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ANISOTROPIC SHEAR STRESS σ_{xy} EFFECTS IN THE BASAL PLANE OF Sr_2RuO_4

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ABSTRACT

In the present paper following the previous work (Walker and Contreras, 2002; Walker, 1980; Walker *et al*., 2001; Contreras, 2006) we calculate the jumps for the thermal expansion $\alpha_{\sigma xy}$, the specific heat $C_{\sigma xy}$, and the elastic compliance $S_{xyxy}^{\sigma_{xy}}$ in the basal plane of Sr_2RuO_4. We use here the 4^{th} rank tensor notation because of the Voigt notation, where the stress and strain are treated differently. Henceforth, we clarify some issues regarding a Ginzburg-Landau analysis suitable to explain the sound speed experiments (Lupien, 2002), and partially the strain experiments (Hicks *et al*., 2014; Steppke *et al*., 2017) in strontium ruthenate. We continue to propose the following: (1) the discontinuity in the elastic constant C_{xyxy} of the tetragonal crystal Sr_2RuO_4 gives an unambiguous experimental evidence that the Sr_2RuO_4 superconducting order parameter Ψ has two components with a broken time-reversal symmetry state, and (2) the γ band couples the anisotropic electron-phonon interaction to the [xy] in-plane shear stress in Sr_2RuO_4 (Walker *et al*., 2001; Contreras, 2006).

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INTRODUCTION

In Sr_2RuO_4, the electrons in the Cooper pairs are bound in spin triplets, where the spins are lying on the basal plane and the pair orbital momentum is directed along the z-direction. Henceforth, the order parameter Ψ is represented by a vector $\mathbf{d}(\mathbf{k})$ (of the type $k_x \pm ik_y$) (Maeno *et al*., 1994; Maeno *et al*., 2001; MacKenzie and Maeno, 2003; Rice and Sigrist, 1995).

Based on the results of the Knight-shift experiment performed through T_c (Ishida *et al*., 1998; Duffy *et al*., 2000), it has been proposed that Sr_2RuO_4 is a triplet superconductor, also it has been reported by Luke *et al*. (1998) that Ψ breaks time-reversal symmetry, which constitutes another key feature of unconventionality. The Sr_2RuO_4 elastic constants C_{xyxy} have been carefully measured as the temperature T is lowered through T_c, showing the existence of small step in the transverse sound mode T[100] (Lupien, 2002). This experimental result theoretically implies that Ψ has two different components with a time-reversal symmetry broken state (Walker and Contreras, 2002). Similar conclusions from a muon-spin relaxation (μSR) experiment were reported by Luke *et al*. (1998). Recently, experiments on the effects of uniaxial strain ϵ_{xy}, were performed by Hicks *et al*. (2014), reporting that for Sr_2RuO_4 the symmetry-breaking field can be controlled experimentally.

Additionally, a most recently experiment (Steppke *et al*., 2017) found that the transition temperature T_c in the superconductor Sr_2RuO_4 rises dramatically under the application of a planar anisotropic strain, followed by a sudden drop beyond a larger strain. Furthermore, recent theoretical work suggests that those recent experiments tuned the Fermi surface topology efficiently by applying planar anisotropic strain emphasizing again, the point of view that in-plane effects (even by means of a more complicated renormalization group theory framework) also shows clear evidence of a symmetry broken stated in Sr_2RuO_4. Furthermore, they reported a rapid initial increase in the superconducting transition temperature T_c, that the authors associated with the evolution of the Fermi surface toward a Lifshitz-Fermi surface reconstruction under an increasing strain (Liu *et al*., 2017).

Here, we aim to clarify some particular concepts and methods following an elastic phenomenological (GL) approach (Walker, 1980; Landau and Lifshitz, 1980; Landau and Lifshitz, 1970; Testardi, 1971; Auld, 1990; Musgrave, 1970; Philip, 1987). First, it is natural to point out the differences between using stress or strain (which is the response of a system to applied stress; also, according

