Hall Conductivity of a Spin-Triplet Superconductor

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We calculate the Hall conductivity for a spin-triplet superconductor, using a generalized pairing symmetry dependent on an arbitrary phase φ. A promising candidate for such an order parameter is Sr_2RuO_4, whose superconducting order parameter symmetry is still subject to investigation. The value of this phase can be determined through Kerr rotation and dc Hall conductivity measurements. Our calculations impose significant constraints on φ.

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Superconducting strontium ruthenate (Sr_2RuO_4) [1] is remarkable for a variety of reasons: It is a layered compound without copper, and, while its transition temperature is relatively low, the symmetry of the superconducting order parameter is most certainly nonconventional [2]. It is believed [3] that Sr_2RuO_4 is a spin-triplet superconductor [4]; thus, the orbital part of the Cooper pair should have odd parity [5]. Moreover, muon spin-relaxation measurements indicate that the superconducting state in Sr_2RuO_4 breaks time-reversal symmetry [6]. The diffraction patterns of Josephson junctions made from Sr_2RuO_4 also illustrate this phenomenon [7]. In the interpretation of these experimental observations, a spin-triplet superconductor with a $(k_x \pm ik_y)$-wave gap symmetry has been used [2]. On the other hand, characteristics of the penetration depth [8] in Sr_2RuO_4 are not consistent with a pure nodeless p-wave gap. Furthermore, ultrasound attenuation measurements [9] in the superconducting state of Sr_2RuO_4 exclude the possibility of a nodeless p-wave gap, while they seem to imply a possible fourfold gap modulation. In this sense, an f-wave gap has also been proposed [10].

Recently, Xia *et al.* [11] have observed a Kerr rotation developing in Sr_2RuO_4 as the temperature is lowered below $T_c = 1.5$ K. They tried to understand this observation based on a theoretical analysis [12] using a nodeless p-wave gap. However, their theoretical estimate gives a Kerr angle of the order of 10^{-3} nanorad, while the measured value is as big as 65 nanorad. Since the Kerr angle is proportional to the imaginary part of the Hall conductivity [11], Yakovenko [13] derived a Chern-Simons-like term in the action associated with the Hall conductivity and estimated a Kerr angle of about 230 nanorad. In Ref. [13], however, the supercurrent (or Cooper pair) contribution to the Hall conductivity is ignored. Another difficulty with this theory is that the Kerr angle obtained by Yakovenko is proportional to the square of the energy gap, while Xia *et al.* have observed that it is linear with the gap.

As explained in Ref. [4], the superconducting state is described by a linear combination of the basis functions for a given representation. For a system with tetragonal symmetry such as Sr_2RuO_4, the superconducting gap can be written in terms of the two-dimensional representation; thus, its momentum dependence would be $\eta_x k_x + \eta_y k_y$, where $\eta_{x,y}$ are complex numbers. By introducing a relative phase φ between η_x and η_y, one can express $\vec{\eta}$ as $(1, e^{i\varphi})$. Based on the Ginzburg-Landau (GL) theory, we examine $\eta_{x,y}$ further. The corresponding fourth-order terms [4] in the GL free energy would be $\beta_1(\vec{\eta}\cdot\vec{\eta}^*)^2 + \beta_2(\vec{\eta}\times\vec{\eta}^*)^2 + \beta_3|\eta_x|^2|\eta_y|^2$, with $\beta_1 > 0$. Depending on β_2 and β_3, we see what values of φ would be possible. For example, if $\beta_2 > 0$ and $4\beta_2 > \beta_3$, $\varphi = \pm\pi/2$. When, however, $\beta_2 = 0$ and $\beta_3 < 0$, one can consider an arbitrary value of the relative phase φ.

In this Letter, we propose a generalized p-wave (we also consider f-wave) gap with a relative phase (φ) between the momenta along the x and y directions: namely, $\Delta_{\mathbf{k}} = \Delta_0(\hat{k}_x + e^{i\varphi}\hat{k}_y)$ for the p-wave gap and $\Delta_{\mathbf{k}} = \Delta_0(\hat{k}_x + e^{i\varphi}\hat{k}_y)(\hat{k}_x^2 - \hat{k}_y^2)$ for the f-wave gap. We derive an expression for the Hall conductivity and show that the Kerr angle is indeed proportional to Δ_0 as experimentally observed. As in the phenomenological model used by Xia *et al.*, our derivation reveals that impurity scattering plays an important role in the problem. The actual value of φ that we use can be identified by comparison with experimental results for the Kerr angle. The dc Hall conductivity at zero temperature is also computed because it is less sensitive to impurity scattering but demonstrates a strong φ dependence. Consequently, the dc Hall conductivity would be another ideal experiment to determine φ. We also discuss the chirality [14,15] and the density of states (DOS) for these gaps. The DOS of the p-wave gap provides a mapping of φ onto a tiny gap [16] associated with the shape of the Fermi surface in Sr_2RuO_4.

