The BCS Pairing Instability in the Thermodynamic Limit

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(Dated: May 22, 2014)

The superconducting pairing instability—as determined by a divergence of the two-particle susceptibility—is obtained in the mean field (BCS) approximation in the thermodynamic limit. The usual practice is to examine this property for a finite lattice. We illustrate that, while the conclusions remain unchanged, the technical features are very different in the thermodynamic limit and conform more closely with the usual treatment of phase transitions encountered in, for example, the mean-field paramagnetic-ferromagnetic transition. Furthermore, by going to the extreme dilute limit, one can distinguish three dimensions from one and two dimensions, in which a pairing instability occurs even for two particles.

I. INTRODUCTION

The Bardeen, Cooper, and Schrieffer (BCS) theory of superconductivity, following the original literature, is typically first presented in textbooks as a proposed variational ground state, whose energy is lower than that of the corresponding normal state. This is followed by a discussion of the excited states, from which, in weak coupling at least, a critical temperature is derived, corresponding to the breakup of pairs.

An alternate view of the transition was put forward by Thouless2 who tracked the BCS instability from above (in temperature) by monitoring the two particle propagator. By including a specific set of processes (denoted by “ladders” in the particle-particle channel of the diagrammatic version of this formulation), one finds an instability of the normal phase. This approach is also explained in many texts and will be briefly summarized below.

Seeing the superconducting transition as an instability of the normal state at some finite temperature highlights the potential importance of pairing fluctuations that occur in the normal state even before the critical transition is reached. The possibility of pairing fluctuations has been important in the elucidation of the so-called pseudo-gap that occurs in the high-\(T_c\) cuprate materials. One school of thought regards the pseudo-gap in these materials as a tell-tale signature of pairing fluctuations in the normal state.

There is now an extensive literature on the presence of pairing fluctuations in the normal state and on their impact on various normal state properties. However, our purpose here is to revisit the simple so-called Thouless criterion for the BCS instability and to reformulate it in the thermodynamic limit. We have always found it peculiar that this instability is signalled by the appearance of two imaginary roots in the denominator of the two-particle propagator, whereas other instabilities appear to be accompanied by the appearance of a real root. It turns out that the two-particle pairing instability is always, to our knowledge, formulated for a finite system; in the thermodynamic limit, as we show below, the criterion behaves quite differently and much more like other instabilities in condensed matter.

For simplicity we focus on the simplest model that exhibits superconductivity (at least at the mean field level), the attractive Hubbard model on a hypercubic lattice in one, two, and three dimensions. While considerable attention has been devoted to single-particle properties, since these are often most related to the measured properties, the two-particle properties are the ones that are key to understanding single-particle properties. For our purposes, we express the two-particle propagator in the non-self-consistent ladder approximation.

\[
g_2(q, i\nu_n) = \frac{\chi_0(q, i\nu_n)}{1 - U\chi_0(q, i\nu_n)},
\]

where \(\chi_0\) is the “noninteracting” pair susceptibility

\[
\chi_0(q, i\nu_n) = \frac{1}{N\beta} \sum_{k,m} G_{0\uparrow}(k, i\omega_m)G_{0\downarrow}(q - k, i\nu_n - i\omega_m),
\]

and \(G_{0\uparrow}(k, i\omega_m) = [i\omega_m - (\epsilon_k - \mu)]^{-1}\) is the noninteracting single-particle propagator. Here, \(k\) and \(q\) are wave vectors, and \(\epsilon_k\) is the single electron dispersion appropriate to tight-binding with nearest neighbour hopping. The Matsubara frequencies are defined as \(\omega_m = \pi T(2m - 1)\) for Fermions and \(\nu_n = i2\pi Tn\) for Bosons. \(\beta = (k_B T)^{-1}\) is the inverse temperature, and \(N\) is the number of lattice sites. All wavevector summations span the entire Brillouin zone, and Matsubara sums go over all integers.

