Feedback effects and the self-consistent Thouless criterion
of the attractive Hubbard model

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We propose a fully microscopic theory of the anomalous normal state of the attractive Hubbard model in the low-density limit that accounts for propagator renormalization. Our analytical conclusions, which focus on the thermodynamic instabilities contained in the self-consistent equations associated with our formulation, have been verified by our comprehensive numerical study of the same equations. The resulting theory is found to contain no transitions at non-zero temperatures for all finite lattices, and we have confirmed, using our numerical studies, that this behaviour persists in the thermodynamic limit for low-dimensional systems.

The anomalous normal state properties of the high temperature superconductors have, amongst other things, highlighted the limitations of present-day many-body physics. In spite of repeated attempts [1–3] to formulate a controlled fully microscopic many-body expansion, at present both microscopic and semi-phenomenological theories require vindication from Monte Carlo or some other “exact” procedure.

To serve as further and concrete motivation for the work described below, consider the paper of Schmitt-Rink, Varma, and Ruckenstein [4]. They proposed, through a simple formulation of the problem, that in two dimensions (2d) any electronic effective two-particle interaction that was attractive would lead to a destabilization of the Fermi surface, and thus to non-Fermi liquid-like physics. One may consider this result as being based on the idea that the Fermi surface is destroyed via the presence of two-particle bound states that “drain away” all electrons to the bound state. The result is a superconducting instability which, at best, occurs only at zero temperature. The \( T = 0 \) predictions of this model are complicated: they found a critical point, corresponding to all electronic densities, with all electrons paired — whether or not these paired electrons were in a phase coherent state was not addressed, although that is what one would expect.

Many questions and criticisms of this approach have appeared [5]. In particular, by including multiple scattering in the electron number equation, Serene [6] claimed that the physics of Ref. [4] was eviscerated, and that Fermi liquid behaviour was in fact robust. Actually, as we show below, at the multiple-scattering level of formulation the physics of Ref. [4] survives such an improvement.

Another criticism of the result of Schmitt-Rink, Varma, and Ruckenstein [4] is that Luttinger’s theorem is not satisfied — this immediately suggests that renormalization of the single-particle propagators is important. As we show below, this is indeed the case, and, in fact, the physics of Ref. [4] is dramatically changed when such renormalization, or self-consistency, is included. The problem with such a proposal is that the renormalization of these propagators is not a simple matter, and in this paper we address the question of the “appropriate” self-consistent theory, and apply our considerations to the attractive Hubbard model (AHM).

The impact of self-consistency on the results of Ref. [4] is related to the more general question of the study of feedback effects on the Thouless criterion. The Thouless criterion arises from the determination, with decreasing temperatures in the normal state, of the superconducting instability [7]. Such a formulation traditionally uses unrenormalized electron propagators — see [8] for a particularly clear discussion of the physics that arises from such an approach. An important advantage of the Thouless approach is that it focuses on the non-superconducting state, so the possibility of non-Fermi liquid physics in the anomalous normal state can be studied simultaneously with the question of the superconducting instability. Thus, the issue of the self-consistent Thouless criterion can be addressed by repeating the analysis of, say, Ref. [8], using renormalized propagators. This provides feedback, i.e. the single-electron propagators will “know” about the pairing tendency of the system as the temperature is lowered, and this in turn will influence, for better or for worse, that pairing tendency.

What self-consistent formulation is appropriate? One suggestion comes from Levin and coworkers [9,10], based on earlier work [11–13], in which only one specific combination of renormalized propagators (in the equations for both the pair susceptibility and the self energy) was proposed. Fresard, et al. [14], and then Haussmann [15] (and several
Green's function. The pair propagator is given by

\[ G_{\mu} = \frac{\alpha}{\alpha^2 + (\Omega - \tilde{\Sigma})^2} \]

very much reminiscent of experiment \[ 19 \]. Further, our results for the single electron spectral functions derived

\[ G = \frac{\alpha}{\alpha^2 + (\Omega - \tilde{\Sigma})^2} \]

by (ignoring, for this publication, the Hartree term)

is well described by the T-matrix approximation \[ 17 \]. The T-matrix approximation corresponds to a self-energy given

\[ G = \frac{\alpha}{\alpha^2 + (\Omega - \tilde{\Sigma})^2} \]

between the self-energy and the renormalized Green's function,

\[ G = \frac{\alpha}{\alpha^2 + (\Omega - \tilde{\Sigma})^2} \]

where the terms in this Hamiltonian have their usual meaning.

