Automated Gap Identification to Uncover Electronic Inhomogeneity in Bi-2212

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Introduction

This project focused on spectral analysis, especially gap extraction into the high-temperature superconductor Bi-2212. To efficiently and correctly process large amount of data, while maintaining flexibility and distributability, Python is chosen as the language to solve this problem.

While an ultimate definition of "gap size" does not exist, we try to match the automatic calculated result with human visual inspection result, while maintaining consistency across different types of spectra.

Why Use an Algorithm?

A powerful tool in its own right, Scanning Tunneling Microscopy or STM allows experimenters to analyze the relative number of electrons at each energy level (density of state) around the Fermi Energy. This spectroscopic data provides information about the electronic properties of a material. However, the measurement must be repeated numerous of times to obtain high signal to noise ratio, ensuring features observed are relevant. This is especially important at room temperature where thermal energy contributes significantly to noise, as shown in some example spectra below.

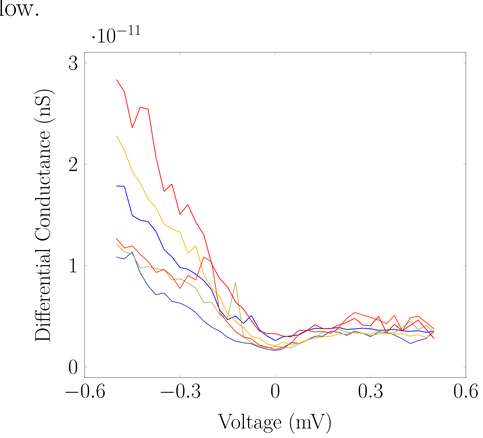


Figure 1: Sample raw spectra from underdoped 78 K

Here we present an algorithm designed to filter through noisy room temperature spectroscopic data to uncover underlying trends and gap sizes in Bi-2212.

High T_C Superconductivity and the Bi-2212

First discovered in the mid 1980s the Bi-2212 is one of the most studied classes of high-temperature superconductors. Much of the research into this material has focused on the relationship and transition between the so called "Pseudogap" phase, named for the gap in the density of states around the Fermi energy, and the superconducting phase which occurs at low temperatures. But not much is known about the transition between the normal metal and psuegogap which occurs around room temperature in some samples. At these temperatures the spectral gap can be difficult to determine since it is not clearly demarcated with a peak as in the low temperature data, therefore we have developed an algorithm to determine the gap size of each individual spectra to study the properties of this gap.

Important Result

This developed program could find the gap sizes of **three types** of spectra, with very good consistency compared to vision inspection values.

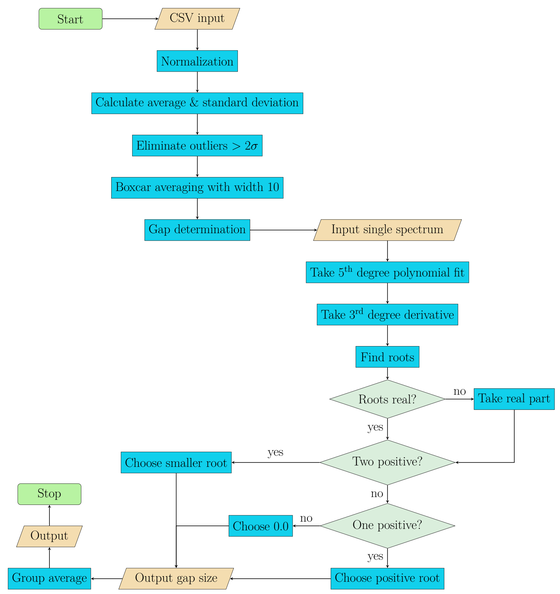
Mathematics

Before gap determination, efforts are made to eliminate as much noise as possible.

To explain this algorithm, consider the definition of the gap. There should be a shoulder, or other types of inflection on the spectroscopic data that hints the edge of the gap. Some examples will be presented in the result section.

To precisely identify this point, we take the fifth degree polynomial fit of the positive section of the spectra, to catch enough meaningful features of the trend without picking up too much noise; and then we take the third derivate of the fitted function, to find the inflection points easily by calculating the roots of the function. The is because inflection point of the curvature indicates an end to the gap. Obviously, only the root lying in the range of search is relevant. For safety we pick the smaller one if more than one is in the range.

Process



Results

Below is the result generated by the program, from flat (upper left), downward (upper right), and upward (lower) ending towards the high positive bias side.

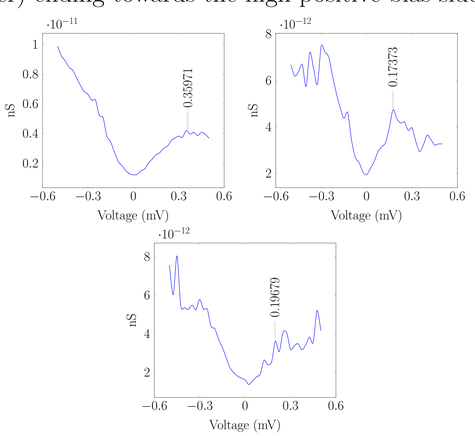


Figure 2: Actual spectra of three types, marked with gap size determined by the program

Conclusion

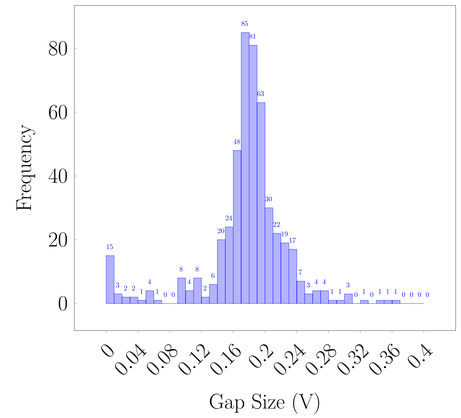


Figure 3: Histogram of gap sizes, 10-boxcared, data size 1476

Above shown is the histogram of captured gap sizes, for 1500 spectra collected from a 78 K underdoped sample. The majority of peaks lies in the expected range.

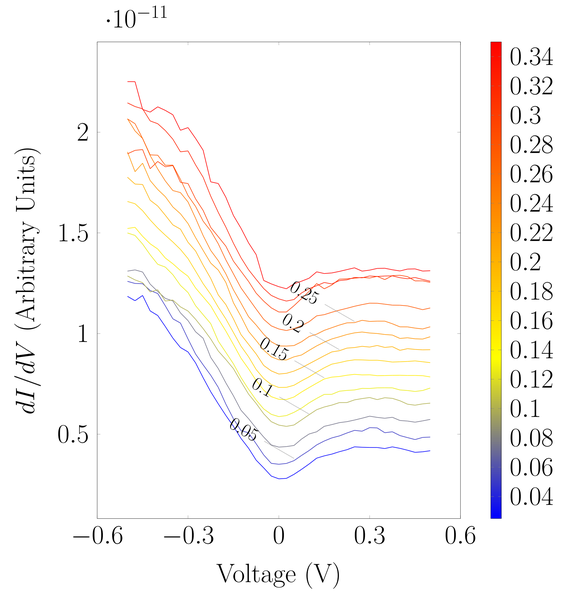


Figure 4: Averaged spectra for different gap sizes, with $y-$offset

Above shown is the group average for all the spcectra, with $y-$offset. The trend of gap sizes could be seen.