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Majorana states and longitudinal NMR absorption in a 3He-*B* **film**

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The topological superfluid 3He-*B* supports massless Dirac spectrum of surface bound states which can be described in terms of the self-conjugated Majorana field operators. We discuss here the possible signature of surface bound states in nuclear magnetic resonance absorption spectrum in a ³He-*B* film. It is shown that transitions between different branches of the surface states spectrum lead to the nonzero absorption signal in longitudinal NMR scheme when the frequency is larger than the Larmour one.

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I. INTRODUCTION

Recently, much attention has been devoted to the investigation of bound fermion states on surfaces and interfaces of topological superfluid 3 He-*B*. The presence of surface states in ³He-*B* can be observed through anomalous transverse sound attenuation, $1-4$ surface specific heat measurements.⁵ Gapless fermion states are supported by the nonzero value of the topological invariant in 3 He- B^{7} B^{7} B^{7} and have two-dimensional relativistic massless Dirac spectrum.[6,8–11](#page-3-0) Such massless fermions can be described in terms of the Majorana selfconjugated field operators which have been intensively studied recently in a number of condensed matter systems.^{[12](#page-3-0)}

It has been suggested that NMR technique can be employed to study the spectrum of surface states. 13 The NMR measurements were implemented recently on superfluid 3 He films demonstrating various frequency shifts associated with the order parameter dynamics both at high-temperature *A* phase as well as with two nonequivalent low-temperature*B* phase states characterized by the different values of the Ising variable.^{[14,15](#page-3-0)}

In this paper, we focus on the contribution of the surface bound states to the ac magnetic susceptibility of 3He-*B* film. We demonstrate that the transitions between different branches of surface states spectrum result in dissipation manifested in the nonzero imaginary part of the χ_{zz} component of magnetic susceptibility, where *z* is the axis normal to the film surface. This effect should provide the contribution to the longitudinal NMR absorption signal absent both in the normal state and the bulk 3He-*B* phase. Under the action of the *z* component of the magnetic field which destroys the self-conjugating Majorana states, the magnetic absorption is suppressed at frequencies smaller than the Larmour one.

II. SPECTRUM OF SURFACE STATES IN 3HE-*B* **FILM**

At first we introduce the basic formalism for treating the spectrum of fermionic quasiparticles. We consider ³He-*B* film confined in a slab at $z > 0$ and homogeneous in the x and *y* directions. The 3He-*B* surface mode is derived from the quasiclassical BdG Hamiltonian

$$
\hat{H} = -i\hbar V_z \hat{\tau}_3 \partial_z + \hat{\tau}_1 \hat{\Delta} - \frac{\gamma}{2} \mathbf{H} \cdot \hat{\boldsymbol{\sigma}}, \tag{1}
$$

where $\hat{\Delta} = A_{ij}q_i\hat{\sigma}_j$, and $\mathbf{q} = \mathbf{k}/k_F$ where $\hat{\tau}_i$ are Pauli matrices of Bogolyubov-Nambu spin, $\hat{\sigma}_{\alpha}$ are Pauli matrices of ³He nuclear spin, and γ is the gyromagnetic ratio of the ³He atom.

The order parameter in ³He-*B* is 3×3 matrix A_{ij} where the first and second indices correspond to the spin and orbital variables. The geometrical confinement induced by the walls destroys the isotropy of the *B* phase order parameter.¹⁶ As a result, for the distorted 3 He-*B* it has the form

$$
A_{ij} = \begin{pmatrix} \Delta_{\parallel} & 0 & 0 \\ 0 & \Delta_{\parallel} & 0 \\ 0 & 0 & \Delta_{\perp} \end{pmatrix},
$$

where Δ_{\perp} is the gap for quasiparticles propagating in the direction along the normal to the wall, and Δ_{\parallel} is the gap for quasiparticles propagating in directions parallel to the wall.

