Semiclassical computational approach to the superconductive transition in twisted bilayer graphene

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I. INTRODUCTION

Studies

- BSc Engineering physics (CFIS)
- BSc Mathematics (CFIS)
- MSc Nanoscience and nanotechnology (UAB)

→ Finishing it right now (in early September). Only the master thesis left. Supervisor: Jordi Boronat.

Main interest: Topological materials

→ NIMS internship in Japan (7/6/23 - 2/8/23): Topological properties in a 2D lattice with disclinations. Supervisor: Toshikaze Kariyado.

Future prospects:

- Start the PhD as soon as possible. Ideally in Japan.

→ Since they start in April, need to find a temporal research job to work and gain experience.

- Probably (but not clear yet) I will be able to start the PhD in Grenoble this October with Prof. Adolfo Grushin.

II. MASTER THESIS

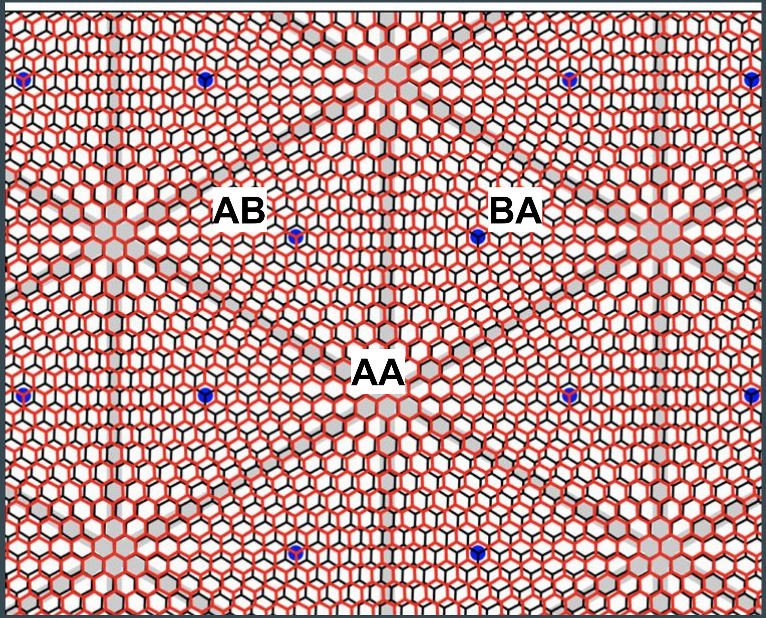
0. Original Motivation

Need of finding a topic which related my supervisor Jordi Boronat and Toshikaze's research.

- Prof. Jordi Boronat study mainly superfluidity in lattices with Monte Carlo.
- Toshikaze works mainly in topological materials but also a bit in superconductivity and van der Waals heterostructures.

→ Final election of the project: Study the superconductive transition in twisted bilayer graphene (tBG).
→ Verify if the (topological) BKT transition temperature of the XY model in a lattice modeling tBG is similar to its superconductive temperature.

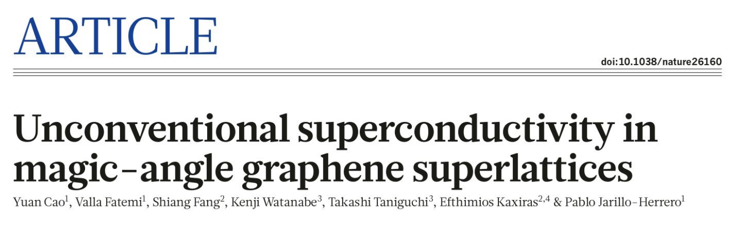
1. Graphene and twisted bilayer graphene (tBG)



[1]

1. Superconductivity (SC) in tBG

[2]



ARTICLE

doi:10.1038/nature26160

Unconventional superconductivity in magic-angle graphene superlattices

Yuan Cao[1], Valla Fatemi[1], Shiang Fang[2], Kenji Watanabe[3], Takashi Taniguchi[3], Efthimios Kaxiras[2,4] & Pablo Jarillo-Herrero[1]

