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THE ROLE OF TRANSVERSE ANISOTROPIC ELASTIC WAVES AND EHRENFEST RELATIONSHIPS IN THE SUPERCONDUCTING STATE OF THE COMPOUND Sr_2RuO_4

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ABSTRACT

In this review, some problems of the unconventional superconductivity in Sr_2RuO_4 are touched. In the strontium ruthenate compound (Sr_2RuO_4), the Ehrenfest relations, the elastic velocity propagation, and ultrasound attenuation find a common point to study elastic lattice effects. This can turn into a new role of the spin and polarization of the transverse phonon fields and their interaction with the conduction electrons in its normal state.

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INTRODUCTION

The physical kinetics (PK) or physics of transport properties (TP) is defined as the science that studies the macro and microscopic transport processes in crystals that are out of thermodynamic equilibrium (Lifshitz and Pitaevskii, 1987). PK is a difficult subject due to its complicated mathematical formalism through the collision integral, or the Green functions. However, the experimental study of low temperature transport properties such as the ultrasound attenuation and electronic heat conduction helps to clarify physical phenomena relevant to superconductivity.

For example, the experimental and theoretical study of the directional ultrasound attenuation below the superconducting temperature (T_c) helps to predict the symmetry properties of the Cooper pair wave function, and the visualization of the nodes in superconducting gap (Pokrovskii and Toponogov, 1961). Additionally, the electronic thermal conductivity accounts for the physics present in superconductors at ultra-low temperatures, such as the relationship between nonmagnetic impurities and superconductivity, allowing to predict whether the superconductor crystal is in Bohr or unit scattering limit as T approaches absolute zero (Griffin, 1965; Hirschfeld *et al*., 1988).

Finally, the Ehrenfest thermodynamic relations, namely the thermal expansion, the specific heat, and the isothermal compressibility are a powerful tool in the study of second-order phase transitions at T_c. Ehrenfest thermodynamic relations occur for example, in the second order transition to superconductivity and ferromagnetism (Landau and Lifshitz, 1980; Walker, 1980). Therefore, in the discussion section of this paper, we will make a brief review of results obtained thanks to the ER and the ultrasound attenuation in the compound Sr_2RuO_4 for a particular model (Walker and Contreras, 2002; Contreras *et al*., 2004; Contreras, 2011; Contreras *et al*., 2016).

Recently, novel experimental and theoretical advances continue to be achieved in the prediction of the broken time-reversal symmetry state. These studies are useful in order to explain the mechanism of superconductivity in this compound (Benhabib *et al*., 2020; Ghosh *et al*., 2020).

In the last section, it is briefly proposed to carry out certain theoretical studies related to three phenomena. First, the propagation of the transverse elastic phonons and their spin in the normal state of Sr_2RuO_4 is touched. Second, the elastic polarization is also discussed. Third, the interaction between the transverse phonons and the conduction electrons at T_c is also treated. These studies could give unexpected results inherent to the propagation, and attenuation of transverse elastic waves by conduction electrons, in compounds with anisotropic lattices such as strontium ruthenate. Let's discuss the subject.

DISCUSSION

The strontium ruthenate crystal (Sr_2RuO_4) has a body-centered tetragonal lattice (D_{4h}) with a layered square structure, according to the lattice shown in Figure 1. In its normal state, it is described by a Fermi liquid, with three metallic conduction sheets. Therefore, the Fermi surface (FS) is composed of three sheets called the α, β, and γ sheets (MacKenzie and Maeno, 2003).

