GW approach to the calculation of electron self-energies in semiconductors

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Various approximation schemes concerning the calculation of the electron self-energy M for a semiconductor in the (bubble) GW scheme of Hedin [Phys. Rev. 139, A796 (1965)] are discussed. It is shown by using a contour-deformation procedure in the complex energy plane that M, as obtained in the first iteration cycle of the GW scheme, is Hermitian for real energies $|\varepsilon| < 3\varepsilon_g/2$, where ε_g is the unperturbed energy gap, and non-Hermitian for $|\varepsilon| > 3\varepsilon_g/2$. The Taylor expansion for M around the midgap energy value $\varepsilon=0$ has a convergence radius of $3\varepsilon_g/2$. Extended use of a (truncated) Taylor series at $|\varepsilon| > 3\varepsilon_g/2$ is not capable of giving the non-Hermitian part of M, while there is also no guarantee that the Hermitian part is correctly obtained in this way.

I. INTRODUCTION

Successful *ab initio* quasiparticle band-structure calculations for semiconductors are well within reach nowadays.[1-5] There is growing evidence that reliable predictions follow already from the relatively simple (bubble) GW approximation scheme of Hedin,[6] in which, moreover, it turns out to be allowed to approximate the single-particle Green function G by its simplified local-density-approximated version $G^{(0)}$.

In such a GW calculation of the electron self-energy M, one is confronted with an integration of the product of G and the screened Coulomb interaction W along the entire real energy axis. Direct evaluation of this integral for, e.g., one of the plane-wave matrix elements of M, reveals that the integrand consists of a sum over wave vectors $\mathbf{k}'$ in the first Brillouin zone (1BZ) of an expression which contains zero denominators for a large variety of combinations of energy and wave vector.

A possible way to deal with this expression is to apply a contour-deformation procedure in the complex energy plane, such that an energy integration results along the *imaginary* energy axis.[6,7] The above denominator problem is then circumvented and the involved $\mathbf{k}'$ summations, after having dealt in an appropriate way with the $1/|\mathbf{k}'|^2$ singularity due to the Coulomb potential and the nonanalytic behavior of W around $\mathbf{k}'=\mathbf{0}$, can be performed by using a special-point–integration procedure.[8,9] It follows, however, that *except for real energies within the energy gap,* the contour-deformation procedure also gives rise to additional pole contributions, the evaluation of which still requires the knowledge of W at (almost) real energies. Though a direct calculation of W at real energies is well within reach,[10] it would certainly be of interest to investigate whether an evaluation of the pole contributions could be avoided. In the approach of Godby, Schlüter, and Sham[5] to this problem, the above-mentioned pole contributions appear to play no role, since these authors advocate the use of the analytical continuation of the Taylor-expanded self-energy M as obtained for purely imaginary energies [see their expression (25)]. One of the interesting questions in this connection, to be discussed below, is to what extent, *for real energy values outside the energy gap* this Taylor-expanded self-energy indeed yields the correct self-energy M.

It is shown that the non-Hermitian part of M *cannot* be obtained in this way. As far as the Hermitian part is concerned, the question can in practical cases be answered by comparing truncated Taylor-series expansions with the exact expressions. the apparent successes of plasmon-pole models suggest that a truncated Taylor expansion may very well be adequate.

In this paper we take the opportunity to rubricate a number of common and uncommon approximations to M in the (bubble) GW scheme.

We have chosen to start from plane-wave matrix elements of the two-point function $M(\mathbf{r}_1,\mathbf{r}_2;\varepsilon)$. Though it is not strictly necessary to do so for all our arguments, it emphasizes the difficulties encountered in performing wave-vector summations over 1BZ.

