Evolution from BCS superconductivity to Bose condensation: Role of the parameter $k_F \xi$

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(Received 5 November 1993)

We argue that the natural variable to establish the crossover from Cooper-pair-based superconductivity to Bose-Einstein condensation of bound-electron pairs is the product $k_F \xi$ of Fermi electron wave vector times the coherence length for two-electron correlation, and that Cooper-pair-based superconductivity is stable against bosonization down to $k_F \xi \approx 2\pi$. We also propose that the experimental plot by Uemura et al., relating the superconducting temperature $T_c$ to the Fermi temperature $T_F$ for a variety of “exotic” as well as conventional superconductors, can be rationalized by correlating the ratio $T_c/T_F$ to $k_F \xi$. It appears in this way that the high-$T_c$ superconductors lie in the plot by Uemura et al. near the “instability” line $k_F \xi = 2\pi$.

Uemura et al.\(^1\) have recently proposed to distinguish a class of “exotic” superconductors (including cuprate, bismuthate, organic, Chevrel-phase, heavy fermions, and fullerene systems) from the more conventional superconductors (like Nb) by the value of the ratio $T_c/T_F$ between the experimental superconducting temperature and the (effective) Fermi temperature, which turns out to be about one hundred times larger for the “exotic” than for the conventional superconductors. Uemura et al. have also suggested that this substantial difference might be an indication that the “exotic” superconductors are in some sense intermediate between conventional BCS superconductors and Bose-condensed systems.

In order to establish a possible connection between the physical consequences of this suggestion and the experimental relation between $T_c$ and $T_F$, one should first try to figure out the appropriate variable to determine the crossover between Cooper-pair-based (BCS) superconductivity and Bose-Einstein (BE) condensation. One could then attempt to use that variable as a sort of “normal” coordinate in the plot constructed by Uemura et al. (hereafter referred to simply as the Uemura plot), by figuring out a phenomenological relation (independent of the underlying superconducting mechanism) between that variable and the ratio $T_c/T_F$, thus encompassing the difference between the “exotic” and conventional superconductors. Completion of this program might further turn out to be useful both experimentally (by suggesting possibly in which direction one should move in the Uemura plot to improve $T_c$) and theoretically (by giving hints on the underlying dynamics related to high-$T_c$ superconductivity). In this paper we shall propose how to meet this program by a rather general argument on the stability of the Cooper-pair-based superconductivity.

Evolution from weak- to strong-coupling superconductivity has been addressed a few years ago by Nozières and Schmitt-Rink\(^2\) (hereafter referred to as NSR) following the pioneering work by Legget.\(^3\) Central to this work is the well-known argument\(^4\) that the BCS wave function has built in the Bose-Einstein condensation as a limiting case, since it reduces to the BE condensate wave function when the (average) occupation numbers $\langle n_{k,\sigma} \rangle$ can be neglected with respect to unity for all wave vectors $k$ (and for both spin projections $\sigma$). NSR follow the evolution from Cooper-pair-based superconductivity to BE condensation through the increase of the coupling strength associated to an effective fermionic attractive potential, and conclude that the evolution is “smooth.” Although this result is appealing from a theoretical point of view, it does not allow for a direct comparison with the Uemura plot since the coupling strength of the effective fermionic attraction is not a quantity that could be realistically inferred from experiments. Besides, associating an effective coupling strength to a given class of superconductors would unavoidably require one to face at the outset the problem of the mechanism responsible for superconductivity,\(^5\) which need not be actually necessary to unravel the kind of message conveyed by the Uemura plot.

We need thus to figure out a more significant variable than the coupling strength to follow the evolution from BCS superconductivity to BE condensation. The new variable should be selected according to the following criteria: (i) the evolution from BCS to BE should turn out to be as much as possible *universal*, i.e., independent of the details of the interaction potential and of the single-particle density of states; (ii) when using the new variable to rationalize the Uemura plot, it should be possible to subject that variable to an *independent* experimental check.\(^6\) We shall illustrate in the following why we propose to identify the product $k_F \xi$ as the desired variable.

