In-Plane Zeeman Field and Rashba SOC

Ethan Lake
(Dated: July 9, 2015)

We investigate unconventional superconductivity in the 2DEG with Rashba SOC and an applied external magnetic field, where $E_R \perp B$. When the Zeeman field is in-plane, pairing with finite center-of-mass momentum is possible, and so we develop a way to formulate the BCS theory with finite momentum pairing.

**Finite COMM Pairing**

Since the introduction of an in-plane magnetic field will generically result in pairing with finite COMM, it is worthwhile to develop the formulation of BCS theory in this situation. We will work with two bands and suppose the existence of two momenta $2q_\parallel$, $2q_\perp$ that optimize the pairing strength on each band. The Hamiltonian reads

$$H = \sum_{k,\lambda} \xi_{k\lambda} a^\dagger_{k\lambda} a_{k\lambda} + \sum_{kk'\lambda\mu} G_{kk'\lambda\mu} a^\dagger_{k+q_\parallel q_\perp} a_{k-q_\parallel q_\perp} a_{k'+q_\perp} a_{k'-q_\perp}$$

We define the anomalous averages on each band as

$$A_{k\lambda} = \langle a_{-k+q_\parallel q_\perp} a_{k+q_\parallel q_\perp} \rangle,$$

and the corresponding order parameters by

$$\Delta_{k\lambda} = \sum_{k'\mu} G_{kk'\lambda\mu} A_{k'\mu}$$

which allows us to write the interaction Hamiltonian in mean-field form as

$$H_{int} = \sum_{k,\lambda} \left( \Delta_{k\lambda} a^\dagger_{k+q_\parallel q_\perp} a_{-k+q_\parallel q_\perp} + \text{h.c.} \right) - \sum_{kk'\lambda\mu} G_{kk'\lambda\mu} A^*_{k'\mu} A_{k\mu}$$

The next step is, as usual, the diagonalization of the Hamiltonian. As before, we introduce the spinor $\Psi_{k\lambda} = (a_{k+q_\parallel q_\perp}, a^\dagger_{-k+q_\parallel q_\perp})^T$. However, our matrix $h$ changes a bit. First, introduce the combinations ($P$ for $+$, $M$ for $-$

$$P_{k\lambda} = \frac{1}{2}(\xi_{k+q_\parallel q_\perp} - \xi_{-k+q_\parallel q_\perp}), \quad M_{k\lambda} = \frac{1}{2}(\xi_{k+q_\parallel q_\perp} + \xi_{-k+q_\parallel q_\perp})$$

and then construct $h$ by

$$h_{k\lambda}(k) = \left( P_{k\lambda} + M_{k\lambda} \quad 2\Delta_{k\lambda} \right) \begin{pmatrix} 2\Delta_{k\lambda} & -P_{k\lambda} + M_{k\lambda} \end{pmatrix}$$

which allows us to write

$$H = \frac{1}{2} \sum_{k,\lambda} \left( \Psi^\dagger_{k\lambda} h_{k\lambda}(k) \Psi_{k\lambda} + \xi_{k\lambda} \right) - \sum_{kk'\lambda\mu} G_{kk'\lambda\mu} A^*_{k'\mu} A_{k\mu}$$

We didn’t have to do this before, since with $q = 0$ we have $\xi_{k+q} = \xi_{-k+q}$.

The next step is, of course, a Bogoliubov transformation. By looking at the eigenvalues of $h$ and recalling that we had $v = \sqrt{(1 - \xi/E)/2}$ in the zero COMM case, it’s natural to choose (again, we look at $2\Delta$ as the quantity of physical interest)

$$E_{k\lambda} = \sqrt{P_{k\lambda}^2 + \Delta_{k\lambda}^2}, \quad v_{k\lambda}^2 = \frac{1}{2} (1 - P_{k\lambda}/E_{k\lambda}), \quad v_{k\lambda}^2 = 1 - v_{k\lambda}^2$$

after which the standard calculation gives

$$H = \sum_{k,\lambda} \left( (E_{k\lambda} + M_{k\lambda}) \gamma^\dagger_{k\lambda} \gamma_{k\lambda} + \frac{\xi_{k\lambda} - E_{k\lambda}}{2} - \sum_{k'\mu} G_{kk'\lambda\mu} A^*_{k'\mu} A_{k\mu} \right)$$

which looks like the usual Hamiltonian, except with an added term in the first sum accounting for the energy created by the finite pairing momentum.