Upon specular reflection from the surface, the quasiparticle momentum projection q_z , and therefore part of the order parameter, changes the sign which leads to the formation of surface bound states. To find the spectrum of this state we employ the usual procedure, considering the two parts of Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}_1$ so that

$$
\hat{H}_0 = -i\hbar V_z \hat{\tau}_3 \partial_z + \hat{\tau}_1 \hat{F}(z) \tag{2}
$$

$$
\hat{H}_1 = \Delta_{\parallel} \hat{\tau}_1 (\hat{\sigma}_x q_x + \hat{\sigma}_y q_y) - \frac{\gamma}{2} \mathbf{H} \cdot \hat{\boldsymbol{\sigma}}, \tag{3}
$$

where $\hat{F}(z) = \Delta_{\perp}(z)\hat{\sigma}_z q_z$ and $\mathbf{q} = \mathbf{p}/p_F$. The Hamiltonian (2) has zero energy eigenvalues corresponding to the degenerate surface bound states. To get into account correction from the perturbation terms \hat{H}_1 , we find the eigenfunctions as a superposition

$$
\psi = \sum_{j=1}^{2} X_j \varphi_j(z),\tag{4}
$$

where X_j are the arbitrary coefficients, and the generic terms $\varphi_i(z)$ are the eigenfunctions of Hamiltonian \hat{H}_0 corresponding to the zero energy $\varepsilon = 0$

$$
\varphi_j(z) = A^{-1/2} \alpha_j \beta_j \exp[-K(z)], \tag{5}
$$

where $A = \langle \varphi_1 | \varphi_1 \rangle = \langle \varphi_2 | \varphi_2 \rangle$ is the normalizing coefficient and

$$
K(z) = \frac{1}{\hbar V_F} \int_0^z \Delta_{\perp}(s) ds.
$$

The Pauli and Nambu spinors β_j and α_j satisfy the relations $\hat{\sigma}_z \beta_{1,2} = \pm \beta_{1,2}$ and $\hat{\tau}_2 \alpha_{1,2} = \pm \alpha_{1,2}$.

Following the standard method, we substitute the solution in the form (4) into the equation $(H_0 + \hat{H}_1)\psi = \varepsilon \psi$ multiply

it by $\psi_j^*(z)$ from the left and integrate over *z*. Then for the spinor $X = (X_1, X_2)^T$, we obtain the two-dimensional Dirac equation

$$
[C\hat{\sigma}\mathbf{p} + \hat{\sigma}_z M]X = \varepsilon X, \tag{6}
$$

with the "light velocity" given by

$$
C = \frac{1}{A p_F} \int_0^\infty dz \Delta_{\parallel}(z) \exp[-2K(z)] \sim \Delta_{\parallel}/p_F,
$$

and "mass" $M = \hbar \omega_H/2$ determined by the Larmour frequency $\omega_H = \gamma H/\hbar$.

For the massless particles we can choose the eigenfunctions of Eq. (6) satisfying the relation

$$
X_{\varepsilon} = i \hat{\sigma}_y X_{-\varepsilon}.
$$
 (7)

As a result, the quasiparticle field operators are self-conjugated analogously to the Majorana fermions in relativistic quantum field theories. In the external magnetic field, the particles described by Eq. (6) become massive¹³ so that the property (7) does not hold and therefore the quasiparticles are no longer self-conjugated Majorana fermions.

The Dirac equation (6) determines the equation for the energy levels in the following form 13

$$
\varepsilon_{1,2} = \pm \sqrt{(Cp)^2 + (\hbar \omega_H)^2/4}.
$$
 (8)

The energy spectrum of surface bound states (8) is sensitive only to the *z* projection of the magnetic field. It can result in a large anisotropy of magnetic susceptibility⁶ if the magnetic field is much smaller then the effective dipole field. However the larger magnetic field will reorient the spin axes eliminating the magnetic anisotropy.¹³ Note that deriving the spectrum (8) , we have neglected the finite thickness of the slab. The size effect due to the overlap of quantum states localized at the opposite surfaces of the slab leads to the splitting of the Dirac $cone¹¹$ even in zero magnetic field. For a sufficiently strong magnetic field, this modification can be neglected.

III. MAGNETIC SUSCEPTIBILITY AND NMR ABSORPTION SPECTRUM

Now we consider the contribution of surface bound states to the imaginary part of ac magnetic susceptibility component *χzz*, which determines the power absorption under the experimental conditions of the longitudinal scheme of magnetic resonance when the total magnetic field is directed along the *z* axis.