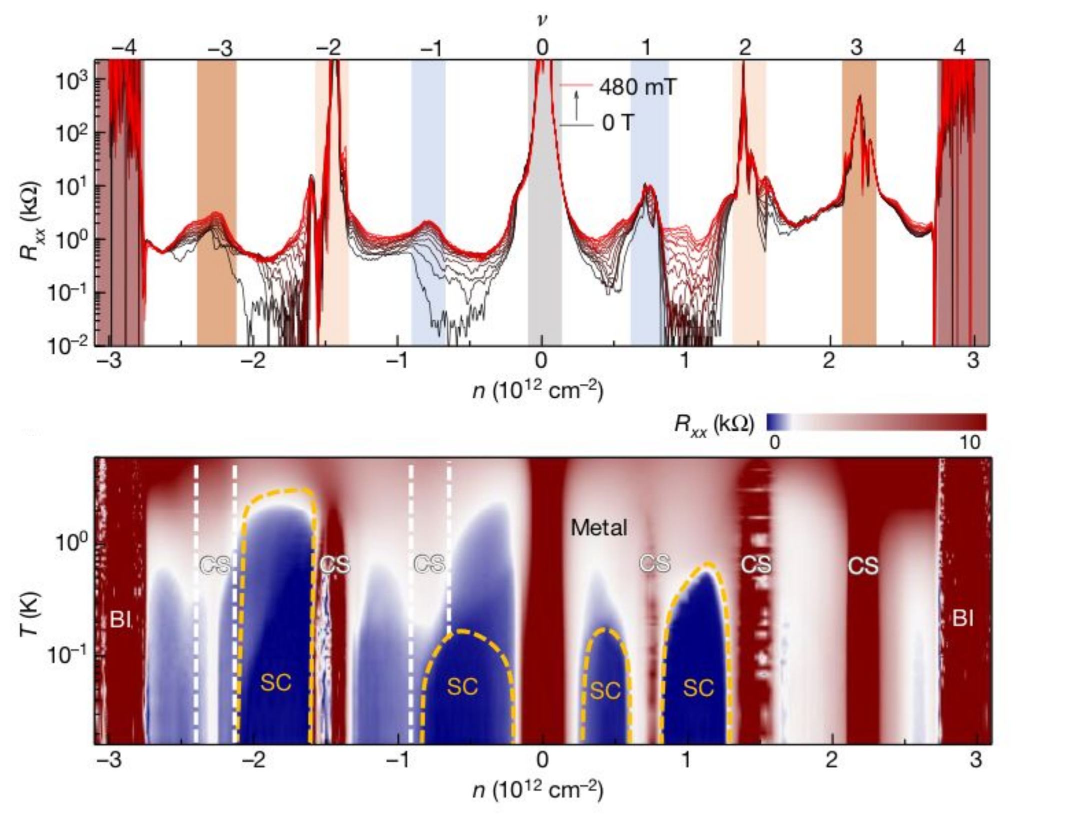
Unconventional SC

→ Platform to study High-T_c SC

(simplicity + easy to dope)

4 SC domains

up to 4e/unit cell: (2 valleys)*(2 spins)



2. XY model, BKT transition and superconductivity

Spins rotate freely in a plane

$$H = -J \sum_{<i,j>} cos(\theta_i - \theta_j)$$

J the exchange interaction

θ the angles of the spins

Phase transition without symmetry breaking ⟶ BKT transition

⟶ Nobel Prize in Physics 2016

Related with superconductivity (similar behaviour)

2. Helicity modulus

$$\Upsilon_\mu = \frac{1}{A} J \left\langle \sum_{<i,j>} cos(\theta_i - \theta_j)(e_\mu \cdot v_{ij})^2 \right\rangle - \frac{1}{A} J^2 \beta \left\langle \left(\sum_{<i,j>} sin(\theta_i - \theta_j)(e_\mu \cdot v_{ij}) \right)^2 \right\rangle$$

[3]

