

Two-dimensional superconductivity with strong spin-orbit interaction

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We consider superconductivity confined at a two-dimensional interface with a strong surface spin-orbit (Rashba) interaction. Some peculiar properties of this system are investigated. In particular, we show that an in-plane Zeeman field can induce a supercurrent flow.

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Most superconductors have their underlying crystal structures and the normal states obeying inversion symmetry. This symmetry allows the classification of superconductors¹⁻³ into singlet and triplet pairing, and correspondingly even and odd symmetry of the order parameter under sign change of momentum $\vec{p} \rightarrow -\vec{p}$, i.e., the opposite sides of the Fermi surface. This classification has played an important role in our current understanding of superconductors and their properties. Most “conventional” superconductors such as Nb and Pb are singlet *s* wave,⁴ oxide superconductors are likely to be singlet *d* wave,⁵ whereas superfluid ³He is triplet *p* wave.⁶

When inversion symmetry is absent in the normal state, such classification is no longer possible. The superconducting pairing can thus be neither singlet nor triplet,⁷ and the order parameter neither even nor odd under $\vec{p} \rightarrow -\vec{p}$. The superconductor can, therefore, have rather peculiar physical properties when compared with those where the above-mentioned classification can be made. This absence of inversion symmetry may be relevant to some known superconductors (see also references cited in Ref. 8). An examination of the list of superconductors in Table 6.1 of Ref. 9 shows that, e.g., Mo₃Al₂C (symmetry *P4*₁32), La₅B₂C₆ (symmetry *P4*), and Mo₃P (symmetry *I* $\bar{4}$) are all without inversion centers. Furthermore, two-dimensional (2*d*) surface superconductivities have been induced by gate electric potentials in C₆₀ and some molecular crystals in the field-effect-transistor geometry.^{10,11} There is no inversion symmetry in these cases since “up” and “down” are different due to the electric gates, substrates, etc.

Some properties of superconductors without inversion centers have already been studied theoretically before (see Refs. 7 and 8, and references therein). For definiteness and motivated by the last mentioned examples above, we here consider, as in Refs. 7 and 8, a 2*d* superconductor at an interface with no up-down symmetry. As pointed out there, one potentially important effect due to the lack of inversion symmetry in such a geometry is the existence of a surface spin-orbit coupling or Rashba¹² term in the Hamiltonian of the form $-\alpha\hat{n} \times \vec{p} \cdot \vec{\sigma}$. Here \hat{n} is the surface normal and $\vec{\sigma}$ are the Pauli spin matrices. This term acts like an effective magnetic field along $\hat{n} \times \vec{p}$ and thus splits the spin degeneracy of the electrons at a given momentum \vec{p} . The energy difference near the Fermi level can be large: in some systems it is known to be of order 0.1 eV (Ref. 13), and is, therefore, expected to be much larger than the superconducting gap Δ

even for a transition temperature ~ 100 K. Rashba splitting of this magnitude hence is expected to have dramatic effects on the superconducting properties in these systems. Some physical consequences due to this spin-orbit coupling term have been considered in Refs. 7 and 8, using Green’s function approach. Gor’kov and Rashba⁷ calculated the spin susceptibility in this system. Edelstein⁸ pointed out an interesting magnetoelectric effect, that a spin polarization can be induced by a supercurrent flow. Here we shall reconsider these physical properties under the most probable case, where

$$\frac{p_F^2}{2m} \gg \alpha p_F \gg |\Delta| \quad (1)$$

using simple physical arguments. [Here p_F is the Fermi momentum and m is the effective mass. The definition of p_F will be made more precise below.] In addition, we give a more complete description of the magnetoelectric effect in this system. More precisely, we shall show the existence of an inverse effect, i.e., a supercurrent can be induced by an applied Zeeman field. The relation of this effect to that proposed by Edelstein and the possibility of its experimental observation is discussed.