II. THE CONTOUR-DEFORMATION PROCEDURE

We start from an expression for the (bubble) GW self-energy, in which G is replaced by $G^{(0)}$, while W may be identified by the random-phase-approximation (RPA) bubble expression $W^{(0)}$ in terms of the Green function $G^{(0)}$. In the $G^{(0)}W^{(0)}$ approximation it is straightforward to show[11] that the self-energy in Fourier-transformed form reads

$$M_{\mathbf{G},\mathbf{G}'}(\mathbf{k};\varepsilon)=\frac{i}{2\pi\hbar^2\Omega}\sum_{\mathbf{k}'}\sum_{\mathbf{K}}\sum_{\mathbf{K}'}F_{\mathbf{K},\mathbf{K}'}(\varepsilon,\mathbf{G},\mathbf{G}',\mathbf{k},\mathbf{k}')\ , \tag{1}$$

where $\mathbf{G},\mathbf{G}',\mathbf{K},\mathbf{K}'$ are reciprocal lattice vectors; $\mathbf{k}$ and $\mathbf{k}'$ are wave vectors in 1BZ; ε is the energy; Ω the crystal volume. The functions F occurring in (1) may be expressed as

$$F_{\mathbf{K},\mathbf{K}'}(\varepsilon,\mathbf{G},\mathbf{G}',\mathbf{k},\mathbf{k}')=\hbar\sum_l d_{l,\mathbf{k}-\mathbf{k}'}(\mathbf{K})d^*_{l,\mathbf{k}-\mathbf{k}'}(\mathbf{K}')\int_{-\infty}^{+\infty}d\varepsilon'\frac{W^{(0)}_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}';\varepsilon')e^{-i\varepsilon'\eta_1/\hbar}}{\varepsilon-\varepsilon'-\varepsilon_l(\mathbf{k}-\mathbf{k}')-i\eta_0\mathrm{sgn}[\mu-\varepsilon_l(\mathbf{k}-\mathbf{k}')]}\ . \tag{2}$$

Here the $d_{l,\mathbf{k}-\mathbf{k}'}(\mathbf{K})$'s are plane-wave coefficients of the Bloch wave functions with band index l and energy $\varepsilon_l(\mathbf{k}-\mathbf{k}')$, as obtained, e.g., in the LDA framework. In what follows the functions $W^{(0)}_{\mathbf{K},\mathbf{K}'}(\mathbf{k}';\varepsilon')$ will be written

$$W^{(0)}_{\mathbf{K},\mathbf{K}'}(\mathbf{k}';\varepsilon')=v_{\mathbf{K},\mathbf{K}'}(\mathbf{k}')+\tilde{W}^{(0)}_{\mathbf{K},\mathbf{K}'}(\mathbf{k}';\varepsilon')\ , \tag{3}$$

where $v_{\mathbf{K},\mathbf{K}'}(\mathbf{k}')$ denotes a matrix element of the bare Coulomb interaction and $\tilde{W}^{(0)}_{\mathbf{K},\mathbf{K}'}(\mathbf{k}';\varepsilon')$ the screening correction. The chemical potential μ lies somewhere in the band gap and separates valence and conduction bands; $\mathrm{sgn}(x)=x/|x|$; η_0 and η_1 are infinitesimally small positive quantities. The function $\tilde{W}^{(0)}_{\mathbf{K},\mathbf{K}'}(\mathbf{k}';\varepsilon')$ is a symmetric function of complex energy ε', and is free of poles in the first and third quadrants in the complex ε' plane. This can for instance be verified from Eq. (C5) of Ref. 12. The asymptotic behavior of $|\tilde{W}^{(0)}(\varepsilon')|$ is $O(|\varepsilon'|^{-2})$ for $|\varepsilon'|\to\infty$. The expression (2) is easily arrived at by starting from Eq. (35) of Ref. 11. It is straightforward to show that Eq. (2) may be transformed into the expression

$$\begin{aligned}F_{\mathbf{K},\mathbf{K}'}(\varepsilon,\mathbf{G},\mathbf{G}',\mathbf{k},\mathbf{k}')=&2\pi i\hbar\sum_l d_{l,\mathbf{k}-\mathbf{k}'}(\mathbf{K})d^*_{l,\mathbf{k}-\mathbf{k}'}(\mathbf{K}')\\&\times\Bigg[\Theta(\mu-\varepsilon_l(\mathbf{k}-\mathbf{k}'))v_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}')+\frac{1}{2\pi i}\int_{-i\infty}^{+i\infty}d\varepsilon'\frac{\tilde{W}^{(0)}_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}';\varepsilon')}{\varepsilon-\varepsilon'-\varepsilon_l(\mathbf{k}-\mathbf{k}')}\\&+[\Theta(\mu-\varepsilon_l(\mathbf{k}-\mathbf{k}'))\Theta(\varepsilon_l(\mathbf{k}-\mathbf{k}')-\varepsilon)-\Theta(\varepsilon_l(\mathbf{k}-\mathbf{k}')-\mu)\Theta(\varepsilon-\varepsilon_l(\mathbf{k}-\mathbf{k}'))]\ ,\\&\times\tilde{W}^{(0)}_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}';\varepsilon-\varepsilon_l(\mathbf{k}-\mathbf{k}'))\Bigg]\ ,\end{aligned} \tag{4}$$

