

Using machine learning to quantify the symmetry breaking of STM twisted bilayer graphene data

William D Taranto

2020 PARADIM REU Intern @ Cornell

Intern Affiliation: Physics, Cornell University (CU)

Program: 2019 Platform for the Accelerated Realization, Analysis, and Discovery of Interface Materials

Research Experience for Undergraduates Program at Cornell University (PARADIM REU @ Cornell)

PARADIM REU Principal Investigator: Dr. Darrell Schlom, Director, PARADIM

PARADIM REU Mentor: Eun-ah Kim, Physics, Cornell University

Primary Source of PARADIM REU @ Cornell Funding: Support for PARADIM is provided under NSF Grant # DMR-1539918 as part of the Materials Innovation Platform

Program Contact: schlom@cornell.edu, eun-ah.kim@cornell.edu

Website: <http://cnf.cornell.edu/education/reu/2020>

Abstract:

Twisted bilayer graphene (TBG) harbors interesting electronic behavior which contributes to its unique prospective states, such as a superconductor or quantum spin liquid. The sensitivity of TBG to its twist angle manifests itself at the ‘magic’ angle of 1.1 degrees where TBG becomes a superconductor but quickly becomes an insulator at neighboring angles. From visual interpretations of scanning tunneling microscopy data, TBG is suspected to have spontaneous symmetry breaking. The exploration of this apparent spontaneous symmetry breaking remains the goal of this research. By using image processing techniques on STM data, simplified features which represent local symmetry are derived. Furthermore, analyzing the structures of the local symmetries via a Gaussian mixture model characterizes the symmetry breaking of the sample. Such analysis appears to prove fruitful, and this research is ongoing.

Motivation:

Discovery of twisted bilayer graphene’s (TBG) unique electron behavior has provoked great interest into exploring such behaviors. Of particular significance is the sensitivity of TBG to its twist angle: showing superconductivity at 1.1 degrees and insulation at others. This twist angle variation “may pave the way towards more exotic correlated systems, such as unconventional superconductors or quantum spin liquids” [1]. Given its unique prospects, TBG promises to be a novel material worthy of investigation.

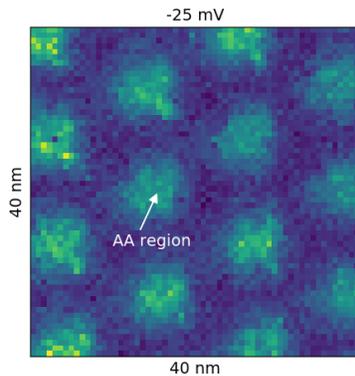
Courtesy of the Nadj-Perge Laboratory [2], scanning tunneling microscopy data (STM) of TBG has been obtained. This data visually appears to exhibit spontaneous rotational symmetry breaking. This apparent spontaneous symmetry breaking would imply the existence of an order parameter and therefore a correlation length of TBG. Both of these are important in describing some of TBG’s unique electronic behaviors. Therefore, this research aims to explore the symmetries of TBG.

Summary of Research:

The TBG data is given as an image from STM. In the collection of the data, there is a range of bias voltages between the STM probe and the TBG. For each of these voltages, the STM provides an image, as shown in Figure 1, with brighter regions

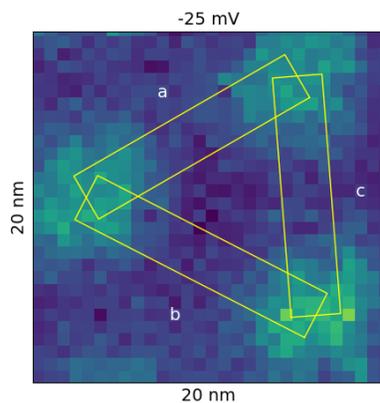
corresponding to the frequency of electron tunneling between the probe and the TBG. The natural first step is to objectively process the data to pull out the particular feature(s) that define local symmetry. There are many ways in which this can be done.

Figure 1: STM data of TBG at magic angle - the bright regions are AA regions where more electrons tunnel to the TBG.



However, the processing used here aims to be simple and interpretable, which are most apt for this research's exploratory goal. To that end, the most notable feature of TBG are the AA regions, where the hexagonal layers are aligned. These occur as brighter sights in the images, and so the common technique of blurring the image then finding the local maxima is done. This gives a set of points which represent the center of AA sights in an equilateral triangular lattice. Considering this lattice, only those triangles which 'point' (are equal under translation) should be considered. This results in a quilted lattice of only triangles which 'point' in the same directions.

