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Anisotropic *s*-wave superconductivity in borocarbides $LuNi_2B_2C$ and YNi_2B_2C

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The symmetry of superconductivity in borocarbides $LuNi_2B_2C$ and YNi_2B_2C is an outstanding issue. Here an anisotropic *s*-wave order parameter (or $s+g$ model) is proposed for $LuNi_2B_2C$ and YNi_2B_2C. In spite of a substantial *s*-wave component, the present superconducting order parameter $\Delta(\mathbf{k})$ has nodes and gives rise to the $\sqrt{H}$ dependent specific heat in the vortex state (the Volovik effect). This model predicts the fourfold symmetry both in the angular dependent thermal conductivity and in the excess Dingle temperature in the vortex state, which should be readily accessible experimentally.

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I. INTRODUCTION

The superconductivity in rare earth (R) transtion metal borocarbides is of great interest,[1,2] in particular its interplay with magnetism and superconductivity is fascinating.[1,3] However in the following we limit ourselves to the nonmagnetic borocarbides $LuNi_2B_2C$ and YNi_2B_2C. They have a relatively high superconducting transition temperature $T_c = 15.5$ K and 16.5 K, respectively. Although a substantial *s*-wave component in $\Delta(\mathbf{k})$ has been established by substituting Ni by a small amount of Pt and subsequent opening of the energy gap,[4,5] a number of peculiarities are not expected in a conventional *s*-wave superconductor.[6] For example, the $\sqrt{H}$ dependence of the specific heat in the vortex state indicates a superconducting state with nodal excitations similar to *d*-wave superconductivity in high T_c cuprates.[7–10] Furthermore the presence of de Haas van Alphen (dHvA) oscillations in the vortex state of $LuNi_2B_2C$ down to $H=0.2H_{c2}$ suggests again nodal superconductivity.[11–13] In a conventional *s*-wave superconductor dHvA oscillations would disappear for $H<0.8H_{c2}$.[11,12] In addition the upper critical field determined for $LuNi_2B_2C$ and YNi_2B_2C for field direction within the *a-b* plane exhibits clear fourfold symmetry somewhat reminiscent to *d*-wave superconductors.[14,15] Furthermore, $1/T_1$ from NMR experiments shows T^3 power law behavior consistent with nodal superconductors.[16] These experiments clearly indicate that $\Delta(\mathbf{k})$ in borocarbides has to be an anisotropic *s*-wave order parameter. Furthermore (i) $\Delta(\mathbf{k})$ has to have a nodal structure with the quasiparticle density of states (DOS) $N(E)\sim|E|$ for $|E|/\Delta \ll 1$, which gives the $\sqrt{H}$ dependence in the specific heat of the vortex state.[6,7] (ii) the nodal structure has to have the fourfold symmetry within the *a-b* plane which is consistent with the tetragonal symmetry of the *a-b* plane. These two constraints appear to suggest almost uniquely

$$\Delta(\mathbf{k}) = \frac{1}{2}\Delta(1+\sin^4\vartheta\cos(4\phi)) \tag{1}$$

or $s+g$-wave superconductivity. Here ϑ,ϕ are the polar and azimuthal angles in $\mathbf{k}$-space, respectively. We show in Fig. 1 $\Delta(\mathbf{k})$, which exhibits clear fourfold symmetry. The four second order nodal points of $\Delta(\mathbf{k})$ are given by $(\vartheta,\phi)=(\pi/2, \pm\pi/4)$ and $(\pi/2, \pm 3\pi/4)$ which dominate the quasiparticle DOS at low energies:

$$\frac{N(E)}{N_0} = \frac{\pi}{4}\frac{|E|}{\Delta} + O\left(\frac{E}{\Delta}\right)^2, \tag{2}$$

where N_0 is the normal state DOS. In constructing $\Delta(\mathbf{k})$, we have made use of a similar approach as in MgB_2.[19–21] In the $s+g$ model of Eq. (1) we assume the equality of s and g amplitudes to have $N(E)\sim|E|$ down to lowest energies. Recent thermal conductivity measurements[17] report a gap anisotropy of at least a factor of 10, the fine tuning of s and g amplitudes in Eq. (1) therefore has a tolerance of 10%. There is no symmetry reason why the amplitudes (or pair potentials) of inequivalent representations like s and g should be very close. However from the bandstructure of