At $T = 0$, the calculation goes through uneventfully. Varying over $\Delta$, the self-consistent equations are

$$\Delta_{k\lambda} = -\sum_{k'\mu} G_{kk'\lambda\mu} \frac{\Delta_{k'\mu}}{2 \sqrt{P_{k'\mu}^2 + \Delta_{k'\mu}^2}}$$

If the dispersion $\xi$ is quadratic and the interaction is momentum-independent, solving the self-consistent equations isn’t so bad. It’s interesting to see what $q_c$ we would need to kill off superconductivity and send $\Delta \to 0$.

For just one band, we have (assuming a momentum-independent interaction $G$ and $\xi_{k+q} = (k+q)^2/2m - \mu$):

$$1 = -G \int_0^{q_c} \frac{dq}{\sqrt{\xi_{k+q}^2 + q_c^2/2m}}$$

We then find, making the usual assumptions, that

$$q_c \approx \sqrt{2m\Delta}$$

Of course, we’ve let $q$ be arbitrary in our analysis. In principle, we can obtain it by varying the thermodynamic potential: $\partial\Omega/\partial q = 0$. However, this is usually easier said than done. With that, we turn to the application to the Rashba + Zeeman problem.

**Introducing an In-Plane Zeeman Field**

When we put the Zeeman field in-plane and introduce non-vanishing SOC, the two Fermi surfaces become distorted away from perfect circular shapes. They become oblong in the direction normal to both the Rashba and Zeeman fields. This means that finite momentum pairing
is possible. Additionally, if the magnetic field dominates over SOC, the spin vectors no longer wind completely about the out of plane direction.

There are two ways of approaching this problem. The first is to orient the Zeeman field along the $\hat{x}$ direction and the Rashba field along the $-\hat{z}$ direction, with the 2DEG in the $x-y$ plane. The free Hamiltonian reads

$$H = \epsilon\sigma^0 + \alpha(k_y\sigma^x - k_x\sigma^y) - B\sigma^z$$

It will again be helpful to transform to the chiral eigenbasis given by the two subbands in the problem. This is accomplished by the transformation

$$c_\uparrow = \frac{\alpha(ik_x + k_y) - B}{\sqrt{2|\alpha k - B\hat{y}|}}(a_+ - a_-)$$

$$c_\downarrow = \frac{1}{\sqrt{2}}(a_+ + a_-)$$

which diagonalizes the free Hamiltonian as

$$H = \sum_{\lambda} \xi_{\lambda\lambda} a_\lambda^\dagger a_\lambda$$

with the dispersion given by

$$\xi_{\lambda\lambda} = \frac{k^2}{2m} \pm \sqrt{\alpha^2 k^2_z + (\alpha k_y - B)^2}$$

where we choose the $+$ sign for $\lambda = 1$ and the $-$ for $\lambda = 2$.

The interaction term is

$$H_{int} = \sum_{\lambda_1,\lambda_2,\lambda_3,\lambda_4} \int \mathcal{G}_{w, x, y, \lambda_1, \lambda_2, \lambda_3, \lambda_4} \mathcal{U}_{w, x, y, \lambda_1} \mathcal{U}_{w, x, y, \lambda_2} \mathcal{U}_{w, x, y, \lambda_3} \mathcal{U}_{w, x, y, \lambda_4}$$

where $\mathcal{U}$ is the matrix that exhibits the diagonalization

$$\mathcal{U} = \frac{1}{\sqrt{2}} \left( \begin{array}{cc} \frac{\alpha(ik_x + k_y) - B}{|\alpha k - B\hat{y}|} & \frac{\alpha(ik_x + k_y) - B}{|\alpha k - B\hat{y}|} \\ \frac{\alpha(ik_x + k_y) - B}{1} & \frac{\alpha(ik_x + k_y) - B}{1} \end{array} \right)$$

we shall also assume a constant repulsive interaction, and let $\mathcal{G}_{w, x, y, \lambda_1, \lambda_2, \lambda_3, \lambda_4} = \mathcal{U}$ (bad notation!).