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to Dr. Grechka explanation, fiber optics yields dynamic fidelity of a fraction of a nanostrain, and tiltmeters yield comparable static fidelity) to explain a time-reversal symmetry broken state. Second, there is a claim (Liu *et al*., 2017) that only the γ band responses to the strain sensitively, and we emphasize that this physical phenomenon is caused by the γ band coupling of the anisotropic electron-phonon interaction to the [xy] plane (Walker *et al*., 2001; Contreras, 2006). Third, we do not expand our analysis to a Lifshitz reconstruction of the Fermi surface mainly because we do not have experimental evidences that show a topological Lifshitz transition in Sr_2RuO_4 even in its normal state, neither we have observed a generalized topological transition in Sr_2RuO_4. In our opinion, a two-dimensional Fermi contour evolution under an applied external strain as the one for the γ band in Sr_2RuO_4 needs further interpretations in terms of a topological electronic Lifshitz phase transition (Lifshitz, 1960; Kaganov and Lifshitz, 1979; Kaganov and Contreras, 1994; Kaganov and Nurmagambetov, 1982). We remember that $\sigma_{ik} = -\,p\delta_{ik}$ shows how pressure and stress are in general related, the stress σ_{ik} becomes the delta function δ_{ik} if a volumetric pressure is applied to a sample (Landau and Lifshitz, 2009).

These experimental results and theoretical interpretations need to clarify moderately in order to unify several theoretical criteria which try to explain the changes occurring in the C_{xyxy} elastic constant at T_c (Lupien, 2002; Hicks *et al*., 2014; Steppke *et al*., 2017).

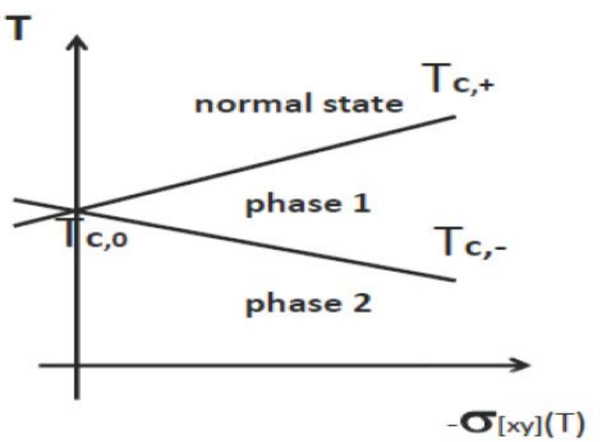

Fig. 1. The phase diagram sketch showing the upper T_{c+}, lower T_{c-}, and zero T_{c0} superconducting transition temperatures as a function of the shear stress $-\,\sigma_{xy}(T)$. Notice that at T_{c0} the derivative $\frac{dT_{c0}}{d\sigma_{xy}}$ does not exist.

Thus, the aim of this short note is to clarify again that an elastic Ginzburg-Landau phenomenological approach partially demonstrates that Sr_2RuO_4 is an unconventional superconductor with a two-component order parameter Ψ (Walker and Contreras, 2002; Contreras, 2006). We based our interpretation on a Sr_2RuO_4 (T[100]) transversal response-impulse mode experimentally measured as the temperature T is lowered through T_c showing only an small step change (Lupien, 2002) (for that particular result, please, see the bottom panel in (Lupien, 2002), namely in Figures 5.7 and 5.8 on pages 138 and 139.) The result clearly shows a discontinuity in the T[100] mode.

Here, let us mention that a different theory of Sr_2RuO_4 elastic properties was presented in (Sigrist, 2002). However, the approach followed does not take into account the splitting of T_c due to the shear σ_{xy}, and directly calculates the jumps at zero stress, where the derivative of T with respect to σ_{xy} does not exist (Walker, 1980), see in Figure 1.

Shear stress σ_{xy} analysis

In this section, we make use of the 4^{th} rank tensor notation because the Voigt notation has a disadvantage; the stress and strain are treated differently. Voigt mapping only preserves the elastic stiffnesses. We also call the uniaxial shear stress as shear stress only because the effect observed is in the basal plane [xy]. As was stated previously (Walker and Contreras, 2002; Contreras, 2006) when shear stress σ_{xy} is applied to the basal plane of Sr_2RuO_4, the crystal tetragonal symmetry is broken, and a second-order transition to a superconducting state occurs. Accordingly, for this case the analysis of the sound speed behavior at T_c also requires a systematic study of the two successive second order phase transitions, see in figure 2. Hence, the C_{xyxy} discontinuity (Lupien, 2002) at T_c, can be explained in this context. Due to the absence of discontinuity in S_{xyxy} for any of the one-dimensional Γ representations, the superconductivity in Sr_2RuO_4 must be described by the two-dimensional irreducible representation E_{2u} of the tetragonal point group D_{4h} (Walker and Contreras, 2002).