We start with the current operator $\mathbf{j}$:

$$\mathbf{j} = \frac{1}{2}e\sum_k \mathbf{v}_k \hat{\psi}_k^\dagger \hat{\psi}_k, \tag{1}$$

where $\hat{\psi}_k^\dagger = (C_{k\uparrow}^\dagger C_{k\downarrow}^\dagger C_{-k\uparrow} C_{-k\downarrow})$. Following the standard formalism, we obtain the current-current correlation $\mathbf{\Pi}(i\Omega)$ in the Matsubara representation as follows:

$$\mathbf{\Pi}(i\Omega) = \frac{1}{4}e^2\sum_k \mathbf{v}_k\mathbf{v}_k T\sum_\omega \mathrm{Tr}[\mathcal{G}_\mathbf{k}(i\omega + i\Omega)\mathcal{G}_\mathbf{k}(i\omega)]. \quad (2)$$

For a spin-triplet superconductor [4], it is necessary to introduce the (4×4) Green function $\mathcal{G}(\mathbf{k}, i\omega)$:

$$\mathcal{G} = \begin{pmatrix} \hat{G} & -\hat{F} \\ -\hat{F}^\dagger & -\hat{G}^\dagger \end{pmatrix}, \quad (3)$$

with

$$\hat{G}(\mathbf{k}, i\omega) = -\frac{i\omega + \xi_\mathbf{k}}{\omega^2 + E_\mathbf{k}^2}\hat{1}, \qquad \hat{F}(\mathbf{k}, i\omega) = \frac{\hat{\Delta}_\mathbf{k}}{\omega^2 + E_\mathbf{k}^2},$$

where $\xi_\mathbf{k} = \mathbf{k}^2/2m - \epsilon_F$, $\hat{\Delta}_\mathbf{k} = i[\mathbf{d}(\mathbf{k}) \cdot \hat{\boldsymbol{\sigma}}]\hat{\sigma}_y$, $\hat{1}$ is the (2×2) unit matrix, and $E_\mathbf{k} = \sqrt{\xi_\mathbf{k}^2 + \mathrm{tr}[\hat{\Delta}_\mathbf{k}\hat{\Delta}_\mathbf{k}^\dagger]/2}$. Since $\hat{\Delta}_\mathbf{k}\hat{\Delta}_\mathbf{k}^\dagger = |\mathbf{d}(\mathbf{k})|^2\hat{1} + i[\mathbf{d}(\mathbf{k}) \times \mathbf{d}^*(\mathbf{k})] \cdot \hat{\boldsymbol{\sigma}}$, depending on $\mathbf{d}(\mathbf{k}) \times \mathbf{d}^*(\mathbf{k})$, the pairing state is called unitary if $\mathbf{d}(\mathbf{k}) \times \mathbf{d}^*(\mathbf{k}) = 0$; otherwise, it is nonunitary. It is commonly assumed [2] that the unitary state is relevant to Sr_2RuO_4 and $\mathbf{d}(\mathbf{k}) = \Delta_\mathbf{k}\hat{z}$:

$$\hat{\Delta}_\mathbf{k} = \begin{pmatrix} 0 & \Delta_\mathbf{k} \\ \Delta_\mathbf{k} & 0 \end{pmatrix}. \quad (4)$$

For this state, the net spin average of a Cooper pair $\mathrm{tr}[\hat{\Delta}_\mathbf{k}^\dagger\hat{\boldsymbol{\sigma}}\hat{\Delta}_\mathbf{k}] = 0$, and $E_\mathbf{k} = \sqrt{\xi_\mathbf{k}^2 + |\Delta_\mathbf{k}|^2}$. It is also possible to represent the d-wave gap in the (4×4) matrix formalism as follows: $\hat{\Delta}_\mathbf{k} = i\Delta_\mathbf{k}\hat{\sigma}_y$, with $\Delta_\mathbf{k} = \Delta_0(\hat{k}_x^2 - \hat{k}_y^2)$.

