Flat-bands and electron-electron correlation properties of graphene with and without twist

Gerardo G. Naumis
Leonardo Navarro-Labastida, Elías Andrade-Amezcua
Depto. De Sistemas Complejos, Instituto de Física, UNAM. Circuito Exterior s/n, Ciudad Universitaria, CP 01000, Coyoacán, CDMX, Mexico
naumis@fisica.unam.mx

FLat bands play a central role in the presence of correlated phases in moiré and other space-modulated graphene lattices. However, their origins and properties are still not well understood, despite the knowledge that they produce complex quantum phase diagrams. This revision aims to present how such bands arise in twisted and untwisted systems and how many-body interactions induce interesting quantum phases like Chern fractional insulator phases.

Starting with a very simple analytically solvable model of an untwisted system, i.e., uniaxially strained graphene, we determine the conditions for having flat bands: a long-wavelength modulation on each of the bipartite graphene sublattices but tagged between neighboring carbon atoms [1]. The origin of such flat bands is the existence of confined, topological wavefunctions at domain walls separating different regions, each characterized by a nonuniform Su-Schriffer-Hegger model (SSH) type of coupling. Subsequently, the Hamiltonian is mapped into a continuum model, allowing to explain the results in terms of the Jackiw-Rebbi model (capable of presenting charge fractionalization) and pseudo-Landau levels [1]. The electron-electron interaction is explored through the Hubbard model, revealing that flat bands induce Néel antiferromagnetic and ferromagnetic domains even with very weak interactions [1]. Furthermore, the repulsive Hubbard interaction results in an effective electron-electron pairing, which is explained as a type of Kohn-Luttinger mechanism believed to be relevant for superconductivity in twisted bilayer graphene at magic angles.

Next, the connection between the quantum Hall effect and zero flat band modes is investigated in twisted bilayer graphene at magic angles. In particular, it is demonstrated that the square of the Hamiltonian, a 2×2 matrix operator, is approximately equivalent to a two-dimensional quantum harmonic oscillator, where the flat bands are mapped into the ground state [2,3]. Interlayer currents between graphene's bipartite lattices are identified with an angular momentum term, while the confinement potential is considered an effective quadratic potential. By analyzing the flat-band mode equations, the boundary conditions, and applying a scaling argument, a magic angle quantization rule is derived [2]. For high-order magic angles, the zero flat band modes converge into almost coherent Landau states [3]. Finally, electron-electron interaction effects are discussed, following the ideas presented for the case of uniaxially strained graphene .

References

[1] E. Andrade, F. López-Urías, G. G. Naumis, Topological origin of flat bands as pseudo-Landau levels in uniaxial strained graphene nanoribbons and induced magnetic ordering due to electron-electron interactions, Phys. Rev. B 107, 235143 (2023).
[2] L. Navarro-Labastida, G.G. Naumis, 3/2 magic angle quantization rule of flat bands in twisted bilayer graphene and its relationship to the quantum Hall effect, Phys. Rev. B 107, 155428 (2023)
[3] L. A. Navarro-Labastida, G.G. Naumis, Self-duality properties, localization centers, and magnetic energy of the electronic wave functions at small magic angles in twisted bilayer graphene, Phys. Rev. B 109, 035402 (2024).