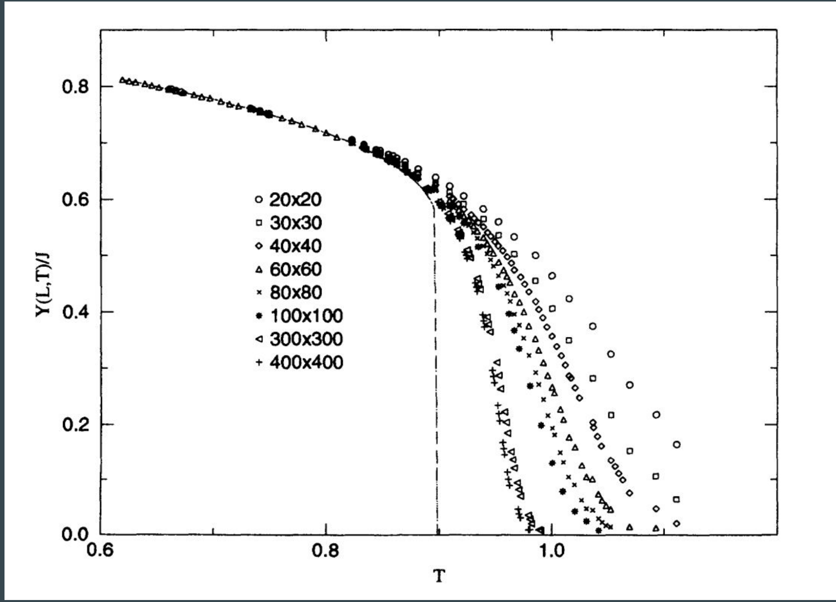
A: parameter that depends on the type of lattice

$\beta = 1/(k_B T)$

e_μ unitary vector of the twist direction

v_{ij} vector between site *i* and *j*

Intuitive idea: Measure of the change of the energy in the system due to a twist of spins along one particular direction μ. Related with the superfluid density.



3. The model

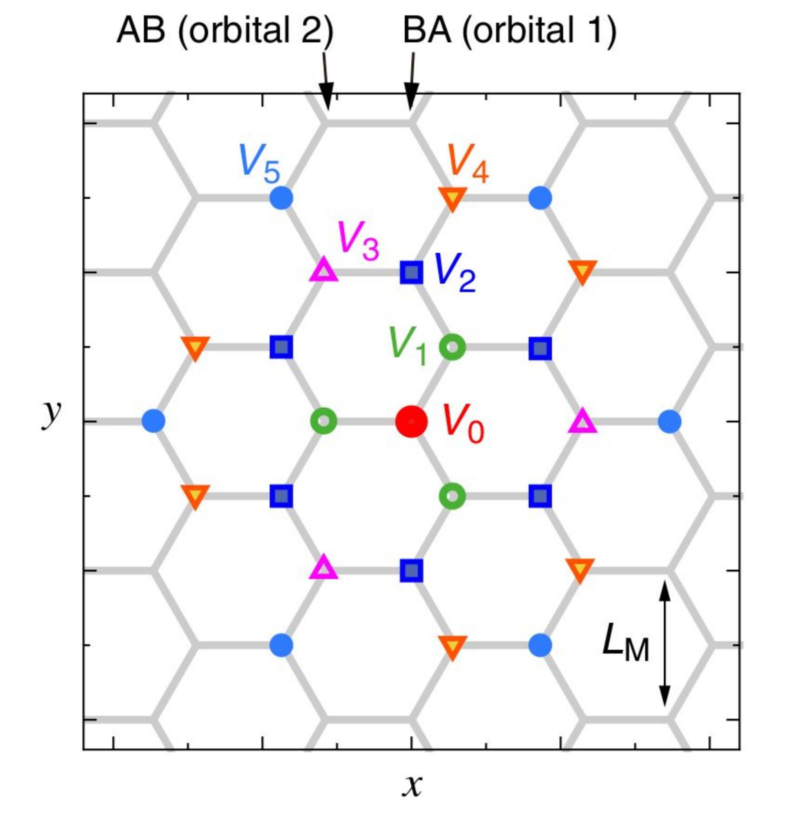
PHYSICAL REVIEW X **8,** 031087 (2018)

Maximally Localized Wannier Orbitals and the Extended Hubbard Model for Twisted Bilayer Graphene

Mikito Koshino,[1,*] Noah F. Q. Yuan,[2] Takashi Koretsune,[3] Masayuki Ochi,[1] Kazuhiko Kuroki,[1] and Liang Fu[2]
[1]*Department of Physics, Osaka University, Toyonaka 560-0043, Japan*
[2]*Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*
[3]*Department of Physics, Tohoku University, Sendai 980-8578, Japan*