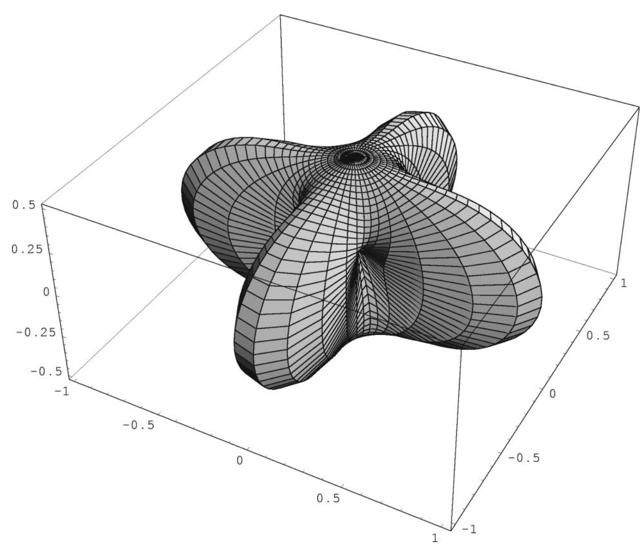

FIG. 1. Normalized gap function $f(\mathbf{k})=\Delta(\mathbf{k})/\Delta$ of the $s+g$ model.

borocarbides[18] it may be argued that the pair potential at the nodal points given above is indeed strongly suppressed. The main Fermi surface sheet shows lobelike structures along the [110] directions which have strong nesting with a wave vector parallel to a. This wave vector appears as the incommensurate ordering vector in the magnetic borocarbides (Lu,Y replaced by rare earth elements). Therefore the lobe states at $(\vartheta,\phi)=(\pi/2,\pm\pi/4)$ and $(\pi/2,\pm 3\pi/4)$ tend to an instability in the particle-hole channel which strongly depresses the effective potential and associated $\Delta(\mathbf{k})$ for Cooper pairing at these points. The approximate fine tuning (up to 10%) of s and g amplitudes may be caused by this peculiar Fermi surface feature of the borocarbides.

In the following we shall first consider thermodynamics and transport of the borocarbides for zero field for the proposed gap function. Then we will study the field angle dependence of specific heat and thermal conductivity which exhibit the fourfold symmetry. We apply the same technique developed in Refs. 7, 22–24. Also we predict the fourfold symmetry in the excess Dingle temperature in the vortex state in borocarbides in a planar magnetic field.

II. THERMODYNAMICS AND TRANSPORT PROPERTIES

First of all $\Delta(\mathbf{k})=\Delta f(\mathbf{k})$ given in Eq. (1) leads to the quasiparticle density of states

$$\frac{N(E)}{N_0}=\frac{1}{4\pi}\int d\Omega \,\mathrm{Re}\frac{|x|}{\sqrt{x^2-f^2}}=|x|\int_0^1 dy F(y)\,\mathrm{Re}\frac{1}{\sqrt{x^2-y^2}}, \tag{3}$$

where $x=E/\Delta$ and

$$F(y)=\frac{2}{\pi}\int_0^{u_0}\frac{dz}{\sqrt{(1-z^2)^4-(1-u_0^2)^4}} \quad \text{with } u_0=(1-\sqrt{|1-2y|})^{1/2}. \tag{4}$$

