Abstract Submitted for the MAR13 Meeting of The American Physical Society

Quantum Monte Carlo study of edge-state magnetism on chiral graphene nanoribbons MICHAEL GOLOR, Institute for Theoretical Solid State Physics, RWTH Aachen University, THOMAS C. LANG, Department of Physics, Boston University, STEFAN WESSEL, Institute for Theoretical Solid State Physics, RWTH Aachen University — We investigate the edge-state magnetism of chiral graphene nanoribbons using projective quantum Monte Carlo (QMC) simulations and a self-consistent mean-field approximation of the Hubbard model. Previous QMC simulations support edge-state ferromagnetism in sufficiently wide zigzag terminated ribbons. We extended these calculations to include the class of chiral graphene nanoribbons and investigate the influence of chirality and ribbon width on spin-spin correlations. The static magnetic correlations are found to rapidly increase with the width of the ribbons for all chiralities, such that already for ribbons of moderate widths we observe a strong trend towards mean-field-type ferromagnetic correlations along the edges. We extract dynamical edge state signatures which can be used to detect edge-state magnetism by scanning tunneling microscopy.

> Thomas C. Lang Department of Physics, Boston University

Date submitted: 09 Nov 2012

Electronic form version 1.4