Quasiparticles in the vortex lattice of unconventional superconductors: Bloch waves or Landau levels?

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A novel singular gauge transformation is developed for quasiparticles in the mixed state of a strongly type-II superconductor which permits a full solution of the problem at low and intermediate fields, $H_{c1} < B << H_{c2}$. For a periodic vortex lattice the natural low-energy quasiparticle states are Bloch waves rather than Landau levels discussed in the recent literature. The new representation elucidates the physics considerably and provides fresh insights into the spectral properties of such systems.

In conventional (s-wave) superconductors the single particle excitation spectrum is gapped and, consequently, no quasiparticle states are populated at low temperatures. The situation is dramatically different in unconventional superconductors which exhibit nodes in the gap. These lead to finite density of fermionic excitations at low energies which then dominate the low-temperature physics. Among the known (or suspected) unconventional superconductors are high-$T_c$ copper oxides, organic and heavy fermion superconductors, and the recently discovered Sr$_3$RuO$_4$. Understanding the physics of the low-energy quasiparticles in the mixed state of these unconventional superconductors is an unsolved problem of considerable complexity. This complexity stems from the fact that (i) in the mixed state superconductivity coexists with the magnetic field $B$ and the quasiparticles feel the combined effects of $B$ and the spatially varying field of chiral supercurrents, and (ii) being composite objects, part electron and part hole, quasiparticles do not carry a definite charge. The corresponding low-energy theory therefore poses an entirely new intellectual challenge [1], which is simultaneously of considerable practical interest.

The initial theoretical investigations were based on numerical computations [3], semiclassical approximations [2] and general scaling arguments [3]. More recently Gorkov and Schrieffer [5] made a remarkable prediction of new singular gauge transformation is developed for quasiparticles in the mixed state of a strongly type-II superconductor which permits a full solution of the problem at low and intermediate fields, $H_{c1} < B << H_{c2}$. For a periodic vortex lattice the natural low-energy quasiparticle states are Bloch waves rather than Landau levels discussed in the recent literature. The new representation elucidates the physics considerably and provides fresh insights into the spectral properties of such systems.

At the heart of our approach is the observation that the collective response of the condensate to the external magnetic field on average exactly compensates its effect on the normal quasiparticles. More formally, the phase of the superconducting order parameter, $\Delta(r) = \Delta_0 e^{i\phi(r)}$, acts as an additional “gauge field” coupled to the quasiparticles. In the vortex state $\phi(r)$ is not a pure gauge: $\nabla \times \nabla \phi(r) = 2\pi \sum \delta(r - R_i)$ where $\{R_i\}$ denotes vortex positions. From the vantage point of a quasiparticle the singularities in $\nabla \times \nabla \phi$ act as magnetic half-fluxes concentrated in the vortex cores with polarity opposing the external field. Flux quantization ensures that on average this “spiked” field exactly cancels out the external applied field $B$. In the mixed state, the quasiparticle therefore can be thought of as moving in an effective field $B_{\text{eff}}$ which is zero on average but derives from a vector potential that is highly nontrivial. The nature of the phenomenon is purely quantum-mechanical, and is closely related to the Aharonov-Bohm effect: classical charged particle would be completely unaffected by the spiked field because the singularities occupy a set of measure zero in the real space.

Our solution consists in finding a gauge in which the Hamiltonian manifestly displays the physical property...
described above. In such a gauge the fermionic excitation spectrum can be found by band structure techniques suitably adjusted to the “off-diagonal” structure of the theory. Besides revealing the nature of the low-energy quasiparticles, this representation leads to new insights into the physics of the mixed state. One surprising finding is that in a perfectly periodic vortex lattice the original Dirac nodes survive the perturbing effect of a weak magnetic field.

We now supply the details. Quasiparticle wavefunction \( \Psi^{f}(r) = [u(r), v(r)] \) is subject to the Bogoliubov-de Gennes equation \( \mathcal{H}\Psi = E\Psi \), where

\[
\mathcal{H} = \left( \begin{array}{cc}
\hat{\mathcal{H}}_{c} & \Delta \\
\Delta^{\ast} & -\hat{\mathcal{H}}_{c}^{\ast}
\end{array} \right)
\]

