Impurity induced density of states and residual transport in nonunitary superconductors

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We obtain general expressions for the residual density of states, electrical conductivity, and thermal conductivity for nonunitary superconductors due to impurity scattering. We apply the results to the so-called "*B* phase" of $PrOs_4Sb_{12}$, which we describe using a nonunitary gap function derived from symmetry considerations. The conductivity tensor has inequivalent diagonal components due to off-axis nodal positions, which may be detectable in experiments.

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I. INTRODUCTION

Nonunitary pairing in superfluids was first described by Leggett,[1] but the A_1 phase of ^{3}He is the only well-established example of this, so far. However, recently, nonunitary pairing was observed in the heavy fermion superconductor $PrOs_4Sb_{12}$ by Aoki *et al.*[2] A physically significant consequence of nonunitary pairing is a lifting of the degeneracy of the superconducting energy gap, so that two different energy gap branches, both of which are anisotropic, are observable. A multigap behavior has been observed in $PrOs_4Sb_{12}$ (Refs. 3–9), but so far this has mainly been attributed to multiband superconductivity, and gap splitting due to nonunitary pairing has received little consideration, in spite of numerous citations of the results of Aoki *et al.*

Superconductivity in $PrOs_4Sb_{12}$ is believed to be unconventional.[2,12–20] The paired electrons are in a spin triplet configuration,[19] and the superconducting state has broken time reversal symmetry and is nonunitary.[2] Low temperature power law behavior, indicative of the presence of nodes in the gap function, has been observed in thermodynamic and transport measurements,[13–15,18,20] but some experiments have found the gap function to be nodeless.[5,21–23] Other experiments observed two superconducting phases, possibly with different symmetries,[2,14,15,24–29] suggesting a multicomponent superconducting order parameter. These two phases are known as the "*A* phase" and the "*B* phase." If it exists, the *A* phase occupies only a small region of the phase diagram just below $H_{c2}(T)$. Thus, most measurements, including those cited above, have probed the *B* phase.

The three dimensional representation T_u of the point group T_h best describes superconductivity in $PrOs_4Sb_{12}$.[30,31] This representation yields several superconducting phases, of which four are accessible from the normal state by a second order phase transition. We have previously identified the states $D_2(C_2)\times\mathcal{K}$ and $D_2(E)$, with order parameter components $(0,0,|\eta_1|)$ and $(0,i|\eta_2|,|\eta_1|)$ as the *A* phase and *B* phase, respectively.[30,31] Here, $D_2(C_2)$ is the symmetry group with elements $\{E,C_2^x,U(\pi)C_2^y,U(\pi)C_2^z\}$, while $D_2(E)=\{E,C_2^x\mathcal{K},U_1(\pi)C_2^y\mathcal{K},U_1(\pi)C_2^z\}$.[30] The corresponding gap functions are unitary for the *A* phase, with two point nodes in the $[00\pm1]$ directions, and nonunitary for the *B* phase, with four nodes on unusual points on the Fermi surface, $[0,\pm\alpha,\pm\beta]$.

Low temperature transport is an effective probe for the symmetry of the gap function.[10,11,32–34] Impurities induce and scatter quasiparticles at the nodes, and the conductance remains finite even in the limit of zero frequency and temperature. Usually, two limiting cases of impurity scattering are considered, the "Born limit" (weak scattering) and the "unitary limit" (strong scattering). The unitary limit is associated with nonmagnetic substitutions of magnetic ions in heavy fermion superconductors.[35–38] The self-energy due to isotropic impurity scattering is obtained from the T matrix,[35,38] $\Sigma(k,\omega)=(n_i/\pi N_n)T(k,k,\omega)$, where n_i is the impurity concentration, N_n is the density of states in the normal state, and the T matrix is the self-consistent solution to $T(\omega)=V+VG_0(\omega)T(\omega)$, where V is the impurity potential, $G_0(\omega)=(1/\pi N_n)\Sigma_{\boldsymbol{k}}G(\boldsymbol{k},\omega)$, and $G(\boldsymbol{k},\omega)$ is the electronic Green's function in the superconducting state. The self-energy is then $\Sigma(\omega)=(n_i/\pi N_n)G_0(\omega)/[c^2-G_0^2(\omega)]$, where c is related to the phase shift, $c=\cot\delta_0$. In the unitary limit $c\to0$, while $c\to\infty$ in the Born limit. The main result of this approach is a renormalization of the frequency $\omega\to\omega-i\Gamma(\omega)$ due to impurity scattering. We will use this result to find impurity induced residual density of states and transport coefficients.

The outline of this paper is as follows: In Sec. II, we define the gap function, the mean field Green's functions, and spectral functions. In Secs. III, IV, and V, we derive general expressions for the impurity induced quasiparticle density of states, the electrical conductivity, and the thermal conductivity in a nonunitary superconducting state. In Sec. VI, we apply our results to the nonunitary *B* phase in $PrOs_4Sb_{12}$, and we summarize our results in Sec. VII.

II. MEAN FIELD RESULTS

In the following, we state the main results of the mean field treatment of an effective pairing Hamiltonian (see Ref. 39 for details).