To find the magnetic susceptibility, let us use a conventional Kubo formula:

$$
\chi_{ij} = \frac{\gamma^2}{4} T \sum_{\omega_n} \int \frac{d^2 \mathbf{p}}{(2\pi\hbar)^2} Tr\{\hat{\sigma}_i \hat{G}(p_+) \hat{\sigma}_j \hat{G}(p_-)\},\qquad(9)
$$

where

$$
\hat{G}(\omega_M, \mathbf{p}) = \sum_{k=1,2} \frac{|\psi_k\rangle \langle \psi_k|}{i\omega_M - \varepsilon_k(\mathbf{p})}
$$

is a temperature Green function and $p_{\pm} = (\omega_n \pm \epsilon_l/2, \mathbf{p})$. Here $\omega_n = \pi(2n + 1)T$ is a fermionic and $\epsilon_l = 2\pi lT$ is a photonic Matsubara frequency. The normalized wave functions $\psi_{1,2}$ are given by the superpositions [\(4\)](#page-0-0) and correspond to the energy branches $\varepsilon_{1,2}$ in Eq. (8). We use the value of the matrix element $|\langle \psi_1 | \check{\sigma}_z | \psi_2 \rangle| = Cp/\varepsilon_1$ and the formula for the sum over fermionic frequencies

$$
\sum_{\omega_n} \frac{T}{[i\Omega_{n+} - \varepsilon_1][i\Omega_{n-} - \varepsilon_2]} = \frac{f_0(\varepsilon_1) - f_0(\varepsilon_2)}{i\epsilon_1 - \varepsilon_2 + \varepsilon_1},
$$

where $\Omega_{n\pm} = \omega_n \pm \epsilon_l/2$ and $f_0(\varepsilon) = \tanh(\varepsilon/2T)$. Then changing the photonic Matsubara frequency by $\epsilon_l \to i\hbar\omega$ from Eq. (9) , we get that

$$
\chi_{zz} = \frac{\gamma^2 C^2}{8\pi\hbar^2} \int p^3 dp \frac{(\varepsilon_2 - \varepsilon_1)[f_0(\varepsilon_1) - f_0(\varepsilon_2)]}{\varepsilon_1^2 [(\hbar\omega)^2 - (\varepsilon_2 - \varepsilon_1)^2]}, \quad (10)
$$

where $\varepsilon_{1,2} = \varepsilon_{1,2}(\mathbf{p})$. We use now the dispersion relation (8) and obtain that when the frequency is larger than the Larmour frequency $\omega > \omega_H$ the susceptibility given by Eq. (10) has a nonzero imaginary part

$$
\mathrm{Im}\chi_{zz} = \left(\frac{\gamma}{4\hbar C}\right)^2 \frac{\hbar \omega}{2} f_0 \left(\frac{\hbar \omega}{4T}\right) \left(1 - \frac{\omega_H^2}{\omega^2}\right). \tag{11}
$$

Note that the nonzero dissipation $Im\chi_{zz} \neq 0$ occurs only when the frequency is larger than the threshold value ω_H , which is similar to the threshold behavior of absorption rate in semiconductors where the absorption edge frequency is determined by the band gap energy. However, in the vicinity of the threshold the frequency dependence of the absorption rate $[Eq. (11)]$ is completely different from that of the electromagnetic wave absorption in the physics of semiconductors.¹⁷

The estimate of imaginary magnetic susceptibility (11) of a unit film area yields

$$
\mathrm{Im}\chi_{zz}\sim \chi_n\xi\frac{\hbar\omega}{\Delta_{\parallel}}f_0\bigg(\frac{\hbar\omega}{4T}\bigg),\,
$$

where $\chi_n \sim \gamma^2 k_F^3 / E_F$ is a normal state susceptibility and $\xi =$ $\hbar V_F/\Delta_{\parallel}$ is a coherence length.