where Θ denotes the Heaviside unit-step function. The first term contributing to (4) is arrived at by closing the integration contour in (2) in the lower half-ε'-plane and by collecting the residues. The remaining terms in (4) are obtained by closing the integration contour in (2) by means of two circular contours in the first and third quadrants and the imaginary ε' axis. Due to the asymptotic character of $\tilde{W}^{(0)}_{\mathbf{K},\mathbf{K}'}(\mathbf{k}';\varepsilon')$ for $|\varepsilon'|\to\infty$ the circular contours do not contribute, such that apart from residue contributions an integral along the imaginary ε' axis results. Note that in case $\varepsilon=\varepsilon_l(\mathbf{k}-\mathbf{k}')$ the integral in (4) is to be considered as a principal-value integral. Consistent with this, we define $\Theta(0)=\frac{1}{2}$. The first term in (4) is relatively easy to evaluate, while the same holds for the integral contribution as the procedure of obtaining $\tilde{W}^{(0)}$ at imaginary energies is *relatively* simple. A special-point–integration technique can be employed here.[8–10] Closer examination of the residue contributions in (4) reveals that valence bands only give rise to pole contributions if $\varepsilon<\varepsilon_{lv}(\mathbf{k}-\mathbf{k}')$, whereas conduction bands contribute only if $\varepsilon>\varepsilon_{lc}(\mathbf{k}-\mathbf{k}')$. Clearly there are no pole contributions at all if ε is located within the (unperturbed) energy gap of the semiconductor. We will make use of this further on, where it will be argued that it is possible (with certain restrictions) by constructing and using the *analytical continuation* of the integral term in (4) as a function of ε, to circumvent the use of the pole contributions in (4) for values of ε exceeding the gap region. Before doing so we first discuss two (static) approximation schemes to M.

III. STATIC APPROXIMATIONS TO M

When considering (2) we might as a first crude approximation set $\tilde{W}^{(0)}_{\mathbf{K},\mathbf{K}'}(\mathbf{k}';\varepsilon)\equiv 0$ for real ε. The resulting expression for $F_{\mathbf{K},\mathbf{K}'}$ reads

$$\begin{aligned}&F_{\mathbf{K},\mathbf{K}'}(\varepsilon,\mathbf{G},\mathbf{G}',\mathbf{k},\mathbf{k}')\\&\simeq 2\pi i\hbar\sum_l d_{l,\mathbf{k}-\mathbf{k}'}(\mathbf{K})d^*_{l,\mathbf{k}-\mathbf{k}'}(\mathbf{K}')\\&\quad\times[\Theta(\mu-\varepsilon_l(\mathbf{k}-\mathbf{k}'))v_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}')]\ ,\end{aligned} \tag{5}$$

with contributions due to the valence bands only; expression (5) has Hartree-Fock *character*. It does not, when used in (1), lead to the Hartree-Fock self-energy, as the $d_{l,\mathbf{k}-\mathbf{k}'}(\mathbf{K})$ coefficients do not belong to self-consistently-obtained Hartree-Fock Bloch wave functions.

As a second approximation to M we might consider the possibility of approximating the function $W^{(0)}_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}';\varepsilon')$ occurring in (2) for real ε', by a constant. In doing so we will discuss two procedures, the second of which [Coulomb-hole plus screened-exchange (COHSEX) approximation] is definitely superior to the first one [statistically screened Hartree-Fock (SSHF) approximation]. In the first procedure we put $W^{(0)}_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}';\varepsilon')=W^{(0)}_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}';0)$ in (2), take this factor out of the integral and perform the remaining ε' integration by closing the integration contour in the lower half-ε'-plane [because of $\exp(-i\varepsilon'\eta_1/\hbar)$], just as in the procedure of obtaining the earlier result (5):

$$\begin{aligned}&F_{\mathbf{K},\mathbf{K}'}(\varepsilon,\mathbf{G},\mathbf{G}',\mathbf{k},\mathbf{k}')\\&\simeq 2\pi i\hbar\sum_l d_{l,\mathbf{k}-\mathbf{k}'}(\mathbf{K})d^*_{l,\mathbf{k}-\mathbf{k}'}(\mathbf{K}')\\&\quad\times\Theta(\mu-\varepsilon_l(\mathbf{k}-\mathbf{k}'))W_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}';0)\ ,\end{aligned} \tag{6}$$

which may be viewed upon as a SSHF expression, or al-

ternatively as a screened-exchange (SEX) expression (see, e.g., Ref. 12, p. 39 for this procedure).

