Hole core in superconductors and the origin of the Spin Meissner effect

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It is proposed that superconductors possess a hidden ‘hole core’ buried deep in the Fermi sea. The proposed hole core is a small region of the Brillouin zone (usually at the center of the zone) where the lowest energy states in the normal state reside. We propose that in the superconducting state these energy states become *singly occupied* with electrons of a definite spin helicity. In other words, that holes of a definite spin helicity condense from the top to the bottom of the band in the transition to superconductivity, and electrons of that spin helicity ‘float’ on top of the hole core, thus becoming highly mobile. The hole core has radius \( q_0 = 1/2\lambda_L \), with \( \lambda_L \) the London penetration depth, and the electrons expelled from the hole core give an excess negative charge density within a London penetration depth of the real space surface of the superconductor. The hole core explains the development of a spin current in the transition to superconductivity (Spin Meissner effect) and the associated negative charge expulsion from the interior of metals in the transition to superconductivity, effects we have proposed in earlier work to exist in all superconductors and to be at the root of the Meissner effect.

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**I. INTRODUCTION**

The Larmor diamagnetic susceptibility for carriers of density \( n \) in orbits of radius \( a \) is \([1]\)

\[
\chi_{\text{Larmor}}(a) = -\frac{ne^2}{4m_e c^2} a^2 \tag{1}
\]

It is remarkable that the normal state Landau diamagnetism of metals is described by this expression for normal state orbits of microscopic radius \( k_F^{-1} \):

\[
\chi_{\text{Landau}} = -\frac{1}{3}\mu_B g(\epsilon_F) = -\frac{ne^2}{4m_e c^2} k_F^2 = \chi_{\text{Larmor}}(k_F^{-1}) \tag{2}
\]

with \( k_F \) the Fermi wavevector, \( g(\epsilon_F) = 3n/2\epsilon_F \) the free electron density of states, and \( \mu_B = e\hbar/2m_e c \) the Bohr magneton. It is equally remarkable that the perfect diamagnetism of the superconducting state is described by the Larmor formula Eq. (1) for orbits of mesoscopic radius \( 2\lambda_L \):

\[
\chi_{\text{London}} = -\frac{1}{4\pi} = -\frac{ne^2}{4m_e c^2} (2\lambda_L)^2 = \chi_{\text{Larmor}}(2\lambda_L) \tag{3}
\]

with the London penetration depth \( \lambda_L \) given by the usual form\([2]\)

\[
\frac{1}{\lambda_L^2} = \frac{4\pi n_s e^2}{m_e c^2} \tag{4}
\]

and \( n_s = n \) the superfluid density. This suggests that (i) the transition to superconductivity involves an *expansion* of electronic orbits from radius \( k_F^{-1} \) to radius \( 2\lambda_L \), and (ii) that the superconducting ground state can be understood as being composed of all electrons \( (n_s = n) \) residing in orbits of radius \( 2\lambda_L \). The latter (iii) is supported by the observation that the angular momentum carried by the electrons in the Meissner current with velocity \( v_s \) in a cylinder of radius \( R >> \lambda_L \) and height \( h \) can be written in the two equivalent forms:

\[
L_{\text{Meissner}} = n_s(2\pi R\lambda_L h) \times (m_e v_s R) = n_s(\pi R^2 h) \times (m_e v_s(2\lambda_L)) \tag{5}
\]

The first form is the conventional description of electrons flowing in a surface layer of thickness \( \lambda_L \), hence cross-sectional area \( 2\pi R\lambda_L \), each moving in a circle of radius \( R \). The second form describes all electrons in the bulk, hence cross-sectional area \( \pi R^2 \), each moving in a mesoscopic orbit of radius \( 2\lambda_L \).