We shall then consider a two-dimensional electronic system lying in the *x*-*y* plane. The one-body part of the Hamiltonian is given by

$$H^{(1)} = \frac{p^2}{2m} - \alpha \hat{n} \times \vec{p} \cdot \vec{\sigma} \quad (2)$$

with $\hat{n} = \hat{z}$. We shall first summarize some consequences of Eq. (2) that we shall need below. As mentioned, the effect of the Rashba term is like a Zeeman field along $\hat{n} \times \vec{p}$. The eigenstates of this spin-dependent part of the Hamiltonian thus correspond to states with spins along and opposite to this direction. We shall label these spin states by $|\vec{p}, +\rangle$ and $|\vec{p}, -\rangle$, respectively. The spinors for these states can be chosen to be (by rotating those for an up and down spin by $-\pi/2$ along \hat{p}),

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ ie^{i\phi_{\vec{p}}} \end{pmatrix} \quad \text{and} \quad \frac{1}{\sqrt{2}} \begin{pmatrix} ie^{-i\phi_{\vec{p}}} \\ 1 \end{pmatrix}, \quad (3)$$

where $\phi_{\vec{p}}$ is the angle between \hat{p} and the \hat{x} axis in the plane. The energy of these states at a given momentum \vec{p} are given

by $\epsilon_{p\pm} = p^2/2m \mp \alpha|p|$. For chemical potential $\bar{\mu}$, the $|+\rangle$ and $|-\rangle$ bands are filled up to Fermi momenta $p_{F\pm} = [(2m\bar{\mu}) + m^2\alpha^2]^{1/2} \pm m\alpha$. The velocities of the particles are $d\epsilon_{p\pm}/dp = p/m \mp \alpha$ and different for the $|\vec{p}, +\rangle$ and $|\vec{p}, -\rangle$ particles. However, at their respective Fermi momenta the Fermi velocities v_{F+} and v_{F-} are equal and given by $[2\bar{\mu}/m + \alpha^2]^{1/2}$. The density of states at $\bar{\mu}$ for the bands are

$$N_{\pm}(0) = (1/2\pi\hbar^2)[p/(d\epsilon_{p\pm}/dp)] \\ = (m/2\pi\hbar^2)\{1 \pm \alpha/[(2\bar{\mu}/m) + \alpha^2]^{1/2}\}.$$

They differ slightly [under condition (1)] by a relative amount of order $\alpha/\bar{\mu}$. In the absence of spin-orbit coupling ($\alpha=0$) they are both given by $N^0(0) = m/2\pi\hbar^2$.

Let us first consider the spin susceptibility of this system in the normal state. For comparison, we note that the spin susceptibility χ^0 in the absence of spin-orbit interaction is isotropic and given by $(m/\pi\hbar^2)\mu^2$, here μ is the magnetic moment. This result can be obtained by elementary considerations, which, however, we shall summarize since we shall use this type of argument repeatedly below. Under a magnetic field B , the energy of spins aligned (antialigned) with the field is lowered (increased) by μB . Since the density of states is $m/2\pi\hbar^2$, the number of particles (per unit area) for these two species are changed by $\pm(m/2\pi\hbar^2)\mu B$, respectively, giving a total magnetic moment of $(m/\pi\hbar^2)\mu^2 B$ and hence the Pauli susceptibility given above.

Now we return to the case with $\alpha \neq 0$. Consider first a magnetic field B perpendicular to the plane (along \hat{z}). Since the spins are originally in the plane, there are no Zeeman energy and thus population changes for either species. The Pauli part of the spin susceptibility χ_{\perp}^P , therefore, vanishes. However, there is also a Van Vleck contribution χ_{\perp}^V . Under the \hat{z} Zeeman field, the $|+\rangle$ state is modified to become

$$|+\rangle' = |+\rangle + \frac{|-\rangle\langle -|\sigma_z|+\rangle\mu B}{2\alpha p} \quad (4)$$

according to perturbation theory. The expectation value of the \hat{z} magnetic moment is given by $\langle +|\sigma_z|+\rangle = (\mu^2 B/\alpha p)$ [using the spinors in Eq. (3)]. Similar expressions apply to $|-\rangle$. A net magnetic moment is present at momentum \vec{p} if $|+\rangle$ is occupied whereas $|-\rangle$ is not. The total magnetic moment of the system is, therefore, given by

$$M_z^V = \frac{1}{2\pi\hbar^2} \int_{p_{F-}}^{p_{F+}} dp p \frac{\mu^2 B}{\alpha p} \\ = \frac{\mu^2}{2\pi\hbar^2} \frac{p_{F+} - p_{F-}}{\alpha} B. \quad (5)$$

Using the expressions for $p_{F\pm}$, we obtain $\chi_{\perp}^V = (m/\pi\hbar^2)\mu^2 = \chi^0$, the same spin susceptibility in the absence of spin-orbit coupling.

