Density Induced Quantum Phase Transitions in Triplet Superconductors

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We consider the possibility of quantum phase transitions in the ground state of triplet superconductors where particle density is the tuning parameter. For definiteness, we focus on the case of one band quasi-one-dimensional triplet superconductors but many of our conclusions regarding the nature of the transition are quite general. Within the functional integral formulation, we calculate the electronic compressibility and superfluid density tensor as a function of the particle density for various triplet order parameter symmetries and find that these quantities are non-analytic when a critical value of the particle density is reached.

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Triplet superconductivity is a very rare, but very rich phenomenon in condensed matter physics. The very few confirmed examples in nature include strontium ruthenate \(^1\) (a Ruthenium oxide) and the Bechgaard salt (TMTSF)\(_2\)PF\(_6\) \(^2\) (an organic molecular compound). Because the full confirmation of triplet superconductivity in solids has occurred only over the last few years, these lattice systems are not yet as fully studied theoretically and experimentally as \(^3\)He, their neutral liquid superfluid counterpart \(^3\). Unlike \(^3\)He, these systems are lattice charged superfluids, and their order parameters are intimately related to the lattice periodicity as in d-wave high critical temperature (\(T_c\)) superconductors \(^4\).

It is known experimentally that electronic properties and ground states of cuprate superconductors (d-wave singlet) \(^4\) and Strontium Ruthenate (p-wave triplet) \(^2\) are very sensitive to chemical doping while these properties for (TMTSF)\(_2\)PF\(_6\) (p-wave triplet) \(^2\) are very sensitive to both external pressure and chemical doping. However, recent experiments have demonstrated that it is possible to change the carrier density electrostatically in cuprate superconductors \(^4\) and amorphous Bismuth \(^5\) without the introduction of additional disorder that often occurs for chemical doping. It is likely that similar electrostatic techniques will be developed for use in other superconductors like Strontium Ruthenate or (TMTSF)\(_2\)X (with X = ClO\(_4\) or PF\(_6\)). Since it may be possible in the near future to tune the carrier concentration with the use of field effect techniques, some important theoretical questions concerning these three types of systems may soon receive an experimental answer. For instance, are there quantum critical points separating magnetic and superconducting order as a function of particle density? Or, are there quantum critical points within the superconducting phase as a function of particle density? In Fig. \(1\) we show the zero temperature density versus interaction phase diagram indicating the existence of quantum critical lines, where the order parameter does not change symmetry but the ground state topology changes. The elementary excitation spectrum also changes from gapless to gapped, and at finite temperatures there are three distinct regions the Fermi liquid, the pseudo-gap, and the Bose liquid regions.

In anticipation of experimental efforts, we propose to study the possible existence of topological quantum phase transitions in lattice triplet superconductors as a function of particle density. We focus on the specific case of the (TMTSF)\(_2\)X family, because they are a single-band triplet superconductors, unlike Strontium Ruthenate where three bands may be necessary to describe triplet superconductivity \(^2\). For this purpose, we study single band quasi-one-dimensional systems in an orthorhombic lattice with dispersion

\[
\epsilon_k = -t_x \cos(k_x a) - t_y \cos(k_y b) - t_z \cos(k_z c),
\]

where \(t_x \gg t_y \gg t_z\). We work with the Hamiltonian

\[
H = H_{\text{kin}} + H_{\text{int}},
\]

where the kinetic energy part is

\[
H_{\text{kin}} = \sum_{k,\alpha} \xi_k \psi_{k,\alpha}^\dagger \psi_{k,\alpha},
\]

with \(\xi_k = \epsilon_k - \mu\), where \(\mu\) may include the Hartree shift. The interaction part is

\[
H_{\text{int}} = \frac{1}{2} \sum_{kk'q} \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta}(\mathbf{k}, \mathbf{k'}) b_{\alpha\beta}^\dagger(k, \mathbf{q}) b_{\gamma\delta}(\mathbf{k'}, \mathbf{q}),
\]

with

\[
b_{\alpha\beta}^\dagger(k, \mathbf{q}) = \psi_{-k+q/2,\alpha}^\dagger \psi_{k+q/2,\beta},
\]

where the labels \(\alpha\), \(\beta\), \(\gamma\) and \(\delta\) are spin indices and the labels \(\mathbf{k}\), \(\mathbf{k}'\) and \(\mathbf{q}\) represent linear momenta. We use units where \(\hbar = k_B = 1\). In the case of weak spin-orbit coupling and triplet pairing, the model interaction tensor can be chosen to be