The gap function is a 2×2 matrix in pseudospin space. For triplet pairing, it can be parametrized in terms of an odd pseudovectorial function $\boldsymbol{d}(\boldsymbol{k})$ as

$$\tilde{\Delta}_{\boldsymbol{k}}=i[\tilde{\boldsymbol{\sigma}}\cdot\boldsymbol{d}_{\boldsymbol{k}}]\tilde{\sigma}_y=\begin{pmatrix}-d_x(\boldsymbol{k})+id_y(\boldsymbol{k}) & d_z(\boldsymbol{k})\\ d_z(\boldsymbol{k}) & d_x(\boldsymbol{k})+id_y(\boldsymbol{k})\end{pmatrix}. \tag{1}$$

When $\tilde{\Delta}_{\boldsymbol{k}}\tilde{\Delta}_{\boldsymbol{k}}^{\dagger}$ is proportional to the unit matrix, the pairing is said to be unitary. Nonunitary pairing occurs only in the

triplet channel and only when $\boldsymbol{q}_k \equiv i\boldsymbol{d}_k \times \boldsymbol{d}_k^* \neq 0$. Nonunitary states necessarily have broken time reversal symmetry. However, note that, for example, pairing of the form $\boldsymbol{d}_k = (k_x + ik_y)\hat{z}$ (proposed for Sr_2RuO_4) breaks the time reversal symmetry but is unitary. The quasiparticle energies are

$$E_{k\pm} = [\varepsilon_k^2 + \Delta_{k\pm}^2]^{1/2}, \tag{2}$$

where

$$\Delta_{k\pm} = [|\boldsymbol{d}_k|^2 \pm |\boldsymbol{q}_k|]^{1/2}. \tag{3}$$

Thus, nonunitary pairing lifts the gap degeneracy.

For triplet pairing, the normal and anomalous quasiparticle Green's functions are[39,40]

$$\tilde{G}(\boldsymbol{k}, i\omega_n) = \frac{-[\omega_n^2 + \varepsilon_k^2 + |\boldsymbol{d}_k|^2]\tilde{\sigma}_0 + \boldsymbol{q}_k \cdot \tilde{\boldsymbol{\sigma}}}{[\omega_n^2 + E_{k-}^2][\omega_n^2 + E_{k+}^2]}[i\omega_n + \varepsilon_k], \tag{4}$$

$$\tilde{F}(\boldsymbol{k}, i\omega_n) = \frac{[\omega_n^2 + \varepsilon_k^2 + |\boldsymbol{d}_k|^2]\boldsymbol{d}_k - i\boldsymbol{q}_k \times \boldsymbol{d}_k}{[\omega_n^2 + E_{k-}^2][\omega_n^2 + E_{k+}^2]} \cdot [i\tilde{\boldsymbol{\sigma}}\tilde{\sigma}_y]. \tag{5}$$

It is useful to expand these expressions as

$$\begin{aligned}\tilde{G}(\boldsymbol{k}, \omega) = \frac{\tilde{\sigma}_0}{2}\Bigg[& \frac{u_{k-}^2}{\omega - E_{k-} + i\delta} + \frac{v_{k-}^2}{\omega + E_{k-} + i\delta} + \frac{u_{k+}^2}{\omega - E_{k+} + i\delta} \\ & + \frac{v_{k+}^2}{\omega + E_{k+} + i\delta}\Bigg] - \frac{\boldsymbol{q}_k \cdot \tilde{\boldsymbol{\sigma}}}{2|\boldsymbol{q}_k|}\Bigg[\frac{u_{k-}^2}{\omega - E_{k-} + i\delta} \\ & + \frac{v_{k-}^2}{\omega + E_{k-} + i\delta} - \frac{u_{k+}^2}{\omega - E_{k+} + i\delta} - \frac{v_{k+}^2}{\omega + E_{k+} + i\delta}\Bigg],\end{aligned} \tag{6}$$

$$\begin{aligned}\tilde{F}(\boldsymbol{k}, \omega) = -\frac{\tilde{\sigma}_0}{2}\Bigg\{ & \frac{\tilde{\Delta}_k}{\Delta_{k-}}\Bigg[\frac{u_{k-}v_{k-}}{\omega - E_{k-} + i\delta} - \frac{u_{k-}v_{k-}}{\omega + E_{k-} + i\delta}\Bigg] \\ & + \frac{\tilde{\Delta}_k}{\Delta_{k+}}\Bigg[\frac{u_{k+}v_{k+}}{\omega - E_{k+} + i\delta} - \frac{u_{k+}v_{k+}}{\omega + E_{k+} + i\delta}\Bigg]\Bigg\} \\ & + \frac{\boldsymbol{q}_k \cdot \tilde{\boldsymbol{\sigma}}}{2|\boldsymbol{q}_k|}\Bigg\{\frac{\tilde{\Delta}_k}{\Delta_{k-}}\Bigg[\frac{u_{k-}v_{k-}}{\omega - E_{k-} + i\delta} - \frac{u_{k-}v_{k-}}{\omega + E_{k-} + i\delta}\Bigg] \\ & - \frac{\tilde{\Delta}_k}{\Delta_{k+}}\Bigg[\frac{u_{k+}v_{k+}}{\omega - E_{k+} + i\delta} - \frac{u_{k+}v_{k+}}{\omega + E_{k+} + i\delta}\Bigg]\Bigg\},\end{aligned} \tag{7}$$

