Collective order-parameter modes for hypothetical *p*-wave superconducting states in Sr_2RuO_4

D. Fay and L. Tewordt
I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstrasse 9, D-20355 Hamburg, Germany
(Received 23 November 1999; revised manuscript received 7 March 2000)

We have calculated all order-parameter collective modes and their contributions to the spin and charge susceptibilities for possible *p*-wave pairing states in Sr_2RuO_4. The susceptibilities are calculated for pairing states having gaps without and with nodes, and for wave vectors $\mathbf{q}=0$ and nesting vector $\mathbf{q}=\mathbf{Q}$ associated with the α and β bands of Sr_2RuO_4. Important for the observability of the spin-fluctuation modes, for example, by spin resonance or neutron scattering, and of the charge-fluctuation modes by ultrasound, is the effect of quasiparticle damping. This effect is taken into account and discussed in connection with recent neutron-scattering data on Sr_2RuO_4.

I. INTRODUCTION

There are numerous experiments that show that the superconducting state in Sr_2RuO_4 (Ref. 1) (below about 1 K) is unconventional. In particular, the ^{17}O nuclear magnetic resonance Knight-shift experiment shows that the spin susceptibility for the magnetic field parallel to the RuO_2 plane does not change as T decreases across T_c.[2] It has been proposed that the superconducting state in Sr_2RuO_4 is formed by spin-triplet *p*-wave Cooper pairs[3] in analogy to superfluid ^{3}He.[4] The possible *p*-wave pairing states have been classified in terms of the pairing states $\mathbf{d}_j$ $(j=1,..,6)$ corresponding to the irreducible representations of the point group D_{4h} for the layered perovskite structure of Sr_2RuO_4.[5] Notice that the 2×2 gap matrix is given by $\hat{\Delta}=\mathbf{d}\cdot(\boldsymbol{\sigma} i\sigma^y)$. The $\mathbf{d}$ vector formed from this basis set $\mathbf{d}_j$, which is directed perpendicular to the basal plane and has a constant magnitude in orbital $\mathbf{k}$ space, seems to be compatible with all the present data on Sr_2RuO_4.[5]

The situation in Sr_2RuO_4 is complicated because one has observed by quantum oscillations[6] three Fermi sheets where the γ band is essentially quasi-two-dimensional isotropic, while the α and β bands are quasi-one-dimensional. Analysis of the London penetration depth and coherence length[7] suggests that the gap associated with the γ band is larger than that of the α and β bands. For the latter bands, one expects sizable nesting effects at the wave vector $\mathbf{Q}=(2\pi/3,2\pi/3)$. It has been shown that the nesting effect on the dynamical spin susceptibility leads to a collective mode at $\mathbf{Q}$ in the normal state and subsequently to a competition between *d*-wave and *p*-wave superconductivity.[8] In fact, neutron scattering in the normal state of Sr_2RuO_4 yields a large peak at wave vector $(0.6\pi,\ 0.6\pi)$ close to the nesting vector $\mathbf{Q}$ with energy transfer of 6.2 meV.[9]

Observation of collective order-parameter modes might be a tool to determine the nature of the superconducting state in Sr_2RuO_4. Recently, the possible order-parameter collective modes for *p*-wave pairing states in the layered perovskite structure like Sr_2RuO_4 have been calculated in terms of fluctuations of the pairing states $\mathbf{d}_j$ $(j=1,...,6)$ corresponding to the irreducible representations of D_{4h}.[10,18] For the $\mathbf{d}$ vector of the nodeless *a*-phase pairing state[5] and for wave vector $\mathbf{q}=0$, one finds, on the one hand, an amplitude fluctuation mode at frequency $\omega=2\Delta_0$ (Δ_0 is the gap), which couples to charge density and can be excited, for example, by ultrasound. On the other hand, one finds spin-fluctuation modes that can be excited by external vector fields coupling to spin density and lying parallel to the basal plane. The resonance frequencies of the latter modes are approximately given by $(\omega/2\Delta_0)^2=x_1-x_6=\ln(T_{c6}/T_{c1})$ where $x_j=(N_0 v_j)^{-1}$ and the pairing strength v_1 (or transition temperature T_{c1}) refers to the in-plane and v_6 (or T_{c6}) refers to the out-of-plane basis vectors $\mathbf{d}_j$. For finite $\mathbf{q}$ and magnetic fields, the latter order-parameter fluctuations give rise to spin-wave excitations that may be observable by electron spin resonance for sufficiently small "pinning frequency" Ω_d.[11] This phenomenological "pinning frequency" Ω_d, which has been introduced as a measure for the tendency to restore the original direction of $\mathbf{d}$ against external perturbations,[11] is nothing else than the resonance frequency $\omega=2\Delta_0(\ln T_{c6}/T_{c1})^{1/2}$ for spin order-parameter fluctuations[10] discussed above.

Among the 12 collective modes given by the coupled Bethe-Salpeter equations in the particle-particle and hole-hole channels,[12,13] one finds the so-called clapping modes with frequency $\omega=\sqrt{2}\Delta_0$ corresponding to the observed clapping modes in ^{3}He-*A*.[15] In recent theories of ultrasound propagation in Sr_2RuO_4, it has been claimed that the clapping modes couple to sound.[16,17] However, it has been shown previously that the coupling of the clapping modes to charge density vanishes.[18] Instead of the clapping mode, we investigate in this paper more closely the contribution of the amplitude fluctuation mode to sound attenuation that may yield a resonance if the coupling due to particle-hole asymmetry at the Fermi surface is appreciable.[10,18] The resonance frequency $\omega=2\Delta_0$ for a nodeless gap becomes about $\omega=\sqrt{3}\Delta_0$ for a gap with nodes, which is similar to that of the amplitude collective mode for *d*-wave pairing.[14]

More recent measurements of the specific heat C in cleaner samples of Sr_2RuO_4 have shown that the residual density of states is very small and $C\propto T^2$.[19] These experiments have been interpreted as consequences of an anisotropic gap caused by a finite range pairing interaction.[20,21] The specific-heat measurements have also led to speculations of *f*-wave pairing order parameters giving rise to vertical line nodes.[22] As has been pointed out above, these states with nodes give rise to a resonance frequency of the amplitude collective mode that lies well below the pair-breaking edge $2\Delta_0$. This may help to make this mode observable by ultrasound attenuation.