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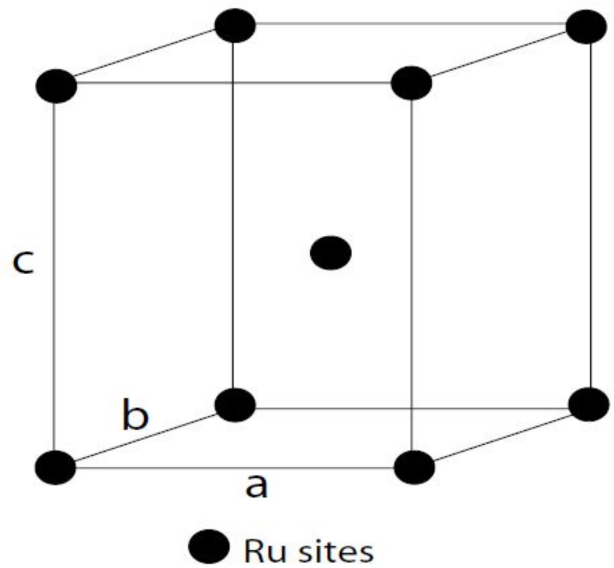

Fig. 1. The body centered tetragonal structure corresponding to an elementary cell of Sr_2RuO_4. Both vectors **a** and **b** are of equal magnitude, the ruthenium atoms are shown at the sites of the 3D lattice.

Sr_2RuO_4 is an unconventional superconductor with $T_c \approx$ 1.5 K. T_c strongly depends on the non-magnetic impurities in the crystal, in addition, it presents some intriguing superconducting properties. For example, temperature power laws were observed in transport experiments measuring the attenuation of phonons by electrons and the electronic heat conductivity. Therefore, from the beginning, it was proposed that Sr_2RuO_4 is an unconventional superconductor (Maeno *et al*., 1994; Rice and Sigrist, 1995; Maeno *et al*., 2001; Wysokinski *et al*., 2003; Liu and Mao, 2015; Yarzhemsky, 2018) with some type of superconducting nodes.

Additionally, a series of theoretical and experimental works proposed the existence of a superconducting gap in the triplet state (Ishida *et al*., 1998; Luke *et al*., 1998; Duffy *et al*., 2000; Tanatar *et al*., 2001) with linear or point nodes, or a combination of them (called accidental nodes) in different sheets of its Fermi surface. A triplet superconductor is defined as a superconductor where the electrons in the Cooper pairs are bound in spin triplets. Spin triplets can have spins parallel to one another rather than antiparallel to one another. In triplet superconductors, the order parameter is represented by a three-dimensional vector.

Moreover, according to several authors, in Sr_2RuO_4 the symmetry of the superconducting gap structure is a state of broken time inversion symmetry, with a point symmetry, that transforms as the irreducible two-dimensional representation E_{2u} of the tetragonal point group (see Table 1). Although many authors considered that the γ sheet of the FS does not have nodes, these works provided experimental agreements with the specific heat $C(T)$, with the electronic heat transport experiments $\kappa_i(T)$, and with the measurements of directional ultrasound $\alpha_j(T)$.

Therefore, all the works indicated in their time, the existence of some type of nodes in addition to the time symmetry breaking state in the Cooper pair wave function. MacKenzie and Maeno (2003) provided a literature review of all the works performed during that period of time. In particular, experimental and theoretical ultrasound studies at low temperatures showed the need for an anisotropic electron-phonon interaction in order to fit the experimental results (Lupien *et al*., 2001; Lupien, 2002; Walker *et al*., 2001; Wu and Joynt, 2001; Contreras *et al*., 2004; Nomura, 2005). This anisotropy was shown to be inherent to the layered square-lattice structure. Therefore, employing an anisotropic tight-binding model, it was shown (Contreras *et al*., 2004) that in strontium ruthenate, different "accidental" superconducting nodes correspond to different sheets of the FS.

Using ultrasound fits, it was found for that the γ band has 8 point nodes symmetrically distributed in the {100} planes, and 8 point nodes symmetrically distributed in the {110} planes. For the α and/or β bands, were found 8 point nodes symmetrically distributed in the {100} planes, and 8 point nodes symmetrically distributed in the {110} planes.

Also, it was found that the nodal structure of the α/β sheets is different from the γ band. The gap on a line along the Fermi surface for α/β bands is an order of magnitude smaller than that on the γ band (see Fig. 2). Furthermore, the exceptionally strong anisotropy in the attenuation of certain modes, which is unique to this material, allowed us to associate the attenuation of the most strongly attenuated modes with their interaction with electrons in the γ band. Finally, we found that this "accidental" nodal model satisfies the two-dimensional E irrepresentation for the triplet state superconducting gap (see Table 1 and Fig. 2).