(2)

with \( \hat{\mathcal{H}}_{c} = \frac{\hbar}{m} (p - \frac{\xi}{2} A) - \epsilon_{F} \) and \( \Delta \) the d-wave pairing operator. Following Simon and Le\[1\] we choose the coordinate axes in the direction of gap nodes, in which case \( \Delta = p_{F}^{2} \{ \hat{p}_{z}, \{ \hat{p}_{y}, \Delta(r) \} \} \), where \( p_{F} \) is the Fermi momentum, \( \hat{p} = -i\hbar \nabla \), and curly brackets represent symmetrization, \( \{ a, b \} = \frac{1}{2}(ab + ba) \). In high-\( T_{c} \) cuprates it is natural to concentrate on the low to intermediate field regime \( H_{\perp} < B \ll H_{c2} \), where the vortex spacing is large and we may assume the gap amplitude to be constant everywhere in space, \( \Delta(r) \simeq \Delta_{0} e^{i\phi(r)} \). Under such conditions the magnetic field distribution is described by a simple London model and superfluid velocity, defined as \( v_{s}(r) = \frac{\hbar}{m} \sum_{i} e^{i\mathbf{k} \cdot (r - \mathbf{R}_{i})} \),

(3)

where \( \lambda \) is the London penetration depth.

In order to diagonalize (2) it is desirable to remove the phase factors \( e^{i\phi(r)} \) from the off-diagonal components of \( \mathcal{H} \). This is accomplished by a unitary transformation

\[
\mathcal{H} \rightarrow U^{-1} \mathcal{H} U, \quad U = \left( \begin{array}{cc}
e^{i\phi_{c}(r)} & 0 \\
0 & e^{-i\phi_{h}(r)}
\end{array} \right),
\]

(4)

where \( \phi_{c}(r) \) and \( \phi_{h}(r) \) are arbitrary functions satisfying

\[
\phi_{c}(r) + \phi_{h}(r) = \phi(r).
\]

(5)

Eq. (4) can be thought of as a singular gauge transformation since it changes the effective magnetic field seen by electrons and holes. We now discuss three specific choices for the functions \( \phi_{c} \) and \( \phi_{h} \).

The most natural choice satisfying (4) is the symmetric one, namely \( \phi_{c}(r) = \phi_{h}(r) = \phi(r)/2 \), resulting in [1]

\[
\mathcal{H}_{S} = \left( \begin{array}{cc}
\frac{\hbar}{2m} (\hat{p} + mv_{s})^{2} - \epsilon_{F} \\
\frac{\hbar}{p_{F}} \hat{p}_{x} \hat{p}_{y} - \frac{\hbar}{2m} (\hat{p} - mv_{s})^{2} + \epsilon_{F}
\end{array} \right).
\]

This particular gauge makes the Hamiltonian very simple but unfortunately is not very useful because, as noted by Anderson [6] and in a different context by Balents et al. [12], the corresponding transformation (4) is not single valued. To see this, consider the situation on encircling the core of a vortex: \( \phi \) winds by \( 2\pi \) but \( \phi_{c} \) and \( \phi_{h} \) pick only a phase of \( \pi \), causing \( U \) to have two branches. Consequently, one is forced to diagonalize \( \mathcal{H}_{S} \) under the constraint that the original wavefunctions are single valued. Clearly, this is a difficult task. Nevertheless, the symmetric gauge reveals the physical essence of the problem: formally, \( \psi_{s} \) enters \( \mathcal{H}_{S} \) as an effective vector potential, which corresponds to an effective magnetic field \( B_{\text{eff}} = \frac{\hbar}{e} (\nabla \times \psi_{s}) \neq \mathbf{B} \). It is easy to show from Eq. (3) that \( B_{\text{eff}} \) vanishes on average \[13\], i.e. that \( (\nabla \times \psi_{s}) = 0 \), where angular brackets denote the spatial average. Aside from the single-valuedness problem, the low-energy physics described by \( \mathcal{H}_{S} \) is that of a quasiparticle in zero average magnetic field. The external field is compensated by the array of magnetic half-fluxes giving rise to a non-trivial vector potential with the periodicity of the vortex lattice.