Following NSR, we introduce the model fermionic
Hamiltonian

\[ H = \sum_{k,\sigma} \epsilon_k c_{k,\sigma}^\dagger c_{k,\sigma} + \sum_{k,\sigma' \neq \sigma} V_{k,k'} c_{k+q/2,\sigma'}^\dagger c_{k+q/2,\sigma}^\dagger c_{k'+q/2,\sigma'}^\dagger c_{k'+q/2,\sigma}, \]

where \( c_{k,\sigma} \) is the destruction operator for fermions with wave vector \( k \) and spin \( \sigma \), \( \epsilon_k \) is a single-particle (or quasiparticle) dispersion relation, and \( V_{k,k'} \) is an "effective" fermionic attraction. In its simplest version, \( \epsilon_k = k^2 / 2m^* - \mu \) where \( m^* \) is an effective (quasi)particle mass and \( \mu \) is the chemical potential.\(^7\) Although the use of the Hamiltonian (1) has obvious shortcomings, by resting on a continuum model (where no effect of the lattice structure is included) and by disregarding dynamical effects, we believe that it is sufficient for our purposes.

The variational procedure with the usual BCS trial wave function

\[ \langle \Phi \rangle = \prod_k \left( u_k + v_k c_{k,\uparrow}^\dagger c_{k,\downarrow}^\dagger \right) |0\rangle \]

leads to the two familiar coupled equations

\[ 2\epsilon_k \phi_k + (1 - 2u_k^2) \sum_{k'} V_{k,k'} \phi_{k'} = 0, \]

\[ n = \frac{1}{\Omega} \sum_k \left[ 1 - \frac{\epsilon_k}{E_k} \right], \]

where \( n \) is the particle density, \( \Omega \) the quantization volume, and \( \phi_k = 2u_k v_k \Delta_k / E_k \) with \( \Delta_k = -\sum_{k'} V_{k,k'} u_{k'} v_{k'} \) and \( E_k = \sqrt{\epsilon_k^2 + \Delta_k^2} \).\(^8\) Note that, provided \( u_k^2 \ll 1 \) for all \( k \), Eq. (3) reduces to the Schrödinger equation for the relative motion of two particles with equal mass \( m^* \) interacting via \( V_{k,k'} \) and with eigenvalue \( 2\mu \). In this limit bosonization of bound-electron pairs is fully achieved.

Solution of Eqs. (3) and (4) gets considerably simplified by considering a separable potential. NSR choose

\[ V_{k,k'} = V w_k w_{k'}, \quad w_k = \frac{1}{\sqrt{1 + (k/k_0)^2}}, \]

where the strength \( V \) \( (< 0) \) and the characteristic wave vector \( k_0 \) are the parameters of the interaction. With this potential, \( \Delta_k = \Delta_0 w_k \) and the associated two-body eigenvalue problem has (in three dimensions) the only eigenvalue \( 2\mu = -\epsilon_0 = -(k_0^2 / m^*) (G - 1)^2 \) for \( G > 1 \), where \( G = -V \Omega m^* k_0 / 4\pi > 0 \) is the dimensionless coupling constant, while the bound-state radius has the asymptotic behavior \( r_0 \sim k_0^{-1} G^{-1/2} \) for \( G \to \infty \).\(^9\) In agreement with the results by NSR, we find that the solutions \( (\Delta_0, \mu) \) of Eqs. (3) and (4) evolve smoothly as functions of \( G \) for given \( k_0 \), although \( (\Delta_0, \mu) \) depend strongly on \( k_0 \) for given \( G \).\(^\text{10}\) No connection with the Uemura plot is evidently possible at this level.

A suggestion to figure out a more significant variable than the coupling strength comes from the observation that "exotic" superconductors of the Uemura plot have a considerable shorter coherence length \( \xi \) (\( -20-50 \text{ Å} \)) than the conventional superconductors (for which \( \xi \sim 10^3-10^4 \text{ Å} \)). Theoretically, \( \xi \) can be obtained from the pair-correlation function with opposite spins

\[ g(r) = \frac{1}{n} \left| \langle \Phi \Psi_{\sigma}^\dagger(r) \Psi_{\sigma}^\dagger(0) \Phi \rangle \right|^2, \]

where \( \Psi_{\sigma}(r) \) is the fermion field operator, by identifying

\[ \xi^2 = \frac{\int d^3 r g(r) r^2}{\int d^3 r g(r)} = \frac{\sum_k |\phi_k|^4}{\sum_k |\phi_k|^2}. \]