In the normal state of Sr_2RuO_4, it was shown that to explain the weakness in the attenuation present in the γ sheet of the FS, the same model yielded the necessary results, since the transverse elastic waves T [100] do not stretch the nearest neighboring bonds. However, they do stretch the second bonds between neighboring atoms (Walker *et al*., 2001).

In recent years, new experimental studies were performed. They took into account the uniaxial elastic tension in order to determine the gap, and also the time symmetry broken state (Hicks *et al*., 2014; Taniguchi *et al*., 2015; Steppke *et al*., 2017).

Table 1. The irreducible basis functions in a tight binding model for the *z* component of a triplet order parameter in a D_4 tetragonal lattice (Contreras, 2006).

Irrepresentation	In plane basis functions	Body-centered basis functions
A_1	×	$\cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_y b}{2}\right)\sin\left(\frac{k_z c}{2}\right)$
A_2	×	×
B_1	×	×
B_2	×	$\sin\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_y b}{2}\right)\sin\left(\frac{k_z c}{2}\right)$
E	$E_{x1} = \sin(k_x a)$ $E_{y1} = \sin(k_y a)$	$E_{x2} = \sin\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_y b}{2}\right)\cos\left(\frac{k_z c}{2}\right)$ $E_{y2} = \cos\left(\frac{k_x a}{2}\right)\sin\left(\frac{k_y b}{2}\right)\cos\left(\frac{k_z c}{2}\right)$

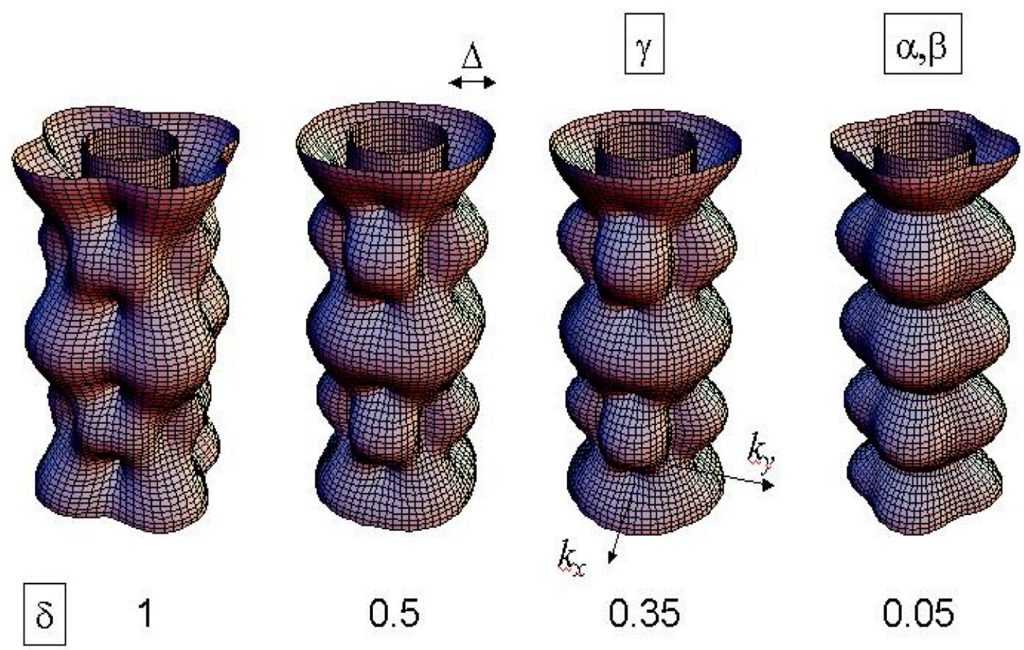

Fig. 2. The anisotropic superconducting triplet gap for Sr_2RuO_4, according to the model with accidental nodes, and which belongs to a gap with E_{2u} body centered basis functions of the point group D_{4h} in a tetragonal crystal (Contreras *et al*., 2004; Contreras, 2006).