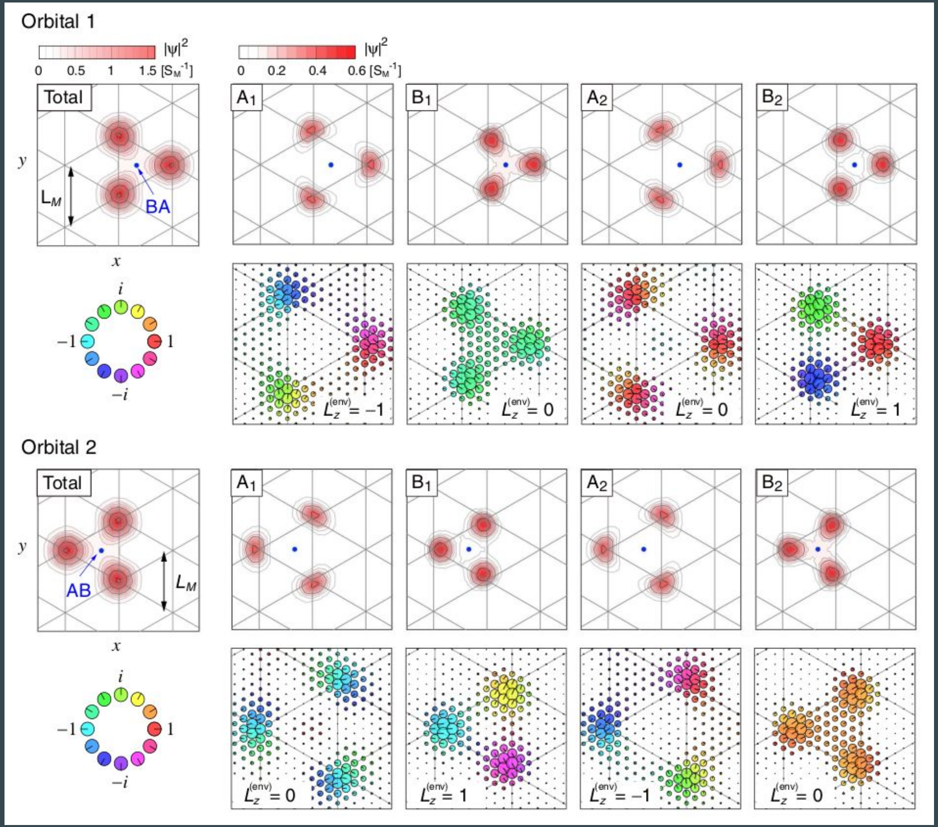
(Received 21 May 2018; published 28 September 2018)

n	0	1	2	3	4	5
V_n	1.857	1.533	1.145	1.068	0.697	0.614
J_n	N/A	0.376	0.0645	0.010	0.014	0.001



[1]