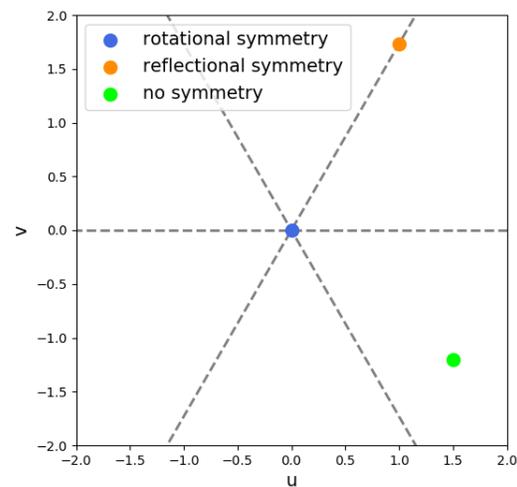
Figure 2: Single unit triangle - An example of a single triangle with the boxes corresponding to each side.



These triangles represent the local symmetry of the TBG sample. Therefore, the local symmetry of a TBG sample requires a measure of a single triangle's symmetry. To do this, a value is assigned to each side which are called a, b and c as in Figure 2. These are equal to the following:

the average of all pixels that fall within a certain longitudinal distance of that side. Therefore, there now exists a characteristic intensity of each side. Depending on the congruence of these three sides, the triangle exhibits different forms of symmetry. For example, if a equals c but a does not equal b, then there exists reflective symmetry with respect to the line perpendicular to the b side. Furthermore, if a is instead approximately equal to c, then there is an approximate reflective symmetry but not exact. This provides a way to establish symmetry measurement. However, this does not allow for easy visualization because plotting an (a, b, c) point is in R^3 . Therefore, a simple linear transform which preserves all symmetries is used: $u = a/2 - (b + c)$, $v = \sqrt{3}/2 * (b - c)$. This transformation can be plotted in R^2 which provides an easier visual interpretation. Additionally, there are lines and points which represent the different symmetries that a triangle could assume. These such locations are shown in Figure 3.

Figure 3: (u, v) space - Each triangle can be mapped into this space. Depending on the location it is mapped to, the triangle may have different symmetries. The origin is a rotationally symmetric and the three lines represent the three reflectional symmetries.



Finally, this gives a readily understandable and visualizable form of local symmetry.

This new space characterizes the local symmetry that the triangle exhibits, which we can relate to two other traits of the triangle: the voltage bias and its location. With the data processed this way, different analyses are possible. As this research is still ongoing, the current analysis clusters different sets of triangles using a Gaussian mixture model (GMM). A mixture model uses an iterative process to group points of data into different distributions. Intuitively, the GMM is fed a set of data with certain characteristics; it then finds different Gaussian distributions which statistically match that set of data. To cluster triangles, they are first preprocessed into (u, v) points which the GMM is able to analyze. The GMM gives results about what the (u, v) clusters look like. Using this process, different sets of triangles, depending on the bias voltage and their location, can be analyzed to find structural relationships between symmetry, location, and voltage bias. There are many different possible sets of triangles that can be chosen. Currently, all triangles within a window of voltages are put into a GMM, and then the GMM results are compared to other GMM results of different voltage windows.

Present Status and Future Direction:

At the present time, this research remains ongoing, and there are two paths being pursued. First, the characteristics of the distributions that the GMM gives us for each voltage window are being analyzed. A distribution can be fully described by a mean vector along with a covariance matrix. For a purely vector description, the covariance matrix can be decomposed into its eigenvalues and eigenvectors. Using a purely vector description aids in measuring the relationship of the distributions with the different symmetry points in (u, v) space.

Second, each triangle is placed into a specific distribution, and the probability of these placements are being analyzed. These probabilities characterize the similarity between different triangles with respect to the whole. As such, this provides a possible order parameter. These results can be mapped back into real space by coloring triangles based on the probabilities.

This provides a way to visualize the local symmetry in real space objectively.

These along with more general processing are still ongoing and as of now are showing novel forms of interpreting and measuring symmetries of TBG.

Acknowledgements:

PARADIM REU Program; Research Advisor: Samuel Lederer; Mentor: Eun-ah Kim; Collaborators: Nadj-Perge Lab

References:

- [1] Cao, Yuan et al. "Correlated Insulator Behaviour at Half-Filling in Magic-Angle Graphene Superlattices." *Nature* 556.7699 (2018): 80–84. Crossref. Web.
- [2] More information regarding the Nadj-Perge Lab can be found at <http://nplab.caltech.edu/>.

Second, the probability of the specific distribution each triangle was placed into are being analyzed. These probabilities characterize the similarity between different triangles with respect to the whole. As such, this provides a possible order parameter. Furthermore, these probabilities can be mapped back into real space by coloring triangles based on this. This provides a way to visualize the local symmetry in real space objectively.