Anisotropic shear stress $\sigma_{xy}$ effects in the basal plane of Sr$_2$RuO$_4$

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In this short note following a previous set of works [3, 4, 16, 17] we repeat the calculations for the jumps for the thermal expansion $\alpha_{\sigma_{xy}}$, the specific heat $C_{\sigma_{xy}}$, and the elastic compliance $S_{\sigma_{xy}xy}$ in the basal plane of Sr$_2$RuO$_4$. 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 [10], and partially the strain experiments [12, 13] in strontium ruthenate. We continue to propose that the discontinuity in the elastic constant $C_{xyxy}$ of the tetragonal crystal Sr$_2$RuO$_4$ gives an unambiguous experimental evidence that the Sr$_2$RuO$_4$ superconducting order parameter $\Psi$ has two components with a broken time-reversal symmetry state, and that the $\gamma$ band couples the anisotropic electron-phonon interaction to the $[xy]$ in-plane shear stress in Sr$_2$RuO$_4$ [16, 17]. Some important words about the roll of the spin equal to one for transversal phonos are added following Levine [34].

Keywords: Shear stress; time-reversal symmetry; Ehrenfest relations; elastic constants; thermal expansion; spin one phonons.

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I. INTRODUCTION

In Sr$_2$RuO$_4$ 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 $\Psi$ is represented by a vector $\mathbf{d}(\mathbf{k})$ (of the type $k_x \pm i k_y$)
Based on the results of the Knight-shift experiment performed through \( T_c \) \[\ref{eq:1}\], it has been proposed that \( \text{Sr}_2\text{RuO}_4 \) is a triplet superconductor, also it has been reported \[\ref{eq:2}\] that \( \Psi \) breaks time-reversal symmetry, which constitutes another key feature of unconventionality. The \( \text{Sr}_2\text{RuO}_4 \) 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 \( T[100] \) \[\ref{eq:10}\]. This experimental result theoretically implies that \( \Psi \) has two different components with a time-reversal symmetry broken state \[\ref{eq:3}\]. Similar conclusions from a muon-spin relaxation (\( \mu \)SR) experiment were reported \[\ref{eq:9}\]. Recently, experiments on the effects of uniaxial strain \( \epsilon_{xy} \), were performed \[\ref{eq:12}\], reporting that for \( \text{Sr}_2\text{RuO}_4 \) the symmetry-breaking field can be controlled experimentally.

Additionally, a most recently experiment \[\ref{eq:13}\] found that the transition temperature \( T_c \) in the superconductor \( \text{Sr}_2\text{RuO}_4 \) 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 state in \( \text{Sr}_2\text{RuO}_4 \). 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 \[\ref{eq:14}\].

Here, we aim to clarify some particular concepts and methods following an elastic phenomenological (GL) approach \[\ref{eq:4, 25, 30}\]. First, the differences between using stress or strain (which is the response of a system to applied stress) \[\ref{eq:31}\] to explain a time-reversal symmetry broken state. Second, there is a claim \[\ref{eq:14}\] that only the \( \gamma \) band responses to the strain sensitively, and we emphasize that this physical phenomenon is caused by the \( \gamma \) band coupling the anisotropic electron-phonon interaction to the \( [xy] \) plane \[\ref{eq:16, 17}\]. 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 \( \text{Sr}_2\text{RuO}_4 \) even in its normal state, neither we have observed a generalized topological transition in \( \text{Sr}_2\text{RuO}_4 \). In our opinion a 2D Fermi contour evolution under an applied external strain as the one for the \( \gamma \) band in \( \text{Sr}_2\text{RuO}_4 \) needs further interpretations in terms of a topological
electronic Lifshitz phase transition [19–22]. We remember that \( \sigma_{ik} = -p \delta_{ik} \) shows how pressure and stress are in general related, the stress \( \sigma_{ik} \) becomes the delta function \( \delta_{ik} \) if a volumetric pressure is applied to a sample [23].

