Strong Anisotropy in Spin Susceptibility of Superfluid $^3$He-B Film Caused by Surface Bound States

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Spin susceptibility of superfluid $^3$He-B film with specular surfaces is calculated. It is shown that, when the magnetic field is applied in a direction perpendicular to the film, the susceptibility is significantly enhanced by the contribution from the surface bound states. No such enhancement is found for the magnetic field parallel to the film. A simplified model with spatially constant order parameter is used to elucidate the magnetic properties of the surface bound states. The Majorana nature of the zero energy bound state is also mentioned.

KEYWORDS: Superfluid $^3$He-B Film, Anisotropic Spin Susceptibility, Surface Bound State

Existence of low-energy midgap states in the vicinity of the surface and/or interface is a universal feature of unconventional superconductors and superfluids. The surface bound states govern the transport properties of superconductors and superfluids, since the system always communicates with its environment through the surface. For example, the zero-bias conductance peak (ZBCP) in the tunneling spectrum of high $T_c$ superconductors has been observed at the zero-energy bound states. ZBCP has been also observed in other superconductors, such as Sr$_2$RuO$_4$, $\kappa$-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br, UBe$_{13}$, and CeCoIn$_5$, and was regarded as evidence of their unconventionality.

The surface bound states in $p$-wave pairing superfluid $^3$He-4 have not been observed until recently, because of the lack of an appropriate probe for the neutral superfluid. It has been recently reported, however, that the transverse acoustic impedance $Z$ provides useful information on the density of states of the surface bound states in superfluid $^3$He-B. The surface bound states in this system have recently attracted much attention as Majorana fermion surface states which characterize the topological symmetry of the bulk BW state. Recently Chung and Zhang suggested that, when the spin quantization axis is taken parallel to the surface, the low energy behavior of the field operators looks like Majorana fermion states solving the Bogoliubov equation

$$\hat{H} = \frac{1}{2} \int d\mathbf{r} d\mathbf{r'} \hat{\Psi}^\dagger(\mathbf{r}) \hat{\mathcal{E}}(\mathbf{r}, \mathbf{r'}) \hat{\Psi}(\mathbf{r'}),$$

where

$$\hat{\Psi}(\mathbf{r}) = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}$$

is the Fermion field operator in the Nambu representation. The energy matrix $\hat{\mathcal{E}}(\mathbf{r}, \mathbf{r'})$ in the presence of magnetic field is a $4 \times 4$ matrix given by

$$\hat{\mathcal{E}}(\mathbf{r}, \mathbf{r'}) = \begin{pmatrix} \xi(\nabla) \delta(\mathbf{r} - \mathbf{r'}) & \Delta(\mathbf{r}, \mathbf{r'}) \\ \Delta^\dagger(\mathbf{r'}, \mathbf{r}) & -\xi(\nabla) \delta(\mathbf{r} - \mathbf{r'}) \end{pmatrix} - \frac{\gamma H}{2} \left( \sigma - \sigma^\dagger \right) \delta(\mathbf{r} - \mathbf{r'})$$

with $\gamma$ the gyromagnetic ratio of the $^3$He atom and $\sigma$ the transpose of Pauli matrix $\sigma$. The order parameter of the BW state with a surface is given by

$$\Delta(\mathbf{r}, \mathbf{r'}) = \sum_p e^{i\mathbf{p} \cdot (\mathbf{r} - \mathbf{r'})} \Delta(z, \mathbf{p})$$

with $\Delta(z, \mathbf{p}) = \begin{pmatrix} \Delta_0(z)(-\hat{p}_z + i\hat{p}_y) \\ \Delta_1(z)\hat{p}_z \\ \Delta_0(z)(\hat{p}_x + i\hat{p}_y) \end{pmatrix}$

where $\mathbf{p}$ is a unit vector along $\mathbf{p}$. We seek surface bound states solving the Bogoliubov equation

$$\int d\mathbf{r'} \hat{\mathcal{E}}(\mathbf{r}, \mathbf{r'}) \hat{\Psi}(\mathbf{r'}) = \lambda \hat{\Psi}(\mathbf{r})$$

under the boundary condition $\hat{\Psi} = 0$ at $z = 0$.

We assume here that $\Delta_0$ and $\Delta_1$ are constant, for simplicity. Using the quasi-classical approximation we can obtain the bound state wave functions (Nambu ampli-
tudes.  