Now consider a magnetic field in the plane, e.g., along the \hat{y} axis. To calculate the spin susceptibility it is convenient, for each momentum \hat{p} , to resolve \vec{B} into components parallel and perpendicular to the momentum direction \vec{p} (see Fig. 1).

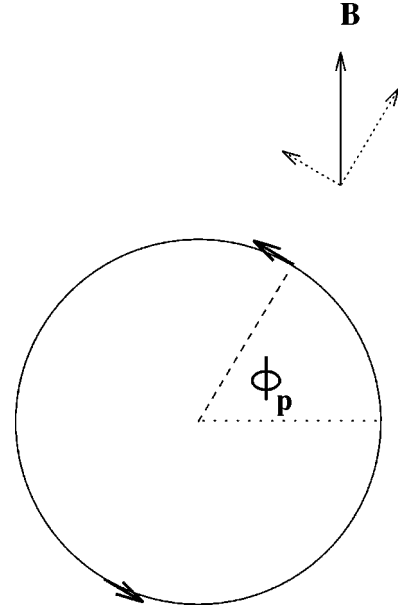


FIG. 1. (1) Spin directions (thick arrows) on the $|+\rangle$ fermi surface at two representative (equal and opposite) momenta. These two electrons form a pair in the superconducting state. (2) An applied magnetic field \vec{B} is resolved into components parallel and perpendicular to the spin direction. The $|-\rangle$ spins are not shown in this figure.

The former (latter) field is perpendicular (parallel) to the original spin direction, and can only give rise to a Van Vleck (Pauli) contribution to the net magnetic moment. One easily finds, using arguments as in the last two paragraphs, the results

$$\chi_{\parallel}^P = [N_+(0) + N_-(0)]\mu^2/2 = \chi^0/2 \quad (6)$$

and

$$\chi_{\parallel}^V = \chi^0/2. \quad (7)$$

The $1/2$ in Eqs. (6) and (7) are due to angular averages. We obtain finally $\chi_{\parallel} = \chi_{\parallel}^V + \chi_{\parallel}^P = \chi^0$. Hence the spin susceptibility is not affected at all by the Rashba term. This result has been obtained also in Ref. 7.

Now we consider the superconducting state. We shall consider the case where the Cooper pairing occurs between the $\pm\vec{p}$ particles from the same band, i.e., between $|\vec{p}, +\rangle$ and $|-\vec{p}, +\rangle$, on the one hand, (see Fig. 1) and between $|\vec{p}, -\rangle$ and $|-\vec{p}, -\rangle$, on the other. We shall also limit ourselves to the case where the energy gaps Δ_{\pm} may be different for the two bands but isotropic in momentum space. That the pairing occurs only within the same band is reasonable since we assume that the energies associated with the pairing Δ_{\pm} are much less than the energy separation between the two bands $2\alpha p_{F\pm}$ for a given momentum \vec{p} near $p_{F\pm}$ [see Eq. (1)]. The assumption of this pairing is consistent with that in Ref. 7. We shall not justify it here and shall simply consider its physical consequences. Situations where Δ_{\pm} are \hat{p} dependent seem also possible and the following results can be generalized to these cases by simple arguments.

Consider now the spin susceptibility in the superconducting state, first for a magnetic field perpendicular to the plane. In this case argument as in the normal state shows that the Pauli susceptibility vanishes. The Van Vleck susceptibility, being generated by virtual processes to states with energy separations much larger than Δ_+ [if Eq. (1) applies], is little affected. We get, therefore, $\chi_{\perp}^V(T) = \chi_{\perp}^V(T > T_c) = \chi^0$ and thus $\chi_{\perp} = \chi^0$ independent of the superconducting transition.