In the second procedure we argue as follows: The exponential factor $\exp(-i\varepsilon'\eta_1/\hbar)$ is *essential* only in the evaluation of the integral of the energy-independent part $v_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}')$ contributing to $\tilde{W}^{(0)}_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}';\varepsilon')$. This ε' integral, as mentioned above, can be done by closing the contour in the lower half-plane. However, when dealing with the function $\tilde{W}^{(0)}_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}';\varepsilon')$ in the integral (2) we easily come to the conclusion, in view of its asymptotic behavior $O(|\varepsilon'|^{-2})$ for $|\varepsilon'|\to\infty$, that the exponential factor may as well be replaced by 1. If then this function $\tilde{W}^{(0)}_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}';\varepsilon')$ is subsequently taken to be a constant, the remaining integral yields $\pi i[\Theta(\mu-\varepsilon_l(\mathbf{k}-\mathbf{k}'))-\Theta(\varepsilon_l(\mathbf{k}-\mathbf{k}')-\mu)]$ instead of $2\pi i\Theta(\mu-\varepsilon_l(\mathbf{k}-\mathbf{k}'))$. The resulting F function is then

$$\begin{aligned}F_{\mathbf{K},\mathbf{K}'}(\varepsilon,\mathbf{G},\mathbf{G}',\mathbf{k},\mathbf{k}')&\simeq 2\pi i\hbar\sum_l d_{l,\mathbf{k}-\mathbf{k}'}(\mathbf{K})d^*_{l,\mathbf{k}-\mathbf{k}'}(\mathbf{K}')\{\Theta(\mu-\varepsilon_l(\mathbf{k}-\mathbf{k}'))[v_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}')+\tfrac{1}{2}\tilde{W}^{(0)}_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}';0)]\\&\qquad-\tfrac{1}{2}\Theta(\varepsilon_l(\mathbf{k}-\mathbf{k}')-\mu)\tilde{W}^{(0)}_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}';0)\}\\&=2\pi i\hbar\sum_l d_{l,\mathbf{k}-\mathbf{k}'}(\mathbf{K})d^*_{l,\mathbf{k}-\mathbf{k}'}(\mathbf{K}')[\Theta(\mu-\varepsilon_l(\mathbf{k}-\mathbf{k}'))W^{(0)}_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}';0)-\tfrac{1}{2}\tilde{W}^{(0)}_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}';0)]\,.\end{aligned}\tag{7}$$

This result may be identified as the COHSEX approximation[6,11] to the electron self-energy. Clearly both valence and conduction bands contribute in this approximation. The additional term involving the factor $\frac{1}{2}\tilde{W}^{(0)}_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}';0)$ represents the so-called Coulomb-hole (COH) correction. Indeed, when transforming the matrix elements $M_{\mathbf{G},\mathbf{G}'}(\mathbf{k}';\varepsilon)$ related to (7) back to real space, both the SSHF and COHSEX contributions are recovered in the form presented earlier by Hedin and Lundqvist.[12]

IV. DYNAMIC APPROXIMATIONS TO M

We now discuss approximations to M in which the ε' dependence of $\tilde{W}^{(0)}$ will not be neglected. In this connection we will concentrate on the function

$$h^l_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k},\mathbf{k}';\varepsilon)=\frac{1}{2\pi i}\int_{-\infty}^{+\infty}d\varepsilon'\frac{\tilde{W}^{(0)}_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}';\varepsilon')}{\varepsilon-\varepsilon'-\varepsilon_l(\mathbf{k}-\mathbf{k}')-i\eta_0\mathrm{sgn}[\mu-\varepsilon_l(\mathbf{k}-\mathbf{k}')]}\,,\tag{8}$$