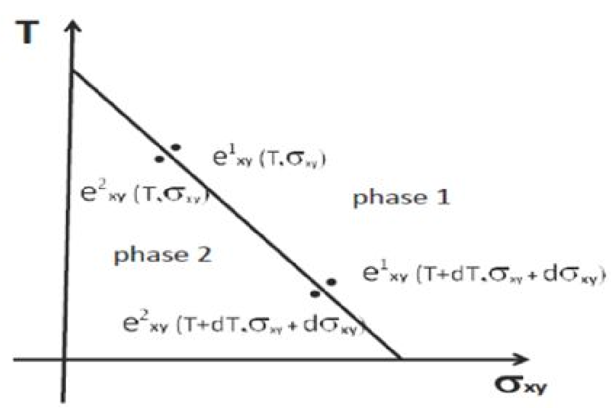

Fig. 2. The sketch showing the line of transition temperatures T_c along of a second order phase transition. The state of the strain e_{xy} shown in the figure, the entropy

S_0, and the volume V are continuous functions along the line of the second order phase transition (Walker, 1980; Contreras, 2006).

If there is a double transition, the derivative of T_c with respect to σ_{xy} (i.e. $dT_c/d\sigma_{xy}$) is different for each of the two transition lines (see the T_c-σ_{xy} phase diagram in Figure 2.) At each of these transitions, the specific heat $C_{\sigma xy}$, the thermal expansion $\alpha_{\sigma xy}$, and the elastic compliance $S^{\sigma_{xy}}_{xyxy}$ show discontinuities (Walker and Contreras, 2002), the sum of them gives the correct expressions for the discontinuities at zero shear stress, where the Ehrenfest relations do not hold.

In the case of an applied shear stress σ_{xy}, the change for the in-plane Gibbs free energy is given by

$$\Delta G_{\sigma_{xy}} = \alpha(|\psi_x|^2 + |\psi_y|^2) + \sigma_{xy} d_{xyxy}(\psi_x\psi_y^* + \psi_x^*\psi_y) + \frac{b_1}{4}(|\psi_x|^2 + |\psi_y|^2)^2 + b_2|\psi_x|^2|\psi_y|^2 + \frac{b_3}{2}(\psi_x^2\psi_y^{*2} + \psi_x^{*2}\psi_y^2) \quad (1)$$

where the d_{xyxy} term couples the stress σ_{xy} to the order parameter, the thermal expansion coefficient $\alpha = \alpha'(T - T_{c0})$, and the minimization of $\Delta G_{\sigma xy}$ is performed by substituting the general expression for Ψ as was previously calculated (Contreras, 2006; Sigrist, 2002). Therefore, $\Delta G_{\sigma xy}$ becomes

$$\Delta G_{\sigma_{xy}} = \alpha(\eta_x^2 + \eta_y^2) + 2\eta_x\eta_y\sigma_{xy}\sin(\phi)\, d_{xyxy} + \frac{b_1}{4}(\eta_x^2 + \eta_y^2)^2 + (b_2 - b_3)\eta_x^2\eta_y^2 + 2b_3\eta_x^2\eta_y^2\sin^2(\phi) \quad (2)$$

In the presence of σ_{xy}, the second order term determines the phase below T_{c+}, which is characterized by ψ_x and by $\psi_y = 0$. As the temperature is lowered below T_{c-}, depending of the value of b_3 a second component ψ_y may appear. If at T_{c-} a second component occurs, the fourth order terms in equation (2) will dominate. Thus, for very low T's, or for $\sigma_{xy} \to 0$, a time-reversal symmetry-breaking superconducting state may emerge. The analysis of equation (2) depends on the relation between the coefficients b_2 and b_3. It also depends on the values of the quantities η_x and η_y, and of the phase ϕ. If $b_3 < 0$, and η_x and η_y are both nonzero, the state with minimum energy has a phase $\phi = \pi/2$. The transition temperature is obtained from equation (2), by performing the following canonical transformations: $\eta_x = (\eta_\mu + \eta_\xi)/2^{1/2}$ and $\eta_y = (\eta_\mu - \eta_\xi)/2^{1/2}$. After their substitution, equation (2) becomes

$$\Delta G_{\sigma_{xy}} = \alpha_+\eta_\xi^2 + \alpha_-\eta_\mu^2 + \frac{1}{4}(\eta_\xi^2 + \eta_\mu^2)^2 + (b_2 + b_3)(\eta_\xi^2 - \eta_\mu^2)^2 \quad (3)$$