In that direction, it is possible to point out two novel analysis of the jump at the transition temperature to the superconducting state (T_c) in the elastic constant C_{66}. It can measure the transverse elastic propagation velocity polarized in the direction [010] (Lupien, 2002; Benhabib *et al*., 2020; Ghosh *et al*., 2020) which expand the studies behavior of the sound velocity at the normal-to-superconducting phase previously developed, see also in Benhabib *et al*. (2020). Jump in the c_{66} shear modulus at the superconducting transition of Sr_2RuO_4: Evidence for a two-component order parameter. arXiv:2002.05916v1).

To complete the picture here, Table 1 lists a theoretical classification of the in-plane and body centered basis functions for a D_4 lattice, (I will use the group D_4 instead of the group D_{4h}. This is possible because the d-vector is an odd function of momentum and the inversion symmetry is already contained in its general form) with the superconducting singlet and 3D triplet states (Contreras, 2006). The irreducible representation *E* is the one that accounts for the triplet state that breaks the time inversion symmetry.

2002) and that took into account the role of the transverse elastic tension using the Ginzburg-Landau theory (Walker *et al*., 2001; Sigrist, 2002; Contreras *et al*., 2016). These

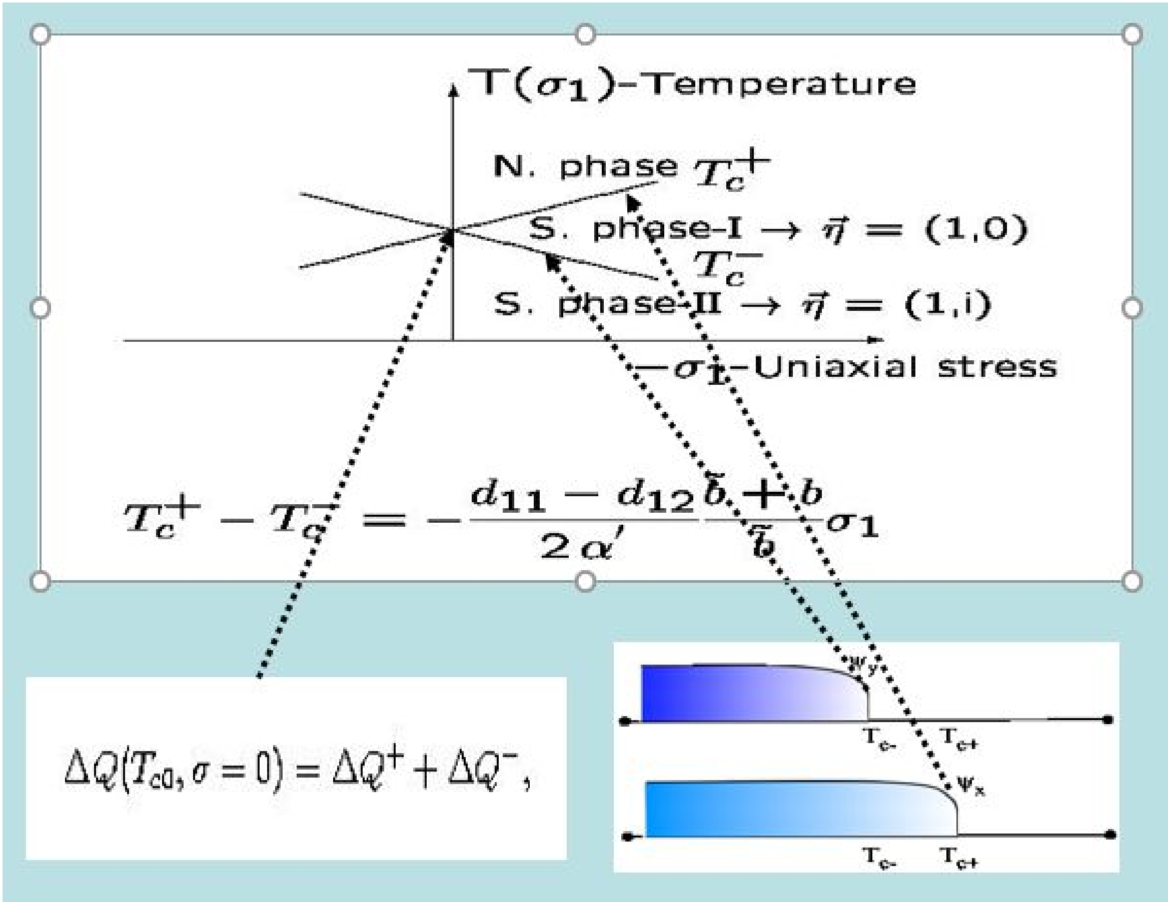

Fig. 3. The phase diagram according to the Ehrenfest relationships for elastic stress at temperatures T_c, 0, T_{c+}, and T_{c-} for a tetragonal crystal (Contreras, 2006).

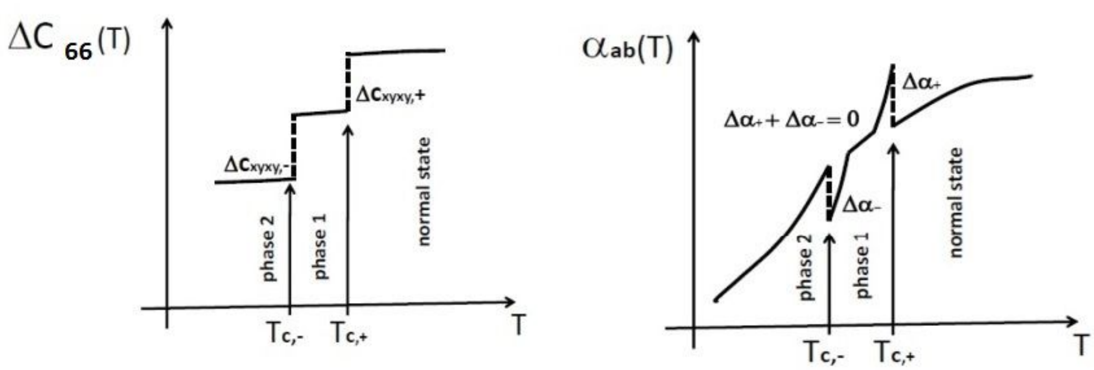

