Comment on "Self-Consistent Calculations of Quasiparticle States in Metals and Semiconductors"

In a recent Letter, Schöne and Eguiluz (SE) [1] present a self-consistent calculation of self-energy in *GW* and polarization in the *GG* approximation. The main progress in [1] is to use full Green's functions (GF's) including damping and renormalization of the one-particle states instead of a simple quasiparticle picture. However, SE find the calculated band gap energies to disagree with experimental results. SE suggested the *GW* approximation to be not appropriate. From our point of view, the reason is less the *GW* approximation, but more the construction of a corresponding polarization function.

The question of self-consistent approximations for self-energy and polarization was discussed by Baym and Kadanoff [2,3]. They stated that the mean field (Hartree) description is consistent with an RPA polarization function. Since the Hartree field vanishes because of electroneutrality, free GF's should be used in this approximation. This is the reason why other authors used a so-called restricted self-consistent approach with a fixed polarization function [2]. More general, Ward's identity [5] connects any frequency dependent damping with vertex corrections. This identity is related to gauge invariance ensuring charge conservation [6] and leads to the f-sum rule for the inverse dielectric function [7], given by

$$F[\varepsilon^{-1}] = -\frac{2}{\pi}\,\Omega_{\mathrm{pl}}^{-2}\int_0^{+\infty} d\Omega\;\Omega\;\mathrm{Im}\varepsilon^{-1}(q,\Omega) = 1\,.$$

It is not our aim to discuss systematically which polarization function is related with the *GW* approximation for the self-energy [8,9], but we show that at least the first vertex correction in the polarization function, given in Keldysh notation by

$$\Pi'(1,1') = G(1,2)G(3,1)W(2,3)G(2,1')G(1',3)$$

has to be taken into account. A self-consistent, iterative calculation of self-energy and polarization (in the *GG* approximation) was already presented [10]. Here, we include the vertex correction Π', calculated with free GF's and a dynamically screened interaction. Figure 1 shows the f sum for an electron gas with $T = 0.6$ Ry and $n_e = 1.5 \times 10^{-5} a_B^{-3}$. Main contributions to the self-energy come from small q values; $q = \sim 0\text{–}5\kappa_D$ (κ_D: inverse Debye radius), where a plasmon exists. In this region, an RPA polarization function with dressed GF's leads to a strong violation of the f-sum rule. From our point of view, this (and not the *GW* approximation for the self-energy) seems to be the main reason why the results in [1] fail to agree with experimental data.

Another method to construct conserving approximations, which is based on a linear response approach, is given in [11]. It allows one to include collisions in the polarization function in such a way that the sum rules are fulfilled within the numerical accuracy.

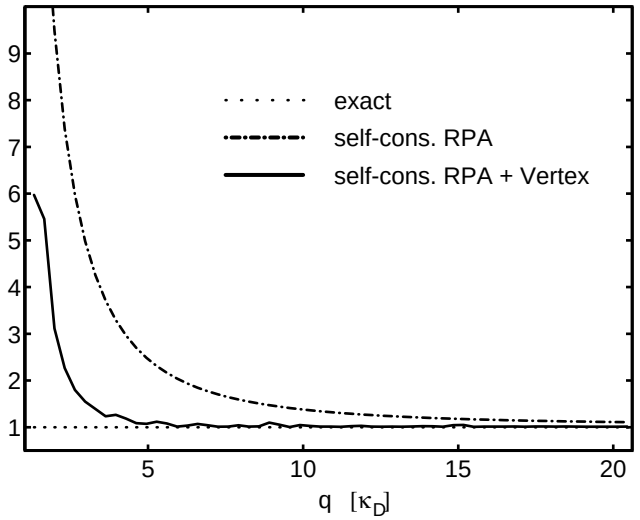

FIG. 1. f-sum rule as a function of q.

The determination of the polarization function from kinetic theory [12] also allows one to fulfill the f-sum rule within numerical accuracy [13].

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Received 30 September 1998
PACS numbers: 71.10.–w, 05.30.Fk, 71.45.Gm

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