As it was before done, $\eta_\xi = \eta\sin(\chi)$ and $\eta_\mu = \eta\cos(\chi)$, equation (3) takes the following form:

$$\Delta G_{\sigma_{xy}} = \alpha_+\eta^2\sin^2(\chi) + \alpha_-\eta^2\cos^2(\chi) + \frac{\eta^4}{4}[b_1 + (b_2 + b_3)\cos^2(2\chi)] \quad (4)$$

$\Delta G_{\sigma xy}$ is minimized if $\cos(2\chi) = 1$, this is, if $\chi = 0$. Also, in order for the phase transition to be of second order, b', defined as $b' \equiv b_1 + b_2 + b_3$, must be larger than zero. Therefore, if σ_{xy} is nonzero, the state with the lowest free energy corresponds to $b_3 < 0$, the phase ϕ equals to $\pi/2$, and Ψ of the form:

$$(\psi_x, \psi_y) \approx \eta(exp(i\phi/2), exp(-i\phi/2)) \quad (5)$$

In phase 1 in Figure 2 there is $\phi = 0$ and T is lowered below T_{c-}. In phase 2, ϕ grows from 0 to approximately $\pi/2$. The two transition temperatures T_{c+} and T_{c-} are obtained to be:

$$T_{c+}(\sigma_{xy}) = T_{c0} - \frac{\sigma_{xy}}{\alpha'} d_{xyxy} \quad (6)$$

$$T_{c-}(\sigma_{xy}) = T_{c0} + \frac{b\sigma_{xy}}{2b_3\alpha'} d_{xyxy} \quad (7)$$

The derivative of T_{c+} with respect to σ_{xy}, and the discontinuity in $C^+_{\sigma_{xy}}$ at T_{c+} are, respectively:

$$\frac{dT_{c+}}{d\sigma_{xy}} = -\frac{d_{xyxy}}{\alpha'} \quad (8)$$

$$\Delta C^+_{\sigma_{xy}} = -\frac{2\alpha'^2 T_{c+}}{b'} \quad (9)$$

After applying the Ehrenfest relations (Landau and Lifshitz, 1980), the results for $\Delta\alpha_{\sigma xy}$ and ΔS_{xyxy} at T_{c+} are:

$$\Delta\alpha^+_{\sigma_{xy}} = -\frac{2\alpha' d_{xyxy}}{b'} \quad (10)$$

$$\Delta S^+_{xyxy} = -\frac{2d^2_{xyxy}}{b'} \quad (11)$$

For T_{c-}, the derivative of this transition temperature with respect to σ_{xy}, and the discontinuities in the specific heat, thermal expansion and elastic stiffness respectively are:

$$\frac{dT_{c-}}{d\sigma_{xy}} = \frac{b d_{xyxy}}{2b_3\alpha'} \quad (12)$$

$$\Delta C^-_{\sigma_{xy}} = -\frac{4\alpha'^2 b_3 T_{c-}}{bb'} \quad (13)$$

$$\Delta\alpha^{-}_{\sigma_{xy}} = \frac{2\alpha' d_{xyxy}}{b'} \quad (14)$$

$$\Delta S^{-}_{xyxy} = -\frac{b d^2_{xyxy}}{b' b_3} \quad (15)$$

For the case of σ_{xy}, because the derivative of T_c with respect to σ_{xy} is not defined at zero stress point (see in Figure 1), the Ehrenfest relations do not hold at T_{c0}. Thus, the discontinuities occurring at T_{c0}, in the absence of σ_{xy}, are calculated by adding the expressions obtained for the discontinuities at T_{c+} and T_{c-},

$$\Delta C^{0}_{\sigma_{xy}} = -\frac{2T_{c0}\alpha'^2}{b} \quad (16)$$

$$\Delta S^{0}_{xyxy} = -\frac{d^2_{xyxy}}{b_3} \quad (17)$$

$$\Delta\alpha^{0}_{\sigma_{xy}} = 0 \quad (18)$$

In this case there is no discontinuity for the thermal expansion of Sr_2RuO_4 at zero stress $\alpha^{0}_{\sigma_{xy}}$ that is another physical feature we previously predicted in (Walker and Contreras, 2002), see in Figure 3. Some experimental studies on the changes in the thermal expansion coefficient α_i below T_c in the HTS reported in (Asahi *et al*., 1997) that an additive lattice jump was found to appear spontaneously at T_c for a high T_c compound with one-component order parameter.

