# Electron-gas self-energy at metallic density

C. Petrillo and F. Sacchetti

Dipartimento di Fisica, Università di Perugia, Perugia, Italy and Istituto di Struttura della Materia del CNR, Via Enrico Fermi 38, 00044 Frascati, Roma, Italy (Received 22 February 1988)

The self-energy of the uniform electron gas is analyzed within the lowest order in the screened potential, using different approximations for the dielectric function. The present numerical analysis reveals that a rather simple approximation for the dielectric function can be used to derive a good estimate for the self-energy.

## I. INTRODUCTION

The study of the electronic properties of a homogeneous electron gas has been of special importance in the development of solid-state physics. It is now well established that electron-gas data can be used as input parameters for application to the real systems of densityfunctional theories.<sup>1-3</sup> At present, quite good knowledge of total energy as well as static properties of electron gas seems to have been achieved.<sup>4-7</sup>

Thanks to the above results, a rather good description of the ground-state properties of real metals has been obtained<sup>8</sup> within the local-density approximation<sup>2,3</sup> (LDA).

Because of the success of LDA calculations of groundstate properties, it is rather obvious to extend such a treatment to one-particle behavior. Such an extension, based on the Sham and Kohn<sup>9</sup> LDA approximation for one-electron self-energy, has been shown to be feasible in the case of real metals<sup>10,11</sup> and in a slightly different form in the case of nonconducting systems.<sup>12</sup> In the work done on metals<sup>10,11</sup> the electron-gas self-energy obtained by Hedin<sup>13</sup> within the random-phase approximation (RPA) has been used, giving quite good results. In the case of nonconducting systems, a proper variant of the same Sham and Kohn approach<sup>9</sup> has been proved to be fairly good.<sup>12</sup> Recently,<sup>14</sup> another variant of the method has been applied to simple metals with very good results.

However, despite the obvious importance of oneelectron self-energy of electron gas, little effort has been devoted to its calculation. To our best knowledge, apart from the calculation by Hedin<sup>13</sup> and co-workers<sup>15,16</sup> within the RPA, there is only one other calculation of the self-energy<sup>17</sup> in a wide range of density, momentum, and energy. It should be remarked that little is known about the accuracy of those calculations.

To get further information on the electron-gas selfenergy, we shall analyze some aspect of practical approaches, confining ourselves to the lowest order (GW)(Refs. 13-16) and GW-like approximations. In fact, most of the available information on self-energy is based on expressions which can be cast into the standard GW form, after a proper definition of the screened potential W. It should be also observed that even the recent approach proposed by Vignale and Singwi<sup>18</sup> and Schreiber and Bross<sup>19</sup> belongs to the same class. In our opinion, to derive a meaningful approximation for the self-energy, it is very important to use fully conserving expressions in the sense of Baym and Kadanoff.<sup>20</sup> This fact has been already recognized,<sup>21</sup> but little has been said about self-energy.

We shall show that GW-like approaches are fully conserving. Moreover, a set of numerical calculations will be used to obtain a guess regarding the accuracy of the selfenergy we derived. In fact, we believe that the quality of a self-energy calculation can be established through a total-energy calculation, performed employing the selfenergy itself. This method to decide the accuracy of the self-energy is based on the fact that there exists an exact relationship between the chemical potential, and hence the self-energy, at the Fermi surface and the total energy. Using such a connection, we can assess the validity of the calculation by comparison with the accurate total energy deduced by means of the variational Monte Carlo approach.<sup>22,23</sup>

It should be also mentioned that in this way we approach the total energy through a perturbative evaluation of the interaction potential. Such a procedure, as observed by Overhauser and  $Tsai^{24}$  is expected to be more accurate than standard models based on interaction strength integration<sup>5</sup> of the interaction potential deduced from the approximate pair-correlation function.

In the following sections, we shall briefly recall the formal framework, which is fairly known, which will be followed by a discussion of the conserving condition with reference to the GW-like approximations. In addition, we shall present a set of numerical calculations of selfenergy based on simple approximations for the dielectric function and hence for the screened potential. The dielectric function will be deduced using static approximations for the *local-field* factor,<sup>5</sup> though the method can be extended to energy-dependent local fields with little numerical effort. The quality of the resulting self-energy will be discussed by comparison to total energy, thus getting a feeling about the validity of the local field itself.

