Quantum criticality in inter-band superconductors

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Abstract
In fermionic systems with different types of quasi-particles, attractive interactions can give rise to exotic superconducting states, such as pair density wave (PDW) superconductivity and breached pairing. In recent years the search for these new types of ground states in cold atoms and in metallic systems has been intense. In the case of metals the different quasi-particles may be the up and down spin bands in an external magnetic field or bands arising from distinct atomic orbitals that coexist at a common Fermi surface. These systems present a complex phase diagram as a function of the difference between the Fermi wavevectors of the different bands. This can be controlled by external means, varying the density in the two-component cold atom system or, in a metal, by applying an external magnetic field or pressure. Here we study the zero temperature instability of the normal system as the Fermi wavevector mismatch of the quasi-particles (bands) is reduced and find a second order quantum phase transition to a PDW superconducting state. From the nature of the quantum critical fluctuations close to the superconducting quantum critical point (SQCP), we obtain its dynamic critical exponent. It turns out to be $z = 2$ and this allows us to fully characterize the SQCP for dimensions $d \geq 2$.

In strongly correlated materials superconductivity can be suppressed in different ways. Most commonly, this is accomplished by an external magnetic field, applied pressure or doping [1–7]. However, the point in the phase diagram where the critical temperature $T_c$ vanishes as a function of the external parameters is not necessarily associated with a superconducting quantum critical point (SQCP). In the case of superconductivity induced by antiferromagnetic fluctuations due to the proximity of an antiferromagnetic quantum critical point (AFQCP) [8], as the system moves away from the AFQCP, these fluctuations change from attractive to repulsive and superconductivity just fades away [9].

Inter-band superconductivity is a long standing problem in condensed matter physics [10, 11]. It can be realized, for example, by applying an external magnetic field in a metallic system. The field splits the band and the phase diagram as a function of the mismatch of the Fermi wavevectors of the up and down spin bands can be investigated. It also occurs for the case of superconductivity mediated by valence fluctuations, where the most relevant correlations are due to inter-band pairing [12]. In multi-band metals, pressure can be used to change the hybridization and the mismatch of the Fermi wavevectors of the different bands coexisting at the common Fermi surface [13]. More recently this problem has received much attention due to the possibility of investigating it in cold atom systems. In this case the attractive interaction between two fermionic systems with different Fermi wavevectors can be tuned by the Feshbach resonance [14]. The Fermi wavevector mismatch $\delta k_F$ in this case is controlled by varying the density of the atoms and this allows the phase diagram to be fully explored. In the core of neutron stars, up and down quarks, in different numbers, with attractive interactions may give rise to color inter-band superconductivity [13, 14].

In the case of a mismatch of the Fermi wavevectors caused by an external magnetic field, we neglect the associated orbital effects [15]. These have to be at least partially quenched to observe the phase transition studied here. Although we consider different driving mechanisms for this instability, we refer generically to the agent causing the mismatch as an external field.

The zero temperature phase diagram for inter-band superconductors with s-wave pairing has been established using mean-field calculations [11]. As the Fermi wavevector mismatch increases, there is a first order phase transition...
from a BCS-like state to an FFLO or PDW state. Further
increase of the mismatch gives rise to a continuous transition
to a normal metallic phase [11]. The discovery of new
systems and the possibility of finding new exotic PDW
phases makes it important to fully understand the nature
of the normal to PDW transition beyond the mean-field
approximation. Here we investigate this transition using a new
approach. It is based on a perturbation theory for retarded and
advanced Green’s functions [16]. We relate the appearance
of superconductivity in the multi-band system to the divergence
of a generalized susceptibility [17] χ(q, ω), like in the Stoner
criterion for ferromagnetism. We start in the normal phase
and calculate the response of the system to a frequency and
wavevector dependent fictitious external field which couples to
the superconducting order parameter [18]. For simplicity we
consider here the case of s-wave superconductivity.

In our approach, at the level of the random phase
approximation (RPA), we have to calculate only single-particle
Green’s functions. This is different and simpler than the usual
linear response theory, which relates the response of the system
to two-particle Green’s functions [16].

At zero temperature, as the Fermi wavevectors mismatch
is reduced, we find a divergence of the static part of the
susceptibility at a finite wavevector q = qo. This occurs at the
critical mean-field value of the mismatch which destroys the
pair density wave superconductivity. This divergence implies
that even in zero fictitious field the system can have a finite
inhomogeneous superconducting order parameter. The condition
for the superconducting instability can be expressed in the
form of a Stoner-like criterion, 1
2
− Uχo(q = qo, δk) = 0.