When the electronic density is either close to zero (\( \langle \tilde{n}_m \rangle \approx 0 \)), or complete filling (\( \langle \tilde{n}_m \rangle \approx 2 \)), the effective interaction is well described by the T-matrix approximation \[ 17 \]. The T-matrix approximation corresponds to a self-energy given by (ignoring, for this publication, the Hartree term)

\[ \Sigma(k,i\omega_n) = -\frac{U^2}{N\beta} \sum_{q,i\Omega_\ell} \mathcal{G}_2(q,i\Omega_\ell) G_{\alpha}(-k+q,i\Omega_\ell - i\omega_n) \]

where \( \mathcal{G}_2 \) is the pair propagator, and \( G_{\alpha} \) can be either \( G_0 \) (the non-interacting) or \( G \) (the renormalized) single-particle Green’s function. The pair propagator is given by

\[ \mathcal{G}_2(q,i\Omega_\ell) = \frac{\chi(q,i\Omega_\ell)}{1 - |U| \chi(q,i\Omega_\ell)} \]

where the pair susceptibility, \( \chi \), is a convolution of two single-particle propagators given by

\[ \chi(q,i\Omega_\ell) = \frac{1}{\beta N} \sum_{k,i\omega_n} G_{\alpha'}(k,i\omega_n)G_{\alpha''}(q-k,i\Omega_\ell - i\omega_n) \]

with \( G_{\alpha'} \) and \( G_{\alpha''} \) either \( G_0 \) or \( G \). In these equations, \( \beta \) is the inverse temperature (\( k_B = 1 \)), \( N \) is the number of lattice sites, and \( \omega_n \) (\( \Omega_\ell \)) are Fermi (Bose) Matsubara frequencies. Finally, Dyson’s equation gives another relation between the self-energy and the renormalized Green’s function, \( G \).

As outlined in Ref. \[ 8 \], the Thouless criterion, signifying the instability of the normal state, corresponds to poles of the zero-centre-of-mass momentum retarded, real-time, pair propagator moving off the real axis into the upper half of the complex plane. From Eq. (3) this simplifies to the condition (defining \( \chi = \chi' + \chi'' \))

\[ \chi'(q = 0, i\Omega_\ell = 0) = 1/|U| \]

(noting that \( \chi''(q = 0, i\Omega_\ell = 0) = 0 \)).

For future reference, let us make clear the instability that is found when propagator renormalization is ignored. Traditionally \[ 8 \], one evaluates Eq. (3) using bare propagators. The divergence of Eq. (3) then leads to an instability at a temperature \( T_c \) which is identical to that predicted by BCS theory (\( e.g., \) see Ref. \[ 8 \)). Below we discuss some of the effects of feedback on this scenario.

As further information on the above no-feedback theory, note that researchers have begun to use the appearance of the pseudogap as an important test for the presence of strong correlations in model systems, and this requires that one obtain the dynamics, and not the static thermodynamic quantities, for the proposed model. However, to obtain the dynamics from even the simple non-self-consistent T-matrix theory involves some hard-to-control extrapolations to the real frequency axis. Recently, we formulated a partial fraction decomposition method, that is described elsewhere \[ 18 \], and which can be evaluated with a precision (with respect to pole locations and residues of the self energy) to a relative accuracy of \( 10^{-80} \). The resulting density of states shows a well-defined pseudogap at low temperatures \[ 18 \], very much reminiscent of experiment \[ 14 \]. Further, our results for the single electron spectral functions derived
from the non-self-consistent T matrix are remarkably similar in character to the quantum Monte Carlo/maximum entropy method spectral functions and density of states determined by the Sherbrooke collaboration [20] (although their calculations are for a much higher electron filling). Thus, from a comparison to either experiment or “exact” Monte Carlo data, it appears that a T-matrix theory with unrenormalized propagators is a reasonable formalism with which to examine this problem. However, as discussed at the start of this paper (with regards to Ref. [4]), and as we now delineate below, this agreement is fortuitous — the predictions for the (static) thermodynamics for such a theory are in error, and thus the dynamics produced by such a formulation are of no value.