Let us first consider the case without magnetic field. We can find both positive and negative energy bound states for each Fermi momentum \((K_\parallel, k)\), where \(K_\parallel\) is the component parallel to the surface and \(k\) is the perpendicular component. The bound states energies are given by \(\pm \Delta_0 \sin \theta\) with \(\theta\) the polar angle of the Fermi momentum with respect to the \(z\) axis.\(^{12}\) For positive energy eigen value \(E = \Delta_0 \sin \theta\), the eigen function is given by

\[
\Psi_{K_\parallel}^{(+)}(r) = e^{iK_\parallel \cdot r}u(k, z)(\Phi_+ - e^{i\phi}\Phi_-),
\]

and for negative energy eigen value \(E = -\Delta_0 \sin \theta\)

\[
\Psi_{K_\parallel}^{(-)}(r) = e^{iK_\parallel \cdot r}u(k, z)(e^{-i\phi}\Phi_+ + \Phi_-),
\]

where \(\phi\) is the azimuthal angle of the Fermi momentum around the \(z\) axis. Here \(\Phi_{\pm}\) are the Nambu amplitudes given by

\[
\Phi_+ = \begin{pmatrix} 1 \\ 0 \\ 0 \\ -i \end{pmatrix}, \quad \Phi_- = \begin{pmatrix} 0 \\ i \\ 1 \\ 0 \end{pmatrix}.
\]

It is worth noting here that \(\Phi_{\pm}\) is the eigenvector of spin operator \(S_z\) in the Nambu representation

\[
S_z = \frac{1}{2} \begin{pmatrix} \sigma_z & -\sigma_z \\ -\sigma_z & \sigma_z \end{pmatrix}, \quad S_z \Phi_{\pm} = \pm \frac{1}{2} \Phi_{\pm}.
\]

The \(z\) dependence of the eigen functions is included in

\[
u(k, z) = au^{-\kappa z}\sin kz
\]

with \(\kappa = \Delta_1/v_F\) and the normalization constant \(a\) is determined so that \(\Psi_{K_\parallel}^{(\pm)}\) are normalized.

Since all the eigen functions of \(\mathcal{E}(r, r')\) form a complete set, we can expand the Fermion field operator \(\hat{\Psi}\):

\[
\hat{\Psi}(r) = \sum_{K_\parallel} \left( \gamma_{K_\parallel} \Psi_{K_\parallel}^{(+)}(r) + \gamma_{-K_\parallel} \Psi_{K_\parallel}^{(-)}(r) \right) + \cdots,
\]

where we have omitted the gapped modes. Since all the eigen functions are orthogonal to each other, we obtain

\[
\gamma_{K_\parallel} = \int dr e^{-iK_\parallel \cdot r} \nu(k, z)
\times \left( <\Phi_+ | \hat{\Psi} > - e^{-i\phi} <\Phi_- | \hat{\Psi} > \right),
\]

\[
\gamma_{-K_\parallel} = \int dr e^{iK_\parallel \cdot r} \nu(k, z)
\times \left( -e^{i\phi} <\Phi_+ | \hat{\Psi} > + <\Phi_- | \hat{\Psi} > \right),
\]

where

\[
<\Phi_+ | \hat{\Psi} > = \psi_\parallel(r) + i\psi_\parallel^*(r),
\]

\[
<\Phi_- | \hat{\Psi} > = (-i) \psi_\parallel(r) + \psi_\parallel^*(r).
\]

We can show that \(\gamma_{K_\parallel}\) and \(\gamma_{-K_\parallel}\) satisfy the Fermion commutation relation

\[
\{\gamma_{K_\parallel}, \gamma_{-K_\parallel}\} = 0, \quad \{\gamma_{K_\parallel}, \gamma_{-K_\parallel}^\dagger\} = \delta_{K_\parallel, K_\parallel'}.
\]

Some caution is necessary about the doubly degenerate zero energy states which happen when \(K_\parallel = 0\). In this case, the system is essentially the polar state\(^2\) and the azimuthal angle \(\phi\) is an irrelevant quantity. We can choose any linear combination of \(\Psi_{K_\parallel}^{(\pm)}\) as an eigen function of the zero energy state. An example is

\[
\hat{\Psi} = \left( \gamma_0 \Phi_- + \gamma_0^\dagger \Phi_+ \right) \sqrt{2u(kF, z) + \text{nonzero energy states}}.
\]

In this case, \(\gamma_0, \gamma_0^\dagger\) are still Fermion operators because \(\Phi_{\pm}\) are mutually orthogonal. Another choice is

\[
\hat{\Psi} = \left( \Gamma_+ (\Phi_+ + \Phi_+) + \Gamma_- (\Phi_- + \Phi_+) \right) \nu(kF, z) + \cdots
\]

with \(\Gamma_+ = (\gamma_0 + \gamma_0^\dagger)/\sqrt{2}, \Gamma_- = (\gamma_0 - \gamma_0^\dagger)/\sqrt{2}\). The new operators \(\Gamma_{\pm}\) have a Majorana property

\[
\Gamma_\dagger_+ = \Gamma_+, \quad \Gamma_\dagger_- = \Gamma_-
\]

and obey the commutation relation

\[
\{\Gamma_+, \Gamma_+\} = \{\Gamma_-, \Gamma_-\} = 1, \quad \{\Gamma_+, \Gamma_-\} = 0.
\]