where

$$u_{k\pm}^2 = \frac{1}{2}\Bigg[1 + \frac{\varepsilon_k}{E_{k\pm}}\Bigg], \quad v_{k\pm}^2 = \frac{1}{2}\Bigg[1 - \frac{\varepsilon_k}{E_{k\pm}}\Bigg],$$

$$u_{k\pm}v_{k\pm} = \frac{\Delta_{k\pm}}{2E_{k\pm}}, \quad u_{k\pm}^2 + v_{k\pm}^2 = 1 \tag{8}$$

are the extended coherence factors for this particular state. Note that the following identity has been used in deriving the above expressions:

$$i(\boldsymbol{q}_k \times \boldsymbol{d}_k) \cdot \tilde{\boldsymbol{\sigma}} = (\boldsymbol{q}_k \cdot \tilde{\boldsymbol{\sigma}})(\boldsymbol{d}_k \cdot \tilde{\boldsymbol{\sigma}}) - \boldsymbol{q}_k \cdot \boldsymbol{d}_k = (\boldsymbol{q}_k \cdot \tilde{\boldsymbol{\sigma}})(\boldsymbol{d}_k \cdot \tilde{\boldsymbol{\sigma}}) \tag{9}$$

where $\boldsymbol{q}_k \cdot \boldsymbol{d}_k = 0$ because $\boldsymbol{q}_k \perp \boldsymbol{d}_k$. The self-energy can be included by replacing $i\omega_n$ with $i\omega_n - \Sigma(i\omega_n)$. The retarded self-energy is $\Sigma_{ret}(\omega) = \Sigma(i\omega_n \to \omega + i\delta) = -i\Gamma(\omega)$, where the real part is assumed to be frequency independent and absorbed in the chemical potential.

The spectral function $\tilde{A}^G(\boldsymbol{k}, \omega)$ [and similarly $\tilde{A}^F(\boldsymbol{k}, \omega)$] is defined by

$$\tilde{G}(\boldsymbol{k}, i\omega_n) = \int_{-\infty}^{+\infty} d\omega \frac{\tilde{A}^G(\boldsymbol{k}, \omega)}{i\omega_n - \omega}. \tag{10}$$

Usually, the spectral function is just $-\frac{1}{\pi}\Im\tilde{G}^{ret}(\boldsymbol{k}, \omega)$, but in this case, because the Green's function has a complex numerator, the spectral function must be extracted more carefully. Using Eqs. (6) and (7), one finds

$$\begin{aligned}\tilde{A}^G(\boldsymbol{k}, \omega) = \frac{\Gamma(\omega)}{2\pi}\tilde{\sigma}_0\Bigg[& \frac{u_{k-}^2}{(\omega - E_{k-})^2 + \Gamma^2(\omega)} \\ & + \frac{v_{k-}^2}{(\omega + E_{k-})^2 + \Gamma^2(\omega)} + \frac{u_{k+}^2}{(\omega - E_{k+})^2 + \Gamma^2(\omega)} \\ & + \frac{v_{k+}^2}{(\omega + E_{k+})^2 + \Gamma^2(\omega)}\Bigg] \\ & - \frac{\Gamma(\omega)}{2\pi}\frac{\boldsymbol{q}_k \cdot \tilde{\boldsymbol{\sigma}}}{|\boldsymbol{q}_k|}\Bigg[\frac{u_{k-}^2}{(\omega - E_{k-})^2 + \Gamma^2(\omega)} \\ & + \frac{v_{k-}^2}{(\omega + E_{k-})^2 + \Gamma^2(\omega)} - \frac{u_{k+}^2}{(\omega - E_{k+})^2 + \Gamma^2(\omega)} \\ & - \frac{v_{k+}^2}{(\omega + E_{k+})^2 + \Gamma^2(\omega)}\Bigg],\end{aligned} \tag{11}$$

$$\begin{aligned}\tilde{A}^F(\boldsymbol{k}, \omega) = \frac{\Gamma(\omega)}{2\pi}\tilde{\sigma}_0\Bigg\{ & \frac{\tilde{\Delta}_k}{\Delta_{k-}}\Bigg[\frac{u_{k-}v_{k-}}{(\omega + E_{k-})^2 + \Gamma^2(\omega)} \\ & - \frac{u_{k-}v_{k-}}{(\omega - E_{k-})^2 + \Gamma^2(\omega)}\Bigg] + \frac{\tilde{\Delta}_k}{\Delta_{k+}}\Bigg[\frac{u_{k+}v_{k+}}{(\omega + E_{k+})^2 + \Gamma^2(\omega)} \\ & - \frac{u_{k+}v_{k+}}{(\omega - E_{k+})^2 + \Gamma^2(\omega)}\Bigg]\Bigg\} \\ & - \frac{\Gamma(\omega)}{2\pi}\frac{\boldsymbol{q}_k \cdot \tilde{\boldsymbol{\sigma}}}{|\boldsymbol{q}_k|}\Bigg\{\frac{\tilde{\Delta}_k}{\Delta_{k-}}\Bigg[\frac{u_{k-}v_{k-}}{(\omega + E_{k-})^2 + \Gamma^2(\omega)} \\ & - \frac{u_{k-}v_{k-}}{(\omega - E_{k-})^2 + \Gamma^2(\omega)}\Bigg] + \frac{\tilde{\Delta}_k}{\Delta_{k+}}\Bigg[\frac{u_{k+}v_{k+}}{(\omega + E_{k+})^2 + \Gamma^2(\omega)} \\ & - \frac{u_{k+}v_{k+}}{(\omega - E_{k+})^2 + \Gamma^2(\omega)}\Bigg]\Bigg\}.\end{aligned} \tag{12}$$

With the spectral functions in hand, we can proceed to calculate the density of states and the transport coefficients.