Now consider a magnetic field in the plane. For the contribution from the pair $\pm \vec{p}$, we argue as in the normal state and resolve the magnetic field into components parallel and perpendicular to \hat{p} . The former again gives only a Van Vleck contribution unaffected by the superconducting transition, thus the total Van Vleck susceptibility $\chi_{\parallel}^V(T) = \chi^0/2$ as in the normal state. The field component perpendicular to \hat{p} again gives only a Pauli contribution, which can be evaluated by arguments as in the case of superfluid ^3He .⁶ Consider first the $|+\rangle$ band. In the absence of the magnetic field the Hilbert space for $\pm \vec{p}$ consists of four possible states: ground pair with energy 0, (two) broken pair with energy $E_{p+} = \sqrt{\xi_{p+}^2 + |\Delta_+|^2}$ [here $\xi_{p+} \equiv \epsilon_{p+} - \bar{\mu}$ is the normal state quasiparticle energy relative to the chemical potential] corresponding to occupied (empty) $|\vec{p}, +\rangle$ and empty (occupied) $|-\vec{p}, +\rangle$, and excited pair with energy $2E_{p+}$. Under the magnetic field, these energies are modified to become 0, $E_p - h_p$, $E_p + h_p$, $2E_p$ where $h_p = \mu B \cos \phi_p$, since the magnetic moment of $|\vec{p}, +\rangle$ along the field is $\mu \cos \phi_p$. (We are leaving out the $+$ subscripts for the moment for easier writing.) The net magnetization along the field direction is, therefore,

$$(\mu \cos \phi_p) \{ \exp[-(E_p - h_p)/T] - \exp[-(E_p + h_p)/T] \} / Z, \quad (8)$$

where $Z \equiv 1 + \exp[-(E_p - h_p)/T] + \exp[-(E_p + h_p)/T] + e^{-2E_p/T}$ is the partition function. For small magnetic field, this reduces to $\mu^2 B \cos^2 \phi_p (1/4T) \text{sech}^2(E_p/2T)$. The total magnetization of the $|+\rangle$ band is given by summing over \vec{p} , which is the same as multiplying by $\frac{1}{2}N_+(0)$, integrate over ξ_p and average over ϕ_p . (the 1/2 factor is to avoid counting the same pair twice). The angular average gives a factor of 1/2. We obtain the contribution to the Pauli susceptibility $\mu^2 N_+(0) Y(T, \Delta_+)/4$ from this band. Here $Y(T, \Delta) \equiv \int d\xi (1/4T) \text{sech}^2(E_p/2T)$ is the Yosida function. The total Pauli susceptibility from both bands is thus $\chi_{\parallel}^P(T) = \mu^2 [N_+(0) Y(T, \Delta_+) + (+ \leftrightarrow -)]/4$. The full susceptibility is given by $\chi_{\parallel}(T) = \chi_{\parallel}^V + \chi_{\parallel}^P(T)$. If $\Delta_+ = \Delta_-$, we get $\chi_{\parallel}(T) = \chi^0(1 + Y(T, \Delta))/2$. The above results agree with those in Ref. 7 under the condition (1).

Now we turn to the electromagnetic effects. We shall show that an applied Zeeman field in the plane, say along \hat{y} , can produce a supercurrent flow along \hat{x} in the superconducting state. To demonstrate this we shall first consider the normal state and show that the net current vanishes due to the cancellation of two contributions that can be identified as ‘‘Pauli’’ and ‘‘Van Vleck.’’ These two contributions are due, respectively, to the change in occupation and the quantum-mechanical wave function of the particles as in the case of

spin susceptibility. We shall then show that the cancellation no longer holds in the superconducting state, giving rise to the mentioned net supercurrent.