By defining $G(\mathbf{k}, i\omega) = \hat{G}_{11}$ and $F(\mathbf{k}, i\omega) = \hat{F}_{12}$, the xy component of the current-current correlation becomes, at the bare bubble level,

$$\Pi_{xy}(i\Omega) = e^2\sum_k v_x v_y T\sum_\omega [G(\mathbf{k}, i\omega + i\Omega)G(\mathbf{k}, i\omega) + F(\mathbf{k}, i\omega + i\Omega)F^*(\mathbf{k}, i\omega)]. \quad (5)$$

By using the symmetry of $\Pi_{xy}(i\Omega)$, one can see that $\Pi_{xy}(i\Omega) = 0$ for a pure nodeless p-wave gap. A similar analysis has been done for order parameters with various symmetries [17]. The Hall conductivity follows readily from this expression: $\sigma_{xy}(\Omega) = \frac{i}{\Omega}\Pi_{xy,\mathrm{ret}}(\Omega) \equiv \sigma'_{xy}(\Omega) + i\sigma''_{xy}(\Omega)$. By introducing the spectral functions $\mathcal{A}(\mathbf{k}, \omega) = -2\mathrm{Im}[G_\mathrm{ret}(\mathbf{k}, i\omega)]$ and $\mathcal{B}(\mathbf{k}, \omega) = -2\mathrm{Im}[F_\mathrm{ret}(\mathbf{k}, i\omega)]$, one obtains

$$\sigma''_{xy}(\Omega) = \frac{e^2}{\Omega}\sum_k v_x v_y \int \frac{d\omega' d\omega''}{(2\pi)^2}\frac{f(\omega'') - f(\omega')}{\omega'' - \omega' + \Omega} \times [\mathcal{A}(\mathbf{k}, \omega')\mathcal{A}(\mathbf{k}, \omega'') + \mathcal{B}(\mathbf{k}, \omega')\mathcal{B}^*(\mathbf{k}, \omega'')]. \quad (6)$$

In the clean limit, the spectral functions are

$$\mathcal{A}(\mathbf{k}, \omega) = 2\pi|u_\mathbf{k}|^2\delta(\omega - E_\mathbf{k}) + 2\pi|v_\mathbf{k}|^2\delta(\omega + E_\mathbf{k}),$$
$$\mathcal{B}(\mathbf{k}, \omega) = 2\pi u_\mathbf{k} v_\mathbf{k}[\delta(\omega + E_\mathbf{k}) - \delta(\omega - E_\mathbf{k})], \quad (7)$$

where $u_\mathbf{k} = \sqrt{(1 + \xi_\mathbf{k}/E_\mathbf{k})/2}$ and $v_\mathbf{k} = \sqrt{(1 - \xi_\mathbf{k}/E_\mathbf{k})/2}$. In this instance, $\sigma''_{xy}(\Omega)$ vanishes regardless of the gap symmetry because the $\mathcal{A}\mathcal{A}$ term (quasiparticle contribution) is exactly canceled by the $\mathcal{B}\mathcal{B}$ term (Cooper pair contribution). Nonetheless, impurity scattering prevents a complete cancellation. With impurity scattering rate γ, the corresponding spectral functions can be approximated by [18]

$$\mathcal{A}(\mathbf{k}, \omega) = |u_\mathbf{k}|^2\mathcal{D}(\omega - E_\mathbf{k}) + |v_\mathbf{k}|^2\mathcal{D}(\omega + E_\mathbf{k}),$$
$$\mathcal{B}(\mathbf{k}, \omega) = u_\mathbf{k} v_\mathbf{k}[\mathcal{D}(\omega + E_\mathbf{k}) - \mathcal{D}(\omega - E_\mathbf{k})], \quad (8)$$

where

$$\mathcal{D}(\omega \pm E_\mathbf{k}) = \frac{2\gamma}{(\omega \pm E_\mathbf{k})^2 + \gamma^2}. \quad (9)$$

When the self-energy Σ due to impurity scattering is considered, $\omega \rightarrow \tilde{\omega} = \omega - \Sigma$. By using the Born approximation for simplicity, one can readily evaluate the frequency integrals in Eq. (6). By taking the low temperature and high frequency limits $T \rightarrow 0$ (or $T \ll \Delta_0$) and $\Omega \gg \Delta_0 \gg \gamma$, as in Ref. [11], we obtain

$$\sigma''_{xy}(\Omega) \simeq \frac{e^2}{2\pi}\frac{\gamma}{\Omega^3}\sum_k v_x v_y \ln\left[1 + \frac{\Omega^4 - 2\Omega^2(E_\mathbf{k}^2 - \gamma^2)}{(E_\mathbf{k}^2 + \gamma^2)^2}\right]. \quad (10)$$