The proposition that the transition to superconductivity involves an expansion of electronic orbits from radius \( k_F^{-1} \) to radius \( 2\lambda_L \) provides a *dynamical* explanation of the Meissner effect through the Lorentz force acting on radially outgoing electrons\([3, 4]\), an effect which does not exist in the conventional theory of superconductivity. We have argued that the conventional theory is untenable\([5]\) because it cannot provide a dynamical explanation of the Meissner effect\([6]\) and because it leads to non-conservation of angular momentum\([7]\).

We showed in Ref.\([8]\) that in the absence of an applied magnetic field this orbit expansion in the presence of the ionic electric field will generate through the spin-orbit interaction a spin current near the surface of the superconductor, with carrier velocity given by

\[
v^\parallel_s = -\frac{h}{4m_e \lambda_L} \sigma \times \hat{n} \tag{6}
\]

with \( \hat{n} \) the normal direction to the surface of the superconductor (Spin Meissner effect). The spin current originates in the superposition of real space orbits of radius \( 2\lambda_L \) for electrons moving with speed Eq. (6), each electron thus carrying orbital angular momentum \( h/2 \).

Electronic orbit expansion and the associated radially outgoing electron flow lead to a non-homogeneous charge
distribution in the superconducting state, with extra negative charge near the surface, as proposed within the theory of hole superconductivity. New electrodynamic equations describe this scenario, that yield a definite relation between the magnitude of the expelled negative charge and resulting electric field in the interior of superconductors, and the velocity of carriers in the spin current Eq. (6) (Ref. 11, Sect. 4). These equations lead to the surprising prediction that the density of carriers of given spin orientation near the surface will change as a function of the magnitude of the applied magnetic field and resulting charge current (Ref. 11, Eq. 26c and 12), leading to a non-zero Knight shift in the superconducting state, consistent with experiments 13.

In addition, we have proposed in earlier work that the gap function in superconductors has a gap slope of universal sign (Ref. 11, Eq. 19 and Fig.7) (which manifests itself experimentally in an observed tunneling asymmetry of universal sign), which gives rise to a shift in the chemical potential in going from the normal to the superconducting state of magnitude determined by the slope of the gap function, and that superconductivity is driven by kinetic energy lowering and undressing of carriers from the electron-electron as well as from the electron-ion interaction.

In this paper we show that all these phenomena can be understood as arising from the existence of a hidden ‘hole core’ buried deep inside the Fermi sea of metals in the superconducting state.

II. HOLE CORE

If an electric field exists in the interior of superconductors (Ref. 11), it is only natural to expect that the Rashba spin-orbit interaction will play an important role. We assume that in the normal state electronic energies are given by the free electron dispersion relation \( \epsilon_k = \hbar^2 k^2 / 2m_e \) and that in the superconducting state spin-split bands develop, with dispersion

\[
\epsilon_{k\sigma} = \frac{\hbar^2 k^2}{2m_e} - \frac{\hbar^2}{2m_e} kq_0 \hat{\sigma} \cdot (\hat{k} \times \hat{n}).
\]  

(7)

where \( \hat{n} \) is the outward-pointing normal to the surface of the superconductor and

\[ q_0 = \frac{1}{2\lambda_L}. \]  

(8)

The energy dispersion Eq. (7) can be understood as arising from the Dirac spin-orbit interaction

\[
H_{s.o.} = -\frac{e\hbar}{4me^2c^2} \hat{\sigma} \cdot (E \times p)
\]  

(9)

with \( p = \hbar k \) and electric field

\[ E = 2\pi \rho_i r \]  

(10)

pointing outward (parallel to \( \hat{n} \)). The electric field Eq. (10) is the radial electric field generated at the surface of a cylinder of radius \( r = 2\lambda_L \) by the ionic charge density \( \rho_i = |e|n_s \) that compensates the superfluid electronic charge density \( en_s (n_s = \text{superfluid density}) \). The equality between Eqs. (9), (10) and the second term in Eq. (7) follows from using the usual relation for the London penetration depth Eq. (4). In this interpretation, the spin-orbit interaction can be understood as arising from the unscreened positive charge density \( |e|n_s \) acting on the macroscopic superfluid wave function. Instead, for a single electron in the presence of the electric field

\[ E_{m\hat{n}} = -\frac{\hbar c}{4e\lambda_L} \hat{n} \]  

(11)

that arises from charge expulsions, the Dirac spin-orbit interaction gives the second term in Eq. (7) reduced by the factor \( r_qq_0 \), with \( r_q = \hbar/2me_c \) the ‘quantum electron radius’.