which apart from the factor $1/2\pi i$ is the contribution to the integral occurring in (2) due to the screening only. As shown before this function can, by the contour-deformation procedure, be written alternatively in terms of an integral along the imaginary ε' axis and an additional pole contribution [see Eq. (4)]. We first want to emphasize that the thus-obtained integral along the imaginary ε' axis is nonanalytic at $\varepsilon=\varepsilon_l(\mathbf{k}-\mathbf{k}')$. This can, e.g., be seen by using the following identity:

$$\frac{1}{2\pi i}\int_{-i\infty}^{+i\infty}d\varepsilon'\frac{\tilde{W}^{(0)}_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}';\varepsilon')}{\varepsilon-\varepsilon'-\varepsilon_l(\mathbf{k}-\mathbf{k}')}=\frac{1}{\pi}\mathrm{sgn}[\varepsilon-\varepsilon_l(\mathbf{k}-\mathbf{k}')]\int_0^\infty dt\frac{1}{1+t^2}\tilde{W}^{(0)}_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}';it[\varepsilon-\varepsilon_l(\mathbf{k}-\mathbf{k}')])\,,\tag{9}$$

from which the discontinuity at $\varepsilon=\varepsilon_l(\mathbf{k}-\mathbf{k}')$ is easily found to be equal to $\tilde{W}_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}';0)$. This discontinuity is, however, precisely canceled by the discontinuity in the pole-contribution term [cf. Eq. (4)] occurring at $\varepsilon=\varepsilon_l(\mathbf{k}-\mathbf{k}')$. Consequently the function $h^l_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k},\mathbf{k}';\varepsilon)$ in (8), with which we started in (2), does not have a discontinuity at all at $\varepsilon=\varepsilon_l(\mathbf{k}-\mathbf{k}')$.

In view of this, let us introduce the following two functions of a complex variable z:

$$f^l_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k},\mathbf{k}';z)=\frac{-1}{2\pi i}\int_{-i\infty}^{+i\infty}d\varepsilon'\frac{\tilde{W}^{(0)}_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}';\varepsilon')}{\varepsilon'+\varepsilon_l(\mathbf{k}-\mathbf{k}')-z}\,,\tag{10}$$

$$\begin{aligned}g^l_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k},\mathbf{k}';z)&=f^l_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k},\mathbf{k}';z)\\&\quad+[\Theta(\mu-\varepsilon_l(\mathbf{k}-\mathbf{k}'))\Theta(\varepsilon_l(\mathbf{k}-\mathbf{k}')-\mathrm{Re}(z))-\Theta(\varepsilon_l(\mathbf{k}-\mathbf{k}')-\mu)\Theta(\mathrm{Re}(z)-\varepsilon_l(\mathbf{k}-\mathbf{k}'))]\\&\quad\times\tilde{W}^{(0)}_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}',z-\varepsilon_l(\mathbf{k}-\mathbf{k}'))\,.\end{aligned}\tag{11}$$

It can easily be verified, using (7), (8), and (11), that for real z the function g^l coincides with the function h^l, i.e.,

$$g^l_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k},\mathbf{k}';\varepsilon)=h^l_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k},\mathbf{k}';\varepsilon)\qquad(\varepsilon\text{ real})\,.\tag{12}$$

The function f^l of (10) is defined as an integral along the imaginary ε' axis. The integrand is analytic in the whole complex z plane except if $z=\varepsilon'+\varepsilon_l(\mathbf{k}-\mathbf{k}')$. According to a well-known theorem of functions of complex variables[13] the function $f^l(z)$ can only be nonanalytic on the line $\mathrm{Re}(z)=\varepsilon_l(\mathbf{k}-\mathbf{k}')$. Indeed, the function f^l *has* a discontinuity[14] across the line $\mathrm{Re}(z)=\varepsilon_l(\mathbf{k}-\mathbf{k}')$ equal to $\tilde{W}_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}';z-\varepsilon_l(\mathbf{k}-\mathbf{k}'))$. On the other hand, the