Consider now a magnetic field B along \hat{y} in the normal state. The physical situation is as shown in Fig 1. Let us first consider the Pauli contribution from the $|+\rangle$ band. The \hat{y} magnetic moment of the electron at \vec{p} is given by $\mu \cos \phi_p$. Hence the extra number of occupied states (per unit area and per unit angle) due to the magnetic field with momentum near \hat{p} is given by $N_+(0) [\mu B \cos(\phi_p)]$. These electrons have velocity v_{F+} along \hat{p} . Hence the current along \hat{x} is equal to the angular average of $N_+(0)(v_{F+} \mu B) \cos^2(\phi_p)$, i.e., $(1/4\pi\hbar^2) p_{F+} (\mu B)$, using $N_+(0)v_{F+} = p_{F+}/2\pi\hbar^2$. [This Pauli contribution is, therefore, due to the fact that states with $p_x > 0$ are more likely to be occupied than $p_x < 0$ under the field B_y .] The reverse situation applies for the $|-\rangle$ band. The total (number) current density from both bands due to these population changes is given by

$$J_x^P = \frac{1}{4\pi\hbar^2} (p_{F+} - p_{F-}) \mu B_y. \quad (9)$$

The superscript P denotes that this is the Pauli contribution. In addition to this, there is also a Van Vleck contribution. The velocity of an electron at \vec{p} , given by $\vec{v} = \partial\epsilon/\partial\vec{p}$, is actually $\vec{p}/m\hat{1} + \alpha(\vec{n} \times \vec{\sigma})$ and thus an operator in spin space. In particular $v_x = p_x/m - \alpha\sigma_y$. Under the magnetic field B_y , the $|+\rangle$ state is modified as in Eq. (4) with $\sigma_z \rightarrow \sigma_y$. Hence the expectation value of v_x is given by $(p/m - \alpha)\cos(\phi_p) - (\mu B/p) \langle -|\sigma_y|+\rangle$. The first term is the velocity of the $|+\rangle$ particle in the absence of B and its contribution to the current was taken into account by the Pauli term evaluated before. The second term, equals $-(\mu B/p)\sin^2(\phi_p)$, is present due to the modification of the state under the Zeeman field. We shall call its contribution to the current a Van Vleck contribution analogous to the case for the spin susceptibility.

A net Van Vleck contribution at \vec{p} is present only if $|+\rangle$ is occupied whereas $|-\rangle$ is empty. The total Van Vleck current is thus $J_x^V = \frac{1}{2}(1/2\pi\hbar^2) \int_{p_{F-}}^{p_{F+}} dp p (-\mu B/p)$ where the factor 1/2 arises from angular average. We hence obtain

$$J_x^V = -\frac{1}{4\pi\hbar^2} (p_{F+} - p_{F-}) \mu B_y \quad (10)$$

giving $J_x = J_x^P + J_x^V = 0$ in the normal state as claimed. [It can be easily shown that J_y^P and J_y^V both vanish due to angular average over the fermi surface.] The vanishing of the total current is reasonable since otherwise dissipation is expected in the presence of disorder.

In the superconducting state the calculation of J is similar to that of the susceptibility. The Van Vleck contribution J^V is unaffected, while the Pauli contribution has to be multiplied by the Yosida functions. We, therefore, get

$$J_x(T) = -\kappa B_y, \quad (11)$$

where

$$\kappa(T) = \frac{\mu}{4\pi\hbar^2} [p_{F+} \{1 - Y(T, \Delta_+)\} - p_{F-} \{1 - Y(T, \Delta_-)\}]. \quad (12)$$

We can similarly investigate the effect pointed out by Edelstein,⁸ i.e., the generation of a magnetic moment by a phase gradient. Under a phase gradient $\nabla\Phi$, say along \hat{x} , the Cooper pairing is no longer between $\pm\vec{p}$ but rather between $\vec{p}+\vec{q}/2$ and $-\vec{p}+\vec{q}/2$, where $\vec{q}=\hbar(\nabla\Phi)$. Let us first calculate the net magnetic moment at $T=0$. In this case the magnetic moment is the same as that of a Fermi sphere (circle) shifted in momentum space by $\vec{q}/2$. The total moment can be found by summing over all the excess (over $\vec{q}=0$) moments over the Fermi surface(s). For the $|+\rangle$ particles, the number of extra particles along \vec{p} is given by $N_+(0)[\epsilon(\vec{p}+\vec{q}/2)-\epsilon(\vec{p})]=N_+(0)v_{F+}q\cos(\phi_{\vec{p}})/2$ since the quantity between the square bracket is the difference in energy between the particles on the new and old Fermi surfaces. These particles carry a \hat{y} magnetic moment of $\mu\cos(\phi_{\vec{p}})$ per particle. Hence the total \hat{y} magnetic moment from the $|+\rangle$ band is given by $\mu N_+(0)v_{F+}q/4$. Therefore the total contribution from the two bands is