This determines either a critical value of the attractive
interaction Uc above which the system is a superconductor
or a critical mismatch below which superconductivity sets
in. The coupling of the order parameter to the electronic
degrees of freedom determines the frequency dependence of
the generalized susceptibility and the nature of the quantum
fluctuations, i.e., the dynamic critical exponent z [19], in
the PDW SQCP. The theory is equivalent to a quantum Gaussian
approach and since the dynamic exponent turns out to be z = 2,
it yields the correct description of the SQCP for dimensions
d ≥ 2.

We start with the following Hamiltonian describing a two-
band system with inter-band attractive interactions:

\[ H_0 = \sum_{i,j} t_{ij}^a a_i^\dagger a_j + \sum_{i,j} t_{ij}^b b_i^\dagger b_j - U \sum_i n_i^a n_i^b. \]  

For simplicity, we omitted spin indices [14]. The bands a and
b can be the up and down spin bands of a metal polarized
by an external magnetic field h [11], different types of atoms
or the hybridized bands of a multi-band metal [13].

The interaction U is an attractive interaction between the fermions
in different bands. We do not consider intra-band interactions
which have been studied in detail in [13]. These interactions
compete with the inter-band term as they favor homogeneous
BCS-like superconducting ground states. Also, higher order
terms which transfer pairs of particles between the bands will
not be included. These terms play a prominent role in the
pnictides [20] and it would be interesting to use the approach
described below to treat them in the future.

We now calculate the response of the normal two-band
system to a wavevector and frequency dependent fictitious field
that couples to the superconducting order parameter of interest, ⟨a_i^\dagger b_j⟩. This is given by

\[ \mathcal{H}_1 = -g \sum_i e^{i q \cdot r} e^{i \omega t} (a_i^\dagger b_i^\dagger + a_i b_i), \]

where the frequency \(\omega_0\) has a small positive imaginary part to
guarantee the adiabatic switching on of the field. The response
of the system to the fictitious field will be obtained using
perturbation theory for the retarded and advanced Green’s
functions [16]. We start in the normal phase where the
superconducting order parameter is zero in the absence of the
external field g. We split the Green’s functions, normal and
anomalous, into two contributions. The first is of order zero
and the second of first order in the field g. For the anomalous
Green’s functions ⟨⟨a_i^\dagger b_j⟩⟩, for example, we write

\[ ⟨⟨a_i^\dagger b_j⟩⟩ → ⟨⟨a_i^\dagger b_j⟩⟩^{(0)} + ⟨⟨a_i^\dagger b_j⟩⟩^{(1)}. \]

In the normal phase and in the absence of the fictitious
field, the relevant zero order Green’s functions can easily be calculated,

\[ G_k^{aa}(\omega) = \langle a_k | a_k^\dagger \rangle_\omega^{(0)} = \frac{\delta_{k,k'}}{2\pi (\omega - \epsilon_k^a)}, \]
\[ G_k^{bb}(\omega) = \langle b_k | b_k^\dagger \rangle_\omega^{(0)} = \frac{\delta_{k,k'}}{2\pi (\omega - \epsilon_k^b)}, \]
\[ \langle a_k | b_k^\dagger \rangle_\omega^{(0)} = 0, \quad \langle a_k^\dagger | a_k \rangle_\omega^{(0)} = 0, \]
\[ \langle b_k^\dagger | b_k \rangle_\omega^{(0)} = 0, \]

and

\[ \langle a_k^\dagger | a_k \rangle_\omega^{(0)} = \langle b_k^\dagger | b_k \rangle_\omega^{(0)} = 0. \]

where \(\epsilon_k^a = \sum_i t_{ij}^a e^{i k \cdot r_j - i \omega t}, (\alpha = a, b).\)

The first order propagators should be obtained more
carefully. Let us consider the equation of motion for the first
order anomalous Green’s function,

\[ \frac{i}{\hbar} \frac{\partial}{\partial t} \langle a_i^\dagger(t) | b_j^\dagger(t') \rangle^{(1)} = - \sum_i \frac{1}{\hbar} \langle a_i^\dagger(t) | b_i^\dagger(t') \rangle^{(1)} \]
\[ - U \langle a_i^\dagger(t) | b_i^\dagger(t) | b_i(t) | b_i^\dagger(t') \rangle^{(0)} \]
\[ - g e^{i q \cdot r} e^{i \omega t} \langle b_i(t) | b_i^\dagger(t') \rangle^{(0)}, \]

where we neglected terms of second order in the perturbation
and used the equation for the zero order propagator
\(\langle a_i^\dagger(t) | b_j^\dagger(t') \rangle^{(0)}.\)