We note that $F(1-y)=F(y)$ holds. The quasiparticle density of states is evaluated numerically and shown in Fig. 2. For $|E|/\Delta \ll 1$ we obtain

$$\frac{N(E)}{N_0}=\frac{\pi}{4}\frac{|E|}{\Delta}\left(1+\frac{9}{4\pi}\frac{|E|}{\Delta}+\cdots\right), \tag{5}$$

then the low temperature specific heat is given by

$$\frac{C_s}{\gamma_N T}=\frac{27}{4\pi}\zeta(3)\left(\frac{T}{\Delta}\right)+\frac{63}{80}\left(\frac{\pi T}{\Delta}\right)^2+\cdots, \tag{6}$$

where γ_N is the Sommerfeld constant. Similarly the spin susceptibility and the superfluid density are given by

$$\frac{\chi}{\chi_N}=\frac{\pi}{2}\frac{T}{\Delta}(\ln 2)+\frac{3\pi^2}{16}\left(\frac{T}{\Delta}\right)^2+\cdots,$$

$$\frac{\rho_s(T)}{\rho_s(0)}=1-\frac{\chi}{\chi_N}. \tag{7}$$

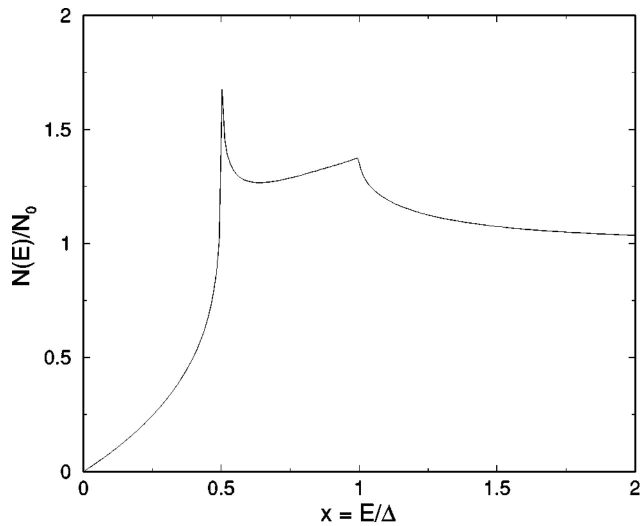

FIG. 2. Quasiparticle density of states. Logarithmic singularity occurs at $E=\Delta/2$ due to the saddle points at $\vartheta=0,\pi$. The cusp at $E=\Delta$ is due to the gap maxima at $(\vartheta,\phi)=(\pi/2,0)$, $(\pi/2,\pm\pi/2)$ and $(\pi/2,\pi)$.

Likewise the electronic thermal conductivity of the $s+g$ model at low temperature is obtained in a universal form as

$$\frac{\kappa}{T}=\frac{\pi^2}{8}\frac{n}{m\Delta}. \tag{8}$$

The prefactor $\pi^2/8$ is specific for the $s+g$ model. Here n, m are the electronic density and mass, respectively. This is equivalent to $\kappa/\kappa_n=3\Gamma/8\Delta$ where κ_n is the normal state thermal conductivity and Γ the quasiparticle scattering rate. The linear T behavior of κ has recently been found[17] in $LuNi_2B_2C$ from which we extract $\Gamma/\Delta \leqslant 0.02$.

III. ANGULAR DEPENDENT SPECIFIC HEAT AND THERMAL CONDUCTIVITY

We are proposing that the angular dependent specific heat and especially thermal conductivity in the vortex state provides a unique window to look for the symmetry of $\Delta(\mathbf{k})$.[22–25] Indeed from the latter Izawa and co-workers have succeded in deducing the symmetry of $\Delta(\mathbf{k})$ in Sr_2RuO_4,[26] $CeCoIn_5$,[27] and more recently $\kappa-(ET)_2Cu(NCS)_2$.[28] First of all we have to construct the equation for the residual density of states in the presence of impurity scattering.[29]

$$g=\mathrm{Re}\left\langle\frac{C_0-ix}{\sqrt{(C_0-ix)^2+f^2}}\right\rangle =\frac{1}{4}\sum_{\pm}\left\langle C_0\ln\left(\frac{2}{\sqrt{C_0^2+x^2}}\right)+x\tan^{-1}\left(\frac{x}{C_0}\right)\right\rangle, \tag{9}$$

where $C_0=\lim_{\omega\to 0}\mathrm{Im}(\tilde{\omega}/\Delta)$ with $\tilde{\omega}$ giving the renormalized frequency and $x=|\mathbf{v}\cdot\mathbf{q}|/\Delta \sim|\sin(\theta\pm\pi/4)|$. Here $2\mathbf{q}$ is the sum of the pair momentum associated with a supercurrent circulating around each vortex and $\mathbf{v}\cdot\mathbf{q}$ is the Doppler shift connected with it. In the first line the brackets mean averag-