By changing the summation to an integration over $\mathbf{k}$, we arrive at the high frequency result

$$\sigma''_{xy}(\Omega) \simeq \frac{e^2}{2\pi}v_f^2 N(0)\frac{\gamma\Delta_0}{\Omega^3}I(\varphi), \quad (11)$$

where v_f is the Fermi velocity, $N(0)$ the DOS of the normal state, and $I(\varphi)$ is, for the p-wave gap,

$$I(\varphi) = \frac{4\cos(\varphi)}{3 - 3|\sin(\varphi)|}\sqrt{\frac{2}{1 + |\sin(\varphi)|}} \times [E(\nu) - |\sin(\varphi)|K(\nu)],$$

where $\nu = [1 - |\sin(\varphi)|]/[1 + |\sin(\varphi)|]$ and K and E are the complete elliptic integrals of the first and the second kind, respectively. The corresponding result for the f-wave gap is

$$I(\varphi) = \frac{8\sqrt{2}}{15}\frac{1 + \frac{3}{2}|\sin(\varphi)|}{1 + |\sin(\varphi)|}[|\sin(\varphi/2)| - |\cos(\varphi/2)|].$$

In Fig. 1, we plot $I(\varphi)$ for the p-wave and f-wave gaps. Using a numerical integration of Eq. (10) with actual values of Ω and γ taken from experiment [2,11] gives results indistinguishable from those in Fig. 1. Note that $I(\varphi)$ changes its sign depending on φ and vanishes at $\varphi = \pi/2$ and $3\pi/2$. From this plot, we estimate $\varphi \approx \pi/\sqrt{2} \sim 5\pi/6$, for which $I(\varphi) \sim 1$. These estimates will depend on the precise symmetry as clearly the p-wave gap gives greater values than the f-wave gap. Since $v_f^2 N(0) \sim \Omega$

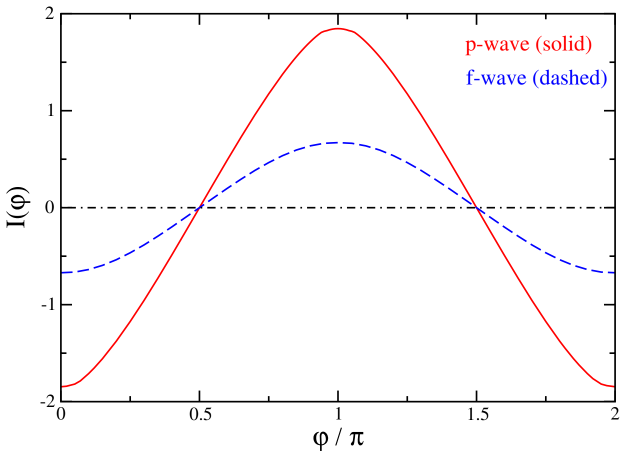

FIG. 1 (color online). $I(\varphi)$ for the p-wave gap (solid curve) and the f-wave gap (dashed curve).

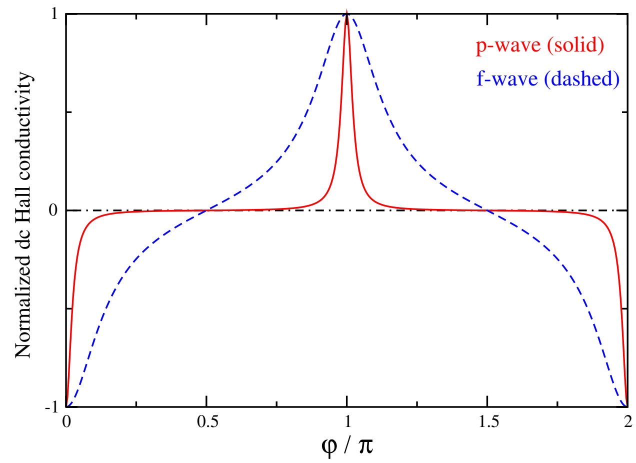

FIG. 2 (color online). Normalized dc Hall conductivity as a function of φ at zero temperature for p-wave and f-wave superconductors with $\gamma/\Delta_0 = 0.05$.

from parameters in Ref. [2], we obtain

$$\sigma''_{xy}(\Omega) \approx \frac{e^2}{2\pi}\frac{\gamma\Delta_0}{\Omega^2}. \tag{12}$$

Note that our result is reduced from that in Ref. [13] by a factor of γ/Δ_0. This revises the theoretical estimate for the Kerr angle to 10–80 nanorad for $\gamma/\Delta_0 \approx 0.05$–0.4. Its value congruous to the measured Kerr angle would be 0.15–0.35. Consequently, Eq. (12) correctly illustrates the observed linear dependence of the Kerr angle on the gap value and supports the phenomenological expression used in Ref. [11].