The dispersion relation Eq. (7) gives rise to two ‘Rashba-like’ bands, given by

\[ \epsilon_k^1 = \frac{\hbar^2 k^2}{2m_e} - \frac{\hbar^2 kq_0}{2m_e} = \frac{\hbar^2}{2m_e}(k - q_0/2)^2 - \frac{\hbar^2 q_0^2}{8m_e} \]  

(12)

\[ \epsilon_k^2 = \frac{\hbar^2 k^2}{2m_e} + \frac{\hbar^2 kq_0}{2m_e} = \frac{\hbar^2}{2m_e}(k + q_0/2)^2 - \frac{\hbar^2 q_0^2}{8m_e} \]  

(13)

corresponding to spin orientations \( \hat{\sigma} \cdot (\hat{k} \times \hat{n}) = \pm 1 \). The bands are shown in Figure 1. There are negative energy states in band 1 in the range \( 0 < k < q_0 \). We postulate that as the system goes superconducting the spin-degenerate band splits into the two bands Eqs. (12), (13) and simultaneously the negative energy states in band 1 fill up with holes, driven by the Coulomb interaction. In other words, electrons in these negative energy states get ejected from the bulk of the superconductor towards the surface. The occupation of the bands in the Brillouin zone is shown in Figure 2. The gap between energy states in both bands for the same wavevector is

\[ \Delta_k = \frac{\epsilon_k^1 - \epsilon_k^2}{2} = \frac{\hbar^2 kq_0}{2m_e} \]  

(14)

as obtained in Ref. 4 using different arguments.

The carrier density for a two-dimensional free electron band structure is given by \( n_s = k_F^2 / 2\pi \), the Fermi energy by \( \epsilon_F = \hbar^2 k_F^2 / 2m_e \), the total energy (per unit area) by

\[ E = \frac{1}{\pi} \frac{\hbar^2}{2m_e} \]  

(15)

and the energy per particle by \( \epsilon = \epsilon_F / 2 = \hbar^2 k_F^2 / 4m_e \). For the spin-split bands, assuming no change in the density of particles, the new Fermi wavevectors are

\[ k_{F1} = \sqrt{\frac{k_F^2 - q_0^2}{4} + q_0 / 2} \]  

(16)
FIG. 1: Spin-split bands below $T_c$ given by Eqs. (12), (13). $k_F$ and $\epsilon_F$ are the Fermi wavevector and Fermi energy (chemical potential) in the normal state with energy dispersion relation indicated by the dot-dashed line. In the superconducting state the Fermi energy shifts down by $\nu$ and the Fermi wavevectors for the two Rashba bands are $k_{F1}$ and $k_{F2}$. The negative energy states in band 1 in the region $k < q_0$ are filled with holes as indicated by the + signs. Note that in the region $k_{F2} < k < k_{F1}$ only electrons of helicity $\vec{\sigma} \cdot (k \times \hat{z}) = 1$ exist.

$$k_{F2} = \sqrt{k_F^2 - q_0^2/4} - q_0/2$$

(17)

and the new Fermi energy is

$$\epsilon_{k_{F1}} = \epsilon_{k_{F2}} = \epsilon_F - \frac{\hbar^2 q_0^2}{4m_e} \equiv \epsilon_F - \nu$$

(18)

Thus, the Fermi energy (or chemical potential) is lowered by $\nu$ in the transition to superconductivity. This change in chemical potential as the system goes superconducting was derived within the theory of hole superconductivity as originating in the slope of the gap function

$$\nu = \frac{1}{2} \frac{\partial}{\partial k} (\Delta k)^2$$

(19)

and coincides with the result Eq. (18) derived here from the condition of constant density of particles.