In the present paper, we give a more complete and detailed account of all the order-parameter collective modes and their contributions to the charge and spin susceptibilities that can possibly occur if p-wave pairing actually exists in Sr_2RuO_4. These include, on the one hand, collective modes for superconducting states without and with nodes in the gap, and, on the other hand, collective modes for wave vector $\mathbf{q}=0$ and for nesting vector $\mathbf{q}=\mathbf{Q}$, which are presumably relevant for the γ band and the α and β bands, respectively.

In Sec. II, we present an outline of the theory of collective order-parameter modes for spin-triplet p-wave pairing in the layered perovskite structure of Sr_2RuO_4. In Sec. III, we give results for the spin- and charge-fluctuation susceptibilities at $\mathbf{q}=0$ and $\mathbf{q}=\mathbf{Q}$ for states without nodes and with nodes in the superconducting energy gap. We calculate the spin susceptibility for the normal state at the nesting vector $\mathbf{Q}$ and make a fit to the neutron-scattering data.[9] In Sec. IV, we discuss the possibilities to observe the spin-fluctuation modes and charge density fluctuation modes, for example, by spin resonance or ultrasound attenuation technique.

II. GENERAL THEORY OF ORDER PARAMETER COLLECTIVE MODES FOR *p*-WAVE PAIRING IN Sr_2RuO_4

The p-wave pairing states $\mathbf{d}_j$ corresponding to the irreducible representations of D_{4h} are the following:[5]

$$A_{1u}:\mathbf{d}_1=\hat{x}k_x+\hat{y}k_y,\quad A_{2u}:\mathbf{d}_2=\hat{x}k_y-\hat{y}k_x,$$

$$B_{1u}:\mathbf{d}_3=\hat{x}k_x-\hat{y}k_y,\quad B_{2u}:\mathbf{d}_4=\hat{x}k_y+\hat{y}k_x,$$

$$E_u:\mathbf{d}_5=\sqrt{2}\hat{z}k_x,\quad \mathbf{d}_6=\sqrt{2}\hat{z}k_y. \tag{1}$$

For simplicity, we take the orbital basis set $\hat{k}_x=\cos\phi$ and $\hat{k}_y=\sin\phi$ on a cylindrical Fermi surface. It should be pointed out that the theory of collective modes[10,18] is essentially unaltered if the basis functions $\hat{k}_i$ are replaced by $\sin k_i$ ($i=x,y$) corresponding to a finite range interaction.[20,21] The weak-coupling pairing interaction can be written as a sum of projection operators onto the basis states $\mathbf{d}_j$ in Eq. (1) with eigenvalues v_j ($v_5=v_6$):

$$V(\mathbf{k},\mathbf{k}')=-\sum_{j=1}^{6} v_j\mathbf{d}_j(\mathbf{k})\mathbf{d}_j^{\dagger}(\mathbf{k}'). \tag{2}$$

The fluctuations $\delta\mathbf{d}$ of the equilibrium pairing state $\mathbf{d}$ are decomposed in terms of the basis vectors in Eq. (1):

$$\delta\mathbf{d}(\mathbf{k};\mathbf{q},i\nu_m)=\sum_j \delta\Delta_j(\mathbf{q},i\nu_m)\mathbf{d}_j(\mathbf{k}). \tag{3}$$

Then the coupled Bethe-Salpeter equations for the order-parameter fluctuations in the particle-particle and hole-hole channels[12] can be decomposed in terms of coupled equations for the fluctuation components $\delta\Delta_j$ and $\delta\Delta_j^*$. These fluctuations are coupled to the charge- and spin-density fluctuations in the particle-hole channels[12] that are excited by external fields U_s and $\mathbf{U}_a$, respectively. These equations are the following:[13,18]

$$\begin{aligned}\delta\Delta_i=v_iT\sum_{\omega_n}\sum_k\Bigg\{\sum_{j=1}^{6}&[G(\mathbf{k},i\omega_n)G(\mathbf{q}-\mathbf{k},i\omega_{m-n})\\&\times(\mathbf{d}_i\cdot\mathbf{d}_j)\delta\Delta_j-\mathbf{F}(\mathbf{k},i\omega_n)\cdot\mathbf{F}(\mathbf{q}-\mathbf{k},i\omega_{m-n})\\&\times(\mathbf{d}_i\cdot\mathbf{d}_j)\delta\Delta_j^*+2(\mathbf{d}_i\cdot\mathbf{F}(\mathbf{k},i\omega_n))\\&\times(\mathbf{F}(\mathbf{q}-\mathbf{k},i\omega_{m-n})\cdot\mathbf{d}_j)\delta\Delta_j^*]+2G(\mathbf{k},i\omega_n)\\&\times[(\mathbf{d}_i\cdot\mathbf{F}(\mathbf{q}-\mathbf{k},i\omega_{m-n}))U_s\\&-i(\mathbf{d}_i\times\mathbf{F}(\mathbf{q}-\mathbf{k},i\omega_{m-n}))\cdot\mathbf{U}_a]\Bigg\}.\end{aligned} \tag{4}$$

Here, G and $\mathbf{F}$ are the normal and anomalous Green's functions, which for unitary states ($\mathbf{d}\times\mathbf{d}=0$) are given by

$$G(\mathbf{k},i\omega_n)=-(i\omega_n+\varepsilon_k)/N,\quad \mathbf{F}(\mathbf{k},i\omega_n)=-\mathbf{d}(\mathbf{k})/N,$$

$$N=(\omega_n^2+\varepsilon_k^2+|\mathbf{d}(\mathbf{k})|^2). \tag{5}$$

First, we consider the so-called a phase[5] with $\mathbf{d}$ vector and squared gap $|\mathbf{d}|^2$:

$$\mathbf{d}=\Delta_0\hat{z}(k_x+ik_y),\quad |\mathbf{d}|^2=\Delta_0^2. \tag{6}$$

