Ground-state Properties of Inhomogeneous Graphene Sheets

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When inter-valley scattering is weak and gauge fields due to e.g. ripples are neglected, doped and gated graphene sheets can be described using an envelope-function Hamiltonian with a new sublattice pseudospin degree-of freedom, an ultrarelativistic massless-Dirac free-fermion term, a pseudospin scalar disorder potential, and a non-relativistic instantaneous Coulombic interaction term. There is considerable evidence from experiment that this simplified description of a honeycomb lattice of Carbon atoms is usually a valid starting point for theories of those observables that depend solely on the electronic properties of $\pi$-electrons near the graphene Dirac point \[1\]. Although the use of this model simplifies the physics considerably it still leaves us with a many-body problem without translational invariance, which we do not know how to solve. In this talk we present a Kohn-Sham-Dirac density-functional-theory (DFT) scheme for graphene sheets that treats slowly-varying inhomogeneous scalar external potentials and electron-electron interactions on an equal footing \[2\]. The theory is able to account for the unusual property that the exchange-correlation contribution to chemical potential increases with carrier density in graphene \[3,4\]. Consequences of this property, and advantages and disadvantages of using the DFT approach to describe it, are discussed. The approach is illustrated by solving the Kohn-Sham-Dirac equations self-consistently for a model random potential describing charged point-like impurities located close to the graphene plane. The influence of electron-electron interactions on these non-linear screening calculations is discussed at length, in the light of recent experiments \[5,6\] reporting evidence for the presence of electron-hole puddles in nearly-neutral graphene sheets.


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