Our definition (7) correctly reduces to the Pippard coherence length \( \xi_0 = (d\epsilon_k/dk)_k / \pi \Delta_k \) in the weak-coupling limit (actually, \( \xi \sim \xi_0 \pi / 2 \sqrt{2} = 1.11 \xi_0 \) when \( G \ll 1 \)) and to the bound-state radius \( r_0 \) in the strong-coupling limit. It turns out that the behavior of \( \xi \) versus \( G \) is also "smooth," although it strongly depends on the parameter \( k_0 \) of the interaction. A reasonable attempt to eliminate the coupling constant \( G \) from further considerations is then to replace it by a dimensionless parameter containing \( \xi \). Since \( k_F^{-1} \) is the only other independent physical length scale in the problem, we replace the original pair of variables \((G, k_0)\) by the alternative pair \((k_F \xi, k_0)\) and study the crossover from BCS superconductivity to BE condensation as a function of \( k_F \xi \) for given \( k_0 \).\(^\text{11}\)

In Fig. 1 we report the chemical potential \( \mu \) versus \( k_F \xi \) for a wide range of values of the reduced density \( n/k_0^3 \) (=10\(^\alpha\) with \( \alpha = -5, -4, \ldots, +4 \)). Positive values of \( \mu \) have been normalized by the Fermi energy \( \epsilon_F \) (=\( k_F^2 / 2m^* \), by our definition), while negative values of \( \mu \) have been normalized by half of the eigenvalue \( \epsilon_0 \) of the

FIG. 1. Chemical potential \( \mu \) versus \( k_F \xi \) (at zero temperature). The normalization of \( \mu \) and the meaning of the different curves are explained in the text. The two limiting curves corresponding to the values \( 10^{-3} \) and \( 10^{6} \) of the reduced density \( n/k_0^3 \) are indicated.
associated two-body problem. The two curves for the
reported extreme values of \( n / k_B^2 \) act as limiting (accumu-
lation) curves for all practical purposes. The striking feature of Fig. 1 is that, when expressed in terms of \( k_F \xi \), the behavior of the chemical potential becomes universal
(i.e., independent of the parameter \( k_0 \) of the interaction
potential), but possibly for an “intermediate” range
\( \pi^{-1} \leq k_F \xi \leq 2\pi \) where the normalization values \( \xi_F \) and \( \xi_0 \)
(depending on the sign of \( \mu \)) actually lose their mean-
ing.\(^{12}\) This remarkable universal behavior of \( \mu \) versus
\( k_F \xi \) strongly suggests that \( k_F \xi \) is indeed the appropriate
variable to follow the evolution from BCS superconduc-
tivity to BE condensation.

Note in addition from Fig. 1 that \( \mu \) gets pinned to
(about) the normal-state value \( \xi_F \) when \( k_F \xi \gg 2\pi \), and
that \( \mu \) drops rather abruptly from \( \xi_F \) at \( k_F \xi \approx 2\pi \). In
other words, Fig. 1 shows that, when the coherence length \( \xi \)
equals the Fermi wavelength \( \lambda_F = 2\pi/k_F \) of the electrons,
the system becomes unstable against bosonization and the
Fermi surface is wiped out. We expect that the instabil-
ity of the Cooper-pair-based superconductivity when
\( k_F \xi \approx 2\pi \), inasmuch as it is consequence of a genuine
quantum-mechanical effect, should actually persist
beyond the limits of validity of the procedure we have
followed to establish it. In this sense, the stability crite-
ron \( k_F \xi \approx 2\pi \) should be regarded as the analog for the
problem at hand of the Ioffe-Regel criterion for transport
in disordered systems.

It still remains to figure out how the Uemura plot for
\( T_c \) versus \( T_F \) could be mapped out in terms of the vari-
able \( k_F \xi \). To this end, we remark that the variable \( k_F \xi_0 \)
appears in the characteristic weak-limit BCS expression
for \( T_c \) obtained from \( k_B T_c / \Delta_{k_F} = e\gamma / \pi \) (\( \gamma \) being Euler's
constant) by eliminating \( \Delta_{k_F} \) in favor of the Pippard
coherence length \( \xi_0 \), namely,

\[
k_B T_c = \frac{2e\gamma}{\pi^2} \frac{\xi_F}{k_F \xi_0},
\]

\( k_B \) being Boltzmann’s constant and \( 2e\gamma / \pi^2 = 0.36 \). The
question naturally arises whether an expression like (8)
could be used not only asymptotically in the weak-
coupling limit, but also down to \( k_F \xi \approx 2\pi \) whenever the
concept of a Fermi surface is still preserved. To answer
this question, we have followed again NSR and evaluated
the thermodynamic potential within the ladder approxi-
mation in the particle-particle channel for the normal
state (i.e., for \( T \geq T_c \)). In this way, \( T_c \) and \( \mu(T_c) \) have
been determined versus \( G \), or alternatively versus \( k_F \xi \), for
given \( k_0 \). The result is that the relation

\[
k_B T_c = 0.40 \frac{\xi_F}{k_F \xi}
\]

holds universally for \( k_F \xi \approx 2\pi \), independent of \( k_0 \).\(^{13}\)