III. DENSITY OF STATES

The quasiparticle density of states can be defined in terms of the spectral function as

$$N(\omega) = \sum_{\boldsymbol{k}} \mathrm{Tr}[\tilde{A}^G(\boldsymbol{k},\omega)]. \tag{13}$$

Using Eq. (11), we find the general expression for the density of states in a nonunitary superconductor,

$$N(\omega) = \sum_{\boldsymbol{k},\pm} [u^2_{\boldsymbol{k}\pm}\delta(\omega - E_{\boldsymbol{k}\pm}) + v^2_{\boldsymbol{k}\pm}\delta(\omega + E_{\boldsymbol{k}\pm})] \tag{14}$$

in the absence of impurities. For small ω, in the vicinity of the gap node, we have $v_{\boldsymbol{k}\pm} \approx 0$, $u_{\boldsymbol{k}\pm} \approx 1$, and Eq. (14) is reduced to[39]

$$N(\omega) \approx \sum_{\boldsymbol{k},\pm} \delta(\omega - E_{\boldsymbol{k}\pm}). \tag{15}$$

When the impurities are included, the density of states becomes

$$N(\omega) \approx \frac{\Gamma(\omega)}{\pi} \sum_{\boldsymbol{k},\pm} \left[\frac{1}{(\omega - E_{\boldsymbol{k}\pm})^2 + \Gamma^2(\omega)} \right]. \tag{16}$$

It is clear from Eq. (16) that the residual density of states depends on the impurity concentration through the self-energy $\Gamma(0)$.

IV. ELECTRICAL CONDUCTIVITY

The dc electrical conductivity is defined by the Kubo formula[41]

$$\tilde{\sigma} = -\lim_{\Omega\to 0} \frac{\Im\tilde{\Pi}_{ret}(\Omega)}{\Omega}, \tag{17}$$

where

$$\tilde{\Pi}(\boldsymbol{q}, i\Omega_n) = -\int_0^\beta d\tau e^{i\Omega_n\tau} \langle T \boldsymbol{j}_{\boldsymbol{q}}(\tau)\boldsymbol{j}_{-\boldsymbol{q}}(0)\rangle \tag{18}$$

is the current-current correlation function. The electrical current is defined by

$$\boldsymbol{j}(\boldsymbol{q},\tau) = \frac{e}{m^*} \sum_{\boldsymbol{k},s} \left[\boldsymbol{k} + \frac{\boldsymbol{q}}{2} \right] c^\dagger_{\boldsymbol{k}+\boldsymbol{q},s}(\tau) c_{\boldsymbol{k},s}(\tau). \tag{19}$$

The current-current correlation function is therefore

$$\tilde{\Pi}(\boldsymbol{q}, i\Omega_n) = \frac{e^2}{m^{*2}} \sum_{\boldsymbol{k}} \left[\boldsymbol{k} + \frac{\boldsymbol{q}}{2} \right]^2 \frac{1}{\beta} \sum_{i\omega_n} \mathrm{Tr}[\tilde{G}(\boldsymbol{k}, i\omega_n)\tilde{G}(\boldsymbol{k}+\boldsymbol{q}, i\omega_n + i\Omega_n) + \tilde{F}(\boldsymbol{k}, i\omega_n)\tilde{F}^\dagger(\boldsymbol{k}+\boldsymbol{q}, i\omega_n + i\Omega_n)]. \tag{20}$$

The conductivity vanishes when the self-energy is absent, and the contribution from the anomalous part vanishes even when the self-energy is included. In the limit $\mathbf{q} \to 0$, the correlation function is

$$\tilde{\Pi}(i\Omega_n) = e^2 \sum_{\boldsymbol{k}} \boldsymbol{v}_F \boldsymbol{v}_F \frac{1}{\beta} \sum_{i\omega_n} \mathrm{Tr}[\tilde{G}(\boldsymbol{k}, i\omega_n)\tilde{G}(\boldsymbol{k}, i\omega_n + i\Omega_n)]. \tag{21}$$

To evaluate this correlation function, we follow the approach of Refs. 41 and 11 and rewrite the Green's function in terms of the spectral function [Eq. (11)] and sum over Matsubara frequencies. This eventually leads to

$$\Im\tilde{\Pi}_{ret}(\Omega) = -\pi e^2 \sum_{\boldsymbol{k}} \boldsymbol{v}_F \boldsymbol{v}_F \int_{-\infty}^{\infty} d\omega' \, \mathrm{Tr}[\tilde{A}^G_{\boldsymbol{k}}(\omega')\tilde{A}^G_{\boldsymbol{k}}(\omega' + \Omega)] \times [n_F(\omega') - n_F(\omega' + \Omega)]. \tag{22}$$

Then, the dc electrical conductivity [Eq. (17)] is

$$\tilde{\sigma} = \pi e^2 \sum_{\boldsymbol{k}} \boldsymbol{v}_F \boldsymbol{v}_F \int_{-\infty}^{\infty} d\omega' \, \mathrm{Tr}[\tilde{A}^G_{\boldsymbol{k}}(\omega')\tilde{A}^G_{\boldsymbol{k}}(\omega')] \left[-\frac{\partial n_F(\omega')}{\partial \omega'} \right]. \tag{23}$$