IV. EFFECT OF SURFACE ROUGHNESS

In general, the quasiparticle energy levels are broadened due to the statistical fluctuations of the film surface which affect the boundary conditions for the wave functions. Different models of surface roughness related to the surface effects in 3 He were developed including the diffusive surface layer, $18,19$ randomly rippled wall (RRW), randomly oriented mirrors (ROM) models, $19,20$ and random scattering matrix model.²¹ Under the conditions of diffusive scattering, the acoustic impedance data demonstrate the presence of surface bound states in 3 He-*B* film,^{[2,3](#page-3-0)} although there is no evidence of the relativistic massless Dirac spectrum. On the other hand, the surface conditions can be varied in the experiments by coating the surface of several layers of 4 He.²² For increased specularity factor, the new features on the temperature dependence of acoustic impedance were observed indicating the formation of [2](#page-3-0)D Dirac energy spectrum.²

Here we employ the ROM model assuming that the surface consists of small randomly oriented specularly scattering facets[.20](#page-3-0) This model is applicable to describe the fluctuations with the scale much larger than k_F^{-1} of the ⁴He coated surface of the film. Within the framework of ROM model, the important characteristic is the angle α_s which constitutes the local normal vector to the wall n_s with the *z* axis. Let us use the new coordinate system rotated by the angle α_s with respect to the axis defined by $v = z \times n_s$. Then we obtain in the new coordinate system the expression for the order parameter matrix $A_{ij} = A_{ik} R_{kj}$, where *R* is the corresponding rotation matrix. Let us assume without loss of generality that the rotation axis coincides with the *y* axis. Then in the Eq. (2) for the Hamiltonian \hat{H}_0 , we obtain $\hat{F} = (\Delta_{\perp} \cos \alpha_s \hat{\sigma}_z - \Delta_{\parallel} \sin \alpha_s \hat{\sigma}_x) q_z$ and the perturbation term is given by

$$
\hat{H}_1 = \hat{\tau}_1 q_x (\Delta_{\parallel} \hat{\sigma}_x \cos \alpha_s + \Delta_{\perp} \hat{\sigma}_z \sin \alpha_s) - \frac{\gamma}{2} \mathbf{H} \cdot \boldsymbol{\sigma}. \quad (12)
$$

To proceed further with analytical calculations we assume that the order parameter does not depend on the space coordinates so that $\Delta_{\perp}, \Delta_{\parallel} = \text{const.}$ Then we obtain easily the zero energy eigenvectors of the Hamiltonian \hat{H}_0 in the form of Eq. (5) with

$$
\beta_1 = \left(\frac{\Delta_{\parallel} \sin \alpha_s}{\Delta_{\perp} \cos \alpha_s + \bar{\Delta}}, 1\right)^T \tag{13}
$$

$$
\beta_2 = \left(1, -\frac{\Delta_{\parallel} \sin \alpha_s}{\Delta_{\perp} \cos \alpha_s + \bar{\Delta}}\right)^T, \tag{14}
$$

where $\bar{\Delta} = \sqrt{(\Delta_{\parallel} \sin \alpha_s)^2 + (\Delta_{\perp} \cos \alpha_s)^2}$. Correspondingly in Eq. (5) , for the zero order wave functions we obtain

$$
K(z) = \frac{1}{\hbar V_F} \int_0^z \bar{\Delta} ds.
$$

The quasiparticle spectrum obtained along the perturbation theory scheme described above yields the spectrum in the form [\(8\)](#page-1-0) but with modified parameters. We will study the modification of the absorption threshold which is determined by the "mass" term and does not depend on the "light velocity." We therefore will neglect the modification of "light velocity" and focus on the "mass" term which is given by

$$
\tilde{\omega}_H = \omega_H \frac{(\Delta_\perp \cos \alpha_s + \bar{\Delta})^2 - (\Delta_\parallel \sin \alpha_s)^2}{(\Delta_\perp \cos \alpha_s + \bar{\Delta})^2 + (\Delta_\parallel \sin \alpha_s)^2}.
$$
 (15)

To proceed further and calculate statistical average over the surface roughness, we assume that $|\alpha_s| \ll 1$ and obtain to the leading order

$$
\tilde{\omega}_H = \omega_H \bigg(1 - \frac{\alpha_s^2 \Delta_\parallel^2}{2\Delta_\perp^2} \bigg). \tag{16}
$$

