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Analytic Local and Total Density of States for Hydrogen Adatoms on Graphene[1] NICHOLAS PIKE, DAVID STROUD, The Ohio State University
— Spin transport through graphene is strongly influenced by the presence of adatoms with unpaired spins, such as hydrogen adatoms. In this work, we calculate the local density of states (LDOS) for a simple model of hydrogen on graphene using a tight binding model. The model includes nearest neighbor hopping between carbon atoms, the value of the hydrogen energy level, hopping between the carbon and hydrogen atoms, and a Hubbard U-term to account for the on-site Coulomb interaction. When $U = 0$, we develop an exact analytic equation for the LDOS on the adatom site, and for the total density of states (DOS). When $U \neq 0$, we carry out the same calculation but treat the Hubbard term using mean-field theory. We find that the hydrogen adatom has a net non-integer spin polarization, and that some of the electronic density is transferred from the hydrogen adatom to the graphene host. Possible implications of these results for spin transport through graphene will be discussed.

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