Mesoscopic Transport in High Temperature Superconductors

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Preface

Mesoscopic Transport in High Temperature Superconductors is specifically written in order to show how simplistic electron transport equations can be used to describe complex HTS phenomena. My goal when writing on high temperature superconductivity is to lean as much as possible about the basics of HTS and solve a variety of electron transport problems. I have consulted several texts in an effort to look at the different pathways that are used when solving for useful quantities such as Pairon densities and coherent lengths.

In order to make sure that I learned something in each chapter, I tried to see if I could use the derived formulae to solve for quantities by looking up properties that could be measured. Thus in each chapter there will be at least one problem worked out causing this text to take on a tutorial approach. A discussion section at the end of each chapter also is included to help reinforce what was learned. This work is broken up into 5 chapters covering the basic foundation of superconductivity with BCS theory through the future of HTS and applications. I have included references to texts and journals that I found useful when writing this work as well as a bibliography that describes how each text was helpful.

Jordan Pommerenck

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Chapter 1

History and Properties of Superconductors

Superconductors display a variety of unique behavior that cannot be described accurately by an independent electron approximation (used to solve the otherwise intractable Hamiltonian in equation (1.1) [1-3].

$$H = -\frac{\hbar^2}{2m}\nabla_1^2 - \frac{2e^2}{4\pi\epsilon_0 r_1} - \frac{\hbar^2}{2m}\nabla_2^2 - \frac{2e^2}{4\pi\epsilon_0 r_2} + \frac{1}{2}\frac{e^2}{4\pi\epsilon_0 r_1} \tag{1.1}$$

Some of the properties that can be observed include no measureable DC resistance, perfect diamagnetism, and energy gap of width 2Δ centered about the Fermi energy. These properties motivated the need for theory that would accurately describe the superconductor system. In the 1950s, Bardeen, Cooper, and Schrieffer formulated a Hamiltonian describing the superconducting system for which they later shared the Nobel Prize. The important result from BCS theory is the relationship between the energy gap at 0 Kelvin and the critical temperature. The critical temperature is the temperature above which the bulk metal behaves normally but below which the material shows superconducting behavior.

$$2\Delta(T=0) = 3.53 k_B T_c \tag{1.2}$$

But all was not well with the theory. The BCS Hamiltonian needed a discussion of the band structure of electrons if the question of which metals are superconductors is to be answered. Generalized BCS theory helped resolve this. Around the same time that BCS was developed, Cooper and Schrieffer arrived at another independent relation for the critical temperature from (1.2) [6]. While electrons are fermions, Pairons are composed of a pair of electrons that move as a boson. A composite particles motion is either fermionic or bosonic if it contains odd or even integer numbers of fermions respectively. Pairons moving in 3D were shown to have an energy momentum relation given by:

$$\varepsilon_q = \frac{1}{2}\nu_F q + \omega_0, \quad \nu_F \equiv \left(\frac{2\varepsilon_F}{m^*}\right)^{1/2} \tag{1.3}$$

The ground state energy in equation (1.3) is given by ω_0. The critical temperature for free Pairons was also found for both 2D and 3D crystals.

$$T_c = 1.01\hbar k_B^{-1}\nu_F n_{3D}^{1/3}, \qquad T_c = 1.24\hbar k_B^{-1}\nu_F n_{2D}^{1/2} \tag{1.4}$$

Both of these expressions (1.2) and (1.4) are in good agreement. The zero temperature BCS coherence length helps to determine the Pairon size.

$$\xi_0 = \frac{\hbar v_F}{\pi\Delta} = 0.18\frac{\hbar v}{k_B T_c} \tag{1.5}$$

We can finally solve for the interpairon distance r_0 by arranging equation (1.4) for number density of the bosons [6].

$$r_0 \equiv n^{-1/3} = 1.01\frac{\hbar v_F}{k_B T_c} = 5.61\xi_0 \tag{1.6}$$

The utility of these formulae can be seen in the ability to determine Pairon density and Fermi velocity by measuring the critical temperature and coherence length. A novel instructional example homework problem is shown below:

<u>Example Problem 1</u>: Find the 2D Pairon density and Fermi velocity for Yttrium Barium Copper Oxide (YBCO).