As in the out-of-plane Zeeman field case, it’s kind of a mess. We have the same sort of terms as before, and will denote $(1222)$ for $a_{k_1 - q_1 + q_2}^\dagger a_{k_2 - q_1 + q_2} a_{k_3 - q_2} a_{k_4 - q_2}$, for example. We have allowed for each band to have its own pair momentum $q_\lambda$, which will need to be determined self-consistently later by minimizing the thermodynamic potential. The intra-band and Josephson terms are (1 is the smaller band)

$$\frac{U}{4} \left( f_{k_1}^* f_{k''_1}^* (1111) + f_{k''_2}^* f_{k''_2}^* (2222) - f_{k_1}^* f_{k''_2}^* (1122) \right)$$

with the notation

$$f_{k\lambda} = \frac{\alpha(ik_x + k_y + q_\lambda) - B}{\sqrt{\alpha^2 k_x^2 + (\alpha k_y + \alpha q_\lambda - B)^2}}$$

where we have assumed that the vector $q = -\hat{y}$ is along the direction of the deformation of the Fermi surface.

While this isn’t so bad, the coefficient of the $(1221)$ term (the one that we want to perform the unitary transform on) is a bit worse. Additionally, we still have many terms with three identical band indices, like $(1112)$. Unlike before, they are not any smaller than the other terms. If we can get rid of them, we need a better justification.

**The Better Approach**

The better approach is to set the spin quantization axis in-plane, aligned with the Zeeman field. This way when we take the $B \gg \alpha$ limit, the spins will be nearly parallel or antiparallel to the quantization axis, allowing more simplification when the resulting terms are treated perturbatively in $\alpha/B$.

To do this, we re-define our coordinate system so that the electrons move in the $x-z$ plane, with the Rashba $E$ field directed in the $-\hat{y}$ direction and the Zeeman field in the $+\hat{z}$ direction. This means that the free Hamiltonian looks like

$$H_f = \epsilon\sigma^0 - B\sigma^z + \alpha(k_x\sigma^x - k_z\sigma^z)$$

The dispersion, as before, is

$$\xi_{\lambda\lambda} = \frac{k^2}{2m} \pm \sqrt{\alpha^2 k_z^2 + (\alpha k_x - B)^2}$$

The diagonalization is a bit trickier in this case, but still doable. The matrix that diagonalizes $H$ is

$$\mathcal{U} = \frac{1}{\sqrt{2}} \left( \begin{array}{cc} \frac{B - \alpha k_x - \xi_1 + \epsilon_k}{\alpha k_z} & \frac{B - \alpha k_x - \xi_1 + \epsilon_k}{\alpha k_z} \\ \frac{B - \alpha k_x - \xi_1 + \epsilon_k}{1} & \frac{B - \alpha k_x - \xi_1 + \epsilon_k}{1} \end{array} \right)$$

where $\xi_1$ is the larger eigenvalue. Of course, the columns of $\mathcal{U}$ aren’t normalized yet. The actual normalization procedure only yields useful expressions in the $\alpha \ll B$ limit, and involves a fair bit of algebra. We’ll skip writing the full thing out, and will just quote the final result:

$$c_\uparrow = \left( 1 - \frac{\alpha^2 k_z^2}{8B^2 - 4B\alpha k_z} \right) a_1 - \frac{\alpha k_z}{2B - \alpha k_z} a_2$$

$$c_\downarrow = \frac{2B - \alpha k_z}{2B - \alpha k_z} a_1 + \left( 1 - \frac{\alpha^2 k_z^2}{8B^2 - 4B\alpha k_z} \right) a_2$$

The above transformation is approximate, but remarkably accurate. For $\alpha k_z/B \sim 0.1$, the above expression agrees with the exact result to about 1 part in $10^4$. As we progress further, we can rest easy knowing that simplifying further will not sacrifice too much accuracy. We
note that in the $\alpha \to 0$ limit, the transformation between spin and band operators is the identity, which was the whole point of choosing the quantization axis to be in-plane in the first place.