To see how the thermodynamics predicted by Refs. [4] make clear the failings of such a theory, consider the following: If one chooses a chemical potential that lies in the band (|μ| < W/2, where W is the single-particle non-interacting bandwidth), and then lowers the temperature, using the original Schmitt-Rink et al. [4] formulation applied to the 2d AHM, we have shown that the electron density actually diverges as the instability is approached (for constant a chemical potential). Use of the correct number equation, as follows from the number-conserving theory of Serene [3], leads to a number density of one at the instability temperature (see below). Then, this leads to the unphysical result that for any fixed electron density less than one, the chemical potential is always driven to half the bound state value (viz. below the band), indicative of the elimination/suppression of the Fermi surface. Further problems abound — while the electron density approaches unity at the instability, the two-particle correlation function ⟨n_m↑, n_m↓⟩ diverges — that is, this formulation has difficulties at “the two-particle level” [14]. This is clearly incorrect, since for the AHM it should be bounded between (⟨n_m⟩)^2/4 and ⟨n_m⟩/2.

We now demonstrate the above-mentioned behaviour analytically: We note that Eq. (5) indicates that near the Thouless curve (Tc) the self-energy (Eq. (2)) is dominated by the q = 0, Ω = 0 term. Thus for all finite lattices one finds

$$\Sigma(k, i\omega_n) \sim -\frac{U^2}{N\beta} \frac{\chi(0,0)}{1 - |U|} G_0(-k, -i\omega_n) \ .$$

(6)

Note the electron density equation is

$$\langle \tilde{n}_m \rangle = 1 + \frac{2}{N\beta} Re \sum_{k, i\omega_n} (i\omega_n - \xi_k - \Sigma(k, i\omega_n))^{-1} \ ,$$

(7)

where ξ_k is the band energy relative to the chemical potential, and that at the Thouless temperature the self-energy diverges (Eq. 3), and thus ⟨n_m⟩ = 1, as stated above [21]. Several example flow lines are shown in a (μ, T) plot for a 2d square lattice in Fig. , in which it is seen that they approach the two-electron (hole) bound state energy below (above) the band as T → 0. This results in a system of bound electrons (holes), and the Fermi surface (and hence the normal state Fermi liquid) is destroyed.

To remedy these deficiencies within a fully microscopic diagrammatic theory, renormalized propagators are required. Unfortunately, there are a variety of different self-consistent T-matrix theories. These different theories are based on the choice of a non-interacting G_0 or a fully renormalized G in the G_s’s that appear in Eqs. (2,4). Based on the consideration of Marčelja [12] and Patton [13], Levin and coworkers [9,10] have argued that the G_s in Eq. 4 must be the non-interacting Green’s function (to avoid states in the superconducting gap, which are absent in the weak coupling limit). While we agree with this “non-derivable” approach, we disagree with the claim that the appropriate combination of Green’s functions in the pair susceptibility should be asymmetric (χ ∼ G G_0). Firstly, these theories do not produce the full two-particle Green’s function, but rather just the pair propagator. One cannot say that a pair propagator is conserving, but one could ask: Is the two-particle Green’s function from which the pair propagator is formed conserving? It follows from Ref. [2] that a symmetric convolution (∼ G G) leads to two-particle quantities that are conserving, and thus it is not required, nor necessarily wise, to use the asymmetric form (∼ G G_0) [4] for the pair propagator.
FIG. 1. Lines of constant density are plotted in the $\mu$-$T$ plane (each quantity shown in units of the bandwidth $W$) for a $14 \times 14$ lattice. The contours shown here (from bottom to top) correspond to electron densities $\langle n \rangle = 0.1, 0.2, 0.3, \ldots, 1.8, 1.9$ and are calculated for $|U|/t = 4$. The Thouless criterion line forms the boundary to the shaded superconducting region. Notice that all the density contours, except the $\langle n \rangle = 1$ line, are deflected away from this area, and never cross into this area, as they proceed to lower temperatures.