The above equation yields the fluctuating correction to the absorption edge in Eq. (11) . It leads to the smoothing out of the sharp absorption edge at the Larmour frequency. To estimate this effect, we assume the Gaussian distribution of angle α_s with the zero average value $\langle \alpha_s \rangle = 0$ and the dispersion $\langle \alpha_s^2 \rangle =$ σ_{α}^2 . After that the average value of the susceptibility in the vicinity of Larmour frequency is given by

$$
\mathrm{Im}\chi_{zz} = \left(\frac{\gamma}{4\hbar C}\right)^2 \left(\frac{\Delta_{\parallel}}{\Delta_{\perp}}\right)^2 \frac{\hbar \omega}{2} f_0\left(\frac{\omega}{4T}\right) S(\alpha_0, \sigma_{\alpha}),
$$

FIG. 1. Plot of the function $S(\alpha_0, \sigma_\alpha)$ for $\sigma_\alpha = 0.01$ (solid line) and $\sigma_{\alpha} = 0.7$ (dashed line).

where $\alpha_0 = 2(\Delta_{\perp}/\Delta_{\parallel})^2[1 - (\omega/\omega_H)^2]$ and

$$
S(\alpha_0, \sigma_\alpha) = \int_{\alpha^*}^{\infty} (\alpha^2 - \alpha_0) \frac{\exp[-(\alpha/\sigma_\alpha)^2]}{\sigma_\alpha \sqrt{\pi}} d\alpha, \qquad (17)
$$

where $\alpha^* = \sqrt{\alpha_0}$ if $\alpha_0 > 0$ and $\alpha^* = 0$ if $\alpha_0 < 0$.

The plots of the function (17) for the different values of σ_{α} are shown in Fig. 1 demonstrating smoothing of the absorption edge with increasing dispersion of surface ripples. Although in general for $\sigma_{\alpha} > 0$ the absorption signal is nonzero at the whole frequency domain, it is exponentially decaying for $\omega \ll \omega_H$. The size of the crossover domain in Fig. 1 is determined by the dispersion $\delta \omega = \omega_H \sigma_\alpha$. Therefore in general we can conclude that the absorption edge should be well observed provided these fluctuations are small so that $\sigma_{\alpha} \ll 1$.

V. CONCLUSION

To conclude, we have calculated the contribution of fermionic surface bound states to the ac magnetic susceptibility of 3He-*B* film. We have shown that in the longitudinal NMR scheme the nonzero absorption signal appears provided the frequency is larger than the threshold one determined by the Larmour frequency $\omega > \omega_H$. Such absorption is absent in the normal state of 3 He and can not occur due to the dynamics of the order parameter spin either. In zero magnetic field, there is no frequency threshold for the dissipation which can be considered as the fingerprint of the gapless Majorana surface bound states. The surface fluctuations are shown to smooth the threshold behavior out providing the small absorption in the frequency domain $\omega < \omega_H$.