#### **II. FORMAL FRAMEWORK**

To study the self-energy of the electron gas we start from the conserving approach of Baym and Kadanoff,<sup>20</sup> instead of using the series expansion in terms of the

38 3834

screened potential.13

In the conserving scheme of Baym and Kadanoff<sup>20</sup> the self-energy is given by

$$M(1,1') = -i \int V(13)G_2(13^-, 23^+)G^{-1}(21')d2d3 ,$$
(1)

where V is the bare Coulomb potential, G and  $G_2$  are the one-particle and two-particle Green's functions, and the numbers stand for space-time coordinates in standard notation. Equation (1) is conserving in the sense that, given an approximate two-particle Green's function, the solution of the Dyson equation

$$G^{-1}(11') = G_0^{-1}(11') - M(11')$$
(2)

and of Eq. (1) allows the number of particles as well as the momentum flux to be conserved. In Eq. (2)  $G_0$  is the one-particle Green's function with the Coulomb potential V switched off.

It should be remarked that, in principle,  $G_2$  can be derived from G. However, in this case, the entire procedure has to be self-consistent. To avoid such a complex selfconsistent procedure, whose feasibility has to be shown,  $G_2$  can be given as input. In this case, all observables connected to  $G_2$  cannot be deduced using  $G_2$  as derived from G, as such a procedure will lead to internal contradictions. Nevertheless, such a contradictory situation appears to be the normal practice of band-structure calculations in solids. For instance, the optical conductivity is generally deduced from one-particle wave functions obtained solving a Schrödinger equation containing approximate exchange-correlation potentials. These potentials can be considered as static approximations for the selfenergy, so that, in view of the above discussion, the calculation of the optical conductivity could be incorrect.

Starting from Eqs. (1) and (2) it is quite natural to *define* a screened potential, using the implicit form

$$G(11')W(1^+1') = -\int V(13)G_2(13^-, 23^+) \times G^{-1}(21')d2d3.$$
(3)

This definition has to be compared to the GW approximation, which implies the following form for the screened potential:

$$W(11') = \int V(12)\epsilon^{-1}(21')d2 , \qquad (4)$$

 $\epsilon(1,2)$  being the dielectric matrix.<sup>5,6,25</sup>

To compare Eqs. (3) and (4) we introduce

$$f(11',3) = \int G_2(13^-, 23^+) G^{-1}(21') d2 .$$
 (5)

For Eq. (4) to be a conserving approximation in the sense we described, the following relationship must hold:

$$f(11',3) = G(11')\epsilon^{-1}(31') .$$
(6)

Such an equation can define a meaningful dielectric matrix or alternatively a meaningful two-particle Green's function, if appropriate symmetry properties of these functions are satisfied.

Unfortunately it is not possible to show that Eqs. (5)

and (6) are compatible with the symmetry properties of  $G_2$ . However, in the case of the uniform electron gas, where  $G_2(1,2,1',2')$  depends only on coordinate differences, Eqs. (5) and (6) can be consistently satisfied.

In the general case, it is not obvious that the GW approximation is a conserving scheme and the corresponding self-energy has to be considered with some care.

### **III. NUMERICAL ANALYSIS OF SELF-ENERGY**

To study numerically the self-energy of the electron gas we use the following form in the reciprocal space for the dielectric function:

$$\epsilon(q,\omega) = 1 + \frac{Q_0(q,\omega)}{1 - G(q,\omega)Q_0(q,\omega)} , \qquad (7)$$

 $Q_0(q,\omega)$  being the Lindhard polarizability and  $G(q,\omega)$  an appropriate local-field factor. Equation (7) is quite general, however, little is known about the actual form of the local-field factor. Although some approximation for the frequency-dependent local field has been proposed,<sup>26–28</sup> we prefer to resort to the more widely employed static approximation.<sup>5</sup>

To perform this numerical study we shall confine ourselves to a number of analytical approximations which appear to be quite reasonable in calculating the total energy by using the standard interaction strength integration algorithm.<sup>5</sup>