In the limit $T \to 0$, we have $-\frac{\partial n_F(\omega')}{\partial \omega'} = \delta(\omega')$, and the conductivity is

$$\tilde{\sigma} = \pi e^2 \sum_{\boldsymbol{k}} \boldsymbol{v}_F \boldsymbol{v}_F \, \mathrm{Tr}[\tilde{A}^G_{\boldsymbol{k}}(0)\tilde{A}^G_{\boldsymbol{k}}(0)]. \tag{24}$$

Using Eq. (11), we finally obtain the conductivity for a nonunitary superconductor,

$$\tilde{\sigma} = \frac{e^2\Gamma_0^2}{\pi} \sum_{\boldsymbol{k}} \boldsymbol{v}_F \boldsymbol{v}_F \left[\frac{1}{(\Gamma_0^2 + E^2_{\boldsymbol{k}-})^2} + \frac{1}{(\Gamma_0^2 + E^2_{\boldsymbol{k}+})^2} \right], \tag{25}$$

where $\Gamma_0 = \Gamma(\omega = 0)$.

V. THERMAL CONDUCTIVITY

The dc thermal conductivity is defined by the Kubo formula[11]

$$\frac{\tilde{\kappa}}{T} = -\frac{1}{T^2} \lim_{\Omega\to 0} \frac{\Im\tilde{\Pi}_{ret}(\Omega)}{\Omega}. \tag{26}$$

The heat current can be written in second quantization form as

$$\boldsymbol{j}_{\boldsymbol{q}}(\tau) = -\frac{1}{2m^*} \sum_{\boldsymbol{k},s} \left[i[\boldsymbol{k} + \boldsymbol{q}] \frac{\partial c^\dagger_{\boldsymbol{k},s}(\tau)}{\partial\tau} c_{\boldsymbol{k}+\boldsymbol{q},s}(\tau) - i\boldsymbol{k} c^\dagger_{\boldsymbol{k},s}(\tau) \frac{\partial c_{\boldsymbol{k}+\boldsymbol{q},s}(\tau)}{\partial\tau} \right]. \tag{27}$$

This form is similar to Eq. (4.17) in Ref. 11, except that we have neglected the term proportional to the gap velocity, which we assume to be much smaller than the Fermi velocity. The current-current correlation function is then

$$\tilde{\Pi}(i\Omega_n) = \frac{1}{\beta} \sum_{\boldsymbol{k}, i\omega_n} \boldsymbol{v}_F \boldsymbol{v}_F \left[i\omega_n + \frac{i\Omega_n}{2} \right]^2 \mathrm{Tr}[\tilde{G}_{\boldsymbol{k}}(i\omega_n + i\Omega_n) \times \tilde{G}_{\boldsymbol{k}}(-i\omega_n) - \tilde{F}_{\boldsymbol{k}}(-i\omega_n)\tilde{F}^\dagger_{\boldsymbol{k}}(i\omega_n + i\Omega_n)]. \tag{28}$$

As in the electrical conductivity, the anomalous part does not

contribute to the thermal conductivity. Finally, the correlation function is expressed in terms of the spectral function as

$$\Im\tilde{\Pi}_{ret}(\Omega) = \sum_{\boldsymbol{k}} \boldsymbol{v}_F \boldsymbol{v}_F \int_{-\infty}^{\infty} d\omega' \, \mathrm{Tr}[\tilde{A}^G_{\boldsymbol{k}}(\omega'+\Omega)\tilde{A}^G_{\boldsymbol{k}}(-\omega')] \times \left[\omega' + \frac{\Omega}{2}\right]^2 [n_F(\omega'+\Omega) - n_F(\omega')]. \quad (29)$$

Substituting this into the Kubo formula [Eq. (26)] and evaluating in the limit $\Omega \to 0$ and $T \to 0$, we find

$$\frac{\tilde{\kappa}}{T} = \frac{\pi^2}{3} k_B^2 \sum_{\boldsymbol{k}} \boldsymbol{v}_F \boldsymbol{v}_F \, \mathrm{Tr}[\tilde{A}^G_{\boldsymbol{k}}(0)\tilde{A}^G_{\boldsymbol{k}}(0)]. \quad (30)$$

Comparing Eqs. (24) and (30), we can see that the Wiedemann-Franz law $\frac{\kappa}{\sigma T} = \frac{\pi k_B^2}{3e^2}$ is satisfied. Explicitly, the thermal conductivity is

$$\frac{\tilde{\kappa}}{T} = \frac{k_B^2}{3} \Gamma_0^2 \sum_{\boldsymbol{k}} \boldsymbol{v}_F \boldsymbol{v}_F \left[\frac{1}{(\Gamma_0^2 + E_{\boldsymbol{k}-}^2)^2} + \frac{1}{(\Gamma_0^2 + E_{\boldsymbol{k}+}^2)^2} \right]. \quad (31)$$