This state is stable if $v_5=v_6>v_j$ ($j=1,...,4$). Comparison of the pairing interaction (2) with the effective intraorbital interaction derived in Ref. 21 shows that the differences between the intraplane eigenvalues v_j ($j=1,...,4$) are caused by spin-orbit coupling.[18] For the state (6) (and all the other states considered later), the system of equations (4) for the fluctuations $\delta\Delta_j$ and $\delta\Delta_j^*$ ($j=1,...,6$) decouples into three sets of four equations each. The first two sets of these equations yield fluctuations being proportional to $(\mathbf{d}_1+\mathbf{d}_3)$ and $(\mathbf{d}_2-\mathbf{d}_4)$, respectively, which are excited by external fields $\mathbf{U}_a$ coupling to spin density that lie in the xy plane and are directed perpendicular to these vectors [see Eq. (4)]. The corresponding contribution to the spin susceptibility for $\mathbf{q}=0$ is the following:

$$\chi_{f1}^{\mu\nu}(0,\omega)=-N_0\frac{\frac{1}{2}[\omega\Delta_0\langle F\rangle]^2}{\frac{1}{2}\omega^2\langle F\rangle-(x_1-x_6)}\quad(\mu\nu=xx,yy,xy). \tag{7}$$

The function $F(\phi,\omega)$ for $\mathbf{q}=0$ and a general state $\mathbf{d}(\phi)$ is defined by

$$F(\phi,\omega)=\frac{|\mathbf{d}(\phi)|^2}{\langle|\mathbf{d}|^2\rangle}\int_{-\infty}^{+\infty}d\varepsilon\,\frac{\tanh(E/2T)}{E[4E^2-(\omega+i\Gamma)^2]}$$

$$[E^2=\varepsilon^2+|\mathbf{d}(\phi)|^2]. \tag{8}$$

In this function F, we have introduced a phenomenological damping constant Γ. The brackets $\langle\cdots\rangle$ in Eq. (7) denote the average over ϕ from 0 to 2π. The term (x_1-x_6) in the denominator of Eq. (7) corresponds to the phenomenological "pinning frequency" Ω_d introduced in Ref. 11:

$$(\Omega_d/2\Delta_0)^2\equiv x_1-x_6=\ln(T_{c6}/T_{c1}),\quad x_j\equiv 1/N_0v_j. \tag{9}$$

Here, T_{cj} are the superconducting transition temperatures corresponding to the pairing coupling constants v_j in Eq. (2).[13] For simplicity, we assume here and in the following that the in-plane pairing constants $v_j\,(j=1,...,4)$ are all equal. It should be pointed out that in Refs. 10 and 18, it was assumed that $v_1=v_2$ and $v_3=v_4$ while v_1 and v_3 are different where the difference (v_3-v_1) arises from spin-orbit coupling terms. Then the pinning frequency (x_1-x_6) in Eq. (7) is replaced by $\frac{1}{2}(x_1+x_3)-x_6$ [note that we have changed the definition of x_j in Refs. 10 and 18 to x_j-x_6 in Eq. (9), which is more convenient for later purposes].

The last set of four equations yields coupled equations for the real and imaginary fluctuation components $\delta\Delta_5$, $\delta\Delta_5^*$, $\delta\Delta_6$, and $\delta\Delta_6^*$ of the two basis vectors $\mathbf{d}_5$ and $\mathbf{d}_6$ along the z axis. From these equations, one obtains the amplitude fluctuation mode with $\omega^2=4\langle|\mathbf{d}|^2\rangle$, the phase fluctuation mode with $\omega^2=0$, and the two clapping modes with $\omega^2=2\langle|\mathbf{d}|^2\rangle$. In recent theories of ultrasound propagation in Sr_2RuO_4, it has been claimed that the clapping mode couples to sound.[16,17] In contrast to these theories, we find that the coupling of the clapping modes to density [external field U_s in Eq. (4)] vanishes. However, we find that the amplitude fluctuation mode couples to density by a term that is small of the order of particle-hole asymmetry at the Fermi surface. This yields at $\mathbf{q}=0$ the following contribution to the charge-density susceptibility:

$$\chi_{f1}^{00}(0,\omega)=-N_0^{-1}\frac{[4\Delta_0\langle N(\varepsilon)\varepsilon F\rangle]^2}{\langle(\omega^2-4|\mathbf{d}|^2)F\rangle}. \tag{10}$$

The coupling term $\langle N(\varepsilon)\varepsilon F\rangle$ in the numerator of Eq. (10) is different from zero if the density of states $N(\varepsilon)$ has an antisymmetric contribution in ε at the Fermi energy $\varepsilon=0$. It has been stressed[17] that in Sr_2RuO_4, the ratio of sound velocity to Fermi velocity, $s=c/v_F$, is small of the order $s\approx10^{-2}$. Therefore, terms of order $\zeta^2=(\mathbf{v}_F\cdot\mathbf{q})^2$ have to be taken into account in the theory of sound propagation and attenuation. This means that the function F in Eq. (10) has to be replaced by the more general function $F(\zeta,\omega)$, which has been derived in the theory of collective modes in ^{3}He-A [see Eq. (18) in Ref. 15]. Furthermore, the term ω^2 in the denominator of Eq. (10) has to be replaced by $(\omega^2-\zeta^2)$. However, for direction $\mathbf{u}$ of sound propagation parallel to the z axis, the correction terms ζ^2 vanish. Thus we conclude that the expression in Eq. (10) remains correct for longitudinal sound waves with $\mathbf{u}\|\mathbf{q}\|\mathbf{z}$.