Based on these (and other [22]) considerations, we examine the self-consistent theory given by Dyson’s equation with $G_\alpha = G_0$ and $G_\alpha' = G_{\alpha''} = G$ in Eqs. (2,4). Following our earlier arguments, for non-zero temperatures and a finite lattice we can write the ansatz [23] near the superconducting instability

$$\Sigma(k, i\omega_n) = \frac{\Delta^2}{i\omega_n + \xi_k},$$

(8)

$$\Delta^2 = \frac{U^2}{N\beta} \frac{\chi(0,0)}{(1 - |U|\chi(0,0))}.$$  

(9)

From Eq. (3) it follows that a $T_c > 0$ instability is indicated by $\Delta \to \infty$. However, evaluating $\chi(0,0)$ using Eq. (8) in Eq. (4) leads to

$$\chi(0,0) = \frac{1}{N\beta} \sum_{k,\omega_n} \frac{\omega_n^2 + \xi_k^2}{(\omega_n^2 + \xi_k^2 + \Delta^2)^2},$$

(10)

and shows in fact, that $\chi(0,0)$ goes to zero in the limit of $\Delta \to \infty$. Thus, there is no self-consistent solution at non-zero temperatures for any finite lattice — this cures an obvious problem that exists for mean-field (non-self-consistent T-matrix) theories [24].

The only self-consistent solution of these equations occurs at $T = 0$. That is, by solving $1 = |U|\chi(0,0)$ in the $T \to 0$ limit we obtain a modified gap equation given by

$$1 = \frac{|U|}{2N} \sum_k \left( \frac{1}{\sqrt{\Delta^2 + \xi_k^2}} - \frac{1}{2} \frac{\Delta^2}{(\Delta^2 + \xi_k^2)^{3/2}} \right).$$

(11)

One finds that in the small $|U|/t$ limit, $\Delta \sim \exp(-4W/|U|)$; this shows, in contrast to what was claimed in Ref. [9,10], that when both propagators in the pair susceptibility are renormalized one still recovers the weak coupling BCS limit [25]. Indeed, the form of the density of states at $T = 0$,
\[
N(\omega) \sim N^0(0) \frac{|\omega|}{\sqrt{\omega^2 - \Delta^2}} \Theta(\omega^2 - \Delta^2),
\]

is that of weak coupling BCS theory, and shows a fully developed gap.

In order to further analyze the predictions of our theory, we have conducted a comprehensive numerical study of the resulting self-consistent equations, and have solved these equations down to the lowest temperatures that we can access (typically, these temperatures are 1/100th of the mean-field BCS temperature). Further, we have obtained convergence of all static quantities to better than 1 part in 10\(^5\) (at low temperatures this requires that our Matsubara frequency sums be performed with a frequency cutoff of 4\(W\), and we have thus used this same cutoff at all temperatures). An example set of data is shown in Figure 2 for \(d = 1\); lattices from 8 \(\times\) 1 to 128 \(\times\) 1 were studied, and it was found that for \(L \times 1\) lattices, for \(L \geq 64\) no changes with lattice size were encountered. Thus, these data represent the quantitative predictions of our renormalized propagator theory for one dimension in the thermodynamic limit (with the shown parameter set). As is clear from this Figure, the \(T \to 0\) limit of \(\chi(0, 0)\) is \(1/|U|\) (in units of \(1/t\)); however, \(\chi(0, 0)\) remains less than \(1/|U|\), and thus no instabilities are encountered, for all nonzero temperatures. Clearly, as is predicted by our analytic theory, there is only a zero temperature transition to a superconducting state.

![Figure 2](image-url)
such a theory accounts for critical effects at $T = 0$, it is clear that this formulation represents a very useful starting point of a fully microscopic theory for the evaluation of, e.g., the spectral functions at non-zero temperatures (albeit for low electronic densities).

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