VI. APPLICATION TO $PrOs_4Sb_{12}$

As discussed in the Introduction, we assume that the gap function for the A phase is

$$\Delta_{\boldsymbol{k}} = |\eta_1|[a^2 k_y^2 + b^2 k_x^2]^{1/2}, \quad (32)$$

where a and b are undetermined constants, while for the B phase it has the form

$$\Delta_{\boldsymbol{k}\pm} = [[|\eta_1|^2 b^2 + |\eta_2|^2 a^2]k_x^2 + |\eta_1|^2 a^2 k_y^2 + |\eta_2|^2 b^2 k_z^2 \pm 2|\eta_1||\eta_2| \times |k_x|\sqrt{a^2 b^2 k_x^2 + a^4 k_y^2 + b^4 k_z^2}]^{1/2}, \quad (33)$$

which is nondegenerate.[31] The gap function in the A phase is unitary and has two cusp point nodes in the $[00\pm1]$ directions. The lower branch of the B phase gap function has four point nodes, which are in the $k_y=0$ plane at the positions $\sqrt{|\eta_1|^2 b^2 - |\eta_2|^2 a^2}k_x = \pm|\eta_2| b k_z$ if $|\eta_1|^2 b^2 > |\eta_2|^2 a^2$; else, they are in the $k_z=0$ plane. We will assume the former in our calculations. Since we are interested in the very low temperature regime, we will consider only the B phase.

The gap function of the B phase in the vicinity of nodes can be linearized as

$$\Delta_{\boldsymbol{k}} \approx v\sqrt{k_\parallel^2 + k_y'^2}, \quad (34)$$

where $v = \sqrt{|\eta_1|^2 b^2 - |\eta_2|^2 a^2}$, $k_y' = \frac{a}{b}k_y$, and

$$k_\parallel = \frac{\sqrt{|\eta_1|^2 b^2 - |\eta_2|^2 a^2}}{|\eta_1| b} k_x \pm \frac{|\eta_2| a}{|\eta_1| b} k_z. \quad (35)$$

$k_\parallel$ and $k_\perp$ (used below) are momenta parallel and perpendicular to the Fermi surface at the node. The upper branch, which is degenerate with the lower branch on the line $k_x=0$ between each pair of nodes, is properly included with this linearization of the gap function. Therefore, we relabel the two branches of the gap function, as shown in Fig. 1. Thus, for any function, we have

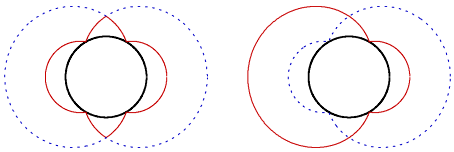

FIG. 1. (Color online) Gap function for the B phase of $PrOs_4Sb_{12}$ drawn in the k_x-k_z plane over a spherical Fermi surface (bold black). Left: the + branch is shown in blue (dashed) and the − branch in red (solid). Right: branch 1 is shown in blue (dashed) and branch 2 in red (solid).

$$f(E_+) + f(E_-) \equiv f(E_1) + f(E_2). \quad (36)$$

Each branch 1 and 2 has two cusp point nodes, and the contribution to the excitation spectrum from each branch is equal. With this picture in mind, we now calculate the density of states and the transport coefficients.

A. Density of states

The density of states was calculated previously in Ref. 31 in the absence of impurities; here, we will include the effect of impurities starting from Eq. (16). Linearizing the gap function as described above, we find

$$N(\omega) = \frac{\Gamma(\omega)}{\pi} 2 \sum_{j=1}^{2} \int \frac{d^3k}{(2\pi)^3} \frac{1}{(\omega - E_{\boldsymbol{k}})^2 + \Gamma^2(\omega)}, \quad (37)$$

where there is a factor of 2 because there are two branches of the gap function, and the sum is over the two nodes in each branch. To perform the integration, we change variables to $p^2 = v^2(k_\parallel^2 + k_y'^2) + v_F^2 k_\perp^2 \approx E_{\boldsymbol{k}}^2$,

$$N(\omega) = \frac{2\Gamma(\omega)}{\pi^3} \frac{b}{a} \frac{1}{[|\eta_1|^2 b^2 - |\eta_2|^2 a^2] v_F} \int_0^{p_0} \frac{dpp^2}{(\omega - p)^2 + \Gamma^2(\omega)} \quad (38)$$

and introduce a cutoff p_0. Performing the integration, we arrive at the result

$$N(\omega) = \frac{2}{\pi^3} \frac{b}{a} \frac{1}{[|\eta_1|^2 b^2 - |\eta_2|^2 a^2] v_F} \Bigg[[\omega^2 - \Gamma^2(\omega)] \times \left[\tan^{-1}\left(\frac{p_0 - \omega}{\Gamma(\omega)}\right) + \tan^{-1}\left(\frac{\omega}{\Gamma(\omega)}\right) \right] + \omega\Gamma(\omega) \ln\left(\frac{[p_0 - \omega]^2 + \Gamma^2(\omega)}{\omega^2 + \Gamma^2(\omega)}\right) - \omega\Gamma(\omega) + p_0\Gamma(\omega) \Bigg]. \quad (39)$$

Setting $\Gamma(\omega)=0$, we obtain our previous result[31]

$$N(\omega) = \frac{b}{a} \frac{2\omega^2}{\pi^2 v_F [|\eta_1|^2 b^2 - |\eta_2|^2 a^2]}, \quad (40)$$

which has a quadratic dependence on frequency as expected for point nodes. In the limit $\omega \to 0$, Eq. (39) becomes

$$N(0) = \frac{2}{\pi^3}\frac{b}{a}\frac{\Gamma_0^2}{[|\eta_1|^2 b^2 - |\eta_2|^2 a^2]v_F}\left[\tan^{-1}\left(-\frac{p_0}{\Gamma_0}\right) + \frac{p_0}{\Gamma_0}\right]. \tag{41}$$