III. RESULTS FOR SPIN AND CHARGE FLUCTUATION SUSCEPTIBILITIES FOR VARIOUS STATES

In this section, we calculate the spin- and charge-fluctuation susceptibilities in terms of the expressions given in Eqs. (7) and (10) for a number of p-wave superconducting states given by the vectors $\mathbf{d}_j$ in Eq. (1). This means that we have to calculate the angle averages $\langle F\rangle$ and $\langle|\mathbf{d}|^2\cdot F\rangle$ where the function F is given by Eq. (8) for wave vector $\mathbf{q}=0$. We shall see that these functions of ω are quite different for states having gaps without or with nodes. Furthermore, these functions depend crucially on the magnitude of the phenomenological damping constant Γ, which has been introduced into the function F. This damping constant takes into account the scattering of quasiparticles by spin fluctuations. It has been shown that for d-wave pairing in the high-T_c cuprates the self-consistently calculated quasiparticle scattering due to spin fluctuations has a large effect on the spin density and order parameter collective modes.[14] We determine also the collective modes at $\mathbf{Q}=(2\pi/3,2\pi/3)$.

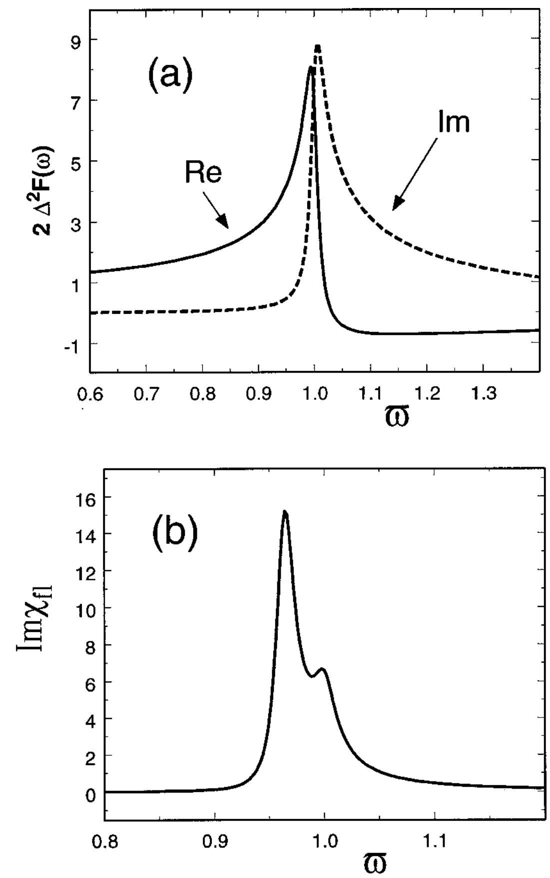

FIG. 1. (a) Real part (solid line) and imaginary part (dashed line) of function $2\Delta_0^2\,F$ for state (1) at $T=0$ [see Eq. (5)] versus reduced frequency $\overline{\omega}=\omega/2\Delta_0$ for reduced quasiparticle damping $\gamma=\Gamma/2\Delta_0=0.01$, (b) Fluctuation-spin susceptibility for state (1), $\mathrm{Im}\,\chi_{fl}^{\mu\nu}$ [see Eq. (2)], versus $\overline{\omega}$, for $T=0$, $\gamma=0.01$, and reduced pinning frequency $(x_1-x_6)=5$.

We start with state (6) having a constant energy gap Δ_0. Then the function $\langle F\rangle\equiv F(\omega)$ can be calculated analytically at $T=0$ and becomes equal to

$$2\Delta_0^2F(\omega)=[1-(\overline{\omega}+i\gamma)^2]^{-1/2}\,\frac{\arcsin(\overline{\omega}+i\gamma)}{(\overline{\omega}+i\gamma)},$$

$$\overline{\omega}=\frac{\omega}{2\Delta_0},\quad \gamma=\frac{\Gamma}{2\Delta_0}. \tag{11}$$

In Fig. 1(a), we have plotted the real and imaginary parts of the function (11) versus $\overline{\omega}$ for $\gamma=0.01$. We find that the maxima occurring near the pair-breaking edge $\overline{\omega}=1$ decrease for increasing values of γ. Analytically, we derive that these maxima are of the order of magnitude $\gamma^{-1/2}$. This means that the real part of the denominator of the spin-fluctuation susceptibility in Eq. (7) has a zero for $\overline{\omega}<1$ only if $\gamma^{-1/2}>(x_1-x_6)$. Here it should be recalled that the pairing strengths $v_1=v_2=v_3=v_4$ (for simplicity we have taken them to be equal) refer to the basis vectors $\mathbf{d}_j$ lying in the basal xy plane while $v_5=v_6$ is the pairing strength of the vectors $\mathbf{d}_5$ and $\mathbf{d}_6$ making up the $\mathbf{d}$ vector in Eq. (6). For large values of the ''pinning frequency,''[11] that is, $(\Omega_d/2\Delta_0)^2=x_1-x_6\gg 1$, the resonance of $\chi_{fl}^{\mu\nu}(0,\omega)$ occurs just below the pair-breaking edge. In Fig. 1(b) we show as an example Im $\chi_{fl}^{\mu\nu}$ versus $\overline{\omega}$ for $\gamma=0.01$ and $(x_1-x_6)=5$. For $(x_1-x_6)\rightarrow 0$ the resonance frequency tends to zero because this collective mode becomes the Goldstone mode for broken rotational symmetry. One recognizes easily that the resonance of the charge-fluctuation susceptibility χ_{fl}^{00} in Eq. (10) occurs for the superconducting state (6) at frequency $\omega=2\Delta_0$. The coupling term of this mode to charge density [see the numerator in Eq. (10)] is small of the order $N_0'=dN(\varepsilon)/d\varepsilon$ at the Fermi energy, which is a measure of the amount of particle-hole asymmetry.