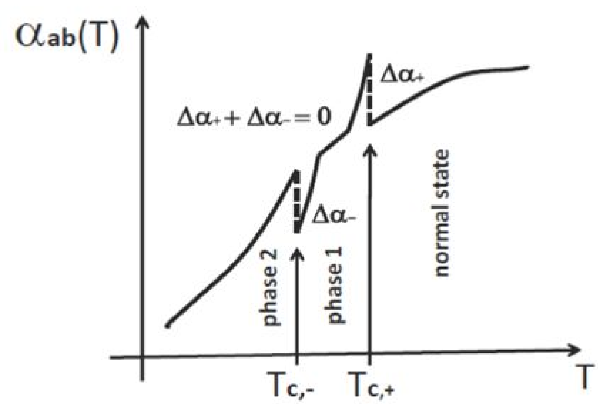

Fig. 3. The schematic dependence of the thermal expansion on the temperature for Sr_2RuO_4. Notice the two jumps in the in plane thermal expansion coefficient near the transition temperatures T_{c+} and T_{c-}. The sketch shows two jumps of the same magnitude but they have opposite signs, and their sum cancels out at T_{c0}. This happens for a two-component order parameter Ψ.

Since the phase diagram was determined as a function of σ_{xy}, rather than as a function of the shear strain ϵ_{xy}, see in Figure 1, in this work, as in (Walker and Contreras, 2002; Contreras, 2006), we make use of the 6 × 6 elastic compliance matrix S, and also of the full range tensor notation. However, the sound speed measurements (Lupien, 2002; Lupien *et al*., 2001) are best interpreted in terms of the elastic stiffness tensor C with the matrix elements C_{ijkl}, which is the inverse of the elastic compliance matrix S (Nye, 1989). However, the strain is easier to measure than the stress because fiber optics yields dynamic fidelity of a fraction of a nanostrain. Here we have to mention the explanation by Dr. Grechka: fiber optics yields dynamic fidelity of a fraction of a nanostrain, and tiltmeters yield comparable static fidelity.

Therefore, it is important to be able to obtain the discontinuities in the elastic stiffness matrix in terms of the elastic compliance matrix for the shear stress case. Thus, close to the transition line we follow (Walker, 1980): $C(T_c + 0^+) = C(T_c - 0^+) + \Delta C$ and $S(T_c + 0^+) = S(T_c - 0^+) + \Delta S$, where 0^+ is positive and infinitesimal. By making use of the fact that $C(T_c + 0^+)\, S(T_c + 0^+) = \hat{I}$, where $\hat{I}$ is the unit matrix, it is shown that, to first order, the discontinuities satisfy, $\Delta C \approx -C\, \Delta S\, C$. In this manner, it is found that, for instance, at T_{c+}, the expressions that define the jumps for the discontinuities in elastic stiffness and compliances, due to an external stress, have either a positive or a negative value. In this way, ΔS_{xyxy} must have a negative sign; while ΔC_{xyxy} must have a positive sign.

Conclusive remarks

The most noteworthy outcome of this short note is that the observation of a discontinuity in the elastic constant C_{xyxy} (Lupien, 2002; Lupien *et al*., 2001) is an evidence that the order parameter Ψ in Sr_2RuO_4 has two components as the theoretical GL analysis predicts. Also, the theoretical indicator that the sum of the jumps $\Delta\alpha^{+}_{\sigma_{xy}} + \Delta\alpha^{-}_{\sigma_{xy}} = 0$ for the in-plane thermal expansion coefficient (Walker and Contreras, 2002), see in Figure 3. Hence, the use of Sr_2RuO_4 as a material in detailed studies of superconductivity symmetry-breaking effects has significant advantages because is described by a two-component order parameter. Nevertheless, determining from Sr_2RuO_4 experimental measurements the magnitude of the parameters in the Ginzburg-Landau model is complicated (Walker and Contreras, 2002).

In the experimental work of the sound velocity measurements (Lupien, 2002; Lupien *et al*., 2001) in Sr_2RuO_4 a discontinuity in the behavior for C_{xyxy} below T_{c0}, without a significant change in the sound speed slope as T goes below 1 Kelvin was understood as a signature of an unconventional transition to a superconducting phase (Walker and Contreras, 2002; Lupien, 2002; Sigrist, 2002). Thus, this set of previous results, and other recent results (Hicks *et al*., 2014; Steppke *et al*., 2017; Liu *et al*., 2017; Acharya *et al*., 2018), considers Sr_2RuO_4 as a strong candidate for a detailed experimental investigation of the effects of a symmetry-breaking field by means of strain or stress experimental measurements. We also suggest that an in-plane thermal expansion measurement at zero uniaxial shear stress might further clarify any previous interpretation.

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