Fig. 4. The jumps the elastic constants C_{66} and in the thermal expansion $\alpha_i(T)$ at the temperatures T_{c+} and T_{c-} for an anisotropic crystal of D_{4h} symmetry. Note that the model predicts zero thermal expansion at the temperature T_c (Contreras and Moreno, 2019).

In the same order of ideas, and in order to account for the time symmetry broken state, it was necessary to propose Ehrenfest relationships capable of predicting the jump in the elastic tensor C_{66} observed experimentally (Lupien, studies allowed the construction of a phase diagram of the compound based on three states: the normal state, the BCS-type singlet state (not seen experimentally yet) and a triplet state (see in Fig. 3 for details).

It is necessary to clarify that to reach the singlet state experimentally, elastic stress different from zero must be applied, capable of splitting the transition temperature into two temperatures, according to the diagram shown in Figure 3, since the effect of an external uniaxial stress on the basal plane of Sr_2Ru0_4 is to break the tetragonal symmetry of the crystal. As a consequence of this, when a second order phase transition to the superconducting state occurs, it splits into two transitions.

In this way, the three quantities calculated using the modified Erenhfest relations can be described in a phase diagram. Experimentally this condition for elastic uniaxial stress is given by $|\sigma_6(T)| << 1$ in agreement with the phase diagram shown in Figure 3. For example, an additional result that is very little discussed in the literature is that the thermal expansion due to this type of jumps is zero for zero elastic stress (Walker and Contreras, 2002). This is shown in Figure 4.

