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Computation of phonon spectra from density-functional perturbation theory in the projector augmented-wave approach MARC TORRENT, FRANCOIS JOLLET, CEA, DAM, DIF. F-91297 Arpajon, France, CHRISTOPHE AUDOUZE, Laboratoire Math. Appliquées. Ecole Centrale de Paris. Grande Voie des Vignes. F-92295 Châtenay-Malabry, France, XAVIER GONZE, Unité PCPM. Université Catholique de Louvain. B-1348 Louvain-la-Neuve, Belgium — The density-functional perturbation theory expressions have been derived within the projector augmented-wave formalism (PAW) and compared to those found in the ultrasoft pseudopotential framework [1]. They have been recently implemented in the ABINIT package [2] in the case of perturbations of the atomic-displacement type. We summarize the key points of this implementation: The variational and non-variational forms of the 2nd-order total energy changes are detailed. The resolution of the variational principle by a generalized Sternheimer equation is explained (the 1st-order wave-function change is found with a band-by-band conjugate gradient algorithm). We focus on some difficulties: metallic electronic occupations, response to incommensurate perturbations of periodic systems ... Results on pure compounds are presented; a comparison with results from pseudopotentials approach is performed in order to highlight the effect of the PAW methodology and its accuracy. [1] Audouze, Jollet, Torrent and Gonze. Phys. Rev. B **73**, 235101 (2006); **78**, 035105 (2008) [2] *http://www.abinit.org.*

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