To avoid the problem of multiple valuedness Anderson [6], suggested taking \( \phi_{c}(r) = \phi(r) \) and \( \phi_{h}(r) = 0 \). This leads to a Hamiltonian of the form [1]

\[
\mathcal{H}_{A} = \left( \frac{\hbar}{2m} (\hat{p} + \frac{\xi}{2} A) + 2mv_{s})^{2} - \epsilon_{F} \right) \frac{\hat{D}}{\hbar} - \frac{\hbar}{2m} (\hat{p} + \frac{\xi}{2} A)^{2} + \epsilon_{F} \right),
\]

with \( \hat{D} = \frac{\hbar}{p_{F}} (\hat{p}_{x} + \frac{\xi}{2} A_{x} + mv_{sx}) (\hat{p}_{y} + \frac{\xi}{2} A_{y} + mv_{sy}) \). In this representation one could consider neglecting in the first approximation the \( \psi_{s} \) terms, on the grounds that they represent a perturbative correction [1]. At low energies, expanding all the terms in \( \mathcal{H}_{A} \) to leading order near the nodes, the Hamiltonian becomes that of massless Dirac fermions in a uniform magnetic field \( \mathbf{B} = \nabla \times \mathbf{A} \) with the energy spectrum \[\mathcal{E}(k)\] given by Eq. (1). The effects of supercurrent field \( \psi_{s} \) can in principle be treated perturbatively. This is, however, difficult in practice, because of the massive degeneracy of the Landau levels and also because \( \psi_{s}(r) \) is not a small perturbation (it diverges as \( 1/r \) at the vortex cores) and will lead to strong LL mixing [9]. In the absence of a reliable scheme to incorporate \( \psi_{s}(r) \), the physical picture of Larmor precessing quasiparticle that leads to Eq. (4) appears incomplete.

We now introduce a new singular gauge transformation that combines the desirable features of the two transformations discussed above but has none of their drawbacks. Consider dividing vortices into two distinct subsets \( A \) and \( B \), each containing an equal number of vortices. Now denote by \( \phi_{A}(r) \) the phase field associated with vortices in the subset \( A \), with the analogous definition of \( \phi_{B}(r) \). The choice \( \phi_{c}(r) = \phi_{A}(r) \), \( \phi_{h}(r) = \phi_{B}(r) \) clearly satisfies the condition (4) and the corresponding transformation \( U \) is single valued. The resulting Hamiltonian is

\[
\mathcal{H}_{N} = \left( \frac{\hbar}{2m} (\hat{p} + mv_{s} A)^{2} - \epsilon_{F} \right) \frac{\hat{D}}{\hbar} - \frac{\hbar}{2m} (\hat{p} - mv_{s} B)^{2} + \epsilon_{F} \right),
\]

with \( \hat{D} = \frac{\hbar}{p_{F}} (\hat{p}_{x} + \frac{\xi}{2} (v_{s} A - v_{s} B)) [\hat{p}_{y} + \frac{m}{2} (v_{s} A - v_{s} B)] \) and

\[
\mathcal{H}_{N} = \left( \frac{\hbar}{2m} (\hat{p} + mv_{s} A)^{2} - \epsilon_{F} \right) \frac{\hat{D}}{\hbar} - \frac{\hbar}{2m} (\hat{p} - mv_{s} B)^{2} + \epsilon_{F} \right),
\]
nodes as described in Ref. [4] we obtain $H$ is the free Dirac Hamiltonian and where excitations. By linearizing becomes more transparent if we focus on the low-energy excitations. This property can be generalized to an arbitrary periodic lattice, such as e.g. triangular. We take vortices and apply to arbitrary distribution of vortices. In the following we illustrate the utility of the new Hamiltonian by finding the excitation spectrum in a periodic square vortex lattice. With minor modifications the same approach can be extended to an equation of the form

$$H = \left( \begin{array}{cc} v_F p_x & v_{\Delta} \hat{p}_y \\ v_{\Delta} \hat{p}_y & -v_F p_x \end{array} \right)$$

is the free Dirac Hamiltonian and

$$H' = m \left( \frac{1}{2} v_F v_{s}^{A} - v_{s}^{B} \right)$$

is the vector potential term, $v_F$ is the Fermi velocity and $v_{\Delta} = \Delta_0 / \hbar v_F$ denotes the slope of the gap at the node.

Our considerations so far have been completely general and apply to arbitrary distribution of vortices. In the following we illustrate the utility of the new Hamiltonian by finding the excitation spectrum in a periodic square vortex lattice. With minor modifications the same approach can be generalized to an arbitrary periodic lattice, such as e.g. triangular. We take A and B subsets to coincide with the two sublattices of the square vortex lattice as illustrated in Figure 1(a). Expanding the quasiparticle wavefunction in the plane wave basis $\Psi(r) = \sum_{q} \Psi_{q} e^{iq \cdot r}$ we arrive at an equation of the form

$$H_0(q)\Psi_q + \sum_{K} H'(K)\Psi_{q+K} = E\Psi_q.$$  

Because of its periodicity, $H'$ only has non-vanishing Fourier components at the reciprocal lattice vectors $K = 2\pi d (m_x, m_y)$, where $(m_x, m_y)$ are integers and $d = \sqrt{2\rho_0 / B}$ is the size of the unit cell. Aside from the $2 \times 2$ matrix structure, Eq. (6) is a standard Bloch equation which we solve by numerical diagonalization for $q$ vectors in the first MBZ, sketched in Figure 1(b).

