously discussed, we have obtained the result that Δ/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 are under way [16]. The value $\Delta(0)/T_c \approx 3.86$, and the temperature behaviour of $\Delta(T)$ at $U/t = -4.0$, $n = 0.1$ are very different from the 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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