The critical temperature and coherence length for YBCO can be looked up on Wikipedia. The critical temperature is around 93 Kelvin. The coherence length is different for along the crystal axis but is given $\xi_0^{ab} \approx 2\,\text{nm}$ and $\xi_0^{c} \approx 0.4\,\text{nm}$. We can now calculate the Fermi Velocity and the Pairon density.

$$\begin{gathered} \xi_0 = \frac{\hbar v_F}{\pi\Delta} = \frac{\hbar v_F}{\pi\left(3.53 k_B T_c\right)} = \frac{\hbar v_F}{\pi\left(3.53 k_B\left(93\,\text{K}\right)\right)} = 20\,\mathring{\text{A}} \\ n^{-1/2} = 1.24\frac{\hbar v_F}{k_B T_c} = 1.24\frac{\hbar v_F}{k_B\left(93\,\text{K}\right)} \end{gathered} \tag{1.7}$$

We can solve these equations simultaneously for the Fermi Velocity and the Pairon density.

$$\boxed{\begin{gathered} v_F \approx 270.1\,\text{km/s} = 2.7\cdot 10^7\ \text{cm/s} \\ n_{2D} \approx 2.44\cdot 10^{10}\ \text{cm}^{-2} \end{gathered}} \tag{1.8}$$

Both of these numbers are reasonable after comparing with values from the literature. □

Discussion

We have learned about basic properties of semiconductors and have gone from an independent electron Hamiltonian to a generalized BCS Hamiltonian to describe our superconducting system. We have learned how to calculate electron transport system specific properties by knowing the critical temperature and the coherence length.

Chapter 2

Type I and II Superconductor Properties

In the last chapter, we discussed type I superconductors. Now we will explore the properties of type II superconductors [1-3]. Compound superconductors have type II magnetic behavior, that is, they form magnetic vortices below a critical temperature and for a critical magnetic field. Type II allows partial penetration of magnetic field below the critical temperature while a type I repels the field. What parameter determines whether a superconductor is type I or II? The coherence length depends on the penetration depth is the answer to this question.

$$\xi > 2^{1/2}\lambda \quad (\text{type }\mathbf{I}), \qquad \xi < 2^{1/2}\lambda \quad (\text{type }\mathbf{II}) \tag{2.1}$$

The coherence length and the penetration depth depend on the material in question, as well, as the temperature and the concentration of impurities. The London penetration depth can be found using the formula:

$$\lambda_L = \left(\frac{m_e}{\mu_0 n q^2}\right)^{1/2} \tag{2.2}$$

Aluminum is a type I superconductor with a critical temperature of 1.2 K. A novel instructional example homework problem that demonstrates Aluminum is indeed type I is shown below:

<u>Example Problem 2</u>: Estimate the London penetration depth of Aluminum and determine the coherence length in order to determine whether Aluminum is a type I or II superconductor.

The number density for Aluminum can be calculated by knowing the lattice constant. The London penetration depth is then easily calculated.

$$\begin{gathered} n \approx \frac{4}{d^3} = \frac{4}{\left(4.050\ \mathring{A}\right)} = 6.02\cdot 10^{28}\ \text{m}^{-3} \\ \lambda_L = \left(\frac{m_e}{\mu_0 n q^2}\right)^{1/2} \approx \left(\frac{10^{-31}}{10^{-6}10^{28}\left(10^{-19}\right)^2}\right)^{1/2} \approx 21.69\ \text{nm} \end{gathered} \tag{2.3}$$

We can estimate the Fermi velocity at about $2\cdot 10^6$ m/s. We can now calculate the coherent length based off of equation (1.7). This gives us the following for the coherent length:

$$\xi_0 = \frac{\hbar \nu_F}{\pi \Delta} = \frac{\hbar \nu_F}{\pi\left(3.53 k_B T_c\right)} = \frac{\hbar\left(2 \cdot 10^6 \text{ m/s}\right)}{\pi\left(3.53 k_B\left(1.2 \text{ K}\right)\right)} \approx 1148 \text{ nm} \tag{2.4}$$

We can compare these to the actual values of 16 nm and 1600 nm for the penetration depth and coherent length respectively.

$$\boxed{\frac{\xi_0}{\lambda_L} = \frac{1148 \text{ nm}}{21.69 \text{ nm}} = 52.92 > 2^{1/2}, \quad \left(\text{type } \mathbf{I}\right)} \tag{2.5}$$

This is quite reasonable and matches up with what is known for Aluminum. □

Discussion

We have learned about type I and II superconductors and their properties. The type of superconductor can be determined by knowing the coherence length and the penetration depth. We have learned how to calculate whether a superconductor is type I or II based off of the penetration depth and coherence length.