function g^l of (11) is continuous across this line since the Θ-function contributions precisely cancel the discontinuity in f^l. Using Riemann's principle[15] it follows that $g^l_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k},\mathbf{k}';z)$ is analytic across the line $\mathrm{Re}(z)=\varepsilon_l(\mathbf{k}-\mathbf{k}')$, and consequently analytic in the whole complex z plane, *except* for singularities of the function $\tilde{W}^{(0)}_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}',z-\varepsilon_l(\mathbf{k}-\mathbf{k}'))$. Because of this analyticity, the function g^l can be expanded in a Taylor series around $z=0$. The radius of convergence of this series, $R_l(\mathbf{k}-\mathbf{k}')$, is determined by the singularity of $\tilde{W}^{(0)}_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}',z-\varepsilon_l(\mathbf{k}-\mathbf{k}'))$ which lies closest to $z=0$. In RPA the closest singularities will be located at $z=z_c=\pm\min_{\mathbf{k}''}\{\varepsilon_{lc}(\mathbf{k}''+\mathbf{k}')-\varepsilon_{lv}(\mathbf{k}'')\}+\varepsilon_l(\mathbf{k}-\mathbf{k}')$ with $\mathbf{k}''$ in 1BZ, where lc and lv indicate the energetically lowest conduction and highest valence band, respectively. This is based on the observation that $\min_{\mathbf{k}''}\{\varepsilon_{lc}(\mathbf{k}''+\mathbf{k}')-\varepsilon_{lv}(\mathbf{k}'')\}$ is the smallest energy ε at which some denominators in the polarization function $P^{(0)}_{\mathbf{K},\mathbf{K}'}(\mathbf{k}',\varepsilon)$ vanish; see, e.g., Eq. (40) of Ref. 11. The apparent nonanalyticity at this ε value is therefore also present in the functions $\tilde{W}^{(0)}_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}';\varepsilon)$. The absolute value of this energy ε is at least equal to the unperturbed energy gap ε_g. Note, incidentally, that this is the minimum energy required to excite an electron-hole pair in the semiconductor. Measuring the band energies from the midgap-energy value, the absolute minimum value for $R_l(\mathbf{k}-\mathbf{k}')$ equals

$$R_l(\mathbf{k}-\mathbf{k}')=\varepsilon_g+\varepsilon_l(\mathbf{k}-\mathbf{k}')\ , \tag{13}$$

if l stands for a conduction band, and

$$R_l(\mathbf{k}-\mathbf{k}')=\varepsilon_g-\varepsilon_l(\mathbf{k}-\mathbf{k}')\ , \tag{14}$$

if l stands for a valence band.

In view of the above considerations we may now write

$$h^l_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k},\mathbf{k}';\varepsilon)=\sum_{m=0}^{\infty} a^l_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k},\mathbf{k}';m)\varepsilon^m\ , \quad |\varepsilon|<R_l(\mathbf{k}-\mathbf{k}') \tag{15}$$

where the coefficients are given by

$$a^l_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k},\mathbf{k}';m)=\frac{1}{m!}\frac{d^m}{dz^m}g^l_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k},\mathbf{k}';z)|_{z=0}=\frac{1}{m!}\frac{d^m}{dz^m}f^l_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k},\mathbf{k}';z)|_{z=0}\ . \tag{16}$$

In order to obtain $M_{\mathbf{G},\mathbf{G}'}(\mathbf{k};\varepsilon)$ we have to perform the summations over $\mathbf{k}',\mathbf{K},\mathbf{K}',l$ as indicated in Eqs. (1) and (2). As a general result we may then write

$$M_{\mathbf{G},\mathbf{G}'}(\mathbf{k};\varepsilon)=M^{\mathrm{HF}}_{\mathbf{G},\mathbf{G}'}(\mathbf{k})+\sum_{m=0}^{\infty} b_{\mathbf{G},\mathbf{G}'}(\mathbf{k},m)\varepsilon^m\ , \tag{17}$$

where the first term in the right-hand side of (17) stands for the Hartree-Fock-like contribution and where the $b_{\mathbf{G},\mathbf{G}'}$ coefficients are related to the above a^l coefficients in an obvious way. The radius of convergence of the series in (17) is determined by the minimum value of all $R_l(\mathbf{k}-\mathbf{k}')$ radii, which is $R=3\varepsilon_g/2$.