We turn now to the possible collective modes at the nesting vector $\mathbf{Q}=(2\pi/3,2\pi/3)$ for the α and β Fermi sheets of Sr_2RuO_4.[8] Making use of the fact that for the band energy $\varepsilon_{k+Q}=-\varepsilon_k$ at $\mathbf{Q}$, we find that the spin-fluctuation susceptibility $\chi_{fl}^{\mu\nu}(\mathbf{Q},\omega)$ is obtained from the expression in Eq. (7) by replacing in the denominator the term $(\omega^2/2)\langle F\rangle$ by $2\Delta_0^2\langle F\rangle$ and the term (x_1-x_6) by x_1. A resonance occurs close to the pair-breaking edge if the condition $\gamma^{-1/2}>x_1$ is satisfied. For parameter values $\gamma=0.01$ and $x_1=5$, the plot of Im $\chi_{fl}^{\mu\nu}(\mathbf{Q},\omega)$ looks very similar to the plot of Im $\chi_{fl}^{\mu\nu}(0,\omega)$ shown in Fig. 1(b). However, it is unlikely that the condition given above is satisfied because, on the one hand, the pairing strengths N_0v_1 of the basis states in the xy plane are much smaller than one, that is, $x_1\gg 1$. On the other hand, the damping Γ of the quasiparticles near $\mathbf{Q}$ is at least in the normal state quite large as has been shown by neutron scattering on Sr_2RuO_4 (Ref. 9) (see discussion below).

For d-wave pairing, a collective mode occurs in the random-phase approximation (RPA) spin susceptibility at the antiferromagnetic nesting vector $\mathbf{Q}=(\pi,\pi)$.[14] This mode has been observed by neutron scattering in the high-T_c superconductors. A similar mode could occur in the dynamical RPA spin susceptibility $\chi_{xx}=\chi_{xx}^0(1-U\chi_{xx}^0)^{-1}$ for p-wave pairing.[10] For the superconducting state (6), we find that at the nesting vector $\mathbf{Q}=(2\pi/3,2\pi/3)$ of the α and β bands with nesting relationship $\varepsilon_{k+Q}=-\varepsilon_k$ the irreducible spin susceptibility χ_{xx}^0 is given by

$$\chi_{xx}^0(\mathbf{Q},\omega)=N_0[x_6+\overline{\omega}^2 2\Delta_0^2F(\omega)]. \tag{12}$$

Recall that at $T=0$ the function $2\Delta_0^2F(\omega)$ is given by Eq. (11), which is plotted in Fig. 1(a) versus $\overline{\omega}$ for $\gamma=0.01$. A zero of the real part of the denominator of the RPA spin susceptibility is, according to Eq. (11), given by the equation $\overline{\omega}^2 2\Delta_0^2\,\mathrm{Re}\,F(\omega)=(N_0U)^{-1}-(N_0v_6)^{-1}$, which means that the right-hand side of this equation has to be positive. For d-wave pairing, it has been shown that this stringent condition for occurrence of a spin density collective mode is drastically weakened if the feedback effect of the quasiparticle self-energy on the dynamical spin susceptibility is taken into account.[14]

For $\Delta_0\rightarrow 0$ in the normal state, Eq. (12) goes over into the following expression for the Lindhard function at the nesting vector $\mathbf{Q}$:

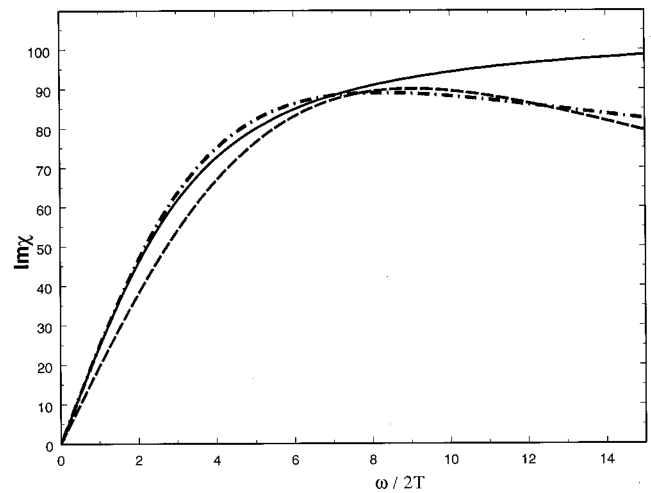

FIG. 2. Fit to neutron-scattering data from Eq. (3) of Ref. 9 on Sr_2RuO_4 at $\mathbf{Q}_0=(0.6\pi,0.6\pi)$ and $T=10.4$ K versus $\omega/2T$ for damping constant $\Gamma=9$ meV (dashed curve). Bare spin susceptibility for normal state at nesting vector $\mathbf{Q}$, Im χ_{xx}^0 [see Eq. (7)], versus $\omega/2T$ for reduced quasiparticle damping $\Gamma/2T=1.8$ (solid curve). RPA spin susceptibility, Im χ_{xx}, for $\alpha=(N_0U)^{-1}-(N_0v_6)^{-1}=1$ and $\Gamma/2T=5$ (dashed-dotted curve).

$$\chi_{xx}^0(\mathbf{Q},\omega)=N_0\left[x_6+(\omega+i\Gamma)^2\int_0^{+\infty}\times\frac{d\varepsilon}{4\varepsilon^2-(\omega+i\Gamma)^2}\,\frac{\tanh(\varepsilon/2T)}{\varepsilon}\right]. \tag{13}$$

The neutron-scattering results for Im $\chi(\mathbf{Q}_0,\omega)$ versus ω at $\mathbf{Q}_0=(0.6\pi,0.6\pi)$ have been parametrized by an expression proportional to $\omega\Gamma/(\omega^2+\Gamma^2)$ (Ref. 9) (see dashed line versus $\omega/2T$ for $T=10.4$ K and $\Gamma=9$ meV in Fig. 2). The curve of Im χ_{xx}^0 in Eq. (13) versus $\omega/2T$, which lies closest to the fit to the experimental points (see solid curve in Fig. 2), is obtained for a ratio of $\Gamma/2T=1.8$. We have also tried to describe the fit to the data points with the full RPA expression (see above). The result for parameter values $\alpha=(N_0U)^{-1}-(N_0v_6)^{-1}=1$ and $\Gamma/2T=5$ is also shown in Fig. 2 (see dashed-dotted curve). This curve shows the experimental decrease for larger ω, and the value of $\Gamma/2T=5$ agrees approximately with the value obtained from the experimental values of Γ and T. This large value of the reduced damping makes it unlikely that the condition $1/\sqrt{\gamma}>x_1$ for obtaining a resonance in $\chi_{fl}^{\mu\nu}(\mathbf{Q},\omega)$ below T_c is satisfied. Therefore, its contribution to $\chi_{xx}^0(\mathbf{Q},\omega)$ may be neglected.