\[
V_{\alpha\beta\gamma\delta}(\mathbf{k}, \mathbf{k'}) = -|V_T| h_{\Gamma}(\mathbf{k}, \mathbf{k'}) \phi_{\Gamma}(\mathbf{k}) \phi_{\Gamma}^*(\mathbf{k'}),
\]

where \(\Gamma_{\alpha\beta\gamma\delta} = v_{\alpha\beta} \cdot v_{\gamma\delta}^\dagger / 2\) with \(v_{\alpha\beta} = (i\sigma y)_{\alpha\beta}\). \(V_T\) is a prefactor with dimensions of energy which characterizes a given symmetry. Furthermore, the term \(h_{\Gamma}(\mathbf{k}, \mathbf{k'}) \phi_{\Gamma}(\mathbf{k}) \phi_{\Gamma}^*(\mathbf{k'})\) contains the momentum and symmetry dependence of the interaction of the irreducible representation \(\Gamma\) with basis function \(\phi_{\Gamma}(\mathbf{k})\) and \(\phi_{\Gamma}^*(\mathbf{k'})\) representative of the orthorhombic group \((D_{2h})\).
A \text{ function that can touch the Brillouin zone boundaries the functions} \ d \text{ is characterized by one of the four states: (1) } |1\rangle, \text{ which means that the fermions are one dimensional and non-degenerate} \ [10], \text{ to the standard thermodynamic potential, and quasiparticle excitation spectrum by considering the vector order parameter for triplet superconductivity through the Hubbard-Stratanovich transformation and integrate out the fermions to obtain the effective action}

\[ S_{\text{eff}} = Q_G + \int_0^\beta d\tau \sum_{k_0} \frac{\xi_k}{2} - \beta^{-1} \text{Tr} \ln \left[ \frac{\beta M}{2} \right], \]

where \( Q_G = \int_0^\beta d\tau \sum_{i} \mathcal{D}_i^\dagger(\mathbf{q}, \tau) \mathcal{D}_i(\mathbf{q}, \tau)/|V| \) and \( M \) is the matrix

\[ M = \begin{pmatrix} \partial_{\tau} + \xi_k & \delta_{k_1 k_2} \delta_{\alpha \beta} & A(k_1, k_2, \tau) \\ A^\dagger(k_1, k_2, \tau) & \partial_{\tau} - \xi_k & \delta_{k_1 k_2} \delta_{\alpha \beta} \end{pmatrix}, \]

where \( A = -\sum_i \phi_\tau(\mathbf{k}_1 + k z_2, \tau) \mathcal{D}_i(k_1 + k z_2, \tau) \mathcal{D}_i(k_1 + k z_2, \tau) \). At the saddle point, \( \mathcal{D}_i(k_1 + k z_2, \tau) \) is taken to be \( \tau \) independent, and to have total Fermion center of mass momentum \( k_1 + k z_2 = 0 \). Thus, \( \mathcal{D}_i(k_1 + k z_2, \tau) = \eta \Delta \Gamma \delta_{k_1 + k z_2, 0} + \delta \mathcal{D}_i(k_1 + k z_2, \tau) \).

The order parameter equation is obtained from the stationary condition \( \delta S_{\text{eff}}^{(0)}/\delta \mathcal{D}_i^\dagger = 0 \), where \( S_{\text{eff}}^{(0)} \) is the saddle point action

\[ 1 = \sum_{k} |V| \mid \phi_\tau(k) \mid^2 \tanh(\beta E_k/2)/2E_k, \]

where \( E_k = \sqrt{\xi_k^2 + |\Delta \Gamma|^2} \), corresponds to the quasiparticle excitation energy. The number equation is obtained from \( N = -\partial \Omega/\partial \mu, \) where \( \beta \Omega = -\ln Z \) is the thermodynamic potential,

\[ N = N_0 + N_{\text{fluct}}, \]

where \( N_0 = \sum_k n_{k} \), and \( n_k = [1 - \xi_k \tanh(\beta E_k/2)/E_k] \) is the momentum distribution. The additional term \( N_{\text{fluct}} = -\beta \Omega_{\text{fluct}}/\partial \mu, \) where \( \Omega_{\text{fluct}} \) are Gaussian fluctuations to saddle point \( \Omega_0 \). These two equations must be solved self-consistently, and quite generally they are correct even in the strong coupling (or low density) regime provided that \( T < T_c \), where \( N_{\text{fluct}} \sim T^4 \) for all couplings \( \mathbf{R} \).