The merit of the expression (17) lies in the fact that as long as we limit ourselves to $|\varepsilon|<3\varepsilon_g/2$, we do not have to evaluate pole contributions to (4) explicitly. The direct calculation of $\tilde{W}^{(0)}$ at such real energies is thus avoided. In practice it is to be expected that only a few terms in the Taylor-expansion expression have to be evaluated.[5]

The question now arises what to do if $|\varepsilon|>3\varepsilon_g/2$. This question is relevant since we know that the exact energy gap in most cases will be larger[3] than the unperturbed LDA gap ε_g, such that in order to obtain a renormalized band structure, we very likely have to consider values of $M_{\mathbf{G},\mathbf{G}'}(\mathbf{k};\varepsilon)$ at $|\varepsilon|$ values exceeding the value $3\varepsilon_g/2$, if at least the band structure in the close vicinity of the energy gap is to be predicted. A first answer to this question might be to use *a truncated* version of the Taylor expansion in (17) for larger $|\varepsilon|$ values [note that the full series expansion in (17) is *divergent* for the latter energy values]. Indeed, it is known that rather good approximations to $\tilde{W}^{(0)}$ exist whose dynamical behavior is completely described in terms of plasmon poles, located at energies far away from the energy-gap region. Extended use of (17), employing a few terms in the expansion only, could therefore very well yield very good approximate renormalized band structures. This has, however, in principle to be verified by comparing the thus-obtained band structures with those obtained in the framework of an exact evaluation of the integral and pole contributions to M. Such a direct evaluation of the various contributing terms in (4) is indeed within reach, including the pole contributions. In this connection we refer to Ref. 10 where a novel and fast method is outlined for a direct calculation of the RPA dielectric function at real energies. The necessary $W^{(0)}$-matrix elements in (4) can then easily be obtained by subsequent inversion of this dielectric function. However, purely on the basis of the apparent nonanalyticity of $\tilde{W}^{(0)}_{\mathbf{K},\mathbf{K}'}(\mathbf{k}';\varepsilon)$ for $|\varepsilon|>\varepsilon_g$ the use of (17) is suspicious and needs further investigation.

Extended use of (17) is of course incapable of giving *the non-Hermitian part* of M at real energies for which $|\varepsilon|>3\varepsilon_g/2$, as the matrix elements $M_{\mathbf{G},\mathbf{G}'}(\mathbf{k};\varepsilon)$ given by (17) belong to a *Hermitian* matrix. This Hermiticity can be traced back to that of the matrix f^l for real z [see Eq. (10)], which gives rise to Hermitian matrix elements $b_{\mathbf{G},\mathbf{G}'}(\mathbf{k},m)$ in (17). In order to show the Hermiticity of f^l for real z, use has to be made of the property $\tilde{W}^{(0)}_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k};\varepsilon')=\tilde{W}^{(0)}_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k};-\varepsilon')$ and of the Hermiticity of the $\tilde{W}^{(0)}$ matrix at purely imaginary energy. Note that these two properties of $\tilde{W}^{(0)}$ hold as well for the exact $\tilde{W}$ function as can easily be verified from Eq. (C5) of Ref. 12.

On the other hand, we know that the function M obtained in the (bubble) $G^{(0)}W^{(0)}$ approximation at real energies $|\varepsilon|>3\varepsilon_g/2$ is a non-Hermitian function indeed. This is a consequence of the pole contribution occurring in (4), which for $|\varepsilon-\varepsilon_l(\mathbf{k}-\mathbf{k}')|>\varepsilon_g$ contains a non-Hermitian part due to the non-Hermiticity of the screening interaction function $\tilde{W}^{(0)}$. Again, this non-Hermiticity is a general property of the exact $\tilde{W}$ func-

tion[12] for energies exceeding the lowest excitation energy of the N-particle system. We repeat, however, that extended use of (17) might very well lead to good predictions for the *real parts* of quasiparticle energies. Note in this connection that the non-Hermiticity of M at real energies $|\varepsilon| > 3\varepsilon_g/2$ is closely related to the finite probability of particles at such an energy to decay through the excitation of electron-hole pairs (via Coulomb interaction), which is impossible if $|\varepsilon| < 3\varepsilon_g/2$. The implications of the Hermitian or non-Hermitian character of M in the respective energy regions $|\varepsilon| < 3\varepsilon_g/2$ and $|\varepsilon| > 3\varepsilon_g/2$ for quasiparticle lifetimes are not immediately obvious: one has first to solve Schrödinger-like quasiparticle equations[11] in which the above $M_{G,G'}(\mathbf{k};\varepsilon)$ matrix elements play their role, leading to eigenvalues $E_{l,\mathbf{k}}(\varepsilon)$, and secondly one has to solve the equation $E_{l,\mathbf{k}}(\varepsilon)=\varepsilon$, the (possibly complex) solutions ε of which are the quasiparticle energies. The possibility that complex solutions are obtained even with $|\mathrm{Re}(\varepsilon)| < 3\varepsilon_g/2$ cannot *a priori* be excluded.