We have employed four different local fields, namely

$$G(q) = 0 , \qquad (8a)$$

$$G(q) = \frac{1}{2} \frac{q^2}{q^2 + 2k_F^2} , \qquad (8b)$$

$$G(q) = \frac{1}{2} \frac{q^2}{q^2 + k_F^2}$$
, (8c)

$$G(q) = A \left[ \frac{q}{k_F} \right]^4 + B \left[ \frac{q}{k_F} \right]^2 + C$$
  
+  $\left[ A \left[ \frac{q}{k_F} \right]^4 + (B + \frac{8}{3}A) \left[ \frac{q}{k_F} \right]^2 - C \right]$   
 $\times \frac{4k_F^2 - q^2}{4k_F q} \ln \left| \frac{2k_F + q}{2k_F - q} \right|,$  (8d)

where the equations refer to the RPA, Ref. 29, Ref. 30, and Ref. 31, respectively,  $k_F$  being the Fermi momentum and A, B, and C appropriate functions of electron density.<sup>5,30</sup> The RPA calculation has been already performed by Hedin<sup>13</sup> and has been repeated here for comparison purposes.

Employing the dielectric function of Eq. (7), the selfenergy is readily deduced as an integral in the energy momentum space

$$M(q,\omega) = \frac{i}{(2\pi)^4} \int d\omega' \int d\mathbf{q}' \frac{4\pi e^2}{q'^2} \epsilon^{-1}(q',\omega') \\ \times (\omega - \omega' - |\mathbf{q} - \mathbf{q}'|^2)^{-1} .$$
(9)

The numerical evaluation of Eq. (9) can be performed

along the lines described in Refs. 13 and 17. No special difficulty is present in performing such a calculation apart from the presence of the plasmon pole contribution. To handle the diverging behavior of  $1/\epsilon(q,\omega)$  when the energy is close to the plasma frequency, we added an imaginary part to the plasmon energy. This imaginary contribution shifts the plasmon pole from the real axis and, in principle, should be taken vanishingly small. Several values for the imaginary part have been tried to derive a converging self-energy within 1 mRy. It should be remarked that special care has been devoted to the calculation of  $M(q,\omega)$  at the Fermi surface, to obtain a chemical potential as accurate as possible. Present numerical accuracy on  $M(k_F, k_F^2)$  is estimated to be of the order of 0.1 mRy.

Finally, we observe that in Eq. (9) the actual oneparticle Green's function is assumed to be well approximated by that of free particles. Therefore, the present calculation is not a self-consistent estimate of Eqs. (3) and (6). However, the main purpose of present analysis is the study of the effect of the local field so that selfconsistency is considered a secondary requirement. As a check, we determined the self-consistent self-energy at selected values of energy, momentum, and density and we found that self-consistency has a little effect on the selfenergy itself, according to Hedin<sup>13</sup> who reached similar conclusions.

Several densities  $n = 3/4\pi r_s^3$  have been considered with  $r_s$  ranging from 0.1 to 50. Typical results are reported in Table I, where the self-energy is given for the different local fields at selected values of the momentum along the free-electron parabola  $\omega = q^2$ .

Comparing present results within the RPA with the self-energy given by  $Hedin^{13}$  we see that they agree to 1 or 2 mRy, so that we expect both calculations to be accurate at least at this level, also in view of the numerical checks we have performed.

Looking at Table I, we see that the effect of the local field is not negligible: the difference between two different calculations being tens of mRy. Moreover the local field also effects the q dependence of the self-energy. As a consequence of the chosen local field we can expect an effect on the shape of the spectral weight function. Before performing a spectral analysis to study the single-particle behavior with different local fields, it is worthwhile to derive the total energy of the system.

First of all we recall that the following exact relationship holds:<sup>13</sup>

$$\boldsymbol{\epsilon}(\boldsymbol{r}_s) = \frac{3}{5} \left[ \frac{1}{\alpha \boldsymbol{r}_s} \right]^2 + 3r_s^3 \int_{\boldsymbol{r}_s}^{\infty} \frac{\boldsymbol{M}_0(\boldsymbol{x})}{\boldsymbol{x}^4} d\boldsymbol{x} \quad , \tag{10}$$

where  $\alpha = (4/9\pi)^{1/3}$ ,  $\epsilon(r_s)$  is the total energy per particle, and  $M_0(r_s) = M(k_F, k_F^2)$  is the self-energy at the Fermi surface.