Therefore, for this part, we conclude that the experimental and theoretical studies mentioned above show that strontium ruthenate is a compound in which an elastic external uniaxial field splits T_c, thanks to the interaction of the transverse elastic waves with the Cooper pairs (Fig. 3). This leads to a gap corresponding to a time reversal symmetry broken state.

Additionally, the study of ultrasound attenuation allowed visualizing the position of the nodes of the superconducting gap using an "accidental" nodes model shown in Figure 2. These point nodes are "accidental" in the sense that they are not required by symmetry but exist only if the material parameters have values in a certain range. Also, these point nodes will degenerate into the line nodes discussed by previous authors. This interpretation led to the determination of a superconducting gap model with different nodal structures on different bands, based on directional ultrasound experiments.

Additional notes

In this note, it is proposed to consider additional theoretical studies in the normal state of Sr_2RuO_4 aiming to expand the knowledge about the role of the polarization of the transverse elastic waves and their interaction with the conduction electrons. These studies would be mostly related to the polarization and the value of the spin of the elastic transverse waves in the mentioned compound.

I start mentioning that due to the need for different approximations of the electron-phonon interaction in different sheets of the Fermi surface, it is clear that the anisotropic electron phonon interaction plays a fundamental role in this compound. It is known for example that only the second neighbors describe the electron-phonon interaction in the transverse direction [010] for elastic waves propagating along [100] direction.

Additionally, in Sr_2RuO_4 the stiffness C_{66} is related to the speed of the elastic transverse wave V_s [100] with polarization direction [010] (Lupien, 2002; Paglione *et al*., 2002). Hereby, it is concluded that Sr_2RuO_4 is a strong candidate to study microscopic phenomena inherent to transversal elastic waves propagation such as the transversal phonon spin value. However, in order to extend any microscopic study of transverse phonons, a second quantization of the elastic field is necessary.

This theoretical program was initially carried out by Vonsovskii and Svirskii (1961) and Levine (1962), see also discussion in Kittel (1958) who showed that for transverse elastic waves in isotropic elastic media, the spin of the phonons is equal to $\pm$ 1 (depending on the polarization of the wave) unlike longitudinal waves which have zero spin value. Therefore, a second quantization program of the elastic field in a tetragonal lattice based on the formalism of the phonon creation and annihilation operators might show that the spin of the transverse waves has an integer value of $\pm$ 1.

Furthermore, in Sr_2RuO_4 there is the breaking of the time inversion symmetry due to the change in velocity of the elastic transverse wave that propagates in the [100] direction with polarization in the [010] direction at T_c, and a transverse spin phonon value of $\pm$ 1. It is worth thinking about.

Additionally, in another order of ideas, a new theory has recently been formulated by Grechka (2020) where the classic Christoffel equation (Musgrave, 1970) is solved in the polarization variables. This finding makes it possible to study the polarization fields due to the propagation of elastic waves for homogeneous anisotropic media. Solving for the slowness vectors (the inverse of the propagation velocity) of the plane waves corresponding to a given polarization, unexpectedly, Grechka found a subset of triclinic solids in which the polarization field contains holes; showing that there are solid angles of finite size with polarization directions unattainable for any plane wave, depending on the value of the elastic constants. Henceforth, the study of the polarization for elastic fields in tetragonal media such as Sr_2RuO_4 can be remarkable.

Finally, a theoretical microscopic study of the change in speed of the transverse elastic waves in a system with tetragonal symmetry such as Sr_2RuO_4 at T_c could be also stunning. For example, the calculation of the real part of the phononic polarization operator would potentially elucidate, if there are singularities in the energy spectrum of the transverse elastic phonon field at T_c. For studies on other compounds, see in Kulik (1963) and Vaskin and Demikhovskii (1968).

CONCLUSION

The phenomenon of superconductivity, particular the unconventional superconductivity in Sr_2RuO_4 was of a great interest for theoreticians and experimentalists during the last century. It is obvious that this century researches will also focus on this phenomenon. Therefore, this short discussion has touched some aspects of the problem, it might be worth exploring.

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