For the BCS instability we can focus on \(q = 0\) and, in fact, \(\nu_n = 0\); nonetheless, we wish to illustrate the instability by monitoring \(g_2\) as a function of (real) frequency. The result for \(\chi_0\) is

\[
\chi_0(q, z) = \frac{1}{N} \sum_k \frac{1 - f(\epsilon_k - \mu) - f(\epsilon_{-k+q} - \mu)}{z - (\epsilon_k - \mu) - (\epsilon_{-k+q} - \mu)},
\]

where we have now analytically continued the result to the upper half-plane \((i\nu_n \rightarrow z)\), and in particular for \(z = \nu + i\delta\), with \(\delta\) a positive infinitesimal. Here \(f(x) \equiv 1/(e^{\beta x} + 1)\) is the Fermi-Dirac distribution function. Equation (3) is the one displayed in textbooks and reviews. We show its real and imaginary parts in...
to those of the noninteracting case, indicated by the ver-
tures the excitation energies occur at energies very close
energy of the top of the band \((4t)\). As the temperature
goes to zero (not evident in (a) because the divergence
is logarithmic). The figures were produced in one dimension
at the band edges in one dimension.

The negative divergences occur at the band edges and
are due to the divergent single electron density of states,
\(g(\epsilon)\)

\[
\chi_0(\nu + i\delta) = -\int_{-|W/2|}^{+|W/2|} d\epsilon \frac{g(\epsilon) \tanh(\beta(\epsilon - \mu)/2)}{\nu + i\delta - 2(\epsilon - \mu)},
\]

(4)

where \(\pm W/2\) is the top (bottom) of the single electron
band \((\pm 2t\) in 1D, \(\pm 4t\) in 2D, and \(\pm 6t\) in 3D), and since
\(q = 0\) we have omitted it from the argument list for \(\chi_0\).
This integral requires a principal value part, which can be
done analytically:

\[
\chi_0(\nu + i\delta) = \frac{1}{2} g(\frac{\nu}{2} + \mu) \frac{\beta \nu}{4} \log \left\{ \frac{W/2 - \mu - \nu + i\delta}{W/2 + \mu + \nu + i\delta} \right\} \\
+ \frac{i}{2} \frac{\pi}{2} g(\frac{\nu}{2} + \mu) \frac{\beta \nu}{4} \\
+ \frac{1}{2} \int_{-|W/2|}^{+|W/2|} d\epsilon \frac{g(\epsilon) \tanh(\beta(\epsilon - \mu)/2) - g(\mu + \epsilon) \tanh(\beta \mu/2)}{\epsilon - \mu - (\nu + i\delta)/2}.
\]

(5)

The integration on the last line is no longer singular and
can be computed by quadrature.

In Figs. 2(a) and 2(b) we show the corresponding
results for an infinite system (1D) at temperatures
\(T = 1, 0.1,\) and \(0.01\) in units of \(t\); hereafter all ener-
gies will be quoted in units of \(t\). The real part of \(\chi_0(\nu)\)
clearly shows a maximum at zero frequency; elsewhere
there are no positive divergences as they have been in-
tegrated to a smooth curve in the principal value sense.
The negative divergences occur at the band edges and
are due to the divergent single electron density of states
at the band edges in one dimension.

As is apparent from the figure, these “band edge”
divergences are present at all temperatures. In fact, for
the lowest two temperatures shown, the curves are essen-
tially the same except for the region near zero frequency,
where the maximum diverges as \(T \to 0\), indicative of a
superconducting/charge-density-wave instability. In fact
at zero temperature the real part is given analytically by the following expression (for $\mu = 0$):

$$\text{Re}\,\chi_0(\nu + i\delta) = \begin{cases} 
\frac{1}{2\pi} \log \left( \frac{1 + \sqrt{1 - \nu^2}}{1 - \sqrt{1 - \nu^2}} \right) & \bar{\nu} < 1, \\
-\frac{1}{2\pi} \arctan \left( \frac{1}{\sqrt{\nu^2 - 1}} \right) & \bar{\nu} > 1,
\end{cases}$$

(6)

where $\bar{\nu} \equiv \nu/(4t)$. The divergence at zero frequency is evident in this expression. At finite temperature an exact analytical expression is not possible, even for zero frequency. However, to a very good approximation one can obtain $\text{Re}\,\chi_0(\nu = 0) = \frac{1}{2\pi} \log \left( 1 + \frac{|U|}{|t|} \right)$. Notice that the argument of the natural logarithm is a factor of 2 larger than what would have been obtained by simply approximating the density of states as a constant at the chemical potential ($\mu = 0$ in this case).

