GW approximation of the many-body problem and changes in
the particle number  FABIEN BRUNEVAL, CEA, DEN, Service de Recherches
de Metallurgie Physique — A stringent test for an exchange-correlation approxima-
tion in electronic structure calculations is the equality between the ionization energy
of the neutral system and the affinity of the singly positively charged system. All
of the commonly used approximations (local, semilocal, hybrid) for the exchange
correlation within density functional theory fail badly with this test. They conse-
quently present a localization or delocalization error, resulting in a highest occupied
molecular orbital or lowest unoccupied molecular orbital gap over- or underestima-
tion [1]. The GW approximation [2] appears as the best available framework to
describe particle number changes [3]. The small remaining error can be further
reduced by devising a DeltaSCF-like method within the GW approximation. The
proposed approach is necessary as soon as localized electrons are involved. We then
show applications to molecules, ions, and defect states in crystals.