Now let us consider the effect by magnetic field. To obtain the low energy spectrum, we consider matrix elements of \(\mathcal{E}\) of Eq. (3) between the eigen functions given by Eqs. (7) and (8). It is quite interesting that only \(S_z\) has a finite matrix element between \(\Psi_{K_\parallel}^{(+)}\) and \(\Psi_{K_\parallel}^{(-)}\). Other spin components \(S_x, S_y\) have no matrix element at all. It implies that the surface bound states respond only to the magnetic field in the direction of the surface normal. This agrees with the recent suggestion by Chung and Zhang.\(^{23}\) When the magnetic field is applied in the \(z\)-direction, the surface bound state wave function is given by

\[
a \Psi_{K_\parallel}^{(+)} + b \Psi_{K_\parallel}^{(-)}
\]

and the energy is obtained from an eigen value equation

\[
\begin{pmatrix}
\Delta_0 \sin \theta & -\gamma H/2 e^{-i\phi} \\
-\gamma H/2 e^{i\phi} & -\Delta_0 \sin \theta
\end{pmatrix}
\begin{pmatrix}
a \\
b
\end{pmatrix}
= E
\begin{pmatrix}
a \\
b
\end{pmatrix}
\]

to be

\[
E = \pm \sqrt{\left(\Delta_0 \sin \theta \right)^2 + \left( \frac{\gamma H}{2} \right)^2}.
\]

In the \(K_\parallel \to 0\) limit, the wave function (22) is reduced to \(\Phi_+\) for the positive energy +\(\gamma H\) and to \(\Phi_-\) for the negative energy -\(\gamma H\). Let us consider the spin susceptibility of the ground state. Contribution from the occupied negative energy bound states to the ground state energy is given by

\[
E_0(H) = \frac{1}{2} \sum_{K_\parallel} \left( \Delta_0 \sin \theta \right)^2 + \left( \frac{\gamma H}{2} \right)^2
\]

\[
= -\frac{k_F^2}{4\pi} \int_0^1 d(cos \theta) \cos \theta \sqrt{\left(\Delta_0 \sin \theta \right)^2 + \left( \frac{\gamma H}{2} \right)^2}
\]

\[
= -\frac{k_F^2}{12\pi \Delta_0^2} \left( \left( \Delta_0^2 + \left( \frac{\gamma H}{2} \right)^2 \right)^{3/2} - \left( \frac{\gamma H}{2} \right)^3 \right)
\]
\[ \sim -\frac{k_F^2}{12\pi} \Delta_0 \left( 1 + \frac{3}{2} \left( \frac{\gamma H}{2\Delta_0} \right)^2 + \cdots \right), \tag{26} \]

where the factor 1/2 in Eq. (25) comes from the prefactor in Eq. (1). We obtain the susceptibility

\[ \chi_{zz} = -\frac{\partial^2}{\partial H^2} E_0(H) = \frac{\gamma^2 k_F^2}{16\pi \Delta_0} \] \tag{27}

which is as large as the normal state susceptibility \( \chi_N \) multiplied by the width \( 1/\kappa \) of the bound states. The susceptibility of the surface BW state at \( T = 0 \) is large but finite, while in the polar state the susceptibility will diverge because \( \Delta_0 = 0 \). The magnetism of the polar state is just Ising spin like because the bound state energy under magnetic field splits into \( \pm \frac{\gamma H}{2} \).

In Fig. 1, we show the local distribution of \( \chi_{zz} \) in \(^3\)He-B film at a temperature \( T = 0.2T_c \), \( \chi_{zz} \) is scaled by the normal state value \( \chi_N \). Fermi liquid correction by \( F_0^a \) is taken into account. Film widths are the same as in Fig. 1. Note that the vertical scale is different from Fig. 2.

\[ \text{Fig. 1. Self consistent order parameter at } T = 0.2T_c \text{ of } ^3\text{He-B film with width } L = 5, 6, 10, 15, 20\xi. \text{ The coherence length } \xi \text{ is defined by } \xi = v_F/\pi T_c, \text{ which is equal to 0.155\mu m at SVP.} \]