This is the zero energy density of states induced by impurities. The cutoff is normally taken to be the size of the Brillouin zone,[11] but it may be more physical to use the reciprocal of the range of the single impurity potential,[34] $p_0 \propto \lambda^{-1}$. In terms of the ratio (p_0/Γ_0), the two limits are

$$\frac{p_0}{\Gamma_0} \gg 1 \quad \text{(unitary)}, \tag{42}$$

$$\frac{p_0}{\Gamma_0} \ll 1 \quad \text{(Born)}. \tag{43}$$

In the unitary limit, the density of states is

$$N(0) = \frac{2}{\pi^3}\frac{b}{a}\frac{p_0\Gamma_0^u}{[|\eta_1|^2 b^2 - |\eta_2|^2 a^2]v_F}, \tag{44}$$

where u refers to unitary scattering. If Γ_c is the critical scattering rate at which the superconductor becomes normal at the node, then we can write Eq. (44) as

$$\frac{N(0)}{N_n} = \frac{\Gamma_0^u}{\Gamma_c^u} = \frac{n_{imp}}{n_{imp}^c}. \tag{45}$$

In the Born limit, the density of states vanishes as Γ_0^2.

The presence of the residual density of states, in general, gives a contribution linear in temperature to the specific heat and the nuclear spin relaxation rate at low temperature. The prefactor dependence on impurity doping may be helpful in identifying the symmetry of the order parameter. The specific heat is[39]

$$C(T) = \frac{2}{T}\int_0^\infty d\omega \omega^2 N(\omega)\left[-\frac{\partial f}{\partial \omega}\right]. \tag{46}$$

At low temperature, this yields

$$\frac{[C(T)/T]}{[C(T)/T]_n} = \frac{\Gamma_0^u}{\Gamma_c^u}, \tag{47}$$

and the nuclear spin relaxation rate is[39]

$$\frac{(1/T_1)_T}{(1/T_1)_n} = 2\frac{T}{T_c}\int_0^\infty d\omega N(\omega)N(\omega-\omega_0)\left[-\frac{\partial f}{\partial \omega}\right],$$

$$\frac{(1/TT_1)_T}{(1/TT_1)_n} = \frac{\Gamma_0^{u2}}{\Gamma_c^{u2}}. \tag{48}$$

B. Electrical and thermal conductivities

Beginning with Eq. (25) and making use of Eq. (36), we divide the integration into four parts, each centered about one node in the gap function. The factor $\boldsymbol{v}_F\boldsymbol{v}_F$ is evaluated at each node; the sum over nodes yields

$$\sum_{j=1}^{4} \boldsymbol{v}_F\boldsymbol{v}_F = 4v_F^2\begin{pmatrix} \frac{|\eta_2|^2 a^2}{|\eta_1|^2 b^2} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{|\eta_1|^2 b^2 - |\eta_2|^2 a^2}{|\eta_1|^2 b^2} \end{pmatrix}. \tag{49}$$

The remaining integration is the same for each part. Performing the same change of variables as in the density of states calculation, we find

$$\tilde{\sigma} = \frac{e^2\Gamma_0^2}{2\pi^3}\frac{b}{a}\frac{\sum_{j=1}^{4}\boldsymbol{v}_F\boldsymbol{v}_F}{[|\eta_1|^2 b^2 - |\eta_2|^2 a^2]v_F}\int_0^{p_0}\frac{dpp^2}{[p^2+\Gamma_0^2]^2}, \tag{50}$$

and completing the integration we get

$$\tilde{\sigma} = \frac{e^2}{\pi^3}v_F\Gamma_0\left[\tan^{-1}\left(\frac{p_0}{\Gamma_0}\right) - \frac{(p_0/\Gamma_0)}{1+(p_0/\Gamma_0)^2}\right] \times \begin{pmatrix} \frac{a|\eta_2|^2}{b|\eta_1|^2[b^2|\eta_1|^2 - a^2|\eta_2|^2]} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{1}{ab|\eta_1|^2} \end{pmatrix}. \tag{51}$$

This is the impurity induced dc electrical conductivity for the B phase of $PrOs_4Sb_{12}$. The thermal conductivity can be easily obtained by using the Wiedemann-Franz law. In the unitary limit $\left(\frac{p_0}{\Gamma_0} \gg 1\right)$, the term which includes $\tan^{-1}\left(\frac{p_0}{\Gamma_0}\right) = \frac{\pi}{2}$ will dominate; the conductivities become

$$\tilde{\sigma} = \frac{e^2}{2\pi^2}v_F\Gamma_0^u\begin{pmatrix} \frac{a|\eta_2|^2}{b|\eta_1|^2[b^2|\eta_1|^2 - a^2|\eta_2|^2]} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{1}{ab|\eta_1|^2} \end{pmatrix} \tag{52}$$

and

$$\frac{\tilde{\kappa}}{T} = \frac{k_B^2}{6\pi}v_F\Gamma_0^u\begin{pmatrix} \frac{a|\eta_2|^2}{b|\eta_1|^2[b^2|\eta_1|^2 - a^2|\eta_2|^2]} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{1}{ab|\eta_1|^2} \end{pmatrix}. \tag{53}$$