3. The model (justification)

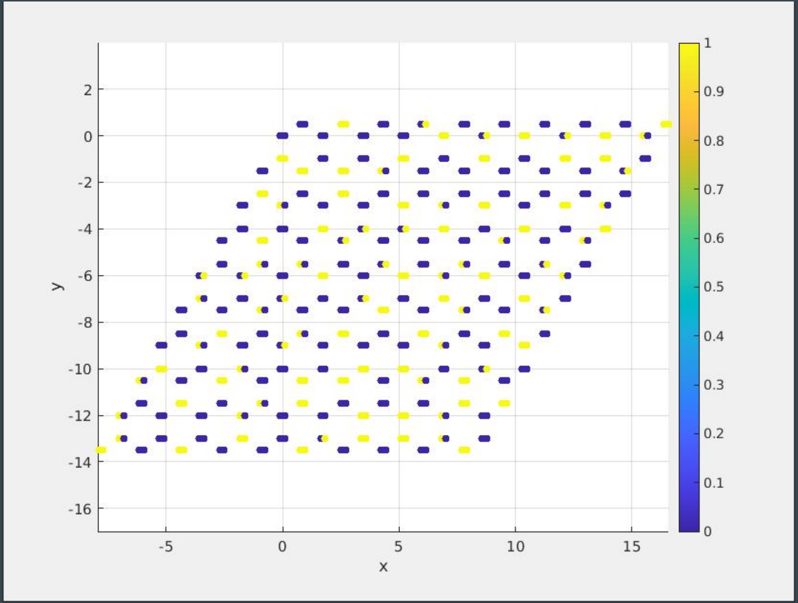


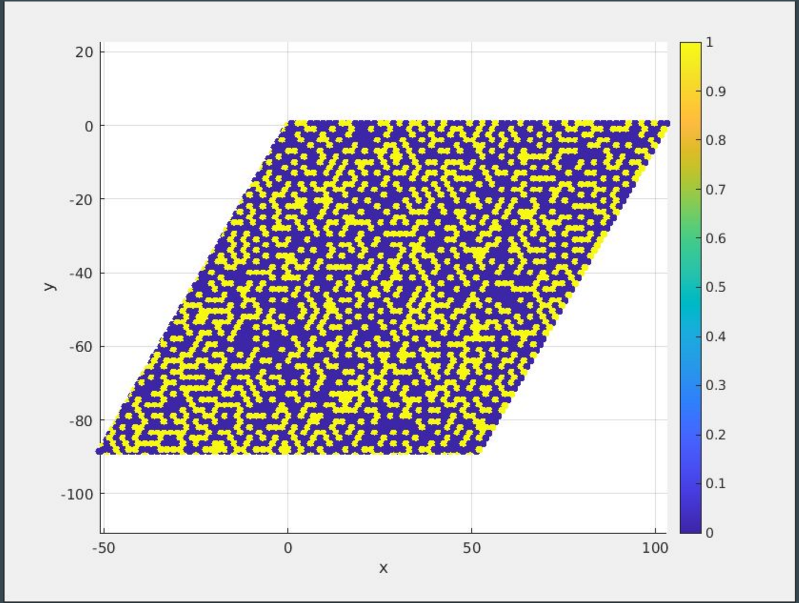
[1]

3. The model: Coulomb step

Not all the sites occupied. How we distribute the electrons?

→ Previous step with Coulomb. Then, XY calculation with that distribution constant





4. Monte Carlo methods: Metropolis

Broad class of stochastic numerical algorithms

Generate states following an appropriate law: The states appear with the same probability as in the real system

The mean magnitudes *A* are just

$$A \approx < A >_{MC} = \frac{1}{N} \sum_{n=1}^{N} A_n$$

For XY, in the “move” we choose a site *i* and propose an update of its angle.

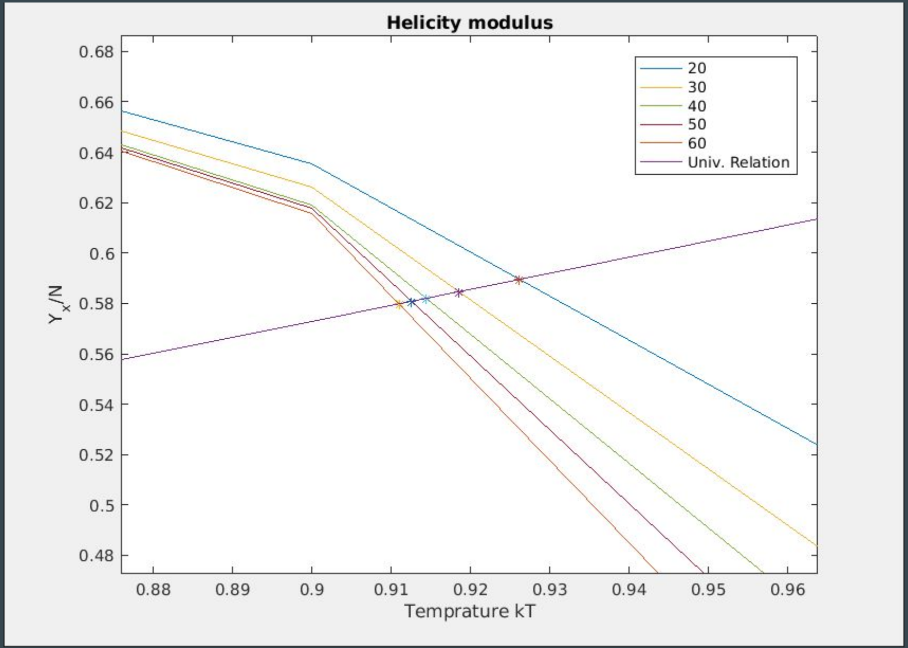
procedure Metropolis
- Choose an initial configuration $S = S_0$
- Thermalize
- **for** $k \in 1, ..., it_{max}$ **do**
  - Propose a move S_k with a probability $T(S \to S_k)$
  - Accept the new state with probability $A = \min\{1, e^{-\beta \Delta E}\}$
  - **if** Accepted **then**
    - $S = S_k$
    - Update $A(S)$
  - **end if**
  - Take statistics of A
- **end for**
- Compute mean values of A