Because of the important role of impurity scattering, the Kerr angle measurement may not be the ideal quantity to determine the phase φ. Moreover, the dependence of $\sigma''_{xy}(\Omega)$ on φ is not sufficiently decisive to pinpoint φ accurately. Since the low-lying quasiparticles behave sensitively to φ, the dc Hall conductivity at zero temperature can be a good measurement to determine the phase. In the dc, low temperature limit we get for the Hall conductivity

$$\sigma'_{xy}(0) = \sigma_0\left\langle\frac{\sin(2\theta)}{[\Delta_\theta^2 + (\gamma/\Delta_0)^2]^{3/2}}\right\rangle_{FS}, \tag{13}$$

where $\sigma_0 = e^2 v_f N(0)\gamma^2/(\pi\Delta_0^3)$, $\Delta_\theta = \Delta_{\mathbf{k}}/\Delta_0$, and $\langle\ldots\rangle$ means the average over the Fermi surface. Figure 2 shows the normalized dc Hall conductivity, $\sigma'_{xy}(0)$ divided by its maximum value, as a function of φ for the p-wave gap and for the f-wave gap when $\gamma/\Delta_0 = 0.05$. The maximum values are about $140\sigma_0$ and $420\sigma_0$ for the p-wave and the f-wave case, respectively. It is understandable that for a given φ the magnitude of the dc Hall conductivity of the f-wave gap is greater than that of the p-wave gap, because there are more quasiparticles in the f-wave case. The strong dependence of $\sigma'_{xy}(0)$ on φ, particularly between $\pi/2$ and π, makes the determination of φ more accurate.

Finally, it is necessary to address the chirality of the p-wave and f-wave gaps because it is interesting to see if φ changes this property. The chirality [14,15] of a superconductor is defined as $\mathcal{N} = \frac{1}{4\pi}\int d^2k\hat{\mathbf{m}}\cdot(\frac{\partial\hat{\mathbf{m}}}{\partial k_x}\times\frac{\partial\hat{\mathbf{m}}}{\partial k_y})$, where $\hat{\mathbf{m}} = \mathbf{m}/|\mathbf{m}|$ with $\mathbf{m} = (\mathrm{Re}[\Delta_{\mathbf{k}}], \mathrm{Im}[\Delta_{\mathbf{k}}], \xi_{\mathbf{k}})$. For the p- wave superconductor, this becomes

$$\mathcal{N}(\varphi) = -\int_0^{2\pi}\frac{d\theta}{2\pi}\frac{\sin(\varphi)}{1 + \cos(\varphi)\sin(2\theta)}. \tag{14}$$

Note that $\mathcal{N}(\varphi) = \pm 1$ except for $\varphi = 0$ and π, for which the chirality is not uniquely defined because $\mathbf{m}$ vanishes at some points on the Fermi surface. The chirality of the f-wave gap cannot be defined uniquely either, because $\mathbf{m}$ goes to zero at the nodal points on the Fermi surface.

The DOS of a superconducting state is defined as $\frac{N(\omega)}{N(0)} = \mathrm{Re}[\langle\omega/\sqrt{\omega^2 - |\Delta_{\mathbf{k}}|^2}\rangle_{FS}]$. For the p-wave gap, we obtain

$$\frac{N(\omega)}{N(0)} = \frac{\pi}{2}\mathrm{Re}\left[\frac{\omega}{\sqrt{\omega^2 - 2\Delta_\varphi^2}}K\left(\frac{2\Delta_0^2\cos(\varphi)}{\omega^2 - 2\Delta_\varphi^2}\right)\right], \tag{15}$$