For completeness of our discussion, we remark that the collective mode corresponding to the Goldstone mode for broken gauge invariance at $\mathbf{q}=0$ (Ref. 10) gives rise at wave vector $\mathbf{Q}$ to a charge-fluctuation susceptibility $\chi_{fl}^{00}(\mathbf{Q},\omega)$, which differs from the spin-fluctuation susceptibility $\chi_{fl}^{\mu\nu}(\mathbf{Q},\omega)$ in that x_1 in the denominator is replaced by x_6. Since $x_6<x_1$, it seems to be more likely that a collective mode at $\mathbf{Q}$ can be excited by external fields coupling to charge density like ultrasound than by external vector fields coupling to spin density.

Next we consider the order-parameter fluctuations for the so-called b-phase state,[5] whose gap has nodes

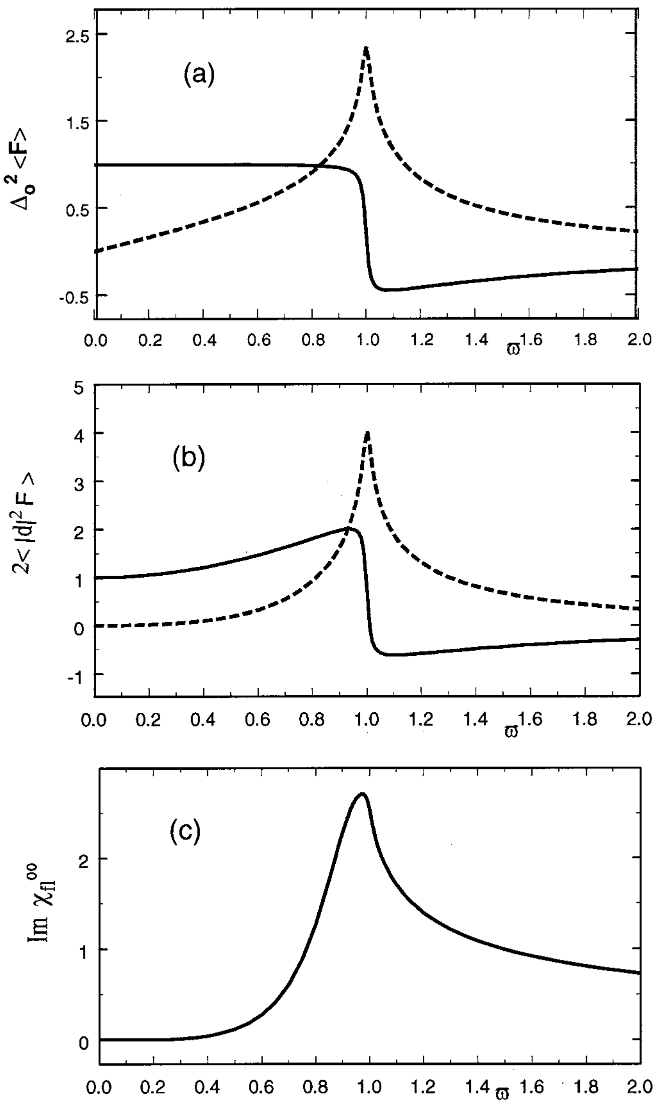

FIG. 3. (a) Real part (solid line) and imaginary part (dashed line) of function $\Delta_0^2\langle F\rangle$ for state (8) [see Eq. (9)] versus $\overline{\omega}$ for $\gamma=0.01$. (b) Function $2\langle|\mathbf{d}|^2F\rangle$ [see Eq. (10)] versus $\overline{\omega}$ for $\gamma=0.01$. (c) Fluctuation-charge susceptibility for state (8), Im χ_{fl}^{00} [see Eq. (3)], versus $\overline{\omega}$ for $\gamma=0.01$.

$$\mathbf{d}=(1/\sqrt{2})\Delta_0\hat{z}(k_x-k_y),\quad |\mathbf{d}|^2=\Delta_0^2(1-\sin 2\phi)/2. \tag{14}$$

For this state, we obtain from Eq. (8) the following angle average $\langle F(\omega)\rangle$ at $T=0$:

$$\Delta_0^2\langle F(\omega)\rangle=1+i(\overline{\omega}+i\gamma)^{-1}[K(\overline{\omega}+i\gamma)-E(\overline{\omega}+i\gamma)]$$

$$(\overline{\omega}=\omega/2\Delta_0,\quad \gamma=\Gamma/2\Delta_0).$$

$$K(\overline{\omega},+i\gamma)\sim\ln\{4[1-(\overline{\omega}+i\gamma)^2]^{-1/2}\}\quad(\overline{\omega}\lesssim 1). \tag{15}$$

Here, K and E are the complete elliptic integrals. One recognizes that the function in Eq. (15) is quite different from the corresponding function $2\Delta_0^2F$ for a constant energy gap in Eq. (11) as can be seen by comparing Figs. 3(a) and 1(a) for $\gamma=0.01$: Re $\Delta_0^2\langle F\rangle$ stays almost constant up to the pair-breaking edge $\overline{\omega}=1$, while Re $2\Delta_0^2F$ exhibits a peak near $\overline{\omega}=1$. On the other hand, Im $\Delta_0^2\langle F\rangle$ increases rapidly with increasing $\overline{\omega}$ in consequence of the gap nodes, while Im $2\Delta_0^2F$ is almost zero up to $\overline{\omega}\lesssim 1$ and then rises steeply to a high peak at the pair-breaking edge $\overline{\omega}=1$. This result for Re $\Delta_0^2\langle F\rangle$ implies that there exists a zero of the real part of the denominator in Eq. (7) only if the reduced pinning frequency squared (x_1-x_6) is smaller than one.