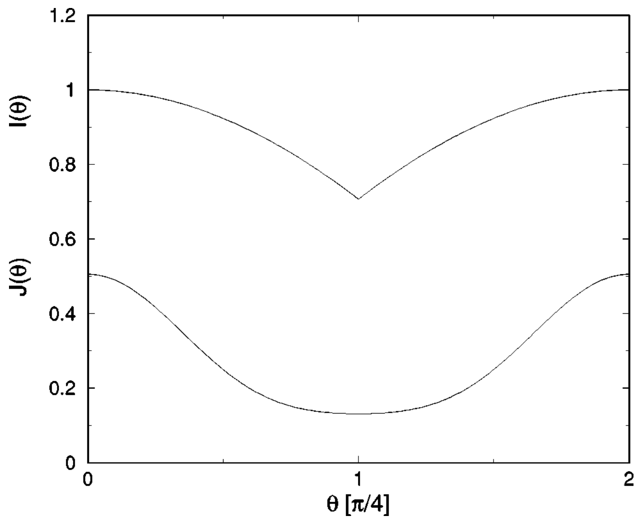

FIG. 3. Angular dependence of specific heat $C_s \sim I(\theta)$ and excess Dingle temperature $\sim J(\theta)$ in an external field in the a-b plane. θ is the angle between field direction and a axis.

ing over both Fermi surface and vortex lattice, in the second line the former is evaluated up to the $\pm$ summation and the latter still remains. In the superclean limit defined by $C_0 \ll \langle x \rangle$ or $\Gamma \ll v_a \sqrt{eH} \ll T \ll \Delta$, Eq. (9) gives

$$g = \frac{\pi}{4} \langle x \rangle = \frac{\tilde{v}\sqrt{eH}}{2\sqrt{2}\Delta} I(\theta), \tag{10}$$

where $\tilde{v} = \sqrt{v_a v_c}$ and $I(\theta) = \max(|\sin\theta|, |\cos\theta|)$ for $0 \leqslant \theta \leqslant \pi/2$. The function $I(\theta)$ is shown in Fig. 3. Here v_a and v_c are Fermi velocities in the a-b plane and along the c axis, respectively. The magnetic field is applied within the a-b plane at an angle θ with respect to the a axis.

In the clean limit with $C_0 \gg \langle x \rangle$ or $v_a \sqrt{eH} \ll \Gamma \ll T \ll \Delta$, on the other hand, we obtain

$$g = g(0)\left(1 + \frac{\tilde{v}^2(eH)}{32\Gamma\Delta}\left[\ln\left(\frac{\Delta}{\tilde{v}\sqrt{eH}} \right) - \frac{1}{8}(1-\cos(4\theta)) \right] \right). \tag{11}$$

From these expressions the field angular dependent specific heat in the vortex state may be derived. In the superclean limit we obtain

$$\frac{C_s}{\gamma_N T} = \frac{\tilde{v}\sqrt{eH}}{2\sqrt{2}\Delta} \; I(\theta). \tag{12}$$

In the clean limit, on the other hand, the above θ dependence is replaced by

$$\frac{C_s}{\gamma_N T} = g(0)\left(1 + \frac{\tilde{v}^2(eH)}{32\Gamma\Delta}\left[\ln\left(\frac{\Delta}{\tilde{v}\sqrt{eH}} \right) - \frac{1}{8}(1-\cos(4\theta)) \right] \right), \tag{13}$$

where $g(0) = N(0)/N_0$ in the absence of magnetic field.