The energy of electrons in the spin-split bands (per unit area) is given by

$$E_i = \frac{\hbar^2}{2m_e} \left( \frac{k_{F1}^i}{4} - \frac{\sigma_1 q_0 k_F^2}{3} \right)$$

(20)

with $\sigma_1 = 1$, $\sigma_2 = -1$. Thus, electrons in band 1 lower their kinetic energy upon spin splitting and those in band 2 raise their kinetic energy. The net change in energy per particle is

$$\Delta \epsilon = \frac{1}{n_s} (E - E_1 - E_2) = \frac{\hbar^2 q_0^2}{4m_e} = \nu$$

(21)

in agreement with the result obtained in Ref.4 using entirely different arguments. Eq. (21) is the condensation energy per particle in the superconducting state. Thus, the condensation energy in this model can be interpreted as arising from kinetic energy lowering (in band 1), in agreement with previous considerations.

The number density in each band is given by

$$n_1 = \frac{n_s}{2} + \frac{q_0 k_F}{4\pi} - \frac{q_0^2}{4\pi}$$

(22)

$$n_2 = \frac{n_s}{2} - \frac{q_0 k_F}{4\pi}$$

(23)

The last term in Eq. (22) is the missing density of carriers in the negative energy states, which we argue is expelled to the surface of the superconductor

$$n_{exp} = \frac{q_0^2}{4\pi}$$

(24)
The speed of carriers in the spin-split bands is given by $v_k = (1/\hbar)\partial k^2/\partial k$, hence

$$v^1_k = \frac{\hbar}{m_e} (k - \frac{q_0}{2})$$

(25)

$$v^2_k = \frac{\hbar}{m_e} (k + \frac{q_0}{2})$$

(26)

Therefore, the speed of the carriers at the large Fermi surface is the same for both bands ($v^1_{kF1} = v^2_{kF2}$). However, at the small Fermi surface ($k = q_0$) we have

$$v^1_k = \frac{\hbar q_0}{2m_e} = v^0 \sigma$$

(27)

Thus, we can interpret Eq. (27) as the spin current speed of the condensate as a whole. In a cylindrical geometry, the carriers near the surface with spin orientation parallel or antiparallel to the cylinder axis will have a ‘drift’ velocity given by $\pm v^0 \sigma$ parallel to the surface and perpendicular to the cylinder axis, as proposed in our paper on the Spin Meissner effect based on entirely different arguments.

When a charge current circulates, we argue that it is only the electrons in band 1 that shift their occupation. This is based on the fact that experiments on rotating superconductors can be interpreted as indicating that the superconducting current is carried by completely ‘undressed’ electrons, suggesting that a shift in the small Fermi surface describing long wavelength free-electron-like carriers is involved. Hence we assume that the current density is given by

$$J_s = e_n \frac{v^1_s}{2} = -\frac{n_s e^2}{m_e c} \lambda_L B$$

(28)

involving only half the superfluid density ($n_s/2$) corresponding to the carriers in band 1, moving with superfluid velocity $v^1_s$. The second equality in Eq. (28) follows from London’s equation. Thus Eq. (28) yields for the drift speed of the carriers in band 1

$$v^1_s = \frac{2e}{m_e c} \lambda_L B$$

(29)

corresponding to a shift in their wavevector

$$\Delta q = \frac{m_e}{\hbar} v^1_s = \frac{2e}{h c} \lambda_L B$$

(30)

When the wavevector shift reaches the value $q_0$ the small Fermi surface crosses the origin and it is reasonable to expect that this corresponds to the critical value of magnetic field where superconductivity will be destroyed. Eq. (30) then yields for the critical field (when $\Delta q = q_0$)

$$B_c = -\frac{\hbar c}{4e \lambda_L^2}$$

(31)

which is essentially $H_{c1}$, the lower critical field of type II superconductors. The result Eq. (31) coincides with the result obtained analyzing the Spin Meissner effect based on entirely different arguments. Figure 3 shows the occupation of the bands in the presence of a charge current.

