ORBITAL MAGNETISM

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I discuss my implementation of the calculation of orbital magnetism, based on the first-order energy change due to an applied magnetic field, in an insulator. The basic formalism was derived in Ref. [1], and has been adapted to the PAW formalism by X. Gonze [2].
Because the orbital magnetism of an insulator at zero magnetic field is zero, I also implemented nuclear magnetic dipole moments as inputs and features of the ground state Hamiltonian. In the presence of an array of such moments, of fixed direction, the orbital magnetization and Chern number are both non-zero, and this provides a way to test the implementation. It is also highly relevant for experimentalists because it allows for the computation of chemical shielding, one of the observables in nuclear magnetic resonance, by the so-called "converse method" [3]. In this method the shielding σ is computed as the change in orbital magnetization as a function of dipole moment strength.
My implementation is parallelized over k points for both magnetization and Chern number, and the Chern number part can also take advantage of spatial symmetries.

References

[1] X. Gonze, J. W. Zwanziger, Phys. Rev. B **84**, 064445 (2011).

[2] X. Gonze, private communication.

[3] T. Thonhauser, D. Ceresoli, A. A. Mostofi, N. Marzari, R. Resta, D. Vanderbilt, J. Chem. Phys. **131**, 101101 (2009).