For the charge-fluctuation susceptibility $\chi_{fl}^{00}(0,\omega)$ in Eq. (10), we need to know the average value of the gap squared. For $T=0$, we obtain from Eq. (8) for the state (14):

$$2\langle|\mathbf{d}|^2F\rangle=1+\tfrac{4}{3}(\overline{\omega}+i\gamma)^2+i\tfrac{4}{3}(\overline{\omega}+i\gamma)^{-1}\{K(\overline{\omega}+i\gamma)\times[1+\tfrac{1}{2}(\overline{\omega}+i\gamma)^2]-E(\overline{\omega}+i\gamma)[1+(\overline{\omega}+i\gamma)^2]\}. \tag{16}$$

This function is plotted in Fig. 3(b) versus $\overline{\omega}$ for $\gamma=0.01$. It turns out that a zero of the denominator of $\chi_{fl}^{00}(0,\omega)$ in Eq. (10) is obtained only if γ is finite and sufficiently large, namely, $\gamma\gtrsim 0.24$. For increasing γ, the zero of the denominator tends to about $\omega_0=\sqrt{3}\Delta_0$. These results are quite similar to those for the amplitude fluctuation mode of the d-wave pairing state in the high-T_c superconductors.[14] The height of the peak of Im χ_{fl}^{00} at the resonance frequency ω_0 increases with increasing γ. In Fig. 3(c), we show Im χ_{fl}^{00} versus $\overline{\omega}$ for $\gamma=0.01$. Here, we have taken a constant value for the small numerator in Eq. (10), which is of the order of magnitude $(dN/d\varepsilon)^2$.

The resonance of the spin- and charge-fluctuation modes at the nesting vector $\mathbf{Q}$ are obtained from the equations where the function $\Delta_0^2\langle F\rangle$ in Eq. (15) is set equal to x_1 or x_6, respectively. Since $\Delta_0^2\langle F\rangle\leqslant 1$ [see Fig. 3(a)], one obtains no solutions.

We have investigated also the collective modes for p-wave pairing states with $\mathbf{d}$ vectors lying in the basal xy plane and obtain analogous results to the foregoing ones. As a first example, we consider $\mathbf{d}=\Delta_0(\hat{x}k_x+\hat{y}k_y)$ with constant energy gap squared, $|\mathbf{d}|^2=\Delta_0^2$. For wave vector $\mathbf{q}=0$, we find a charge-fluctuation contribution χ_{fl}^{00} corresponding to Eq. (10) with resonance frequency $\omega=2\Delta_0$. Furthermore, we obtain spin-fluctuation contributions $\chi_{fl}^{\mu\nu}$ corresponding to Eq. (7) where the reduced pinning frequency (x_1-x_6) is replaced by (x_6-x_1) for $\mu\nu=xx$, and by (x_2-x_1) for $\mu\nu=zz$. Recall that $x_j=1/N_0v_j$. Since the stable pairing state has the largest pairing strength, N_0v_1, the inequalities $x_6>x_1$ and $x_2>x_1$ hold. For nesting vector $\mathbf{Q}$ of the α and β bands, we find again that in the expressions for $\chi_{fl}^{\mu\nu}$ in Eq. (7), the term $(\omega^2/2)\langle F\rangle$ has to be replaced by $2\Delta_0^2\langle F\rangle$, and that (x_1-x_6) has to be replaced by x_6 for $\mu\nu=xx$, and by x_2 for $\mu\nu=zz$. Otherwise the results are the same as for state (6), in particular, F is given by Eq. (11) [see Fig. 1(a)].

As a second example, we consider the polar state, $\mathbf{d}=(\Delta_0/2)(\mathbf{d}_1+\mathbf{d}_3)=\Delta_0\hat{x}k_x$ with squared gap $|\mathbf{d}|^2=\Delta_0^2\cos^2\phi$. We obtain analogous results to the previous ones for the fluctuation susceptibilities in Eqs. (7) and (10) apart from the fact that now angle averages over ϕ have to be taken with the function $|\mathbf{d}(\phi)|^2/\langle|\mathbf{d}|^2\rangle=2\cos^2\phi$ in $F(\phi,\omega)$ [see Eq. (8)]. The reduced pinning frequency (x_1-x_6) in Eq. (7) has now to be replaced by (x_6-x_1) for $\mu,\nu=y,y$, and by (x_4-x_1) for $\mu\nu=zz$. The averages $\langle F(\omega)\rangle$ and $\langle|\mathbf{d}|^2F\rangle$

are given again by Eqs. (15) and (16). Thus the results for the state $\mathbf{d}=\Delta_0 \hat{x} k_x$ are analogous to those for the b-phase state (14).

IV. CONCLUSIONS

We have studied the large variety of order-parameter collective modes for possible p-wave superconducting states in Sr_2RuO_4. These modes may be observable if their coupling to spin or charge density is sufficiently large and if their resonance frequencies ω fall below the pair-breaking threshold $2\Delta_0$. The dynamics of the Cooper pair modes is given by the function $F(\omega)$ defined in Eq. (8). The sharp pair-breaking threshold $\omega=2\Delta_0$, which can be seen in $\mathrm{Im}\,F(\omega)$ for a state with constant gap Δ_0 [see Fig. 1(a)] is largely washed out for a state with a node in the gap [see Fig. 3(a)]. Recent specific heat measurements on cleaner samples of Sr_2RuO_4 (Ref. 19) have led to speculations that the gap is very anisotropic[20] or has nodes.[22] We obtain for these proposed gap functions very similar results as those shown in Fig. 3. The pair-breaking edge of $\mathrm{Im}\,F(\omega)$ is washed out also by scattering of quasiparticles on spin fluctuations[10,14] and impurities.[20] This quasiparticle damping is simulated here by a damping constant Γ. Our fit of the neutron-scattering data on Sr_2RuO_4 (Ref. 9) (see Fig. 2) shows that Γ is rather large at least in the normal state.