where $\Delta_\varphi = \Delta_0\sin(\varphi/2)$. Figure 3 shows the DOS of the case with a p-wave gap. It is interesting that the peak does not occur at $\omega = \Delta_0$ except for $\varphi = \pi/2$, for which the DOS is s-wave-like. In fact, its location is $\omega/\Delta_0 = \sqrt{1 + |\cos(\varphi)|}$. As mentioned earlier, the DOS illustrates a tiny gap obtained in a different context [16]. When $\varphi \simeq 5\pi/6$, the tiny (minimum) gap is about $0.3\Delta_0$, while the maximum gap (peak) about $1.37\Delta_0$. Note that this value of φ also explains the Kerr angle measurement. It is not possible to express the DOS of the case with the f-wave gap for general φ in an analytic form. We plot the DOS in Fig. 4 for values of $\varphi = 3\pi/4, 4\pi/3$, and π. The location of the peak is not $\omega = \Delta_0$ either; for example, the peak is at $\omega/\Delta_0 = (4/3)\sqrt{2/3}$ for $\varphi = \pi$. As one can see, the DOS is more or less like the DOS of the d-wave gap. When $\varphi = \pi/2$, the DOS is exactly d-wave-like. However, for $\varphi = \pi$ the DOS is definitely not a linear

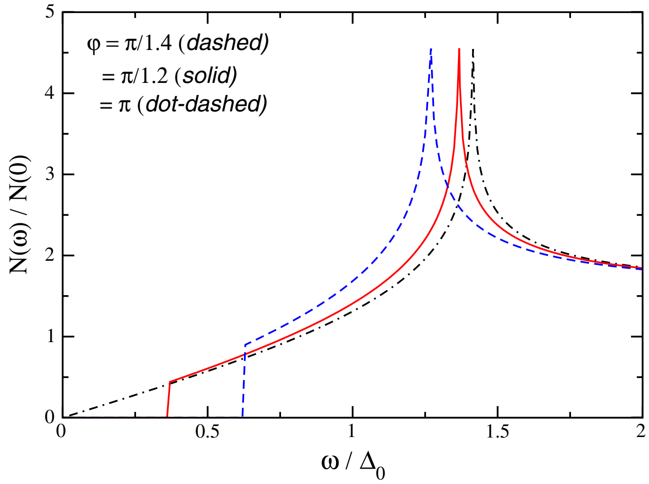

FIG. 3 (color online). The density of states of the p-wave gap as a function of energy ω.

function of ω at low frequency ($\omega \ll \Delta_0$). This is due to the quadratic behavior of the corresponding f-wave gap as a function of the wave vector near the nodes. In addition, because of this, the nodal approximation breaks down for $\varphi \approx \pi$.

In conclusion, we have proposed a novel type of superconducting order parameter symmetry, with a relative phase φ in the definition of the order parameter symmetry. We then showed that the spontaneous Hall conductivity can be reduced by rotational symmetry breaking as well as time-reversal symmetry breaking. We have used the Kerr angle θ_K expression in terms of the Hall conductivity as in Ref. [13]: $\theta_K = (4\pi/\Omega)\,\mathrm{Im}[\sigma_{xy}/(n^3 - n)]$, where n is the complex index of refraction. It is apparent that the actual magnitude and phase of n are important to determine the angle. Another difficulty for a proper theoretical understanding is the issue of the detailed experimental setup discussed recently in Ref. [19]. In fact, we think that the validity of the above expression for θ_K is still an open question for Sr_2RuO_4. Our simple analysis is an initial attempt to understand the recent Kerr angle experimental results [11]. Because of these complications, a measurement of the low-frequency Hall conductivity is most desirable—it will provide a definitive guideline for the theoretical modeling of Sr_2RuO_4. Our p-wave model is compatible with the small gap due to the salient shape of the Fermi surface.

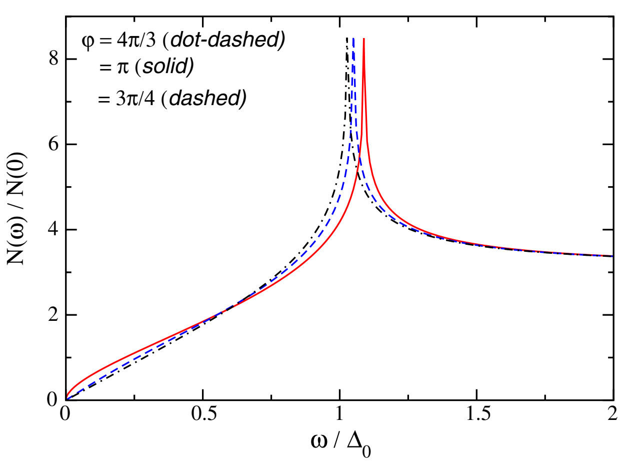

FIG. 4 (color online). The density of states of the f-wave gap as a function of energy ω.

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