Thus, the conductivities in the B phase of $PrOs_4Sb_{12}$ are nonuniversal (dependent on impurity concentration) for unitary scattering but vanish in the Born limit. The conductivity tensor has two inequivalent components, σ_{xx} and σ_{zz}, due to the off-axis nodal positions *and* the choice of a particular domain of superconducting phase. This domain is represented by order parameter components $(0, i|\eta_2|, |\eta_1|)$. If all six domains are present, then all diagonal components of the conductivity tensor will be equal. The σ_{xx} component is pro-

portional to the parameter $|\eta_2|$, which is absent in the unitary A phase. Therefore, the measurement of residual conductivities in a domain-pinned setup, such as the one used in directional dependent thermal conductivity measurements[14] could determine the direction of nodes. Of all the possible SC states in tetrahedral systems, $D_2(E)$, with OP components $(0, i|\eta_2|, |\eta_1|)$, is the only one with off-axis nodes.[30,31]

C. Discussion

There have been several studies on Ru and La doped samples,[6,17,42–44] with the surprising result that Ru substitution leads to a doping-dependent residual density of states and resistivity,[17,42] while La substitution does not.[6] In $PrOs_4Sb_{12}$, it is speculated that quadrupolar fluctuations of the Pr ions play a role similar to the magnetic fluctuations of Ce and U ions in other heavy fermion superconductors; thus, substitution of the Pr ions by La would be expected to produce unitary scatterers. However, in contrast to Eq. (48), there is no dependence on doping on the NQR relaxation rate beyond the La concentration $x=0.05$.

Both $Pr_{1-x}La_xOs_4Sb_{12}$ and $Pr(Os_{1-x}Ru_x)_4Sb_{12}$ are superconducting for the entire range of x, and both become s-wave superconductors at some intermediate value of x. In the Ru doped series, T_c has a minimum at $x=0.6$, with a leveling off of the specific heat at the same value. This suggests that a phase transition between triplet and singlet superconductivity occurs at $x\approx 0.6$, with possibly a region of coexistence of these two phases.[45] A 0.4% change in lattice constant occurs between $PrOs_4Sb_{12}$ and $PrRu_4Sb_{12}$,[42] and effects due to quadrupolar fluctuations appear to be absent in $PrRu_4Sb_{12}$. In the La doped series, T_c decreases linearly along the entire range of x, while the specific heat levels off at $x\approx 0.3$.

According to Eqs. (44) and (52), the dependence of the residual density of states and resistivity on Ru doping suggests that the scattering from Ru ions is unitary. Unitary scattering due to the substitution of Os by Ru may be explained by noting that quadrupolar fluctuations of the Pr ions are charge density fluctuations and will couple to, and possibly be enhanced by, quadrupolar lattice vibration modes. The change in lattice constant that accompanies Ru doping will alter the quadrupole moment of those modes. In addition, Ru substitution has a strong effect on the low-lying crystal electric field (CEF) levels of the Pr ions, which eventually removes quadrupole fluctuations.[44] La substitution produces a much smaller change in lattice constant and has a much weaker effect on the Pr CEF levels. Nevertheless, it is still difficult to explain why there is no dependence at all on the La concentration.

VII. SUMMARY AND CONCLUSIONS

It is evident from Eqs. (16), (25), and (31) that the main effect of a nonunitary superconducting state is a lifting of the gap degeneracy and that this would be observed as a multigap behavior similar to what could be expected for multiband superconductivity. There are, however, some differences which we outline here. We base the following discussion on the unitary state $D_2(C_2)\times\mathcal{K}$ and the nonunitary state $D_2(E)$, with order parameter components $(0,0,|\eta_1|)$ and $(0,i|\eta_2|,|\eta_1|)$, respectively. There are many other states, but all the rest are either nodeless, or else they have a C_3 symmetry element, which has been positively ruled out by experiment.[16]

In a multiband superconductor with a single T_c, the symmetry of the superconducting order parameter should either be the same on both bands, or, possibly, superconductivity on one band is a secondary order parameter to superconductivity on the other. The alternative, which is the simultaneous appearance of two different order parameters, would be unprecedented. This means that the symmetries of superconducting states on the different bands should either be the same, or have a group-subgroup relation. For example, in MgB_2, the archetypal multiband superconductor, s-wave superconductivity is observed as a full gap for both bands. The best candidates for nodal superconductivity in the triplet channel in $PrOs_4Sb_{12}$ are the unitary state $D_2(C_2)\times\mathcal{K}$ and the nonunitary state $D_2(E)$, and neither of these has secondary order parameters.[30] Therefore, multiband superconductivity entails nodes at the same places for both gaps, unless that part of the Fermi surface is missing. On the other hand, the nonunitary superconducting state has nodes in the lower branch and a fully gapped upper branch. This difference may help to distinguish these two possibilities.

To summarize, we have found general expressions for the residual density of states and electrical and thermal conductivities due to impurity scattering, and we have applied the results to the nonunitary B phase of $PrOs_4Sb_{12}$. The nodal positions of the nonunitary state $D_2(E)$ are unique among all the superconducting states for crystals with tetrahedral symmetry[30,31] in that they are not found on a symmetry axis. Inequivalent diagonal components of the conductivity tensor would be an unmistakable signature of such a state.

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