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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 approximation 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 consequently present a localization or delocalization error, resulting in a highest occupied molecular orbital or lowest unoccupied molecular orbital gap over- or underestimation [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 *Delta*SCF-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.

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