Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Wannier interpolation study of the Elliot-Yafet spin relaxation in metals ERIC ROMAN, IVO SOUZA, University of California, Berkeley, JONATHAN YATES, Cambridge University, United Kingdom — Energy states of nonmagnetic metals may be chosen to be purely spin up and down in the absence of spin-orbit coupling. Spin-orbit coupling mixes the two states by a small amount b^2. A spin-conserving interaction (e.g. electron-phonon) causes transitions between the two states, and flips the electron's spin. Some insight into this Elliot-Yafet spin relaxation mechanism can be obtained by averaging b^2 over the Fermi surface. In trivalent metals, such as aluminum, $b^2 \ll 1$ almost everywhere on the Fermi surface, except at small "hot spot" regions. [1] Although the small regions of large b^2 dominate the spin relaxation process, they are difficult to capture numerically. We describe a Wannier interpolation strategy [2] to compute $\langle b^2 \rangle$. We validate it by performing *ab initio* calculations on aluminum, finding good agreement with previous results.[1] We also discuss interpolating *ab initio* electron-phonon matrix elements to compute the spin relaxation rate.

[1] J. Fabian and S. Das Sarma, Phys. Rev. Lett. **81**, 5624 (1998).
[2] X. Wang, J. Yates, I. Souza, and D. Vanderbilt, Phys. Rev. B, in press (cond-mat/0608257).

Eric Roman
University of California, Berkeley

Date submitted: 20 Nov 2006

Electronic form version 1.4