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 \( T_c \) [10, 12, 13].

Thus, the aim of this short note is to clarify again that an elastic Ginzburg-Landau phenomenological approach partially demonstrates that \( \text{Sr}_2\text{RuO}_4 \) is an unconventional superconductor with a two-component order parameter \( \Psi \) [3, 17]. We based our interpretation on a \( \text{Sr}_2\text{RuO}_4 \) [\( T[100] \)] transversal response-impulse mode experimentally measured as the temperature \( T \) is lowered through \( T_c \) showing only an small step change [10] (for that particular result please see bottom panel on Fig 5.7 and Fig 5.8 pp. 138-139 [10]). The result clearly shows a discontinuity in the \( T[100] \) mode.

Here, let us mention that a different theory of \( \text{Sr}_2\text{RuO}_4 \) elastic properties was presented [24]. However, the approach followed does not take into account the splitting of \( T_c \) due to shear \( \sigma_{xy} \), and directly calculates the jumps at zero stress, where the derivative of \( T \) with respect to \( \sigma_{xy} \) does not exist [4] (see fig.1).

FIG. 1: 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.
II. SHEAR STRESS $\sigma_{xy}$ ANALYSIS

In this section, we make use of the 4th 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 [3, 17] when shear stress $\sigma_{xy}$ is applied to the basal plane of Sr$_2$RuO$_4$, 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 fig 2). Hence, the $C_{xyxy}$ discontinuity at $T_c$, can be explained in this context. Due to the absence of discontinuity in $S_{xyxy}$ for any of the one-dimensional $\Gamma$ representations, the superconductivity in Sr$_2$RuO$_4$ must be described by the two dimensional irreducible representation $E_{2u}$ of the tetragonal point group $D_{4h}$ [3].

If there is a double transition, the derivative of $T_c$ with respect to $\sigma_{xy}$ i.e. $dT_c/d\sigma_{xy}$ is different for each of the two transition lines (see the $T_c-\sigma_{xy}$ phase diagram in fig 2). At each of these transitions, the specific heat $C_{\sigma_{xy}}$, the thermal expansion $\alpha_{\sigma_{xy}}$, and the elastic compliance $S_{\sigma_{xyxy}}$ show discontinuities [3], the sum of them gives the correct expressions for the discontinuities at zero shear stress, where the Ehrenfest relations do not hold.

![FIG. 2: 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 $S$, and the volume $V$ are continuous functions along the line of the second order phase transition.](image)

In the case of an applied shear stress $\sigma_{xy}$, the change for the in-plane Gibss free energy
\[
\Delta G_{\sigma_{xy}} = \alpha(|\psi_x|^2 + |\psi_y|^2) + \sigma_{xy} d_{xyxy}(\psi_x\psi_y^* + \psi_y^*\psi_x) + \frac{b_1}{4}(|\psi_x|^2 + |\psi_y|^2)^2 + b_2|\psi_x|^2|\psi_y|^2 + \frac{b_3}{2} (\psi_x^2\psi_y^2 + \psi_y^2\psi_x^2),
\]

(1)

where \(d_{xyxy}\) term couples the stress \(\sigma_{xy}\) to the order parameter, the thermal expansion coefficient \(\alpha = \alpha'(T - T_c)\), and the minimization of \(\Delta G_{\sigma_{xy}}\) is performed by substituting the general expression for \(\Psi\) as was previously calculated \([17, 24]\). Therefore \(\Delta G_{\sigma_{xy}}\) becomes

\[
\Delta G_{\sigma_{xy}} = \alpha(\eta_x^2 + \eta_y^2) + 2\eta_x\eta_y \sigma_{xy} \sin \phi d_{xyxy} + \frac{b_1}{4}(\eta_x^2 + \eta_y^2)^2 + (b_2 - b_3)\eta_x^2\eta_y^2 + 2b_3\eta_x^2\eta_y^2 \sin^2 \varphi.
\]

