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Diffusion Monte Carlo study of the metal-insulator transition in stretched graphene[1] LI CHEN, LUCAS K. WAGNER, University of Illinois at Urbana Champaign — At low energies and equilibrium geometries, graphene is well-described by a single-band Hubbard model[1], with U/t 1.4, which is well within the semimetal regime. One would expect that under tensile stress, U/t should increase and a transition from semimetal to Mott insulator should occur. However, the bonding σ electrons are also affected by the stretching and may affect the applicability of the single-band model. At the same time, the critical region near the metal-insulator transition is a highly multi-determinantal ground state which is a challenging case for fixed node diffusion Monte Carlo simulations. We address progress on both these points by assessing a number of wave functions for the critical region around the transition and assessing the validity of the single-band Hubbard model using the method of Ref 1. [1]. Changlani, Zheng, and Wagner, J. Chem. Phys. 143, 102814 (2015).

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