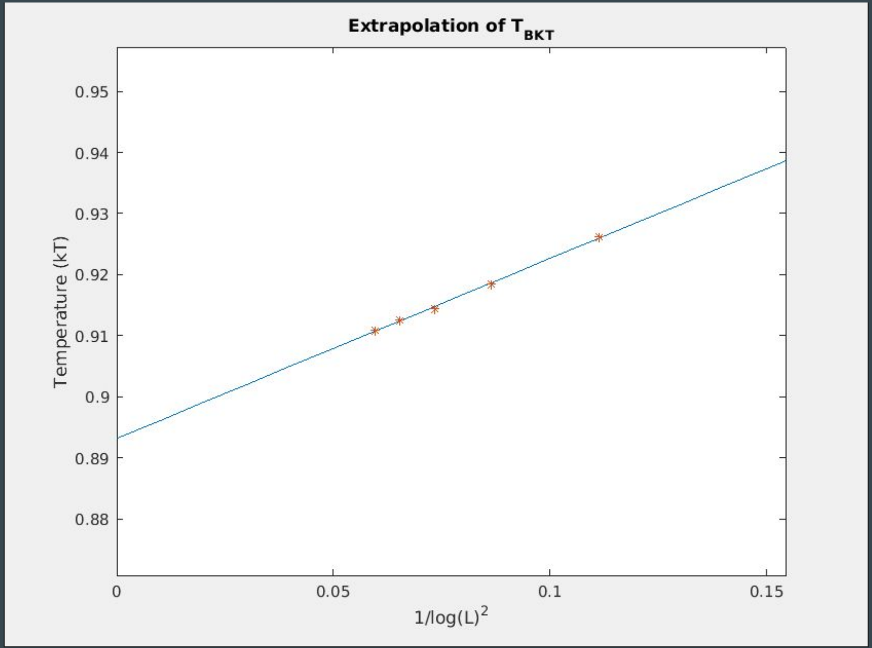
end procedure

4. Our algorithm

```
procedure Main Algorithm
    Define the main parameters J_1, J_2, V_0, V_1, V_2 and the filling ν
    Choose the number of repetitions n_r and iterations it_max.
    Choose the temperatures T_i
    for L ∈ {8, 16, 32, 44, 60} (for example) do
        Get zeroth, first and second neighbours
        for each repetition do
            Define a seed and set the random number generator
            for each temperature T_i do
                Compute the distribution of electrons: occupation = Coulomb(L, T_i, V, ν)
                Do the XY step: ϒ = XY(L, T_i, occupation, J, ν)
                Save the results in a text file
            end for
        end for
    end for
    Plot the results
end procedure
```