Again, we write (1122) for $a_{k+q_1}^\dagger a_{k+q_2}^\dagger a_{-k'+q_1} a_{-k'+q_2}$ and compute the intra-band terms as (dropping terms of order three and higher in $\alpha k/B$):

\[
\begin{align*}
(1111) & \left( \frac{U\alpha^2 k_z k'_z}{4B^2 + 2Ba(k_z + k'_z) + \alpha^2 k_z k'_z} \right) \\
(2222) & \left( \frac{U\alpha^2 k_z k'_z}{4B^2 - 2Ba(k_z + k'_z) + \alpha^2 k_z k'_z} \right)
\end{align*}
\]

The Josephson terms are

\[
(1122) \left( \frac{U\alpha^2 k_z k'_z}{4B^2 + 2Ba(k_z - k'_z) - \alpha^2 k_z k'_z} \right) \\
(2211) \left( \frac{U\alpha^2 k_z k'_z}{4B^2 + 2Ba(k_z - k'_z) - \alpha^2 k_z k'_z} \right)
\]

Finally, the (1221) term is

\[
(1221) U \left( 1 - \sum_{k_x \in w} \frac{\alpha^2 k_x^2}{8B^2 - 4Ba k_x} \right)
\]

As before, the idea is to perform a unitary transform on the (1221) term. We can see that after this is over, all terms except the 1 in the front will go as at least $U^2 \alpha^2 k_x^2 / B^2$. The extra factor of $U$ on the front will just drop them, and so we can take the coefficient of the (1221) term to just be $U$ for now.

The susceptibility then has the same form as usual:

\[
\chi_{\pm}(Q) = \int \frac{d^2 p}{(2\pi)^2} \frac{f(p) - f(p + Q)}{\xi_{\pm}(p) - \xi_{\pm}(p + Q)}
\]

which is valid in the limit we’re working in. We write the susceptibility as

\[
\chi_{\pm}(Q) = \int \frac{d^2 p}{(2\pi)^2} \left\{ \frac{f(p)}{\xi_{\pm}(p) - \xi_{\pm}(p + Q)} + \frac{f(p)}{\xi_{\pm}(p) - \xi_{\pm}(p - Q)} \right\}
\]

To actually do the integral, we need to also approximate the Fermi surface as a circle. This of course isn’t strictly true, but greatly aids in the calculation. With these assumptions, we can do the $p_z$ component of the integral right away, which integrates to $2\sqrt{k_F^2 - p_z^2}$.

We make the following definition:

\[
m_* = \left( \frac{1}{m} \pm \frac{\alpha^2}{B} \right)^{-1}
\]

And introduce the parameters

\[
A_+ = \frac{Q^2 \pm 2 \alpha Q m_*}{2Q k_F}, \quad A_- = \frac{Q^2 \mp 2 \alpha Q m_*}{2Q}
\]

which means that we can write, after a bit of manipulation,

\[
\chi_{\pm}(Q) = -\frac{k_F m_*}{2\pi^2 Q} \int_{-1}^{1} dx \left\{ \frac{\sqrt{1 - x^2}}{x + A_+} + \frac{\sqrt{1 - x^2}}{-x + A_-} \right\}
\]

We’ll omit the calculation of the integrals for brevity, which are standard but fairly involved. When the smoke clears, we find that

\[
\chi_{\pm}(Q) = \frac{m_*}{2\pi} \left\{ 1 - \frac{1}{2} \left\{ \frac{2k_F}{Q} \right\}^2 + \frac{4m_* Q_\pm \alpha}{Q^2} + \frac{4m_*^2 Q_\pm^2 \alpha^2}{Q^4} \right\} - \frac{1}{2} \left( 1 - \frac{2k_F^2}{Q} \right) - \frac{4m_* Q_\pm \alpha}{Q^2} + \frac{4m_*^2 Q_\pm^2 \alpha^2}{Q^4}
\]

which reduces to our previous expression for $\chi$ when $\alpha \to 0$, as it should. Plots of $\chi$ for two different SOC strengths are shown in the figures. Of interest here is that $\chi$ is not a constant for the smaller Fermi surface, as it was before.

The Self-Consistent Equations

Our task now is to solve the self consistent equations. By looking at the coefficients in front of each interaction term, we are led to make the following definition:

\[
g_{\lambda}(k) = \frac{k \sin \phi}{2B/\alpha \pm k \sin \phi}
\]

where we use the + sign for $\lambda = 1$ and the − sign for $\lambda = 2$. This means that the interaction potential is (excluding the susceptibility)

\[
G_{\lambda' \lambda} = U g_{\lambda}(k) g_{\lambda'}(k')
\]

To begin, let us consider $U$ to be very small and ignore the intra-band susceptibility term $\chi_{\lambda}$ for each band. The self-consistent equations are then

\[
\Delta_{\lambda}(k) = -\frac{U}{2} \int \frac{d^2 k'}{(2\pi)^2} \left\{ \frac{g_{\lambda}(k) g_{\lambda'}(k') \Delta_{\lambda}(k')}{E_{k'\lambda}} + \frac{g_{\lambda}(k) g_{\lambda'}(k') \Delta_{\lambda}(k')}{E_{k'\mu}} \right\}
\]
with

\[ E_{k\lambda} = \sqrt{P^2_{k\lambda} + \Delta^2_{\lambda}(k)} \]

where the function \( P \) is as defined in the first section and \( \mu \) is the opposite index as \( \lambda \).