We decouple the higher order Green’s function in the spirit
of the RPA to obtain in the normal phase,
\[ \frac{\partial}{\partial t} \langle a_i^\dagger(t) | b_j^\dagger(t') \rangle \rangle \] 

where we absorbed the \( \omega_0 \) dependence in the Green’s function index. Notice that spatial translation invariance is lost due to the spatial dependence of the external field. Now, we go on to write the equations of motion for the other Green’s functions. Proceeding like before we arrive at the following equations:

\[ \langle a_i^\dagger(t) | b_k^\dagger(t') \rangle \rangle = \langle a_i^\dagger(t) | b_k^\dagger(t') \rangle \rangle \] 

where we have finally omitted the index \( t' \) because all the first order Green’s functions can be completely determined in terms of the zero order, equilibrium Green’s functions obtained previously. Finally, the inter-band anomalous Green’s function, can be written explicitly as

\[ \langle a_k^\dagger(t) | b_k^\dagger(t) \rangle \rangle = -\delta_{k+q,k} \frac{(U \delta \Delta^{ab}_q + g)}{2 \pi (\omega + \epsilon_k^a)(\omega + \omega_0 - \epsilon_k^{b+q})}. \] 

Since the first order propagators are given in terms of equilibrium Green’s functions, we can use the fluctuation-dissipation theorem [16] to obtain the correlation function \( \delta \Delta^{an} \) from the above anomalous Green’s functions. We get

\[ \delta \Delta^{ab}_q = \sum_k F_{\omega}(\langle a_k^\dagger | b_k^\dagger \rangle \rangle) \]

where \( F_{\omega}(G(\omega)) = -\int d\omega f(\omega)G(\omega+ie) - G(\omega-ie) \) is the statistical average of the discontinuity of the Green’s functions \( G(\omega) \) on the real axis [16]. The function \( f(\omega) \) is the Fermi–Dirac distribution.

We define the generalized inter-band susceptibility by

\[ \chi^{ab}_0(q, \omega) = \frac{1}{\Delta \chi^{ab}_0(q, \omega_0)} \left[ \frac{1}{(\omega + \epsilon_k^a)} \right] \]

where \( \chi^{ab}_0(q, \omega_0) \) is given by

\[ \chi^{ab}_0(2q, \omega_0) = \frac{1}{2\pi} \sum_k \left[ 1 - \frac{f(\epsilon_k^{a+q}) - f(\epsilon_k^{b+q})}{\epsilon_k^{a+q} - \epsilon_k^{b+q} - \omega_0} \right]. \]

Let us consider the case of a metal polarized by an external magnetic field \( h \). In this case the \( a- \) and \( b- \) bands are given by the dispersion relations of the up and down spin bands, respectively,

\[ \epsilon_k^{a,b} = h(k^2 - k_f^2) \frac{2m}{\hbar}, \]

where \( k_f \) is the original Fermi wavevector of the unpolarized band \( (h = 0) \). The mismatch of the new Fermi wavevectors is given by \( \delta k_f = k_f^a - k_f^b = h/v_F \), where \( v_F \) is the Fermi velocity. At zero temperature, the generalized susceptibility \( \chi^{ab}_0(2q, \omega_0 = 0) \) can be calculated and we get

\[ \chi^{ab}_0(2q, 0) = \rho \left[ 1 - \ln \left( \frac{\hbar}{v_F k_F} \right) - \frac{1}{2} \left( \frac{1}{\tilde{q}} + i \frac{1}{\tilde{q}} \right) + \ln(\tilde{q}^2 - 1) \right], \]

where \( \tilde{q} = v_F q / h = q / (k_f^a - k_f^b) \) and \( \rho = 3/(8\pi^3 E_F) \) is the density of states of the unpolarized system. The quantum critical point separating the normal metal from the superconducting PDW state is obtained from the condition

\[ \ln \left[ \frac{1}{\Delta_0} \right] \left( 1 - \ln \left( \frac{\hbar}{v_F k_F} \right) \right) + \ln(\tilde{q}^2 - 1) \right] = 0, \]

where \( \Delta_0 = v_F k_F \exp(-1/\rho U) \). Notice that a PDW state is only possible for \( \tilde{q} > 1 \). The equation above determines the critical field \( h_N \) (or mismatch) for a fixed value of \( \tilde{q} \). This is given by

\[ h_N = \frac{e}{\Delta_0} \left( \frac{1}{\tilde{q}} + \frac{1}{\tilde{q}} \right). \]

The maximum value of \( h_N \) for which the instability occurs is denoted by \( h_c \). It is easily obtained by differentiating \( h_N(\tilde{q}) \) with respect to \( \tilde{q} \). From the equation \( (\delta \ln h_N/\delta \tilde{q})_{\tilde{q}=\tilde{q}_c} = 0 \), we find that

\[ \tilde{q}_c = \frac{1}{2} \ln \left( \frac{\tilde{q} + 1}{\tilde{q} - 1} \right). \]

