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Fermi surfaces and quantum oscillations in underdoped high-T_c superconductors $YBa_2Cu_3O_{6.5}$and $YBa_2Cu_4O_8$ HYUNGJU OH, HYOUNG JOON CHOI, Department of Physics and IPAP, Yonsei University, STEVEN G. LOUIE, MARVIN L. COHEN, UC Berkeley and Lawrence Berkeley National Laboratory — We study the underdoped high-T_c superconductors $YBa_2Cu_3O_{6.5}$ and $YBa_2Cu_4O_8$ using first-principles pseudopotential methods with additional Coulomb interactions at Cu atoms and obtain Fermi-surface pocket areas in close agreement with measured Shubnikov-de Haas and de Haas-van Alphen oscillations. With antiferromagnetic order in CuO_2 planes, stable in the calculations, small hole pockets are formed near so-called Fermi-arc positions, reproducing the low-frequency oscillations. A large electron pocket, necessary for the negative Hall coefficient, is formed in $YBa_2Cu_3O_{6.5}$, giving rise to the high-frequency oscillation as well. Effective masses and specific heats are also calculated and compared with measurements. Our results highlight the crucial role of magnetic order in the electronic structure of underdoped high-T_c superconductors. This work was supported by the KRF Grant No. KRF-2007-314-C00075, the KOSEF Grant No. R01-2007-000-20922-0, NSF Grant No. DMR07-05941, and DOE under Contract No. DE-AC02-05CH11231. Computational resources have been provided by KISTI Supercomputing Center (Project No. KSC-2008-S02-0004), NSF through TeraGrid resources, and DOE NERSC.

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