Those fluctuations $\delta\mathbf{d}$ of the pairing state $\mathbf{d}$, which couple to spin density, can be excited by external vector fields $\mathbf{U}_a$ that are directed perpendicular to $\mathbf{d}$. Their resonance frequencies for wave vector $\mathbf{q}=0$ fall below the pair-breaking threshold $\omega=2\Delta_0$ if the pinning of the $\mathbf{d}$ vector by the anisotropic pairing interaction [see Eq. (2)] is sufficiently weak. This pinning frequency Ω_d is given by $(\Omega_d/2\Delta_0)^2=\ln(T_c/T_{cj})$ [see Eq. (9)], where T_c is the transition temperature corresponding to the stable state $\mathbf{d}$, and T_{cj} is the transition temperature of the state $\mathbf{d}_j$ lying in the direction of $\mathbf{U}_a$ and $\delta\mathbf{d}$. One might speculate that the additional transition feature below 0.8 K that has been recently observed in the in-plane anisotropy of the upper critical field in Sr_2RuO_4 (Ref. 23) corresponds to the in-plane T_{cj}, while T_c corresponds to the stable state $\mathbf{d}$ along the c axis. Then, we would obtain for $T_{cj}=0.8\,\mathrm{K}$ and $T_c=1.46\,\mathrm{K}$ a squared ratio $(\Omega_d/2\Delta_0)^2\simeq 0.6$, which means that Ω_d falls far below the pair-breaking threshold and might be observable by spin resonance.

For nesting vector $\mathbf{q}=\mathbf{Q}$ associated with the α and β bands of Sr_2RuO_4, the resonance frequencies of the collective modes are close to $2\Delta_0$ or larger and, therefore, it is unlikely that they can be observed. However, the full RPA spin susceptibility (without the fluctuation contribution) may exhibit at $\mathbf{q}=\mathbf{Q}$ a resonance below $2\Delta_0$ if the on-site Coulomb repulsion U is smaller than the BCS pairing interaction constant. This is very similar to the RPA spin susceptibility for d-wave pairing in the high-T_c cuprates, where a resonance has been actually observed by neutron scattering around the antiferromagnetic wave vector.[14] It is promising that one has observed already in the normal state of Sr_2RuO_4 a broad peak in the neutron-scattering intensity close to the nesting vector $\mathbf{Q}$.[9]

In contrast to recent theories of ultrasound propagation and attenuation in Sr_2RuO_4,[16,17] we find that the coupling of the clapping mode with frequency $\omega=\sqrt{2}\Delta_0$ to charge density vanishes.[18] However, the fluctuation $\delta\mathbf{d}$ in the direction of $\mathbf{d}$ couples to charge density with a coupling strength that is small of the order of particle-hole asymmetry of the density of states at the Fermi energy. This amplitude fluctuation mode has a resonance frequency $\omega=2\Delta_0$ for a state with constant gap Δ_0 and a resonance frequency $\omega\simeq\sqrt{3}\Delta_0$ for a state with nodes in the gap. Since the specific heat measurements favor a state with a strongly anisotropic gap,[19] it seems possible that for sound propagation perpendicular to the basal plane, a resonance can be detected in ultrasound attenuation provided that the amount of particle-hole asymmetry at the Fermi surface is not too small.

[1] Y. Maeno, H. Hashimoto, K. Yoshida, S. NishiZaki, T. Fujita, J. G. Bednorz, and F. Lichtenberg, Nature (London) **372**, 532 (1994).

[2] K. Ishida, H. Mukuda, Y. Kitaoka, K. Asayama, Z. Q. Mao, Y. Mori, and Y. Maeno, Nature (London) **396**, 658 (1998).

[3] T. M. Rice and M. Sigrist, J. Phys.: Condens. Matter **7**, L643 (1995).

[4] A. J. Leggett, Rev. Mod. Phys. **47**, 331 (1975).

[5] M. Sigrist, D. Agterberg, A. Furusaki, C. Honerkamp, K. K. Ng, T. M. Rice, and M. E. Zhitomirsky, Physica C **317–318**, 134 (1999).

[6] A. P. Mackenzie, S. R. Julian, A. J. Diver, G. G. Lonzarich, Y. Maeno, S. NishiZaki, and T. Fujita, Phys. Rev. Lett. **76**, 3786 (1996).

[7] T. M. Riseman, P. G. Kealy, E. M. Forgan, A. P. Mackenzie, L. M. Galvin, A. W. Tayler, S. L. Lee, C. Ager, D. McPaul, C. M. Agterberg, R. Cubitt, Z. Q. Mao, S. Akima, and Y. Maeno, Nature (London) **396**, 242 (1998).

[8] I. I. Mazin and D. J. Singh, Phys. Rev. Lett. **82**, 4324 (1999).

[9] Y. Sidis, M. Braden, P. Bourges, B. Hennion, S. NishiZaki, Y. Maeno, and Y. Mori, Phys. Rev. Lett. **83**, 3320 (1999).

[10] L. Tewordt, Phys. Rev. Lett. **83**, 1007 (1999).

[11] H. Y. Kee, Y. B. Kim, and K. Maki, Phys. Rev. B **61**, 3584 (2000).

[12] L. Tewordt, D. Fay, P. Dörre, and D. Einzel, J. Low Temp. Phys. **21**, 645 (1975).

[13] H. Monien, K. Scharnberg, L. Tewordt, and N. Schopohl, J. Low Temp. Phys. **65**, 13 (1986).

[14] T. Dahm, D. Manske, and L. Tewordt, Phys. Rev. B **58**, 12 454 (1998).

[15] L. Tewordt and N. Schopohl, J. Low Temp. Phys. **34**, 489 (1979).

[16] S. Higashitani and K. Nagai, Physica B **284-288**, 539 (2000).

[17] H. Y. Kee, Y. B. Kim, and K. Maki, cond-mat/9911131 (unpublished).

[18] L. Tewordt, J. Low Temp. Phys. **117**, 1 (1999).

[19] S. Nishizaki, Y. Maeno, and Z. Q. Mao, J. Low Temp. Phys. **117**, 1581 (1999).

[20] K. Miyake and O. Narikiyo, Phys. Rev. Lett. **83**, 1423 (1999).

[21] K. K. Ng and M. Sigrist, cond-mat/9911325 (unpublished).

[22] Y. Hasegawa, K. Machida, and M. Ozaki, cond-mat/9909316 (unpublished).

[23] Z. Q. Mao, Y. Maeno, S. NishiZaki, T. Akima, and T. Ishiguro, Phys. Rev. Lett. **84**, 991 (2000).