From this, we see that \( \Delta_{\lambda}(k) \) must be of the form \( g_{\lambda}(k)C(\lambda) \), where \( C \) is a constant function that only depends on the band index \( \lambda \). That is, the only momentum dependence in \( \Delta \) must be of the form \( g(k) \). If this were not the case, we could vary \( k \) on one side of the equation without changing the other side, and the self-consistent equations would not hold. We are thus lead to the following ansatz for \( \Delta \):

\[ \Delta_{\lambda}(k) = \Delta_{\lambda}e^{i\theta_{\lambda}}g_{\lambda}(k) \]

where \( \Delta_{\lambda} \) is a real positive constant. If we plug this into the self-consistent equations and cancel out the \( k \) dependent terms on either side, we obtain the two equations

\[ 1 = -U \int \frac{d^2k'}{(2\pi)^2} \frac{g_{\lambda}^2(k')}{2E_{k',1}} - U \int \frac{d^2k'}{(2\pi)^2} \frac{\Delta_{\lambda}^2g_{\lambda}^2(k')e^{i(\theta_{\lambda}-\theta_{1})}}{2\Delta_1E_{k',2}} \]

\[ 1 = -U \int \frac{d^2k'}{(2\pi)^2} \frac{g_{\lambda}^2(k')}{2E_{k',2}} - U \int \frac{d^2k'}{(2\pi)^2} \frac{\Delta_{\lambda}^2g_{\lambda}^2(k')e^{-i(\theta_{\lambda}-\theta_{1})}}{2\Delta_2E_{k',1}} \]

Since \( g_{\lambda}^2(k') \) and \( E_{k',\lambda} \) are both positive-definite, we must require that \( \theta_{\lambda} = \theta_{1} \). However, in this case, we see that we also require

\[ \int \frac{d^2k'}{(2\pi)^2} \frac{g_{\lambda}^2(k')}{E_{k',1}} < \int \frac{d^2k'}{(2\pi)^2} \frac{g_{\lambda}^2(k') \Delta_{2}}{E_{k',2} \Delta_{1}} \]

and

\[ \int \frac{d^2k'}{(2\pi)^2} \frac{g_{\lambda}^2(k')}{E_{k',2}} < \int \frac{d^2k'}{(2\pi)^2} \frac{g_{\lambda}^2(k') \Delta_{1}}{E_{k',1} \Delta_{2}} \]

which can not be simultaneously satisfied. Evidently, the only solution to the self-consistent equations is the trivial one.

We could have predicted this earlier, based on some results from my last set of notes. There, we saw that a superconducting ground state was only possible if the product of the two Josephson coefficients was larger than the product of the two intra-band coefficients. Since the two products are equal in this case, a nontrivial solution cannot be found.

The main point here is that including the intra-band susceptibility \( \chi \) is essential to realize a superconducting state. If \( \chi \) is negative the criterion mentioned above will be satisfied, and a superconducting state can be realized. However, introducing \( \chi \) into the self-consistent equations makes finding a nice ansatz for the order parameter a bit trickier, especially since \( \chi \) doesn’t factorize into functions of each momentum.

FIG. 1: A plot of the susceptibility as a function of \( Q \), the momentum transfer. The color scale is normalized to the value at \( Q = (0, 0) \). Although \( m_\ast \) is different for each band, for reasonable values of \( \alpha^2/B \) this affect is small. In this plot \( \alpha \) is taken to be rather small, and so we see a mostly circular appearance as in the \( \alpha = 0 \) case.

FIG. 2: The same as in the last figure, but with a larger value of \( \alpha \).

If there was no \( \Delta_{\lambda}(k) \) in \( E_{k\lambda} \), we could solve the self-consistent equations (in principle) by using a Neumann integral series, although the actual procedure would likely be a bit messy. Barring an expansion into angular harmonics like last time, we’ll need to come up with a better way of approaching the problem.