The saddle point vector \( \mathcal{D}_i^{(0)} = \eta \Delta \Gamma \) is related to the standard \( \mathbf{d} \)-vector via the relation \( \mathbf{d}(k) = \sum_k \mathcal{D}_i^{(0)} \phi_\tau(k) \). In the \( \mathcal{D}_{2h} \) point group all representations are one dimensional and non-degenerate \[ \text{[10]}, \] which means that the \( \mathbf{d} \)-vector in momentum space for unitary triplet states in the weak spin-orbit coupling limit is characterized by one of the four states: (1) \( 3A_{1u} \), with \( \mathbf{d}(k) = \eta \Delta \Gamma_{f \tau z} X Y Z \) ("fz" state); (2) \( 3B_{1u} \), with \( \mathbf{d}(k) = \eta \Delta \Gamma_{p \tau z} \) ("pz" state); (3) \( 3B_{2u} \), with \( \mathbf{d}(k) = \eta \Delta \Gamma_{p \tau n} \) ("pn" state); (4) \( 3B_{2u} \), with \( \mathbf{d}(k) = \eta \Delta \Gamma_{p \tau n} \) ("pn" state). Since, the Fermi surface can touch the Brillouin zone boundaries the functions \( X, Y, \) and \( Z \) need to be periodic and can be chosen to be \( X = \sin(k_\tau a), \) \( Y = \sin(k_\rho b), \) and \( Z = \sin(k_\phi c). \) The unit vector \( \eta \) defines the direction of \( \mathbf{d}(k) \). From here on we scale all energies by \( t_z \). The parameters used are \( t_x = 1.0000, \ t_y = 0.2144 \) and \( t_z = 0.0083. \) It will be easier to discuss the properties of the Fermi surface and quasiparticle excitation spectrum by considering the chemical potential \( \mu \) instead of the filling factor \( \bar{N}. \) Consider the "normal state" Fermi surface defined in the first Brillouin zone (BZ) by \( \xi_k = 0, \) keeping in mind the periodicity in \( k \)-space. Let us define the following characteristic values \( \mu_1^* \equiv t_x + t_y + t_z, \ \mu_2^* \equiv t_x + t_y - t_z, \ \mu_3^* \equiv t_x - t_y + t_z, \ \mu_4^* \equiv t_x - t_y - t_z. \) For \( \mu < \mu_1^* \) the chemical potential is below the bottom of the band and there is no Fermi surface. For \( \mu < \mu_2^* \) the Fermi surface consists of one connected sheet contained entirely in the first BZ and is topologically equivalent to a sphere of genus zero. For \( \mu_2^* < \mu < \mu_3^* \) the Fermi surface is one connected sheet touching the edges of the BZ on the planes \( k_\tau = \pm \pi \) equivalent to a torus of genus one. For \( \mu_3^* < \mu < \mu_4^* \) the Fermi surface is one connected sheet touching the edges of the BZ on the planes \( k_\tau = \pm \pi \)
and $k_y = \pm \pi$ equivalent to a torus of genus two. Lastly for $\mu^*_4 < \mu$, the Fermi surface consists of two disconnected sheets each of which touch the BZ boundary and is equivalent to two disconnected tori each of genus one.

For the superconducting state, the intersection of the Fermi surface and order parameter nodes constitute the loci of gapless quasiparticle excitations. For the $p_i$ symmetry (where $i$ is $x$, $y$, or $z$) the order parameter nodes are on the planes $k_i = 0, \pm \pi$. For the $f_{xyz}$ symmetry, the order parameter nodes are on the union of the planes $k_i = 0, \pm \pi$, where $i$ is $x$, $y$, and $z$. For all symmetries, the quasiparticle excitations are fully gapped for $\mu < \mu^*_1$ since there is no Fermi surface. For $\mu^*_1 < \mu < \mu^*_2$, the order parameter nodes for all symmetries intersect the Fermi surface and hence quasiparticle excitations are gapless. For $\mu^*_1 < \mu$ the Fermi surface splits into two sheets that separate along $k_z$ so that the $p_z$ nodes no longer intersect the Fermi surface opening a gap in the quasiparticle excitation spectrum. However, the $f_{xyz}$, $p_x$, and $p_y$ nodes still intersect the Fermi surface so quasiparticle excitations remain gapless.