Assuming that  $\epsilon(r_s)$  is known as a result of the Monte Carlo calculation,<sup>4</sup> Eq. (10) can be used to derive a rather accurate estimate of  $M_0(r_s)$ . In fact, we have

$$M_0(r_s) = \frac{2}{3} r_s^2 \epsilon(r_s) - \frac{1}{3} r_s^2 \frac{d\epsilon}{dr_s} - \frac{4}{5} \frac{1}{\alpha^2 r_s} .$$
(11)

To evaluate  $M_0(r_s)$  from the accurate Monte Carlo data, we employed the analytical fit suggested by Vosko, Wilk, and Nusair,<sup>23</sup> thus deducing an estimate of the Fermisurface self-energy, which can be considered as a reference for other calculations.

Comparison between the different self-energies as deduced from Eqs. (9) and (11) is given in Table II. It is apparent that the simple local field introduced by Geldart and Vosko<sup>29</sup> gives the best estimate of  $M_0(r_s)$  in the whole metallic density region.

It is somewhat surprising that the local field of Ref. 31 does not supply a good evaluation of  $M_0(r_s)$  even though it gives a reasonable approximation for the pair-correlation function.<sup>5</sup> We consider the wrong behavior of such a local field in the present context as an indication that a static local field is not very useful in deriving accurate dielectric functions. Furthermore, we can note that Eq. (8d) gives rise to a result which is increasingly in error as the density is lowered.

Looking at Table II we also see that the result of Ref. 17 is rather wrong at high density, while its accuracy increases at low density. This suggests that the local field has to be such that correct high-density limits can be always derived.

To gain a better insight about the relevance of the local field, we also used Eq. (10) directly to get an estimate of the correlation energy through the integration of  $M_0(r_s)$ . To this purpose we calculated  $M_0(r_s)$  up to  $r_s = 50$  performing a numerical integration and then deriving the correlation energy through subtraction of the Hartree-Fock contribution to the total energy

$$\epsilon_c = \epsilon(r_s) - \frac{3}{5} \left[ \frac{1}{\alpha r_s} \right]^2 + \frac{3}{2\pi \alpha r_s} . \tag{12}$$

The results of this calculation are given in Table III. Once again the local field of Geldart and Vosko<sup>29</sup> is in very good agreement with the correlation energy deduced by Ceperley and Alder.<sup>22</sup> To check the quality of present numerical integration and, in turn, the quality of the self-energy we obtained from the Monte Carlo data through Eq. (11), we used this last estimate to again derive  $\epsilon_c$ . We employed the same numerical approach used in obtaining the results of Table III. The correlation energy so derived is reported in the second column of Table III and compares fairly well with the original data, the error being less than 0.4 mRy in all cases.

Further effort could be devoted in deducing a better local field, still within the present approach. However, we consider very interesting the present conclusion that the simple local field of Eq. (8b) allows us to obtain such a good estimate of the self-energy. It is also worthwhile to point out that Eq. (8b) does not fulfill special requirements<sup>5</sup> which are thought to be important. Nevertheless, present good results are obtained and this can be considered in agreement with the observation that accurate high-momentum behavior of G(q) is not important in many respects.<sup>32</sup> On the other hand, a similar, almost phenomenological, local field has been employed recently to analyze the electron gas even as a function of temperature<sup>33</sup> with rather reasonable results. To get further information on the effect of the local field on the one-particle behavior of the electron gas, we also analyzed the spectral weight function,  $^{13,25}$  which is defined by

$$\mathcal{A}(q,\omega) = -\frac{1}{\pi} \lim_{\eta \to 0^+} \{ \omega + M_0 + i\eta \operatorname{sgn}(\omega - k_F^2) - q^2 - M[q,\omega + i\eta \operatorname{sgn}(\omega - k_F^2)] \}^{-1}.$$
(13)

It should be remarked that when the energy is different from the chemical potential, the imaginary part of the self-energy is nonzero so that the limit in Eq. (13) is easily carried out. On the other hand, when  $\omega$  is close to  $k_F$ , the imaginary part of  $M(q,\omega)$  vanishes as  $(\omega - k_F^2)^2$  and  $\mathcal{A}(q,\omega)$  approaches a  $\delta$  function of energy, so that well defined one-particle states exist.