This gives \( \tilde{q}_c \equiv 1.2 \), that substituted in equation (12) for \( h_N \) yields

\[ h_c = h_N(\tilde{q}_c) \approx 1.5 \Delta_0. \]

This agrees with the results of Takada and Izyumura [22] for the vanishing of the FFLO phase starting from this phase.
As discussed in [13], an FFLO phase can also be induced by hybridization ($V$). The results above can be easily extended for the case of hybrid bands [13]. The Fermi wavevector mismatch is given by $k_{F}^0 - k_{F}^C = 4V/v_F(1+\alpha)$, where $\alpha < 1$ is the ratio of the effective masses of the quasi-particles. The mismatch is proportional to the hybridization $V$ (or pressure), which now plays the role of the magnetic field.

In order to study the fluctuations close to the PDW SQCP we have to expand equation (9) for small frequencies $\omega_0$, $h \cong h_C$ and $q \cong q_C$. At the same level of approximation as for $q$ of equation (10), we get for the denominator of the generalized susceptibility in equation (8)

$$1 - U\chi_{ab}^{0}(2q, \omega_0) = U\rho \left[ \frac{h - h_C}{h_C} + i \frac{\omega_0}{v_F q_C} + \frac{1}{q_C^2} - \frac{1}{q_C^2} (q - q_C)^2 \right].$$

The coupling of the superconductor order parameter to the electronic degrees of freedom gives rise to Landau damping of the superconductor quantum fluctuations. These modes are purely evanescent with an imaginary dispersion relation.

As in Hertz’s approach [19] to quantum phase transitions, we can construct from the dynamical susceptibility a quantum Gaussian action for this problem [21], which can be written as

$$S = \int d^d q \int d\omega [g + \omega + q^2] |\psi(q, \omega)|^2,$$

where $g = h - h_C$ measures the distance to the PDW SQCP, $\psi(q, \omega)$ is the PDW superconductor order parameter and $q - q_C \to q$. The scaling properties of the free energy associated with this action allow us to identify the dynamic exponent of the SQCP at which the FFLO instability occurs. This is easily found as $z = 2$. The knowledge of the dynamic exponent and the quantum hyperscaling relation [21, 23], $2 - \alpha = v(d+z)$, allows us to fully characterize the universality class of the FFLO quantum phase transition. Since $d_{\text{eff}} = d+z$, for $d = 2$ and 3, the critical exponents are Gaussian with possible logarithmic corrections for $d = 2$. The reason is that for $d \geq 2$, interactions between the fluctuations are irrelevant in the renormalization group sense and the Gaussian action, equation (14), gives the correct description of the quantum phase transition [21].

The next step in the calculations is to extend the results to finite temperatures and particularly to obtain the correction to the mean-field value of the shift exponent $\psi$ of the critical line at very low temperatures close to the PDW SQCP. $T_C(h) \propto |h - h_C|^{1/\psi}$. It turns out that $[24] \psi = z/(d + z - 2)$ for $d_{\text{eff}} > 4$ and can be determined from our knowledge of the dynamic exponent, which yields $\psi = 2/d$. In the same way, scaling [21] gives the contribution of quantum critical fluctuations to the specific heat, $C/T \propto T^{(d-2)/2}$, along the critical trajectory (CT) shown in figure 1. Also shown in this figure is the crossover line [21], $T_C \propto |h - h_C|$, below which the system enters a Fermi liquid regime. We have used that $v z = 1$ for $d \geq 2$.

We have studied the zero temperature instability of a normal two-band system with inter-band attractive interactions as the Fermi wavevector mismatch is reduced. The model describes a superconductor in an external field in the absence of orbital effects, a cold atom system with two atomic species or a two-band metal with mixing tuned by pressure. We find that as the mismatch of the Fermi wavevectors is reduced, the system becomes unstable to an inhomogeneous, FFLO-like, superconducting phase characterized by a wavevector $\bar{q} = \bar{q}_C$. We have introduced a new method to deal with systems coupled to a space and time dependent external field that respond adiabatically to this perturbation. The appearance of superconductivity is related to the divergence of a static generalized susceptibility for $\bar{q} = \bar{q}_C$ at an SQCP. The results obtained are valid to first order in the perturbation and coincide with those of linear response. However, in our approach the basic elements to be calculated are single-particle Green’s functions and not the usual two-particle propagators of linear response theory. The present theory extends the mean-field treatment to include fluctuations close to this SQCP. We have obtained the dynamical critical exponent at the PDW SQCP and from that we have identified the universality class of this quantum critical point for $d \geq 2$. This allows several predictions to be made for the thermodynamic and transport properties close to the quantum phase transition and for the shape of the critical line for dimensions $d \geq 2$.

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