$$M_y(T=0)=\frac{\mu}{8\pi\hbar^2}(p_{F+}-p_{F-})q. \quad (13)$$

It can be easily seen that the \hat{x} magnetic moment vanishes due to angular average over \hat{p} .

The above result, Eq. (13), is when all electrons remained paired. At finite temperatures, we need to take into account the contribution from broken pairs. For this it is essential to note that, under the phase gradient, the energies for a broken pair with particles occupied at \vec{p} is given by $E_{\vec{p}}+\vec{v}_F(\vec{p})\cdot\vec{q}/2$, where $E_{\vec{p}}$ is the energy given before for no phase gradient. The thermal-averaged magnetic moment for the $\pm\vec{p}$ states is given by an expression similar to Eq. (8) in the susceptibility calculation with $-\hbar_{\vec{p}}\rightarrow\vec{v}_F(\vec{p})\cdot\vec{q}/2=v_{F+}q\cos(\phi_{\vec{p}})/2$, giving the final result $-(\mu/8\pi\hbar^2)\times(p_{F+}q)Y(T,\Delta_+)$. [This negative contribution from the quasiparticles is, therefore physically due to the ‘‘backflow,’’ that it is easier to thermally excite quasiparticles with momentum opposite to the superfluid flow. These particles have a net magnetic moment along $-\hat{y}$ for the $|+\rangle$ band.] A similar expression applies for the $|-\rangle$ band. Combining these with Eq. (13), we, therefore, have finally

$$M_y(T)=\frac{\mu}{8\pi\hbar^2}[p_{F+}\{1-Y(T,\Delta_+)\}-p_{F-}\{1-Y(T,\Delta_-)\}]q \\ =\frac{\kappa}{2}q_x \quad (14)$$

with $\kappa(T)$ already defined in Eq. (12). For T near T_c , we can perform an expansion in Δ . [$1-Y\rightarrow[7\zeta(3)/4\pi^2](\Delta^2/T_c^2)$]. Our expression then agrees with that given by Edelstein,⁸ who investigated the effect only near T_c .

The two magnetoelectric effects above are related. They are connected by the fact that there is a cross term in the free energy density $F(T;q_x,B_y)$ given by $-(\kappa(T)/2)q_xB_y$. Equations (14) and (11) can be reproduced by using the relations $M_y=-\partial F/\partial B_y$ and $J_x=2\partial F/\partial q_x$.

Generally, the current J_x and magnetization M_y are given by the constitutive equations,

$$J_x=\rho_s\frac{q_x}{2m}-\kappa B_y, \quad (15)$$

$$M_y=\frac{\kappa}{2}q_x+\chi_{\parallel}B_y, \quad (16)$$

where ρ_s is the superfluid (number) density.

The supercurrent induced by the in plane Zeeman field given in Eq. (11) can be sizeable and should be experimentally observable. The order of magnitude of the electric current I at $T\ll\Delta$ for a sample of width w induced by the magnetic field is given by

$$\left[\frac{I}{A}\right]=10^{-2}\left[\frac{\alpha p_F}{\bar{\mu}}\right]\left[\frac{B}{G}\right]\left[\frac{1}{l/\text{\AA}}\right]\left[\frac{w}{\text{cm}}\right], \quad (17)$$

where we have defined a length l of order of interparticle distance through the two-dimensional number density n by $n=l^{-2}$. If $\alpha p_F/\bar{\mu}$ is not too small, say ~ 0.1 , a current of order of milliampere seems easily achievable for samples of millimeter size under a magnetic field of order 100 G if $l\sim 10$ \AA, say. Measurement of this current seems much easier than the induced magnetization predicted by Edelstein.⁸

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