In connection with the Spin Meissner effect we showed that the spin current with speed Eq. (6) develops when carriers expand their orbits from a microscopic length to radius $2\lambda_L$ and are deflected azimuthally by the spin-orbit interaction. This corresponds in the current scenario to the dropping of holes in band 1 from the top to the bottom to form the hole core. The two representations of the same physics are shown in Fig. 4. Furthermore we showed in refs. [3, 4] that the orbit expansion in the presence of a magnetic field gives rise to the charge current needed for the Meissner effect, and argued that the orbit expansion is driven by kinetic energy lowering. Clearly, in the current scenario this corresponds to the carriers in band 1 developing a charge current as the holes condense from the top of the band to the hole core in the presence of a magnetic field, with the kinetic energy of carriers in band 1 being lowered as described by Eq. (21).

The scenario depicted in Fig. 3 also shows that when a charge current circulates the magnetization of the system will change. Assuming that the ejected electrons from the states indicated by ‘+’ in Fig. 3 represent the excess electrons giving rise to the negative charge density $\rho_-$ predicted to exist near the surface by the modified electrodynamic equations. Fig. 3 shows that as the critical magnetic field is approached the excess electrons...
expelled charge density for spin different arguments. We found in that work that the by the electrodynamic analysis of ref. [11] using entirely zero (since all the holes have moved to the branch on the density of opposite spin orientation has been depleted to have the same spin orientation, and the excess electron moving in direction opposite to the charge current all in the hole core indicated schematically.

FIG. 4: In real space, orbits expand from a microscopic length to radius $2\lambda_L$ (upper left). The upper right picture shows the electronic orbits in a cylinder viewed along the axis, electrons with spin out of (into) the paper circulate clockwise (counterclockwise) with speed $v^0_\sigma$ (Eq. (1)). The lower left panel shows pairs of holes of helicity $\hat{\sigma} \cdot (\hat{k} \times \hat{n}) = 1$ dropping from the top of band 1 to the bottom to form the hole core, shown in the lower right panel, with directions for $\mathbf{k}$ and $\hat{\sigma}$ for holes in the hole core indicated schematically.

moving in direction opposite to the charge current all have the same spin orientation, and the excess electron density of opposite spin orientation has been depleted to zero (since all the holes have moved to the branch on the right in Fig. 3). This is precisely the situation predicted by the electrodynamic analysis of ref. [11] using entirely different arguments. We found in that work that the expelled charge density for spin $\hat{\sigma}$ is

$$\rho_\sigma = \frac{en_s v^0_\sigma}{2c} \frac{1}{8\pi \lambda_L} \hat{\sigma} \cdot \hat{B}$$

(32)

so that the expelled charge density for $\hat{\sigma}$ parallel to $\hat{B}$ goes to zero at the critical field Eq. (31), in agreement with Fig. 3. The variation of spin density with magnetic field indicates that the superconducting state has a triplet component and will give rise to a non-zero Knight shift at zero temperature [12]. It is remarkable that the electrodynamic analysis of Ref. [11] predicted this ‘Edelstein effect’ [28], which we can now understand as originating in the locking of spin and momentum variables in the Rashba-like bands.