(2)

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

\[
\Delta G_{\sigma_{xy}} = \alpha_+\eta_\xi^2 + \alpha_-\eta_\mu^2 + \frac{1}{4}(\eta_\xi^2 + \eta_\mu^2)^2 + (b_2 + b_3)(\eta_\xi^2 - \eta_\mu^2)^2.
\]

(3)

As it was before done, \(\eta_\xi = \eta \sin \chi\) and \(\eta_\mu = \eta \cos \chi\), eqn. (3) takes the form

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

(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 \(\sigma_{xy}\) is non zero, the state with the lowest free energy corresponds to \(b_3 < 0\), phase \(\varphi\) equal to \(\pi/2\), and \(\Psi\) of the form:

\[
(\psi_x, \psi_y) \approx \eta (e^{i\varphi}, e^{-i\varphi}).
\]

(5)
In phase 1 of fig. (2), \( \varphi = 0 \), and as \( T \) is lowered below \( T_{\text{c}_-} \), phase 2, \( \varphi \) grows from 0 to approximately \( \pi/2 \). The two transition temperatures \( T_{\text{c}_+} \) and \( T_{\text{c}_-} \) are obtained to be:

\[
T_{\text{c}_+}(\sigma_{xy}) = T_{c0} - \frac{\sigma_{xy}}{\alpha'} d_{xyxy},
\]

\[
T_{\text{c}_-}(\sigma_{xy}) = T_{c0} + \frac{b}{2 b_3 \alpha} \sigma_{xy} d_{xyxy}.
\]

The derivative of \( T_{\text{c}_+} \) with respect to \( \sigma_{xy} \), and the discontinuity in \( C_{\sigma_{xy}}^+ \) at \( T_{\text{c}_+} \) are respectively:

\[
\frac{dT_{\text{c}_+}}{d\sigma_{xy}} = -\frac{d_{xyxy}}{\alpha'},
\]

\[
\Delta C_{\sigma_{xy}}^+ = -\frac{2 T_{c+} \alpha'^2}{b}.
\]

After applying the Ehrenfest relations the results for \( \Delta \alpha_{\sigma_{xy}} \) and \( \Delta S_{xyxy} \) at \( T_{\text{c}_+} \) are:

\[
\Delta \alpha_{\sigma_{xy}}^+ = -\frac{2 \alpha' d_{xyxy}}{b'},
\]

\[
\Delta S_{xyxy}^+ = -\frac{2 d_{xyxy}^2}{b'b}.
\]

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

\[
\frac{dT_{\text{c}_-}}{d\sigma_{xy}} = \frac{b d_{xyxy}}{2 b_3 \alpha'},
\]

\[
\Delta C_{\sigma_{xy}}^- = -\frac{4 T_{c-} \alpha'^2 b_3}{b b'},
\]

\[
\Delta \alpha_{\sigma_{xy}}^- = \frac{2 \alpha' d_{xyxy}}{b'},
\]

\[
\Delta S_{xyxy}^- = -\frac{d_{xyxy}^2 b}{b'b_3}.
\]

Since for the case of \( \sigma_{xy} \), the derivative of \( T_c \) with respect to \( \sigma_{xy} \) is not defined at zero stress point (see fig.1), the Ehrenfest relations do not hold at \( T_{c0} \). Thus, the discontinuities occurring at \( T_{c0} \), in the absence of \( \sigma_{xy} \), are calculated by adding the expressions obtained for the discontinuities at \( T_{\text{c}_+} \) and \( T_{\text{c}_-} \) in elastic stiffness fig. (3), elastic compliances and
thermal expansion are given by:

\[ \Delta C_{\sigma_{xy}}^0 = -\frac{2 T_c \alpha'^2}{b}, \]  

\[ \Delta S_{xyxy}^0 = -\frac{d_{xyxy}^2}{b_3}, \]  

\[ \Delta \alpha_{\sigma_{xy}}^0 = 0, \]

in this case, there is no discontinuity for the thermal expansion of \( \text{Sr}_2\text{RuO}_4 \) at zero stress.