We plot representative phase diagrams for the $f_{xyz}$ and $p_x$ symmetries in Fig. 1. From the discussion above, the $p_y$ and $p_z$ phase diagrams are qualitatively similar to the $f_{xyz}$ phase diagrams. There are three distinct phases characterized by Fermi surface connectivity and quasiparticle excitation spectrum: (1) no Fermi surface and fully gapped $E(k)$ for all symmetries ($\mu < \mu^*_1$), (2) one sheet Fermi surface and gapless for all symmetries ($\mu^*_1 < \mu < \mu^*_2$), (3a) two sheet Fermi surface and gapless for $f_{xyz}$, $p_y$ ($\mu^*_1 < \mu$) (3b) two sheet Fermi surface and fully gapped for $p_x$ ($\mu^*_2 < \mu$). In addition, the (2) phase splits into three regions using the finer classification of Fermi surface topological genus: (2i) genus zero ($\mu^*_1 < \mu < \mu^*_2$), (2ii) genus one ($\mu^*_2 < \mu < \mu^*_3$), (2iii) genus two ($\mu^*_3 < \mu < \mu^*_4$). There are several qualitative features of interest in the phase diagrams. For a fixed density and all symmetries, the chemical potential does not go below the bottom of the band ($\mu < \mu^*_1$) until a critical coupling is reached. This critical coupling is $V_{f_{xyz}}/t_x = 14.8021$, $V_{p_y}/t_x = 1.8150$, $V_{p_y}/t_x = 2.3952$, $V_{p_z}/t_x = 3.5052$ for $\bar{N} = 0$. In addition, consider the approach to the strict one-dimensional limit ($t_y, t_z \to 0$). If $t_z \to 0$, the $\mu^*_2$ ($\mu^*_3$) boundary merges with $\mu^*_1$ ($\mu^*_2$) leaving only the (2ii) region. If in addition $t_y \to 0$, the $\mu^*_1$ boundary merges with $\mu^*_2$ producing only one boundary between the (1) and (3) phases.

We now turn our attention to thermodynamic quantities that provide signatures of the topological changes discussed above. In the following calculations we fix the interaction strength to be $V_{f_{xyz}}/t_x = 91.7202$, $V_{p_y}/t_x = 11.8747$, $V_{p_y}/t_x = 11.7781$, $V_{p_z}/t_x = 10.8297$, which forces $\mu = \mu^*_1$ at $\bar{N} = 0.5$. In contrast, $\mu = \mu^*_1$ at $\bar{N} = 0.706$, $\bar{N} = 0.674$, $\bar{N} = 0.672$, $\bar{N} = 0.719$ for the $f_{xyz}$, $p_z$, $p_y$, $p_z$ symmetries, respectively. The $T = 0$

electronic compressibility $\kappa = N^{-2}(\partial N/\partial \mu)_{T,V}$ is

$$\kappa = \frac{2}{N^2} \sum_k \frac{1}{2E_k} \left( 1 - \frac{\xi^2_k}{E_k} \right),$$

(7)

which we plot in Fig. 2. Although the compressibility does not formally diverge, there are clear anomalies (non-analyticities) when the Fermi surface topology and quasiparticle excitation spectrum change. As $\bar{N}$ increases, $\mu$ increases and crosses the boundaries $\mu^*_i$ where the first derivative of $\kappa$ decreases discontinuously. Within the $p$-symmetries, the magnitude of this jump is largest for $p_x$. The $f_{xyz}$ symmetry, with the presence of double or even triple nodes compared to the single nodes for the $p$ symmetries, has the largest jumps in the derivative of $\kappa$ clearly identified as the four cusps in Fig. 2. These non-analyticities in $\kappa$ at $T = 0$ are indicative of a quantum phase transition. At finite temperatures the cusps in $\kappa$ are smeared-out, but clear peaks are still present so long as one remains in the quantum critical region. The measurement of the electronic compressibility may be achieved in a field effect geometry through the relation

$$\kappa = V C_d/Q^2,$$

(8)

where $C_d = [\partial Q/\partial V_e]_{T,V}$ is the differential capacitance, $V_e$ is the applied voltage, $Q$ is the absolute value of the total charge of carriers, and $V$ is the sample volume.