Chapter 3

Electron Transport in HTS

We now turn our attention to high temperature superconductors, that is, superconductors with an unusually high temperature critical point such as $La_{2-x}Sr_xCuO_4$ which has a critical temperature of 38 Kelvin. We are interested in the electron transport properties around the critical temperature such as resistivity. Also, we will look at the Seebeck coefficient for HTSs. Above the critical temperature, optimally doped superconductors show linear dependence on the temperature while overdoped superconductors display quadratic dependence on the temperature. Starting from the Drude-Sommerfeld model, we can write the conductivity in terms of a scattering rate. We will define n_1 and n_2 as hole densities [6].

$$\sigma_1 = \frac{n_1 e^2 \tau_1}{m_1} = \frac{n_1 e^2}{m_1}\left(\frac{1}{\gamma_1}\right), \qquad \gamma_1 = n_{ph} \nu_F S_1 \tag{3.1}$$

In equation (3.1), S_1 is the scattering diameter. The number phonon density can be calculated if the acoustic phonon energies are small compared to $k_B T$.

$$n_{ph} = \frac{n_a}{\exp\left(\alpha_0 \hbar\omega_D / k_B T\right) - 1} \approx n_a \frac{k_B T}{\alpha_0 \hbar\omega_D}, \qquad n_a = \left(\frac{1}{2\pi}\right)^2 \int d^2 k \tag{3.2}$$

We have assumed that the parameter $\alpha_0 \approx 0.20$. Now we can solve by substituting (3.2) into (3.1) to obtain the following equation:

$$\boxed{\begin{gathered} \sigma_1 = \frac{n_1 e^2}{m_1}\left(\frac{1}{n_{ph} \nu_F S_1}\right) = \frac{n_1 e^2}{m_1}\left(\frac{1}{n_a \dfrac{k_B T}{\alpha_0 \hbar\omega_D} \nu_F S_1}\right) = C_1 \frac{n_1 e^2}{T}, \quad C_1 = \frac{\alpha_0 \hbar\omega_D}{n_a m_1 k_B \nu_F S_1} \\ \rho_1 = \frac{1}{C_1}\frac{T}{n_1 e^2} \end{gathered}} \tag{3.3}$$

Now for an overdoped system we consider a positively charged Pairon $+2e$ and a linear dispersion relation. Using Newton's Law of motion, we can write the following:

$$F = m\frac{d}{dt}\nu_x = \frac{mc^2}{c^2}\frac{d}{dt}\nu_x = \frac{pc}{c^2}\frac{d}{dt}\nu_x = \frac{\varepsilon}{c^2}\frac{d}{dt}\nu_x = 2eE, \quad \varepsilon \equiv pc \tag{3.4}$$

We can solve this differential equation with τ_2 being the Pairon mean free time and do a thermal average to obtain the following:

$$\nu_2^d = 2ec^2\tau_2 E\left\langle \varepsilon^{-1} \right\rangle \tag{3.5}$$

Now we can write the conductivity using Ohm's law:

$$\sigma_2 = \frac{n_2 (2e)\nu_2^d}{E} = \left(2n_2 e\right) 2ec^2 \tau_2 \left\langle \varepsilon^{-1} \right\rangle = \left(2e\right)^2 c^2 \left\langle \varepsilon^{-1} \right\rangle n_2 \gamma_2^{-1}, \quad \gamma_2 \equiv \tau_2^{-1} \tag{3.6}$$

We can then use the Equipartition theorem claiming that the total kinetic energy is shared equally among the constituent parts.