FIG. 3: Schematic dependence of the elastic constant on the temperature for \( \text{Sr}_2\text{RuO}_4 \). Notice the two jumps in the in plane elastic constant \( C_{xyxy} \) near the transition temperatures \( T_{c+} \) and \( T_{c-} \). The sketch shows two jumps of the same magnitude. This happens for a two component order parameter \( \Psi \).

\( \alpha_{\sigma_{xy}}^0 \) which is another physical feature we previously predicted (see fig.4). Some experimental studies on the changes in the thermal expansion coefficient \( \alpha_i \) below \( T_c \) in HTS reported that an additive lattice jump was found to appear spontaneously at \( T_c \) for a high \( T_c \) compound with one-component order parameter.

Since the phase diagram was determined as a function of \( \sigma_{xy} \), rather than as a function of the shear strain \( \epsilon_{xy} \), (see fig.1), in this work, as in refs. [3, 17], we make use of the 6 \( \times \) 6 elastic compliance matrix \( S \), and also of the full range tensor notation. However, the sound speed measurements \([10, 11]\) are best interpreted in terms of the elastic stiffness tensor \( C \), with matrix elements \( C_{ijkl} \), which is the inverse of \( S \). \([32]\) However, the strain is easier to measure than the stress because fiber optics yields dynamic fidelity of a fraction of a nanostrain \([31]\).

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
FIG. 4: Schematic dependence of the thermal expansion on the temperature for Sr$_2$RuO$_4$. 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 $\Psi$.

transition line we follow $[4]$: $C(T_c+0^+)=C(T_c-0^+)+\Delta C$ and $S(T_c+0^+)=S(T_c-0^+)+\Delta S$, where $0^+$ is positive and infinitesimal. By making use of the fact that $C(T_c+0^+)$ $S(T_c+0^+)$ $= \hat{1}$, where $\hat{1}$ 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, $\Delta S_{xyxy}$ are negative; while $\Delta C_{xyxy}$ are positive.

III. REMARKS

The most noteworthy outcome of this short note is that the observation of a discontinuity in the elastic constant $C_{xyxy}$ $[10, 11]$ is an evidence that the order parameter $\Psi$ in Sr$_2$RuO$_4$ has two components as the theoretical GL analysis predicts. Also the theoretical indicator that the sum of the jumps $\Delta \alpha_{xy}^+ + \Delta \alpha_{xy}^- = 0$ for the in-plane thermal expansion coefficient $[3]$ (see fig.4). Hence, the use of Sr$_2$RuO$_4$ 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$_2$RuO$_4$ experimental measurements the magnitude of the parameters in the Ginzburg-Landau model is complicated $[3]$. 
In the experimental work of the sound velocity measurements \[10, 11\] in \( \text{Sr}_2\text{RuO}_4 \) a discontinuity in the behavior for \( C_{xyxy} \) below \( T_c \), 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 \[3, 10, 24\]. Thus, this set of previous results, and other recent results \[12–15\], considers \( \text{Sr}_2\text{RuO}_4 \) 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.

However, according to Levine \[34\], transversal phonons may have spin equal to one for certain point group symmetries. It could be that it occurs to the \( D_{4h} \) tetragonal group of strontium ruthenate, this could be the key to understand superconductivity and the time-reversal symmetry broken state in \( \text{Sr}_2\text{RuO}_4 \). The possible fact that phonons in the jump observed in the sound transversal mode \( T[100] \) and \( T[110] \) \[10, 11\] have spin equal to one. As a consequence it could be that these symmetry breaking strain or stress fields effects are due the transversal spin waves in certain point group symmetries in metallic solids. Some words about the roll of the magnetic interaction should be added.
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