Next, we analyse the effect of phase fluctuations given by the action

$$\Delta S = \frac{1}{8} \sum_{q,\omega_n} [A(\omega_n)^2 + \rho_{ij} q_i q_j] \phi(q) \phi(-q),$$

(9)

where $A = N^2 \kappa/V$ is proportional to $\kappa$ and

$$\rho_{ij} = \frac{1}{V} \sum_k [n_k \partial_i \xi_k \partial_j \xi_k],$$

(10)

is the superfluid density. Here, $n_k$ is the momentum distribution. In Fig. 3 we show the $\bar{N}$ dependence of
the \( \tilde{\rho}_{\text{zz}} \) component of \( \rho_{ij} \). In the case of the \( D_{2h} \) group only diagonal components \( \rho_{ij} \) exist, but they are highly anisotropic due to the quasi-one-dimensionality of \( \xi_k \).

From Eq. (10) it is clear that the zero-temperature superfluid density is the curvature of the dispersion weighted by the momentum distribution. We find the \( xx \) component is a monotonically increasing function of \( \tilde{N} \) which is best understood as a consequence of quasi-one-dimensionality. Neglecting the curvature of the Fermi surface due to finite \( t_x \), \( t_y \), as \( \tilde{N} \) increases, the Fermi surface encloses a monotonically increasing pocket of \( k \)-space around \( k_z = 0 \). In addition, below half filling the curvature of \( \xi_k \) is of the same sign in this regime so there is little cancellation between different regions of \( k \)-space. We find \( \rho_{yy} \) is also smooth but peaks in the region bounded by \( \tilde{N} \approx 0.5 - 0.8 \) corresponding to \( \mu \approx \mu^* - \mu^s \). No longer neglecting the curvature of the Fermi surface due to finite \( t_y \), we see that for \( \tilde{N} \approx 0.5 - 0.8 \), the Fermi surface encloses an increasing pocket of \( k \)-space around \( k_y = 0 \) up to the edge of the BZ. Since the curvature of \( \xi_k \) changes sign at \( k_y = \pi/2 \), cancellations between different regions of \( k \)-space eventually occur. The \( zz \) component is the most interesting as it exhibits clear anomalies such as those seen in \( \kappa \). The Fermi surface varies rapidly along the \( k_z \) direction as a function of \( \tilde{N} \) so that no simple analysis in terms of contributing regions of \( k \)-space is possible. It appears that the \( \rho_{zz} \) is a more direct probe of the anomalies seen in \( \kappa \) with clear kinks as a function of \( \tilde{N} \). These non-analyticities again indicate the existence of a quantum phase transition as \( \mu \) is tuned below the bottom of the band.

Lastly, it is easy to extract from \( \Delta S \) the phase-only collective mode frequencies via the substitution \( i\omega_n \to \omega + i\delta \). In this case \( \omega(q) = \sqrt{(c_{xx} q_x^2 + c_{yy} q_y^2 + c_{zz} q_z^2)} \), where \( c_{xx} = \rho_{xx}/A \), \( c_{yy} = \rho_{yy}/A \), and \( c_{zz} = \rho_{zz}/A \). These collective mode frequencies also show similar anomalies to those of \( \kappa \) and \( \rho_{ij} \), and can be used to characterize the quantum phase transition as well [9]. Notice that \( \omega(q) \) is anisotropic reflecting the orthorhombic structure. For instance, \( \omega(q_x, 0, 0) = c_x q_x \), \( \omega(0, q_y, 0) = c_y q_y \), and \( \omega(0, 0, q_z) = c_z q_z \), where \( c_i \) is the speed of sound along the \( i \)-th direction. However, these modes may be plasmonized in a charged superfluid.

In summary, we studied possible quantum phase transitions in triplet superconductors, as the density of carriers is changed, provided that the Cooper pairing interaction is sufficiently attractive. For organic quasi-one-dimensional conductors (Bechgaard salts) only one quantum phase transition may be accessible experimentally as the interaction strength is too weak to cross both phase boundaries as a functions of filling factor (See Fig. 1). However, these quantum phase transitions may be possible in optical lattices where the attractive interaction may be changed via Feshbach resonances, thus allowing the system to cross the phase boundary separating the weak and strong interaction regimes [11]. In order to identify these quantum phase transitions (QPT) where the symmetry of the order parameter does not change, we classified Fermi surface topologies and excitation spectrum properties as a function of filling factor for weak spin-orbit coupling symmetries \( f_{xyz} \), \( f_z \), \( p_y \) and \( p_z \). We then related non-analyticities in the electronic compressibility and superfluid density to quantum phase transitions between various phases. We would like to thank NSF (Grant No. DMR-0304380) and NDSEG for support.

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