Now we turn to the susceptibility of films. To calculate the susceptibility, we use the quasi-classical Green function method developed for dealing with the boundary problems.\(^{12, 25-27}\) Within the quasi-classical Green function theory, however, it is not straightforward to calculate the linear response in finite systems because the quasi-classical Eilenberger equation needs an initial condition at some point. We instead start from the linear response formula for the Gor’kov Green function and rewrite the result using the quasi-classical Green functions and the evolution operator.\(^{26, 27}\) When we apply the formulation to the case with the constant order parameter \( \Delta_0, \Delta_1 \), we obtain the susceptibility (per unit volume) \( \chi_{zz}(0) \) at the surface

\[ \frac{\chi_{zz}(0) - \chi_N}{\chi_N} = \int_0^{\pi/2} d\theta \sin \theta \pi T \sum_{n>0} f(\theta, \omega_n) \tag{28} \]

where \( f(\theta, \omega_n) = \frac{\Delta_1^2 \cos^2 \theta}{(\omega_n^2 + \Delta_1^2 \sin^2 \theta)\sqrt{\omega_n^2 + \Delta_0^2 \sin^2 \theta + \Delta_1^2 \cos^2 \theta}}. \tag{29} \]

where \( \chi_N \) is the normal state Pauli susceptibility and \( \omega_n \) is the Matsubara frequency.

In the presence of surfaces, the order parameter is modified cdas can be seen in Fig. 1.\(^{12, 13}\) Near the specular surface, the perpendicular component \( \Delta_1(z) \) is suppressed to zero, while the parallel component \( \Delta_0(z) \) is somewhat enhanced to compensate the pairing energy. In this report, we show the results of numerical calculations using the self-consistent order parameter of Fig. 1.

The details of the calculation shall be reported elsewhere.

\[ \text{Fig. 2. Local distribution of } \chi_{zz} \text{ in } ^3\text{He-B film at a temperature } T = 0.2T_c, \chi_{zz} \text{ is scaled by the normal state value } \chi_N, \text{ Fermi liquid correction by } F_0^a \text{ is taken into account. Film widths are the same as in Fig. 1.} \]

\[ \text{Fig. 3. Local distribution of } \chi_{zz} \text{ in } ^3\text{He-B film at a temperature } T = 0.2T_c, \chi_{zz} \text{ is scaled by the normal state value } \chi_N, \text{ Fermi liquid correction by } F_0^a \text{ is taken into account. Film widths are the same as in Fig. 1.} \]

In Fig. 2, we show the local distribution of \( \chi_{zz}(z) \) at a low temperature \( T = 0.2T_c \) for several width films. The Fermi liquid correction by \( F_0^a \) is taken into account. The vertical axis is the local susceptibility normalized by the normal state susceptibility. The enhancement of the susceptibility can be clearly seen at the end surfaces. The bottom value is almost equal to the bulk B-phase susceptibility. In sufficiently thin films, the overall enhancement is found rather than the surface enhancement. This is because the bound state wave functions extend.
over the entire width of the film. In contrast to $\chi_{zz}$, the susceptibility $\chi_{xx}$ for the magnetic field parallel to the surface is not enhanced at the surfaces as can be seen in Fig. 3. The surface value of $\chi_{xx}$ is even smaller than the bulk susceptibility and is nearly equal to that of the planar state with the Fermi liquid correction. These results clearly demonstrate that the surface bound states respond to the magnetic field only in the direction of the surface normal.

Finally we show in Fig. 4 the susceptibility $\chi_{zz}$ and $\chi_{xx}$ averaged over the film width. We can find that $\chi_{zz}$ even exceeds the normal state Pauli susceptibility for sufficiently thin films. In thicker films, $\chi_{zz}$ is still larger than the B-phase bulk value, while $\chi_{xx}$ remains smaller. The anisotropy is large enough to be observed.

![Graph](image)

**Fig. 4.** Film width dependence of $\chi_{zz}$ and $\chi_{xx}$ averaged over the film width at $T = 0.2T_c$.

In conclusion, we have shown that the spin susceptibility of superfluid $^3$He-B film has a strong anisotropy caused by the surface bound states. The anisotropy is sufficiently large to observe experimentally. We have considered, however, films with specular end surfaces. In actual films on the substrate, the surface scattering by the substrate will be diffusive. One of the methods to avoid the diffuse scattering is to coat the substrate by $^4$He layer. In fact, recent experiments of the transverse acoustic impedance showed that the specularity of the surface is considerably enhanced by the coating. On the other hand, the susceptibility of the film with diffusive surfaces is itself of interest. The density of state at zero energy is known to be increased by the diffusive scattering, which might lead to further enhancement of the susceptibility.

We thank Ryuji Nomura for bringing our attention to Refs. 19-24. This work is supported in part by a Grant-in-Aid for Scientific Research Priority Area (No. 17071009) and a Grant-in-Aid for Scientific Research (No. 21540365) from the Ministry of Education, Culture, Sports, Science and Technology of Japan.

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