Using the various self-energies we have considered, we found that the overall shape of  $\mathcal{A}(q,\omega)$  is almost independent of the local field. In all cases we also recovered the

TABLE I. Self-energy along the quasiparticle dispersion relation  $\omega = q^2$  as calculated using various local fields. The RPA results have already been presented in Ref. 13.

<b>r</b> <sub>s</sub>	q/k <sub>F</sub>	0	0.2	0.4	0.6	0.8	1	1.2
				Local field of	Ref. 29			
1	$\operatorname{Re}(M)$ $\operatorname{Im}(M)$	-1.4582 0.2583	-1.4505 0.2345	-1.4326 0.1751		-1.3957 0.0302	-1.3647 0	
2	$\operatorname{Re}(M)$	-0.6816	-0.6830	-0.6891	-0.7004	-0.7126	-0.7201	-0.7251
	$\operatorname{Im}(M)$	0.1123	0.1009	0.0726	0.0390	0.0116	0	-0.0117
3	$\operatorname{Re}(M)$	-0.4516	0.4542	0.4622	-0.4745	-0.4880	-0.4995	-0.5094
	$\operatorname{Im}(M)$	0.0629	0.0565	0.0407	0.0219	0.0065	0	-0.0067
4	Re( <i>M</i> )	-0.3434	-0.3458	-0.3530	-0.3637	-0.3757	-0.3868	-0.3971
	Im( <i>M</i> )	0.0401	0.0361	0.0262	0.0142	0.0042	0	-0.0045
5	$\operatorname{Re}(M)$	0.2804	-0.2825	-0.2886	-0.2976	-0.3079	-0.3181	-0.3277
	$\operatorname{Im}(M)$	0.0277	0.0251	0.0184	0.0101	0.0030	0	-0.0033
6	$\operatorname{Re}(M)$ $\operatorname{Im}(M)$	-0.2389 0.0203	-0.2408 0.0184	-0.2459 0.0136 Local field of	-0.2535 0.0075 Ref 30	-0.2624 0.0023	-0.2715 0	-0.2803 -0.0025
1	$\mathbf{D}_{\mathbf{a}}(\mathbf{M})$	1 2020	1 2950	1 2702	1 2506	1 2525	1 2227	1 2114
1	$\operatorname{Im}(M)$	0.2835	0.2575	0.1918	0.1064	0.0324	-1.3327	-0.0319
2	$\operatorname{Re}(M)$	-0.6244	-0.6270	-0.6370	-0.6554	-0.6763	-0.6921	-0.7050
	$\operatorname{Im}(M)$	0.1286	0.1153	0.0824	0.0436	0.0128	0	-0.0129
3	$\operatorname{Re}(M)$	-0.4025	-0.4063	-0.4180	-0.4361	-0.4565	-0.4747	-0.4908
	$\operatorname{Im}(M)$	0.0737	0.0660	0.0471	0.0249	0.0073	0	-0.0075
4	$\operatorname{Re}(M)$	0.3007	-0.3043	-0.3146	-0.3301	-0.3478	-0.3645	-0.3799
	$\operatorname{Im}(M)$	0.0477	0.0428	0.0308	0.0165	0.0048	0	-0.0051
5	$\operatorname{Re}(M)$	-0.2427	-0.2458	-0.2546	-0.2677	-0.2828	0.2977	0.3117
	$\operatorname{Im}(M)$	0.0333	0.0301	0.0218	0.0118	0.0035	0	0.0037
6	$\operatorname{Re}(M)$	0.2052	-0.2079	-0.2154	-0.2265	-0.2395	-0.2527	-0.2654
	$\operatorname{Im}(M)$	0.0246	0.0223	0.0163	0.0089	0.0027	0	-0.0029
		1 4056	1 4001		Rei. 31	1 25/2	1 2 2 2 1	1 2050
1	$\operatorname{Re}(M)$ $\operatorname{Im}(M)$	-1.4076 0.2783	- 1.4001 0.2526	- 1.3834 0.1879	- 1.3689 0.1044	- 1.3563 0.0319	- 1.3321 0	-0.0315
2	$\operatorname{Re}(M)$	-0.6209	-0.6230	-0.6311	-0.6463	-0.6639	-0.6780	-0.6893
	$\operatorname{Im}(M)$	0.1276	0.1147	0.0825	0.0442	0.0131	0	-0.0133
3	$\operatorname{Re}(M)$ $\operatorname{Im}(M)$	-0.3869 0.0740	-0.3902 0.0668	$-0.4002 \\ 0.0484$	-0.4157 0.0263	-0.4339 0.0078	-0.4516 0	-0.4677 -0.0082
4	$\operatorname{Re}(M)$	0.2768	-0.2799	-0.2887	-0.3020	-0.3181	-0.3350	0.3514
	$\operatorname{Im}(M)$	0.0484	0.0440	0.0325	0.0181	0.0055	0	0.0060
5	$\operatorname{Re}(M)$	-0.2128	-0.2154	-0.2227	-0.2338	-0.2477	-0.2632	-0.2788
	$\operatorname{Im}(M)$	0.0342	0.0313	0.0236	0.0135	0.0042	0	-0.0047
6	$\operatorname{Re}(M)$	-0.1706	-0.1728	-0.1789	-0.1882	-0.2002	-0.2143	-0.2289
	$\operatorname{Im}(M)$	0.0255	0.0235	0.0180	0.0106	0.0034	0	-0.0040