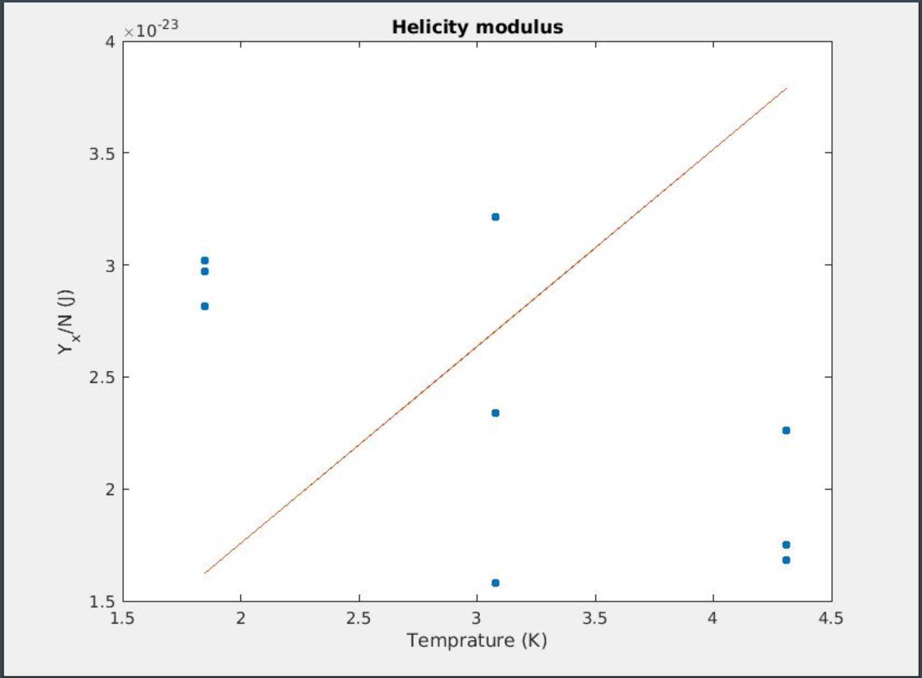
4. Determination of T_{BKT} (squared)

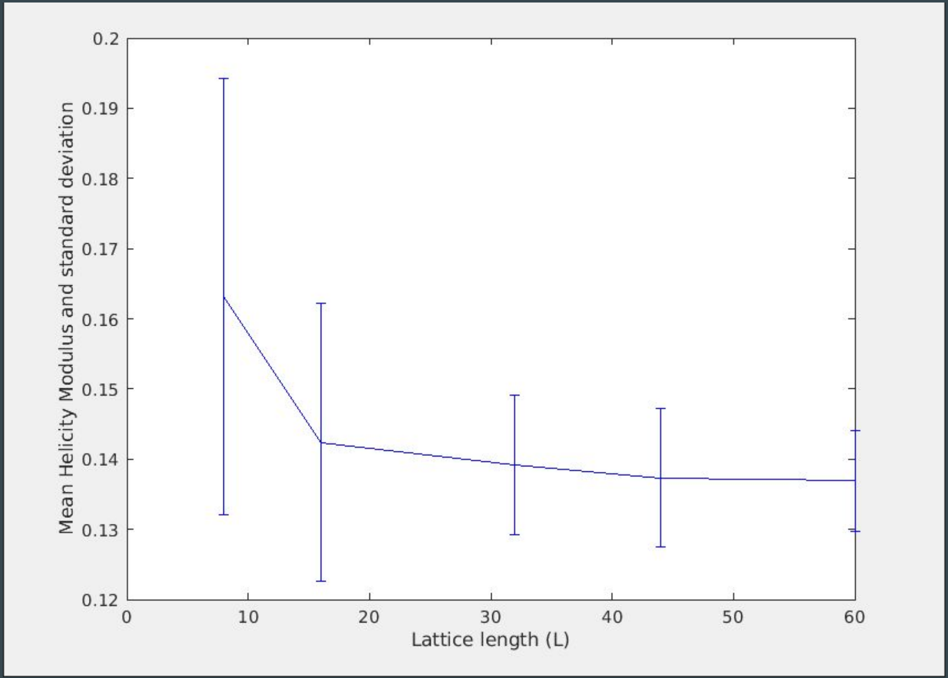




T = 0.893181553363876, very close to 0. 89016(4) from the article [3]

5. Results/Conclusions up to now





Thank you!