$$\boxed{\begin{gathered} \left\langle \varepsilon \right\rangle = k_B T, \qquad \sigma_2 = \frac{\left(2e\right)^2 c^2 n_2}{k_B T \gamma_2} = \frac{2e^2 C_2 n_2}{T^2}, \qquad C_2 \equiv \frac{8}{\pi^2}\frac{\alpha_0 \hbar\omega_D \nu_F}{n_a k_B^2 S_2} \\ \rho_2 = \frac{T^2}{2e^2 C_2 n_2} \end{gathered}} \tag{3.7}$$

We have now found the conductivity in both cases and the total conductivity is equal to the sum.

$$\rho = \frac{1}{\sigma} = \frac{1}{\sigma_1 + \sigma_2} = \frac{T^2}{e^2 \left(C_1 n_1 T + 2C_2 n_2 \right)} \tag{3.8}$$

Thus, the resistivity dependence on temperature correlates with the doping concentration. □

<u>Discussion</u>

After the critical temperature (before which the resistivity is equal to zero), the resistivity dependence can be found using the Drude-Sommerfeld model. The dependence will be either linear or quadratic depending on the doping concentrations. Quadratic dependence occurs for highly overdoped samples indicating that $C_2 n_2 \gg C_1 n_1$. The other regime gives linear temperature dependence.

Chapter 4

The Seebeck Effect in HTS

We will now discuss the Seebeck effect. This effect explains the conversion thermal gradients into a current density. Our discussion will begin with the Seebeck Coefficient (thermopower) which depends on material properties [1], [3], [6].

For a metal we can write classically

$$\mathbf{j} = \sigma\left(-\nabla V\right) + A\left(-\nabla T\right) = \sigma \mathbf{E} - A\nabla T \tag{4.1}$$

For a metal rod, with a thermal gradient between the ends, no current will flow. Mathematically this is given as:

$$\sigma \mathbf{E}_q - A\nabla T = 0, \qquad \mathbf{E}_q = Q\nabla T, \qquad Q \equiv \frac{A}{\sigma} \tag{4.2}$$

We have defined Q as the Seebeck coefficient or thermopower. The Seebeck Coefficient can be related to the specific heat capacity. Classically $c_V = 3nk_B/2$ and for a statistical Fermi heat capacity $c_V = \left(\pi^2/3\right)k_B^2 T N_0$.

$$Q_{classical} = -\frac{k_B}{2e} = -0.43 \cdot 10^{-4}\,\frac{V}{K}, \qquad Q_{Fermi} = -\frac{\pi^2}{3}\frac{k_B}{2e}\left(\frac{k_B T}{\varepsilon_F}\right) \tag{4.3}$$

In order to gain some physical insight into the range of statistical Fermi Seebeck coefficients let us examine a specific case.

Example Problem 3: Estimate the Seebeck coefficient for Bismuth. What is the Seebeck Coefficient for Copper? Compare with experimental measurements.

The Fermi energy for Bismuth is about 9.90 eV. Also, we must remember to make this calculation relative to Platinum in order to compare with measured results. At room temperature Platinum is about $-5\,\mu\mathrm{V/K}$.

$$Q_{F,\mathrm{Bismuth}} = -\frac{\pi^2}{3}\frac{k_B}{2e}\left(\frac{k_B T}{\varepsilon_F}\right) \approx -36.8\,\mu\mathrm{V/K} + 5\,\mu\mathrm{V/K} = -31.8\,\mu\mathrm{V/K} \tag{4.4}$$

Bismuth at room temperature is about $-72\,\mu\mathrm{V/K}$. We are then off by about a factor of two from the measured value, but the sign is correct. Now for copper we have a Fermi energy of about 7 eV.

$$Q_{F,\mathrm{Copper}} = -\frac{\pi^2}{3}\frac{k_B}{2e}\left(\frac{k_B T}{\varepsilon_F}\right) \approx -52.0\,\mu\mathrm{V/K} + 5\,\mu\mathrm{V/K} = -47.0\,\mu\mathrm{V/K} \tag{4.5}$$