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- ¹K. Nagai, Y. Nagato, M. Yamamoto, and S. Higashitani, [J. Phys.](http://dx.doi.org/10.1143/JPSJ.77.111003) Soc. Jpn. **77**[, 111003 \(2008\).](http://dx.doi.org/10.1143/JPSJ.77.111003)
- 2S. Murakawa, Y. Tamura, Y. Wada, M. Wasai, M. Saitoh, Y. Aoki, R. Nomura, Y. Okuda, Y. Nagato, M. Yamamoto, S. Higashitani, and K. Nagai, Phys. Rev. Lett. **103**[, 155301 \(2009\).](http://dx.doi.org/10.1103/PhysRevLett.103.155301)
- 3J. P. Davis, J. Pollanen, H. Choi, J. A. Sauls, W. P. Halperin, and A. B. Vorontsov, Phys. Rev. Lett. **101**[, 085301 \(2008\).](http://dx.doi.org/10.1103/PhysRevLett.101.085301)
- 4Y. Aoki, Y. Wada, M. Saitoh, R. Nomura, Y. Okuda, Y. Nagato, M. Yamamoto, S. Higashitani, and K. Nagai, [Phys. Rev. Lett.](http://dx.doi.org/10.1103/PhysRevLett.95.075301) **95**, [075301 \(2005\).](http://dx.doi.org/10.1103/PhysRevLett.95.075301)
- ⁵H. Choi, J. P. Davis, J. Pollanen, and W. P. Halperin, *[Phys. Rev.](http://dx.doi.org/10.1103/PhysRevLett.96.125301)* Lett. **96**[, 125301 \(2006\).](http://dx.doi.org/10.1103/PhysRevLett.96.125301)
- 6Y. Nagato, S. Higashitani, and K. Nagai, [J. Phys. Soc. Jpn.](http://dx.doi.org/10.1143/JPSJ.78.123603) **78**, [123603 \(2009\).](http://dx.doi.org/10.1143/JPSJ.78.123603)
- 7G. E. Volovik, JETP Lett. **90**[, 587 \(2009\).](http://dx.doi.org/10.1134/S0021364009200089)
- 8M. M. Salomaa and G. E. Volovik, Phys. Rev. B **37**[, 9298 \(1988\).](http://dx.doi.org/10.1103/PhysRevB.37.9298) 9G. E. Volovik, JETP Lett. **90**[, 398 \(2009\).](http://dx.doi.org/10.1134/S0021364009170172)
- 10Suk Bum Chung and Shou-Cheng Zhang, [Phys. Rev. Lett.](http://dx.doi.org/10.1103/PhysRevLett.103.235301) **103**, [235301 \(2009\).](http://dx.doi.org/10.1103/PhysRevLett.103.235301)
- 11Y. Tsutsumi, M. Ichioka, and K. Machida, [Phys. Rev. B](http://dx.doi.org/10.1103/PhysRevB.83.094510) **83**, 094510 [\(2011\).](http://dx.doi.org/10.1103/PhysRevB.83.094510)
- 12F. Wilczek, Nat. Phys. **5**[, 614 \(2009\).](http://dx.doi.org/10.1038/nphys1380)
- 13G. E. Volovik, JETP Lett. **91**[, 215 \(2010\).](http://dx.doi.org/10.1134/S0021364010050024)
- ¹⁴R. G. Bennett, L. V. Levitin, A. Casey, B. Cowan, J. Parpia, and J. Saunders, [J. Low. Temp. Phys.](http://dx.doi.org/10.1007/s10909-009-9941-8) **158**, 163 (2010).
- 15L. V. Levitin, R. G. Bennett, A. Casey, B. Cowan, J. Parpia, and J. Saunders, [J. Low. Temp. Phys.](http://dx.doi.org/10.1007/s10909-009-9946-3) **158**, 159 (2010).
- ¹⁶D. Vollhardt and O. Wölfle, *The superfluid phases of helium 3* (Taylor and Francis, London, 1990).
- 17R. A. Smith, *Semiconductors* (Cambridge University Press, Cambridge, 1961).
- 18N. B. Kopnin, P. I. Soininen, and M. M. Salomaa, [J. Low Temp.](http://dx.doi.org/10.1007/BF00681972) Phys **85**[, 267 \(1991\).](http://dx.doi.org/10.1007/BF00681972)
- 19L. J. Buchholtz and D. Rainer, Z. Phys. B **35**[, 151 \(1979\).](http://dx.doi.org/10.1007/BF01321241)
- ²⁰E. V. Thuneberg, M. Fogelström, and J. Kurkijärvi, *[Physica B](http://dx.doi.org/10.1016/0921-4526(92)90195-X)* 178, [176 \(1992\).](http://dx.doi.org/10.1016/0921-4526(92)90195-X)
- 21Y. Nagato, S. Higashitani, K. Yamada, and K. Nagai, [J. Low Temp.](http://dx.doi.org/10.1007/BF00754654) Phys **103**[, 1 \(1996\).](http://dx.doi.org/10.1007/BF00754654)
- 22S. M. Tholen and J. M. Parpia, [Phys. Rev. Lett.](http://dx.doi.org/10.1103/PhysRevLett.68.2810) **68**, 2810 (1992); D. Kim, M. Nakagawa, O. Ishikawa, T. Hata, T. Kodama, and H. Kojima, *ibid.* **71**[, 1581 \(1993\);](http://dx.doi.org/10.1103/PhysRevLett.71.1581) M. R. Freeman and R. C. Richardson, Phys. Rev. B **41**[, 11011 \(1990\).](http://dx.doi.org/10.1103/PhysRevB.41.11011)