Positive interplay between Coulomb interaction and Jahn-Teller effect in magic angle twisted bilayer graphene

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Twisted Bilayer Graphene, characterized by unique and puzzling electronic properties, has drawn the attention of the condensed matter scientific community since the discovery of its superconducting behaviour at low temperature [1]. The presence of extremely flat bands around the Fermi energy makes the system prone to develop exotic states of matter, since even a small perturbation can induce a great modification of the band structure.

So far, the insulating character of the ground state at integer filling has been investigated only in term of electronic correlation induced by Coulomb repulsion [2], with little or no attention on lattice vibrations, whose role is known to be crucial to separate the flat bands from other higher and lower ones [3]. Moreover, in Twisted Bilayer Graphene the sole Coulomb repulsion seems unable to stabilize Cooper pairs [4], thus pointing toward a superconducting mechanims dominated by phonons.

Among all possible lattice modes, Twisted Bilayer Graphene displays a set of twofold degenerate optical vibrations that resemble the breathing of the whole Moiré cell. These modes Jahn-Teller couple with the electronic flat bands, favouring a spontaneous lattice deformation that efficiently removes the valley degeneracy [5].

In this poster, I present detailed Hartree-Fock results including for the first time the effects of such phonons on the electronic properties of Twisted Bilayer Graphene.
At first, I focus on the "frozen phonon approximation", where the lattice is statically distorted in accordance to the phonon wavefunction, and how it can stabilize insulators at integer fillings.
Next, I introduce an unretarded effective electron-electron attraction mediated by such high-energy phonons. Surprisingly this term enhances the electronic correlation induced by the sole Coulomb repulsion, with the stabilization of a symmetry broken insulator that strongly couples to the phonon degrees of freedom. Due to the Jahn-Teller instability of the band structure, this insulator becomes the true ground state of the system even for a small electron-phonon coupling.
Eventually, I discuss the link of this results to band topology, observable quantities and superconductivity.

References

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