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Ground-state Properties of Inhomogeneous Graphene Sheets[1]

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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 π-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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