References

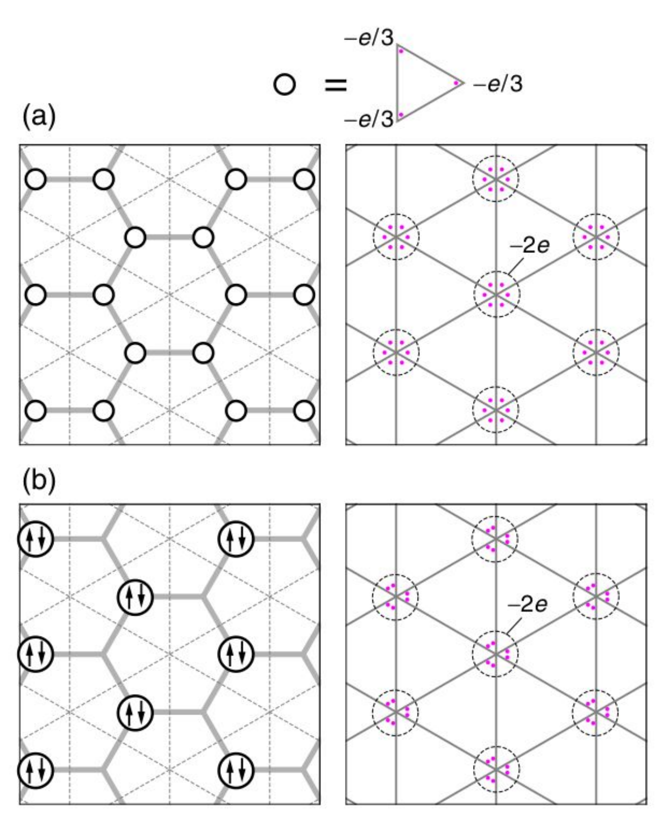
[1] Mikito Koshino, Noah F.Q. Yuan, Takashi Koretsune, Masayuki Ochi, Kazuhiko Kuroki, and Liang Fu. Maximally Localized Wannier Orbitals and the Extended Hubbard Model for Twisted Bilayer Graphene. Physical Review X, 8(3):031087, September 2018.

[2]Xiaobo Lu, Petr Stepanov, Wei Yang, Ming Xie, Mohammed Ali Aamir, Ipsita Das, Carles Urgell, Kenji Watanabe, Takashi Taniguchi, Guangyu Zhang, Adrian Bachtold, Allan H. MacDonald, and Dmitri K. Efetov. Superconductors, orbital magnets and correlated states in magic-angle bilayer graphene. Nature, 574(7780):653–657, October 2019.

[3] Norbert Schultka and Efstratios Manousakis. Finite-size scaling in two-dimensional super-fluids. 49(17):12071–12077

Appendix

3. Coulomb step (justification)



[1]

III. Topological materials at NIMS

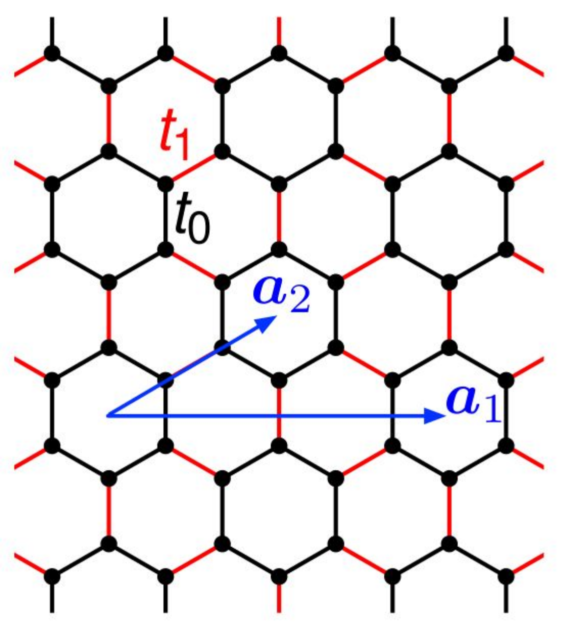
- 2D lattice with disclinations with an intra- (t0) and an inter- (t1) hopping term.

- First month: Tight binding hamiltonian solved by numerical diagonalization in Octave.

→ Play with the relation of both to observe topological or trivial in-gap states.

- Second month: Addition of non-linearities. Time evolution of eigenfunctions solving Schrodinger equation with Runge-Kutta in Octave.

→ Play with the nonlinear coefficient to see interesting dynamics.



Toshizake Kariyado and Xiao Hu. Topological States Characterized by Mirror Winding Numbers in Graphene with Bond Modulation. Scientific Reports. 2017