Finally we would like to show that the expelled electrons from the negative energy states of band 1 correspond to the excess negative charge near the surface derived from the electrodynamic equations, given by [11]

$$\rho_- = en_s v^0_\sigma \frac{1}{c}.$$  

(33)

This excess charge is distributed over a surface layer of thickness $\lambda_L$, hence the ‘surface charge density’ $\Sigma$ is

$$\Sigma = \rho_- \lambda_L = en_s \frac{\hbar}{4m_e c}$$

(34)

The charge content of the hole core (Eq. 24) is

$$n_{exp} = \frac{q_0^2}{4\pi} = n_s \frac{\hbar}{4m_e c} \frac{e^2}{\hbar c} = (\Sigma/e) \times \alpha$$

(35)

with $\alpha = e^2/\hbar c = 1/137$ the fine structure constant. Thus, Eq. (35) implies that the expelled negative charge density $\rho_-$ originates in the hole core of 137 lattice planes, which itself is of the order of $\lambda_L$, as first suggested by Slater [29].

Alternatively we can argue: if $\Delta z$ is the spacing between lattice planes parallel to the surface, the three-dimensional charge density resulting from Eq. (24) is

$$n_{exp} = \frac{q_0^2}{4\pi \Delta z}$$

(36)

and setting $n_{exp} = \rho_-/e$ yields $\Delta z = \alpha \lambda_L$. Taking for the spacing between lattice planes $\Delta z = 2a_0$, with $a_0 = \hbar^2/m_e e^2$ the Bohr radius yields

$$n_s = \frac{1}{2\pi (2a_0)^3} \frac{1}{\alpha \lambda_L}$$

(37)

corresponding, for a simple cubic lattice of lattice constant $a = 2a_0$, to a band filling $1/2\pi = 0.16$ holes per atom, an almost filled band, consistent with the assumptions of the theory of hole superconductivity.

### III. DISCUSSION

Within the theory of hole superconductivity, negative charge is expelled from the interior to the surface of a metal in the transition to superconductivity. A spin current exists in the superconductor near the surface, and the superconducting state can be understood as a superposition of electronic orbits of radius $2\lambda_L$. Superconductivity is driven by kinetic energy lowering, the chemical potential drops in the transition to superconductivity by an amount $\nu$ related to the slope of the gap function versus energy which has universal sign, and $\nu$ also gives the condensation energy per carrier. The spin density near the surface varies with the applied magnetic field and associated superfluid velocity. Carriers ‘undress’ from the electron-ion interaction, expand their wavelength and become free-electron-like as the system becomes superconducting.

All these properties were deduced in earlier work based on different arguments. In this paper we have shown that they can all be understood within a scenario where a ‘hole core’ of radius $q_0 = 1/2\lambda_L$ with hole carriers of helicity $\hat{\sigma} \cdot (\hat{k} \times \hat{n}) = 1$ develops at the bottom of the electronic energy band. The direction $\hat{n}$ is the direction of the interior
electric field pointing towards the closest surface. The electric field arises due to negative charge being expelled from the hole core states to the surface of the superconductor. Thus, the scenario proposed here is consistent with and supports the Spin Meissner effect scenario\cite{3} and its relation with negative charge expulsion deduced from the electrodynamic equations\cite{11}. The ‘hole core’ is the k-space representation of this physics.

Note that in the scenario proposed here, ‘Cooper pairs’ formed by time-reversed carriers, $(\mathbf{k} \uparrow, -\mathbf{k} \downarrow)$, are essential, with the spin directions $\uparrow$ and $\downarrow$ corresponding to $\hat{\sigma} \cdot (\hat{k} \times \hat{n}) = \pm 1$ rather than being fixed in space. Note also that the number of holes in the hole core is only $\sim 10^{-6}n_s$, so that the energy cost in promoting those electrons to the Fermi energy is only of order $\mu eV$ per superfluid electron.

We believe that a full description of the superconducting state of matter has to include the physical elements discussed here (which are not part of conventional BCS theory) and that this physics should be experimentally verifiable. In a planar geometry, the direction of the electric field in the interior and the direction of the majority electron spin for given $\mathbf{k}$ direction is shown in Fig. 5. The k-space scenario shown in Figure 2 should be testable by high resolution spin-resolved angle-resolved photoemission\cite{30,31}, keeping in mind that depending on the particular band structure the location of the spin-split regions could be different from those shown in Figure 2.

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