The thermal conductivity tensor in the vortex phase has been calculated in Ref. 23 and in a planar magnetic field it is given by

$$\frac{\kappa_{xx}}{\kappa_n} = \frac{3}{32}\frac{\tilde{v}^2(eH)}{\Delta^2} I^2(\theta),$$

$$\frac{\kappa_{xy}}{\kappa_n} = -\frac{3}{64}\frac{\tilde{v}^2(eH)}{\Delta}\sin(2\theta) \tag{14}$$

in the superclean limit and

$$\frac{\kappa_{xx}}{\kappa_0} = 1 + \frac{\tilde{v}^2(eH)}{32\Gamma\Delta}\ln\left(\sqrt{\frac{2\Delta}{\Gamma}} \right)\left[\ln\left(\frac{\Delta}{\tilde{v}\sqrt{eH}} \right) - \frac{1}{8}(1-\cos(4\theta)) \right],$$

$$\frac{\kappa_{xy}}{\kappa_0} = -\frac{\tilde{v}^2(eH)}{32\Gamma\Delta}\sin(2\theta)\ln\left(\sqrt{\frac{2\Delta}{\Gamma}} \right)\ln\left(\frac{\Delta}{\tilde{v}\sqrt{eH}} \right) \tag{15}$$

in the clean limit. Here κ_0 is $\kappa_{xx}(H=0)$. Therefore we expect the fourfold symmetry in the thermal conductivity in the vortex state should be readily accessible in future experiments. On the other hand κ_{xx} has recently been measured for field oriented along c.[17] In this case a similar calculation in the superclean limit for $H \ll H_{c2}$ leads to

$$\frac{\kappa_{xx}(H)}{\kappa_n} = \frac{3}{16}\frac{v_a^2(eH)}{\Delta^2(0)} \simeq \frac{H - H_{c1}}{H_{c2}(0)}. \tag{16}$$

This behavior was indeed experimentally observed in Ref. 17. In the clean limit $\kappa_{xx}(H)$ is no longer exactly linear but has a logarithmic correction in H. Since $\Gamma/\Delta \leqslant 0.02$ for $LuNi_2B_2C$ we can use the above equation for the superclean limit except for very small fields.

IV. EXCESS DINGLE TEMPERATURE

It is well known that dHvA oscillations can be seen in the vortex state as well when the quasiparticle damping is much less than the cyclotron frequency.[11,30,31] However in conventional s-wave superconductors the dHvA oscillation becomes invisible when $H \leqslant 0.8\ H_{c2}$. Therefore if dHvA oscillations are seen even for $H \sim 0.2 H_{c2}$ as in the case of $LuNi_2B_2C$,[13] this can be taken as a signature of a nodal superconductor. Since the excess Dingle temperature in the vortex state is due to quasiparticle damping caused by the Andreev scattering it should also exhibit the fourfold symmetry of the order parameter. The excess damping due to Andreev scattering is evaluated as

$$\Gamma_A = \frac{\pi}{2\tilde{v}}\frac{1}{\sqrt{eH}}\langle \Delta^2 \rangle = \frac{\pi}{2}\frac{1}{\tilde{v}\sqrt{eH}}\Delta^2 J(\theta), \tag{17}$$

where we defined

$$J(\theta)=\frac{1}{4\pi}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} d\vartheta(1+\sin^4\vartheta\cos(4\theta))^2$$
$$=\frac{1}{4}\left(1+\frac{3}{4}\cos(4\theta)+\frac{35}{128}\cos^2(4\theta)\right). \qquad (18)$$

That is we average $\Delta^2(\mathbf{k})$ on the Fermi surface sliced perpendicular to $\mathbf{H}$. The angular dependence of $J(\theta)$ is shown in Fig. 3 together with $I(\theta)$. In particular we find $I(\pi/4)/I(0)=1/\sqrt{2}$ and $J(\pi/4)/J(0)=0.2587$. The excess damping is reduced by a factor of $\frac{1}{4}$ for $\mathbf{H}\|[1,1,0]$ as compared to the one for $\mathbf{H}\|[1,0,0]$ for example.

V. CONCLUDING REMARKS

Here we propose a simple model for $\Delta(\mathbf{k})$ for nonmagnetic borocarbide superconductors with fourfold symmetry. The angular dependence of the specific heat, thermal conductivity, and the excess Dingle temperature are worked out with this model. We hope that this work will stimulate further experiments on borocarbide superconductors.

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