Copper at room temperature is about $6.5\,\mu\mathrm{V/K}$. The theory clearly does not accurately predict a sign change for various materials. The classical and even semi-quantum theory introduced so far made assumptions about the Fermi degeneracy and chemical potential being independent of temperature. Also, the sign cannot account for positive Seebeck coefficients. Ashcroft and Mermin attempt to correct this in equation [13.62] in their classical text, but the formula is difficult to use because of the tensor in [13.65] denoted $\mathcal{M}$! We shall therefore follow a derivation by Fujita and Godoy [6] that yields a more easily applied result. Let us begin by writing the thermally excited electron number density:

$$N_{ex} \equiv \int_{\varepsilon_F}^{\infty} d\varepsilon \mathrm{Dos}(\varepsilon)\frac{1}{\exp(\beta(\varepsilon-\mu))+1} = k_B T\,\mathrm{Dos}(\varepsilon_F)\ln(2), \qquad n \equiv N_{ex}/V \tag{4.6}$$

Now we will use Fick's law of diffusion to write the following where D is the diffusion coefficient and d is the dimensionality in this case equal to 2.

$$\mathbf{j} = q\,\mathbf{j}_{\mathrm{particle}} = -qD\nabla n = -q\left(\frac{\nu\ell}{d}\right)\nabla n = -q\left(\frac{\nu_F^2\tau}{d}\right)\nabla n \tag{4.7}$$

We can use equation (4.6) and take the gradient in order to find ∇n.

$$\nabla n = \frac{\ln(2)}{dV} k_B \mathrm{Dos}(\varepsilon_F)\nabla T \tag{4.8}$$

We can use equations (4.1), (4.7), and (4.8) to write an expression for A and then Q. We will also need the Drude-Sommerfeld model for conductivity.

$$\boxed{\begin{aligned} &A = \frac{\ln(2)}{d^2 V} q v_F^2 k_B \tau \mathrm{Dos}(\varepsilon_F), \qquad\qquad v_F^2 = d\varepsilon_F / m^* \\ &Q = \frac{A}{\sigma} = \frac{\frac{\ln(2)}{d^2 V} q v_F^2 k_B \tau \mathrm{Dos}(\varepsilon_F)}{n q^2 \tau / m^*} = \frac{\ln(2)}{d}\left(\frac{1}{qn}\right)\varepsilon_F k_B \frac{\mathrm{Dos}(\varepsilon_F)}{V} \\ &Q < 0 \quad (\text{for } \textbf{electrons}), \quad Q > 0 \quad (\text{for } \textbf{holes}) \end{aligned}} \tag{4.9}$$

In two dimensions the density of states is given by the following (also an example is given for copper):

$$\mathrm{Dos}(\varepsilon_F) = \frac{m^*}{\pi\hbar^2} = \frac{m^* c^2}{\pi(\hbar c)^2} = \frac{1.3\,mc^2}{\pi(\hbar c)^2} = \frac{1.3(0.51\,\mathrm{MeV})}{\pi(1240\,\mathrm{eV}\cdot\mathrm{nm})^2} \tag{4.10}$$

We can now calculate the Seebeck coefficient. A novel instructional example homework problem that demonstrates the correct calculation for copper based off of the refined theory.

<u>Example Problem 4</u>: What is the Seebeck Coefficient for Copper using the theory presented in equation (4.9)? Compare with experimental measurements.

Both gold and copper are hole-dominant [4]. Thus we know that the sign will be positive. This is a critical feature of this theory.

$$\begin{aligned} Q &= \frac{\ln(2)}{d}\left(\frac{1}{qn}\right)\varepsilon_F k_B \frac{\mathrm{Dos}(\varepsilon_F)}{V} = \frac{\ln(2)}{d}\left(\frac{1}{qN}\right)\varepsilon_F k_B \mathrm{Dos}(\varepsilon_F) \\ Q &\approx \frac{\ln(2)}{2}\left(\frac{1}{e\cdot 4/(135\,\mathrm{pm})^2}\right)(7\,\mathrm{eV})\,k_B \frac{1.3(0.51\,\mathrm{MeV})}{\pi(1240\,\mathrm{eV}\cdot\mathrm{nm})^2} \\ Q &\approx 0.048\,\mu\mathrm{V/K} + 5\,\mu\mathrm{V/K} = 5.048\,\mu\mathrm{V/K} \end{aligned} \tag{4.11}$$