As long as $\lambda \gg d$ the results are independent of $\lambda$ and the only free parameter in the low-energy theory is the Dirac cone anisotropy $\alpha_D = v_F / v_{\Delta}$. The band structure for the isotropic case, $\alpha_D = 1$ is presented in Figure 2. When compared to the unperturbed Dirac bands the periodic potential has precisely the expected effect of opening up band gaps at the MBZ boundaries. The surprising finding is that the magnetic field does not destroy the original nodal point, but merely renormalizes the slope of the dispersion. This finding can be understood as a consequence of the exact electron-hole symmetry of the linearized Hamiltonian $H_{H}$ (6). The associated DOS vanishes at the Fermi level, in contrast to the peak expected from the LL scenario (cf. Figure 2). The peaks which appear in DOS are van Hove singularities related to the band structure and have nothing to do with LL quantization at the Fermi level.

In Figure 3 we display the band structure for $\alpha_D = 20$, a value perhaps more relevant for the optimally doped YBa$_2$Cu$_3$O$_{7-\delta}$. The striking new feature is the formation of additional lines of nodes on the Fermi surface [see also Figure 1(b)] which give rise to a finite DOS at the Fermi surface. This structure can be understood by considering the $\alpha_D \rightarrow \infty$ limit (7). The lines of nodes first appear at $\alpha_D \approx 15$ and with increasing nodal anisotropy their number increases. This finding is consistent with the prediction of a finite residual DOS based on the semiclassical approach (6), which is expected to be valid when
\[ \Delta_0 \ll \epsilon_F, \text{ or equivalently } \alpha_D \gg 1. \] Qualitatively similar results are found for different orientations of the vortex unit cell with respect to underlying ionic lattice.

In conclusion, we have shown how the collective superfluid response of a superconductor ensures that the effective magnetic field \( B_{\text{eff}} \) seen by a fermionic quasiparticle (and distinct from the physical field \( B \)) is zero on average, even in the vortex state. The physics of a low energy quasiparticle in a superconductor with gap nodes is that of a massless Dirac fermion moving in a vector potential associated with physical supercurrents but zero average magnetic field. For a periodic vortex lattice the appropriate description is in terms of familiar Bloch waves. A mathematically equivalent description could be given (in a different gauge) in terms of Landau levels \( \frac{1}{2} \) strongly scattered by supercurrents \( \frac{3}{2} \). The fact that no trace of LL structure remains in the exact spectrum of excitations suggests that the former is a more useful starting point. The LL quantization remains a domain of relatively high fields \( \frac{2}{4} \). Our conclusions are corroborated by the absence of LL spectra in the numerical computations \( \frac{2}{4} \) as well as in the experimental tunneling data on cuprates \( \frac{5}{6} \) and are consistent with scaling arguments given previously \( \frac{5}{6} \).

In the present study we have focused on the leading low-energy, long-wavelength behavior of the quasiparticles as embodied by the linearized Dirac Hamiltonian \( \frac{1}{4} \) and \( \frac{5}{6} \). In real materials and at higher energies our results may be modified by the corrections to the linearization, electron-hole asymmetry, possible internode scattering, ionic lattice effects and the vortex core physics. These issues, as well as a more rigorous discussion of the singular gauge transformation, are best addressed within the framework of a tight binding calculation to be reported in a forthcoming publication.

We emphasize that the central idea of this paper, i.e. that upon proper inclusion of the condensate screening the quasiparticles experience effective zero average magnetic field, is completely general and robust against any effects of short length scale physics. Consequently, our method is applicable to any pairing symmetry and arbitrary distribution of vortices and could be useful for understanding the physics of vortex glass and liquid phases, as well as the zero-field quantum phase-disordered states such as the nodal liquid \( \frac{12}{13} \). We expect that disorder in the vortex positions will smear the structure apparent in Figures \( 2 \) and \( 3 \) resulting in smooth DOS. Of obvious interest are implications for the quasiparticle thermodynamics, transport and localization properties in statically disordered or fluctuating vortex arrays.

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