For completeness we mention still another approach to (4) in which the $\tilde{W}^{(0)}$ functions occurring in the pole contributions are replaced by their static values at $\varepsilon-\varepsilon_l(\mathbf{k}-\mathbf{k}')=0$, while the integral along the imaginary axis is computed in full detail for all ε. We call this the static-pole approximation (SPA). The computational advantage is obvious: We only need to calculate $\tilde{W}^{(0)}$ along the imaginary ε' axis (including $\varepsilon'=0$). Improved versions in which the $\tilde{W}^{(0)}_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k}';\varepsilon-\varepsilon_l(\mathbf{k}-\mathbf{k}'))$ functions are replaced by Taylor expansions around $\varepsilon-\varepsilon_l(\mathbf{k}-\mathbf{k}')=0$ may be considered as well.

V. CONCLUSIONS

This paper deals with a variety of static and dynamic approximations to the electron self-energy matrix elements $M_{G,G'}(\mathbf{k};\varepsilon)$ in the GW-approximation scheme. While the static approximations are very likely to be of limited value when considering, e.g., quasiparticle band-structure calculations, the method of analytically continuing the functions $h^l_{\mathbf{G}-\mathbf{K},\mathbf{G}'-\mathbf{K}'}(\mathbf{k},\mathbf{k}';z)$ of (8) looks promising. The procedure advocated by Godby *et al.*[5] is in fact very similar to this method. As it is not *a priori* certain to what extent the method applies for $|\varepsilon|$-values exceeding the value $3\varepsilon_g/2$, the recommendation is that an evaluation of $M_{G,G'}(\mathbf{k};\varepsilon)$ in the spirit of Eq. (17) should be carefully compared with results to be obtained from an exact evaluation of all terms in (4). Anyhow, whether one wants to make use of the analytical-continuation method or not, the expression (4) in itself has calculational advantage over expression (2), and as such is useful if one aims at explicit evaluation of $M_{G,G'}(\mathbf{k};\varepsilon)$ matrix elements. We are currently calculating the respective contributions to M as given in (4) for the semiconductor Si. It will enable us, among other things, to investigate the eventual merits of an extrapolation polynomial obtained by truncating the Taylor expansion in (17).

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[14] In general, let $L(z)$ be a function which on $\mathrm{Re}(z)=C$ satisfies the Hölder condition, $|L(C+iy_1)-L(C+iy_2)| < A|y_1-y_2|^{\gamma}$ with both $A>0$ and $\gamma>0$. Further let $L(z)$ have the asymptotic behavior $L(C+iy)=O(|y|^{-p})$ as $|y|\to\infty$, with $p>0$. Then for the functions

$$L^+(z)\equiv -(1/2\pi i)\int_{C-i\infty}^{C+i\infty} dz'\, L(z')/(z'-z), \quad \mathrm{Re}(z)>C\ ,$$

$$L^-(z)\equiv -(1/2\pi i)\int_{C-i\infty}^{C+i\infty} dz'\, L(z')/(z'-z), \quad \mathrm{Re}(z)<C\ ,$$

holds $L^+(\zeta)-L^-(\zeta)=L(\zeta)$, in which $\mathrm{Re}(\zeta)=C$ and

$$L^+(\zeta)=\lim_{z\to\zeta,\ \mathrm{Re}(z)>C} L^+(z)\ ,$$

$$L^-(\zeta)=\lim_{z\to\zeta,\ \mathrm{Re}(z)<C} L^-(z)\ .$$

We note also that $L^+(z)$ is *analytic* in $\mathrm{Re}(z)>C$ whereas $L^-(z)$ is *analytic* in $\mathrm{Re}(z)<C$. In our case $\tilde{W}$ satisfies both the Hölder condition and the required asymptotic behavior.

[15] See Ref. 13, p. 157.