TABLE II. Self-energy at the Fermi surface in various approximations. The result of column 1 is derived from the fit (Ref. 23) to the Monte Carlo data (Ref. 22) as described in the text. Columns 2, 4, 5, and 6 refer to the local fields of Eqs. (8a), (8b), (8c), and (8d), respectively. Column 3 is deduced from Ref. 17.

r <sub>s</sub>		$M_0(r_s)$ (Ry)						
1	-1.3574	-1.3937	-1.307	-1.3327	- 1.3647	-1.3313		
2	-0.7141	-0.7483	-0.691	-0.6921	-0.7201	-0.6776		
3	-0.4933	-0.5259	-0.482	-0.4747	-0.4995	-0.4514		
4	-0.3803	-0.4115	-0.373	-0.3645	-0.3868	-0.3349		
5	-0.3111	-0.3411	-0.309	-0.2977	-0.3181	-0.2632		
6	-0.2642	-0.2932	-0.263	-0.2527	-0.2715	-0.2143		

double-peak structure observed by Lundqvist<sup>15,16</sup> with a little effect on the relative intensities. Typical results are shown in Fig. 1 in the case of RPA and in the case of the local field of Geldart and Vosko. As we can see, only the peak position is affected by the change of the local field.

The fact that the peak position is affected by the local field could have some relevance in explaining recent photoemission data on sodium.<sup>34</sup> Assuming that sodium is reasonably modeled by an electron gas at  $r_s = 4$ , we expect a bandwidth reduction with respect to the free-electron gas as due to self-energy effects. This reduction amounts to 12% and 18% of the free-electron bandwidth using the RPA and Geldart and Vosko local fields, respectively. These numbers should be compared with the observed value of 25%. Therefore it is seen that the Geldart and Vosko local field gives rise to a better agreement as compared to RPA. It is quite clear that the comparison with experimental data cannot be considered as a check for electron-gas theory, however the above estimates are rather gratifying.

The relative position of the auxiliary peak to the main (one-particle) peak is almost independent of the local field. This fact is expected, as such an auxiliary peak should be due to the coupled propagation of the electron

TABLE III. Correlation energy deduced from the chemical potential. Column 1 is taken from Ref. 23, column 2 is derived from the chemical potential of Ref. 23 throughout present numerical procedure, column 3 is the correlation energy within RPA as deduced by Hedin (Ref. 13), and column 4 is the RPA result derived from the present chemical potential. The last column has been obtained from the chemical potential resulting from the local field of Eq. (8b).

r <sub>s</sub>	$\epsilon_c(r_s)$ (mRy)						
1	-120.0	-119.6	- 157.8	-154.8	-125.7		
2	- 89.6	- 89.5	-123.8	-122.3	-95.6		
3	-73.8	- 74.0	105.8	- 104.9	- 80.6		
4	-63.6	-63.7	-93.8	-93.0	- 70.8		
5	- 56.3	- 56.2	-85.1	- 84.3	-63.8		
6	- 50.7	50.6	- 78.4	-77.5	- 58.6		
10	- 37.1	- 37.0	-61.5	- 60.7	-45.8		

and the plasmon<sup>16</sup> and the plasmon dispersion relation is slightly affected by the local field. We found that the solution of the equation

$$\epsilon(q,\omega) = 0 \tag{14}$$



FIG. 1. Spectral weight function as a function of energy at selected values of  $q/k_F$  at  $r_s=2$  and 4 [(a)  $q/k_F=0$ , (b)  $q/k_F=0.5$ , (c)  $q/k_F=1.5$ ]. The data have been calculated within the RPA (left-hand side) and using the local-field approximation of Ref. 29 (right-hand side).

