Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Dielectric function by FLAPW method. TATSUYA SHISHIDOU, TAMIO OGUCHI, Hiroshima University — Response functions, which describe how electrons respond to external fields, are the central quantity in solid state physics. Many physical properties, such as optical spectra, phonon spectra, dielectric constant, magnetic and structural instabilities, and so on, are accessible if one can calculate the corresponding response function. Moreover, the response functions play important role in the application of many-body perturbation theory. In this paper, we present a way to calculate dynamical inverse dielectric function $\varepsilon^{-1}(r, r', \omega)$ within the framework of the all-electron full-potential linearized augmented plane wave (FLAPW) method. We work with the random phase approximation (RPA) instead of the plasmon pole approximation. Local field effects are taken into account. Details of our method and implementation will be given, focusing on its efficiency and the treatment of the Coulomb singularity at Γ point. Calculations for semiconductors, ferromagnetic $3d$ transition metals, and insulating antiferromagnetic transition-metal oxides will be presented and compared with available experiments and theories.

Tatsuya Shishidou
Hiroshima University

Date submitted: 19 Nov 2006 Electronic form version 1.4