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Improved GW Γ scheme for the first-principles calculation of the electron self-energy¹ YASUTAMI TAKADA, ISSP, Univ. of Tokyo — Improvements are made on the self-consistent calculation scheme for the electron self-energy with the vertex function Γ satisfying the Ward identity, originally proposed in 2001 [1]. Although it is basically equivalent to the original one, this improved scheme not only shortens the computational time by about one hundredth but also opens new horizons in its applications: (i) If it is applied to semiconductors and insulators, the obtained quasiparticle dispersion is virtually the same as that in the one-shot GW approximation (or G_0W_0A), indicating that the G_0W_0A actually takes proper account of both vertex and high-order self-energy corrections in a mutually cancelling manner [2]. (ii) If it is applied to the Tomonaga-Luttinger model, it is reduced to the Dzyaloshinskii-Larkin theory, implying that it is a unified theory to treat both Fermi- and Luttinger-liquids on the same footing. (iii) In contrast with the original one, it can provide the convergent self-consistent solution for the low-density electron liquid where an intrinsic difficulty arises due the dielectric catastrophe associated with the negative electronic compressibility. [1]YT, PRL87, 226402 (2001). [2] S. Ishii, H. Maebashi, and YT, unpublished.

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