TABLE IV. Ratio between the actual compressibility and independent electron compressibility. Column 1 refers to Hartree-Fock approximation to the total energy, column 2 refers to the total energy of Ref. 23, column 3 is taken from Ref. 35, and columns 4 and 5 are deduced from the chemical potential of approximations of Eqs. (8b) and (8d). Column 6 is derived from the dielectric function of Eq. (8b).

r <sub>s</sub>	κ₀/κ							
0.01	1.0016	1.0016		1.0016	1.0016	1.0017		
0.1	1.0168	1.0169	1.017	1.0169	1.0170	1.0169		
1	1.1988	1.2093	1.206	1.2098	1.2118	1.1988		
2	1.4663	1.5485	1.524	1.5484	1.5683	1.4964		
3	1.9901	2.1985	2.045	2.1912	2.2847	1.9904		
4	2.9706	3.9279	3.067	3.8611	4.3602	2.9712		
5	5.8556	20.4970	5.988	17.8925	67.0938	5.8581		
6	203.1731	-6.1812	200	-6.6480	-4.8513	206.3838		
10	- 1.5186	-0.9758	- 1.058	- 1.0086	-0.8331	-1.5184		

(q fixed) is affected by the local field only when q is close to the critical momentum.

In view of the behavior of the spectral function, the analysis of energy-dependent local fields appears rather interesting.<sup>26-28</sup> However, the inherent formal complexity of available energy-dependent local fields makes the numerical calculation much more time consuming, while no clear check on the quality of the spectral function is available.

## **IV. CONCLUDING REMARKS**

The most relevant conclusion we can derive from present calculation is that the electron-gas self-energy is appreciably affected by the local field and that the totalenergy calculation can be employed to get some idea on the quality of the calculation. Furthermore, even simple local fields such as that proposed by Geldart and Vosko can be used to produce a rather good estimate of the total energy, whereas the much more involved phenomenological suggestion of Ichimaru and Utsumi<sup>31</sup> appears not to be adequate especially when  $r_s$  increases. In particular, we found that the local field of Ref. 31 does not give a good estimate of the self-energy at the chemical potential (see Table II) because of the rather high peak present around  $q = 2k_F$ . We believe that our result gives an indication of the inadequacy of the static approximation in deriving accurate dielectric functions.

Further development of the GW-like approximation could be the analysis of the effect of the compressibility sum rule.<sup>5,6</sup> However, to satisfy such a sum rule, a complex self-consistency condition has to be taken into account. Within the present description the compressibility sum rule can be written as

$$\epsilon(q,0) = 1 + n \frac{\omega_p^2 \kappa}{q^2} = 1 + \frac{k_s^2}{q^2}, \quad q \to 0$$
(15)

where  $\omega_p$  is the plasma energy,  $\kappa$  is the isothermal compressibility, and  $k_s$  is the screening wave vector. Thus, such a condition is not straightforward; however, we checked to what extent it is satisfied within various approximations. The results of this evaluation are given in Table IV, where the ratio of the actual compressibility to the noninteracting one  $\kappa_0 = 2\pi \alpha^2 r_s^5$  is reported in comparison with that derived from the Monte Carlo data<sup>22</sup> and other available approximations.<sup>35</sup> As expected, our best approximation to the self-energy [Eq. (8b)] gives a rather good estimate of the compressibility as deduced directly from the chemical potential derivative. However, the corresponding dielectric function is poorer than that derived by Ichimaru and Utsumi.<sup>31</sup> In any case, this behavior is in the spirit of a perturbative approach, as an approximate screened potential is used to derive a reasonable self-energy, while the dielectric function is only a rough approximation.

