Abstract Submitted for the MAR09 Meeting of The American Physical Society

Spin-Current-Density Functional Theory with SU(2) Potentials: the Local Approximation<sup>1</sup> SAEED H. ABEDINPOUR, GIOVANNI VIGNALE, Department of Physics and Astronomy, University of Missouri, Columbia, Missouri 65211, USA — In order to study spin-orbit coupled systems, spin-transfer torque devices, or even systems with pseudospin coupling like graphene, non-Abelian vector potentials and their conjugate variables, the spin-current densities, should be incorporated in the density functional theory. The general formalism for doing this has been known for some time [K. Bencheikh, J. Phys. A: Math. Gen. **36** 11929 (2003)], but explicit functionals of the spin currents are not known. Here we identify the most general form of an exchange-correlation (xc) functional of the spin-currents, which satisfies the SU(2) gauge invariance and construct the local density approximation (LDA) for it. As an illustration we present the LDA functional for a two-dimensional (2D) electronic system, using as reference system a homogeneous 2D electron gas subjected to isotropic SU(2) vector potentials (*i.e.*, linear spin-orbit coupling). The numerical results for the xc energy of this reference system will be presented.

<sup>1</sup>This work supported by NSF Grant No. DMR-0705460.

Saeed H. Abedinpour Department of Physics and Astronomy, University of Missouri, Columbia, Missouri 65211, USA

Date submitted: 02 Dec 2008

Electronic form version 1.4