Anisotropic Phonon-Limited Transport in Sr_2RuO_4 from First Principles

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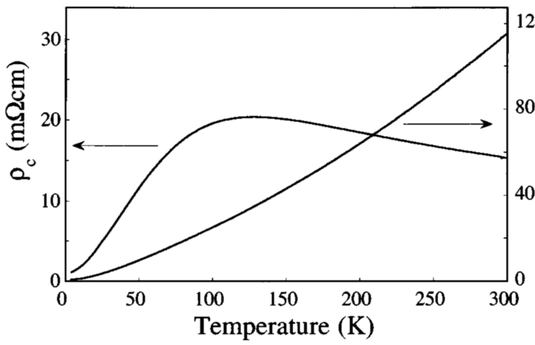
Sr_2RuO_4's Strange Behavior

Sr_2RuO_4 is an unconventional superconductor with $T_c = 1.5$K and is isostructural to the cuprate superconductor LSCO. Though it was exhaustively studied experimentally, computationally and theoretically, it's superconducting gap symmetry is still debated[1].

A peculiar property of Sr_2RuO_4's normal state is its resistivity in function of T. So far, no one can explain its behavior. We'd like to shed light on this phenomenon by using first principles calculations.



Sr_2RuO_4's experimental resistivity[2].

Theoretical Framework

We concentrate on phonon-limited resistivity from first principles approaches. A standard way to compute the resistivity of metals is by using the Ziman's resistivity formula:

$$\rho(T) = \frac{4\pi m_e}{n_c\, e^2 k_B T} \int_0^\infty d\omega \hbar\omega \alpha^2_{\text{tr}} F(\omega) n_B[1 + n_B].$$

Despite giving good results in simple metals[3], this formula is not appropriate for Sr_2RuO_4 because:

- it is an isotropic formula (Sr_2RuO_4 is BCT);
- it is only valid for spherical Fermi surfaces (Sr_2RuO_4 bears three quasi-cylindrical distinct Fermi sheets);
- it has an undefined parameter n_c which is the carrier density.

IBTE Formalism

Our approach uses instead the state-of-the-art **I**terative **B**oltzmann **T**ransport **E**quation formalism which yielded promising results in semiconductors[4]. In this formalism, the current is:

$$\boldsymbol{J} = -\frac{e}{\Omega}\sum_n \int \frac{d^3\boldsymbol{k}}{\Omega_{BZ}} f_{n\boldsymbol{k}}(T, \boldsymbol{E}) \boldsymbol{v}_{n\boldsymbol{k}}.$$

Assuming Ohm's law, the conductivity tensor is derived from the current:

$$\sigma_{ij}(T) = \frac{\partial J_i}{\partial E_j}\bigg|_{\boldsymbol{E}=0} = -e\sum_n \int_{\Omega_{\text{BZ}}} \frac{d^3\boldsymbol{k}}{(2\pi)^3} v^i_{n\boldsymbol{k}} \partial_{E_j} f_{n\boldsymbol{k}}.$$

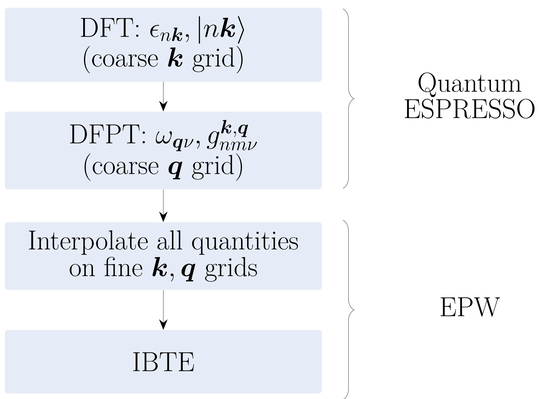
Then, we compute $\partial_{E_j} f_{n\boldsymbol{k}}$ from the BTE assuming only electron-phonon (EPH) interactions:

$$\partial_{E_j} f_{n\boldsymbol{k}} = e\frac{\partial f^0_{n\boldsymbol{k}}}{\partial \epsilon_{n\boldsymbol{k}}} v^j_{n\boldsymbol{k}} \tau^0_{n\boldsymbol{k}} + \frac{2\pi\tau^0_{n\boldsymbol{k}}}{\hbar}\sum_{m\nu}\int \frac{d^3\boldsymbol{q}}{\Omega_{BZ}} |g^{\boldsymbol{k},\boldsymbol{q}}_{mn\nu}|^2 W^{\boldsymbol{k},\boldsymbol{q}}_{nm\nu}\, \partial_{E_j} f_{m\boldsymbol{k}+\boldsymbol{q}}\,.$$

Advantages and Disadvantages:

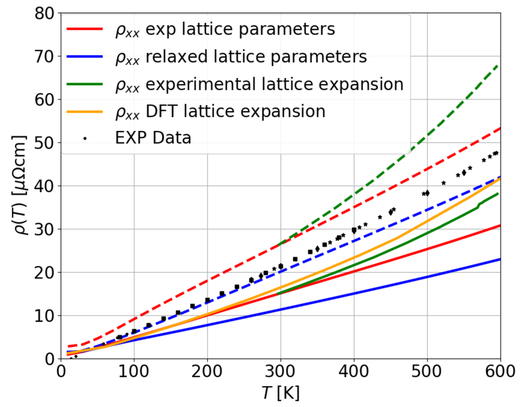
- ☑ less approximations;
- ☑ does not rely on arbitrary parameters;
- ☑ in principles, can integrate more interactions (electron-electron, electron-defects, $\mathbf{B} \neq 0$, etc.);
- ☒ implicit equation ⇒ iterative solution;
- ☒ requires very high $\mathbf{k}$ and $\mathbf{q}$ resolution to converge;
- ☒ semi-classical (because of the BTE);

Computational Scheme

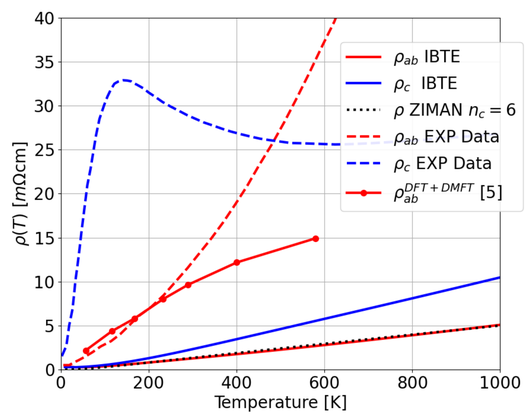


Results

Testing IBTE in Pb seems to give a correct behavior in function of T. Results are close to experimental but not quite the same. Lattice parameters seem to have a big effect. Thus, we explored IBTE with lattice thermal expansion. It turns out it brings a lot of non-linearity at high temperature.



IBTE results in Pb vs experiments. Dashed curves include SOC.



Resistivity of Sr_2RuO_4 in function of temperature. In-plane resistivity ρ_{ab} enhanced by a factor of 100.

From these results, EPH interactions does not seem sufficient to explain the strange resistivity behavior of Sr_2RuO_4. Despite this, IBTE correctly displayed strong anisotropy.

Conclusion

- Resistivity calculations in metals seem sensitive to lattice parameters;
- EPH interactions don't seem sufficient to explain Sr_2RuO_4's properties;

Outlook:

- Including electron correlations (DFT+DMFT) could improve results.
- Test of IBTE scheme in other anisotropic metals (Mg, Zn, Cd, etc.).

References

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