We can now envisage interpreting the Uemura plot in
terms of the variable \( k_F \xi \), by assuming Eq. (9) to hold
phenomenologically (that is, irrespective of the assump-
tions used to derive it) and thus superimposing on the
\( \log_{10} T_c \) versus \( \log_{10} T_F \) plot (with \( T_F = \xi_F / k_B \)) the
straight lines with \( k_F \xi = \text{constant} \). The result is reported
in Fig. 2 where the lines with \( k_F \xi = 10, 10^2, 10^3, 10^4 \), and
\( 10^5 \) are drawn (full lines) together with the “instability”
line \( k_F \xi = 2\pi \) (broken line). We note the following features
from Fig. 2: (i) a linear trend of \( \log_{10} T_c \) versus
\( \log_{10} T_F \) results for any given value of \( k_F \xi \); (ii) the line
with \( k_F \xi = 2\pi \) remarkably appears to be the natural upper
boundary for the experimental data, suggesting that the
systems near the boundary are close to a Fermi surface
instability; (iii) what distinguishes the “exotic” from the
conventional superconductors in the Uemura plot is the
smaller value of \( k_F \xi \) associated to the former ones (apart
from a possible difference in \( m^* \)); (iv) high values of \( T_c \),
result when \( k_F \xi \) is “small” (~10) and \( m^* \) is not too
large.\(^{14}\)

To obtain an independent check on whether our propo-
sal to interpret the Uemura plot is correct, one should
compare the values of \( k_F \xi \) associated via Eq. (9) to the
various samples in the Uemura plot with independently
measured values of \( k_F \xi_{\text{exp}} \) (as obtained by critical
magnetic-field measurements).\(^{15}\) Preliminary checks with
the experimental data available to us give indeed en-
couraging results for this comparison. A complete list of
data on \( T_c, T_F, k_F, \) and \( \xi_{\text{exp}} \) for all samples reported in
the Uemura plot is, however, required to draw a definite
conclusion about the success of the comparison.

Some final comments are in order. First, we remark
that intrinsic to the procedure of how the values of \( T_F \)
are located in the Uemura plot is an effective angular
averaging which washes out all nonspherical features of
the Fermi surface. Otherwise, no meaningful connection
between the Uemura plot and our expression (9) could
even have been attempted. It may thus be possible that
more specific criteria for instability toward bosonization,
which would take into account the asymmetry of the Fer-
mis surface (especially in reduced dimensionality), could

![FIG. 2. Uemura plot with superimposed lines of \( \log_{10} T_c \)
versus \( \log_{10} T_F \) according to Eq. (9) of the text for the values
\( 2\pi \) (broken line) and \( 10, 10^2, 10^3, 10^4, 10^5 \) (full lines) of \( k_F \xi \). Experimental points are reproduced from Ref. 1.](image-url)
result in smaller values (than $2\pi$) for the product of the relevant values of $k$ and of the coherence size. Second, we emphasize that in our approach we have not taken into account any lattice effect. It is likely that the tendency toward bosonization may result in an instability of the coupled electron-lattice system (such as the onset of a charge-density wave or a structural modulation) that could actually overwhelm superconductivity. This could possibly be the reason why no physical system appears to cross the "forbidden" boundary at $k_F\xi = 2\pi$ in the Uemura plot. A consequence of this sort of speculation would thus be that producing samples with even higher $T_c$ would require one to move along the line $k_F\xi = 2\pi$ in the Uemura plot.

We are indebted to A. Bianconi, C. Di Castro, and J. Ranninger for valuable discussions. One of us (F.P.) gratefully acknowledges partial research support from Europa Metalli-LMI S.p.A.