- <sup>1</sup>P. Hohenberg and W. Kohn, Phys. Rev. 136, B864 (1964).
- <sup>2</sup>W. Kohn and L. J. Sham, Phys. Rev. 140, A1133 (1965).
- <sup>3</sup>W. Kohn and P. Vashishta, in *Theory of the Inhomogeneous Electron Gas*, edited by S. Lundqvist and N. H. March (Plenum, New York, 1983), p. 79.
- <sup>4</sup>J. G. Zabolitzky, Phys. Rev. B 22, 2353 (1980).
- <sup>5</sup>S. Ichimaru, Rev. Mod. Phys. 54, 1017 (1982).
- <sup>6</sup>K. S. Singwi and M. P. Tosi, Solid State Phys. 36, 177 (1981).
- <sup>7</sup>V. Contini, G. Mazzone, and F. Sacchetti, Phys. Rev. B 33, 712 (1986).
- <sup>8</sup>V. L. Moruzzi, J. F. Janak, and A. R. Williams, Calculated

Electronic Properties of Metals (Pergamon, New York, 1978).

- <sup>9</sup>L. J. Sham and W. Kohn, Phys. Rev. 145, 561 (1986).
- <sup>10</sup>F. Sacchetti, J. Phys. F **12**, 281 (1982).
- <sup>11</sup>C. Petrillo and F. Sacchetti, J. Phys. F **15**, 91 (1985).
- <sup>12</sup>W. E. Pickett and C. S. Wang, Phys. Rev. B 30, 4719 (1984).
- <sup>13</sup>L. Hedin, Phys. Rev. 139, A796 (1965).
- <sup>14</sup>J. E. Northrup, M. S. Hybertsen, and S. G. Louie, Phys. Rev. Lett. **59**, 819 (1987).
- <sup>15</sup>B. I. Lundqvist, Phys. Kondens. Mater. 6, 206 (1967).
- <sup>16</sup>B. I. Lundqvist, Phys. Kondens. Mater. 7, 117 (1968).
- <sup>17</sup>H. Suehiro, Y. Ousaka, and H. Yasuhara, J. Phys. C 17, 6685

(1984).

- <sup>18</sup>G. Vignale and K. S. Singwi, Phys. Rev. B 32, 2156 (1985).
- <sup>19</sup>M. Schreiber and H. Bross, J. Phys. F 13, 1895 (1983).
- <sup>20</sup>G. Baym and L. P. Kadanoff, Phys. Rev. **124**, 287 (1961).
- <sup>21</sup>L. W. Bifferman and H. Ehrenreich, Phys. Rev. B 2, 364 (1970).
- <sup>22</sup>D. M. Ceperley and B. J. Alder, Phys. Rev. Lett. 45, 566 (1980).
- <sup>23</sup>S. H. Vosko, L. Wilk, and M. Nusair, Can. J. Phys. 58, 1200 (1980).
- <sup>24</sup>A. W. Overhauser and J. T. Tsai, Phys. Rev. B 13, 607 (1976).
- <sup>25</sup>L. Hedin and S. Lundqvist, Solid State Phys. 23, 1 (1969).
- <sup>26</sup>J. T. Devreese, F. Brosens, and L. F. Lemmens, Phys. Rev. B 21, 1349 (1980).

- <sup>27</sup>A. Holas, P. K. Aravind, and K. S. Singwi, Phys. Rev. B 20, 4912 (1979).
- <sup>28</sup>J. E. Alvarellos and F. Flores, J. Phys. F 14, 1673 (1984).
- <sup>29</sup>D. J. W. Geldart and S. H. Vosko, Can. J. Phys. 44, 2137 (1966).
- <sup>30</sup>J. Hubbard, Proc. R. Soc. London, Ser. A 243, 336 (1958).
- <sup>31</sup>S. Ichimaru and K. Utsumi, Phys. Rev. B 24, 7385 (1981).
- <sup>32</sup>R. Taylor, J. Phys. F 8, 1699 (1978).
- <sup>33</sup>R. G. Dandrea, N. W. Ashcroft, and A. E. Carlsson, Phys. Rev. B 34, 2097 (1986).
- <sup>34</sup>E. Jensen and E. W. Plummer, Phys. Rev. Lett. 55, 1918 (1985).
- <sup>35</sup>W. M. Alberico, R. Cenni, P. de Chiara, and A. Molinari, Nuovo Cimento 3, 1 (1980).