This is in close agreement with the measured value for copper that was given earlier in the chapter. □

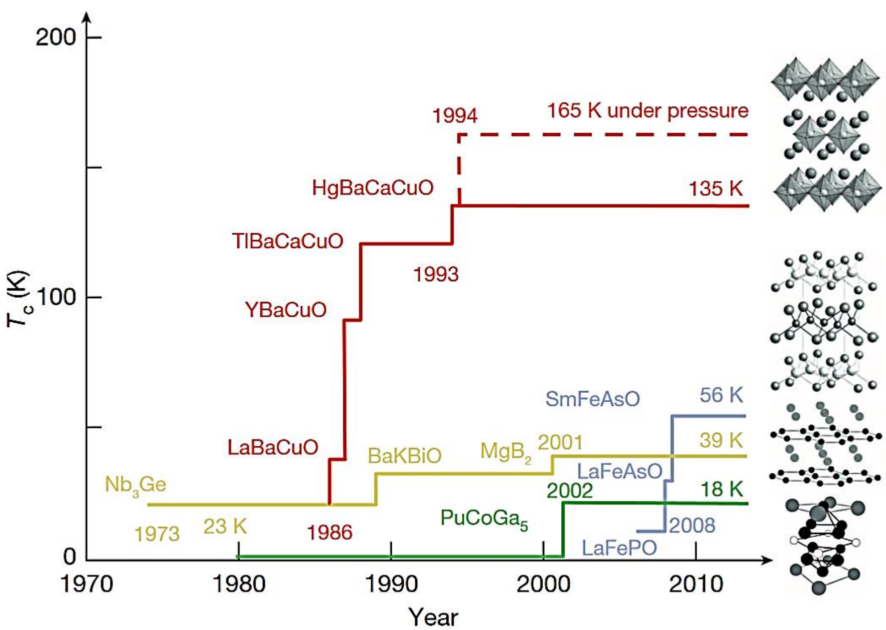
Discussion

We have been introduced to the classical and semi-quantum theory for the Seebeck coefficient. The full quantum discussion has been presented and the shortcomings of the classical expressions have been addressed. We have calculated the Seebeck coefficient for a well-known metal.

Chapter 5

Research and the Future of HTS

High temperature superconductivity discovered in copper oxide perovskite $La_{2-x}Ba_xCu$ ushered in a tremendous growth in high temperature superconductivity [5]. A historical graphic of HTS is also given in the same Nature review article.



The highest confirmed temperature reached for a HTS is about 135 K. As new materials are explored and critical temperatures are increased, new applications continue to develop. Current applications include: MRI, NMR, high energy accelerators, and plasma fusion reactors. A major application is in the medical field particularly with superconducting quantum interference devices (SQUIDs) that are able to measure weak magnetic fields from the human brain. The primary emerging technology available from HTS is power generation systems. These include fusion technology, motors, and energy storage.

Discussion

We have briefly introduced a variety of applications in HTS in an effort to motivate the study of basic electron transport properties in HTS. High temperature superconductors will play a significant role in future technological applications as the higher critical temperatures of new materials are discovered.

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[5] B. Keimer, S.A. Kivelson, M.R. Norman, S. Uchida, and J. Zaanen, Nature **518**, 179 (2015). doi:10.1038/nature14165

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Bibliography

I found Ashcroft and Mermin particularly helpful when writing chapters 1 and 2 and for chapter 4 covering the Seebeck Effect. I also tried to be consistent with the notation.

I used Kittel for several of the ideas and to gather information as well as to check formulas for consistency (there were several typos in the Theory of High Temperature Superconductivity).

I found Fujita's book on HTS the most useful for derivations and learning the basic theory (much of the text follows sections from this book). I found the quantum mechanical treatment in many of the chapters intractable as it was simply quoted from various journals that I had no access to. This caused me to consider electron transport that was also covered in other texts.

I found the solid state physics text by Ibach and Lǖth useful particularly in the discussion of type II superconductors and London penetration.

Hyper Physics was useful in looking up Fermi energies and velocities for materials. Also, Wikipedia was useful when looking up superconductor properties such as for YBCO.