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4Cf., e.g., J. R. Schrieffer, Theory of Superconductivity (Benjamin, New York, 1964), Chap. 2.
5Reduction to an effective fermionic attractive potential may not be possible whenever dynamical (retardation) effects are important. For recent developments see L. Pietronero and S. Strässler, Europhys. Lett. 18, 627 (1992).
6These two criteria were borne out in the original BCS suggestion to express their theoretical results in the form of ratios of experimentally accessible quantities, which are independent of the interaction potential and of the single-particle density of states.
7As in the BCS approach, we rely on a description of the normal state in terms of quasiparticles.
8We have eliminated at the outset the Hartree-Fock-like terms by setting $V_{\text{dia}} = 0$ for the diagonal components. This choice will by no means invalidate our results, since it turns out that these terms are irrelevant in the parameter region of physical interest.
9NSR (Ref. 2) state instead that $r_0 \sim k_0^{-1}$ for $G \to \infty$. Since bosonization can be achieved only when $r_0 \ll n^{-1}$, NSR are able to follow the evolution from BCS to BE condensation as a function of $G$ only in the "dilute limit" $n/k_0 \ll 1$ for the reduced (three-dimensional) density, that is, for given density $n$ only when $k_0 \gg k_F$. This limitation has prevented NSR from connecting the two physical limits (BCS and BE) irrespective of $k_0$. Our finding that $r_0 \sim k_0^{-1} G^{-1/2}$, on the other hand, enables us to satisfy the bosonization condition $(n/k_0^2)/G^{1/2} \ll 1$ even in the "dense limit" $n/k_0^2 \gg 1$, provided $G$ is large enough.
10Probably the most suited quantity to follow the evolution from BCS superconductivity to BE condensation is the chemical potential $\mu$, which almost coincides with the Fermi energy in the weak-coupling limit and reduces to (half of) the lowest eigenvalue of the associated two-body problem in the strong-coupling limit. Furthermore, $\mu$ can also be the object of direct measurements: cf. G. Rietveld, N. Y. Chen, and D. van der Marel, Phys. Rev. Lett. 69, 2578 (1992), and references quoted therein.
11A physical quantity directly related to $k_F\xi$ is the (average) number of electrons $N_G$ within a correlation volume in $d$ dimensions. When $d = 3$ one gets $N_G = (k_F\xi)^d/18\pi$, while when $d = 2$ one gets $N_G = (k_F\xi)^2/8$. Since in the Uemura plot three-dimensional as well as (quasi-)two-dimensional systems are treated on the same footing, we prefer to use simply $k_F\xi$ as the variable replacing $G$.
12We have verified that the universal behavior shown in Fig. 1 for $k_F\xi \geq 2\pi$ and $k_F\xi \leq \pi^{-1}$ is independent of the choice of the single-particle dispersion relation $\varepsilon_k$ and of the shape of the interaction potential embodied by the function $w_k$, provided obviously that these functions do not behave in a pathological way in $k$ space.
13The difference between the numerical prefactors of Eqs. (8) and (9) is due to the difference between our definition (7) for $\xi$ and the Pippard coherence length $\xi_0$. We have also verified that Eq. (9) holds for $k_F\xi \approx 2\pi$ both in three and in two dimensions. This is a requisite to apply Eq. (9) to the Uemura plot, since the data there reported pertain to fully three-dimensional as well as to (quasi-)two-dimensional systems.
14It is interesting to apply Eq. (9) also to superfluid $^3$He, for which $k_F = 0.78$ $\AA^{-1}$, $m^*/m = 2.76$ (where $m$ is the bare mass of the $^3$He atom), and $\xi \approx 200$ $\AA$. Equation (9) then provides for $T_c$ the value 4.5 mK, which compares reasonably well with the experimental value (2.6 mK) if we consider the fact that Eq. (9) applies to $s$-wave pairing while the pairing in $^3$He is known to be $p$-wave. It is thus essentially the large value of $k_F\xi$ ($\approx 160$) which accounts for the three orders of magnitude difference between the superfluid temperature of $^3$He and $^4$He. One should also mention in this context that common features between $^3$He and heavy-fermion systems have already been pointed out by R. Tournier et al., J. Magn. Magn. Mater. 76-77, 552 (1988) (see especially their Fig. 6).
15When comparing the values of the coherence length $\xi$ obtained by our definition (7) with the experimental values, one should be aware of the fact that different numerical factors (of order unity) plague alternative definitions of the (zero-temperature) coherence length. The relation between our $\xi$ and the experimentally determined $\xi_{\text{exp}}$ can be determined by relating $\xi_{\text{exp}}$ to the Pippard coherence length $\xi_0$, in the limit when a microscopic derivation of the Ginzburg-Landau equation from BCS is justified. From the clean-limit expression $\xi_{\text{exp}} = 0.87\xi_0$ [cf. E. Helfand and N. R. Werthamer, Phys. Rev. 147, 288 (1966), and references quoted therein] we then obtain $\xi = 1.25\xi_{\text{exp}}$, which we assume to apply for all materials reported in the Uemura plot.