For a nonzero attractive interaction, an instability is signalled by the maximum crossing the black horizontal line positioned at $1/|U|$. This signals the onset of an instability in a way that is familiar from studies in mean-field ferromagnetism for example. It appears as though two real roots are emerging; in fact a careful analysis of Eq. (1), using $\chi_0(\nu + i\delta) \approx a_0 + c_0\nu$, with $a_0$ and $c_0$ positive real constants [see Figs. 2(a) and (b)] near $\nu \approx 0$ shows that as $a_0$ traverses $1/|U|$, the same root with negative imaginary part becomes a root with a positive imaginary part. As in the finite lattice case, then, the two particle propagator becomes unstable in time.

Figure (2b) shows the spectral function, $B_0(q, \nu) \equiv -\text{Im}\,\chi_0(q, \nu + i\delta)/\pi$ as a function of frequency. Aside from the asymmetrization, this quantity provides an image of the single electron density of states. This remains true in any dimension, as can be seen from taking the imaginary part of Eq. (5):

$$B_0(q = 0, \nu) = -\frac{1}{2} \tanh \left( \frac{\beta \nu}{4} \right) g(\frac{\nu}{2} + \mu).$$

(7)

As the temperature approaches zero, the hyperbolic tangent function simply changes the sign of the density of states at the origin. In Fig. (1b) the delta function structure was merely providing an image of the finite system’s discretized density of states.

As mentioned, this calculation can be done in any dimension, and Fig. (3a) and (3b) show the real and imaginary parts of the pair propagator in three dimensions, with nearest neighbour hopping only, at half filling. Once again the essential feature is that the real part diverges at zero frequency with decreasing temperature; thus, within mean field theory, Eq. (1) guarantees a transition when the real part crosses $1/|U|$. Of special note is the lack of
a negative divergence at the band edges in three dimensions; this affects the extreme dilute limit, and we will comment further below.

Finally, while half-filling gives rise to symmetric results, more often than not some other instability intervenes to suppress the pairing instability in this case. A result illustrating the pairing instability at a chemical potential away from half-filling is shown in Fig. 4, where the real part of the susceptibility is shown in two dimensions for (a) $\mu = -2.5t$ and (b) $\mu = -5.0t$. Note that the divergence in the real part persists in (a) at $\nu = 0$ as the temperature is lowered. The negative divergences associated with the band edge discontinuities (in 1D and 2D) remain, but at a frequency $\pm W - 2\mu$. The discontinuity at $\nu = -2\mu$ ($5t$ for this case) is only present here because of the logarithmic divergence in the 2D density of states at the origin and is absent for other band structures that lack singularities. In (b) the chemical potential is below the bottom of the band; now there is a positive divergence at $\nu = -W - 2\mu$ (here at $2t$). This divergence is peculiar to 2D and 1D only and shows that any $|U|$, no matter how small, will lead to an instability in the extreme dilute limit. This is not the case in higher dimension. For 3D, there is no band edge divergence, and it is well-known that an attractive potential must exceed some threshold before it will support a bound state for two particles.

Results in other dimensions away from half-filling are similar, albeit with differences reflecting the different densities of states, as already noted at half-filling, and the critical difference just noted regarding band edge divergences in 3D vs. 2D and 1D. Furthermore, completely symmetric results occur for $\mu = +2.5$ (compared to $\mu = -2.5$), due to the particle-hole symmetry in the problem.

In summary we have computed the two particle pairing susceptibility in the thermodynamic limit, in a variety of dimensions and for any filling. We have shown how the BCS instability comes about with decreasing temperature and how the nature of the instability more closely resembles the one usually discussed in the context of mean-field ferromagnetism. Technically, at the instability temperature, a single pole passes from the lower half-plane to the upper-half-plane in complex frequency. This is in contrast to the finite lattice result, where two real roots become two pure imaginary roots, one of which leads to the instability. In either case the change at the instability signals a two-particle propagator that diverges with increasing time.

The calculations in the thermodynamic limit enable one to see the dependence on dimensionality. Some quantitative differences occur due to the very different single-particle densities of states in 1D, 2D and 3D. However, in the extreme dilute limit, the different physics in 3D vs. 1D and 2D is highlighted in the thermodynamic limit, and leads, in a natural way, to the necessity in 3D for Cooper’s famous calculation.\textsuperscript{15}

\section*{ACKNOWLEDGMENTS}

This work was supported in part by the Natural Sciences and Engineering Research Council of Canada (NSERC), and by the Canadian Institute for Advanced Research (CIfAR).
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