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Aspects on diagrammatic expansion for models related to a homogeneous electron gas

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Abstract. In a previous paper we have studied the expansion of the irreducible self-energy of an electron gas and found it to give unreliable results for the satellites of the one-electron spectral function. This was due to the incorrect analytic properties of the corresponding Green function. Here we confirm and extend these results by studying a simple model (S-model) which allows us to demonstrate clearly the nature of different approximation schemes.

We also develop a consistent iterative expansion method for the Green function, which, in addition to giving a one-electron Green function with correct analyticity and a spectral function fulfilling the sum rule, is computationally simple enough to be used for an electron gas and possibly for simple metals. The method gives quite reasonable results for the S-model when developed to second order in the screened interaction. From comparison with our and other electron gas calculations we conclude that the method should also give reasonable results for an electron gas.

1. Introduction

In this paper various approximations to obtain properties of a free electron gas are investigated. The investigation is intended as a guide to future uses and improvements of these approximations. The approximation schemes are presented in a fashion which suggests such improvements. We examine the relative merits of different diagrammatic expansions applied to models of an electron gas by testing the expansions on a particularly simple model, the S-model, arguing that some general features of diagrammatic expansions are common to the S-model and more realistic models of the electron gas. The point in using the S-model is that for this particular model we are able to obtain self-consistent Green functions to low order of approximation for the self-energy, as well as the exact solution. We make comparisons with results from the approximation schemes. In §2 models related to a homogeneous electron gas are outlined. §3 describes approximation schemes. In §4 a comparison between various approximations are made considering the lowest-order diagrams. In §5 the second-order diagrams are considered, while §6 contains conclusions.

2. Model related to a homogeneous electron gas

2.1. General

The single-particle properties of the electron gas—that is, the properties when one electron has been added or subtracted—are described by the one-electron Green function $G(k) = G(\boldsymbol{k}, \omega)$. The one-electron Green function in the case of a non-interacting electron gas is $G^0(k) = (\omega - E(\boldsymbol{k}) - i(k_F - |\boldsymbol{k}|)\delta)^{-1}$, where $E(\boldsymbol{k}) = \boldsymbol{k}^2/2m$ (we have put $\hbar = 1$, $\Omega\,(=\text{volume}) = 1$).

In the case of an interacting homogeneous electron gas, $G(k)$ may formally be given as the solution to a coupled set of integral equations:

$$G(k) = G^0(k) + G^0(k)\Sigma(k)G(k) \tag{1a}$$

$$\Sigma(k) = i(2\pi)^{-4} \int d^4q \, \exp(-i\delta q_0)\, G(k-q)\, \Gamma(k,q)\, W(q) \tag{1b}$$

$$W(q) = v_q[\epsilon(q)]^{-1} = v_q[1 - v_q P(q)]^{-1} \tag{1c}$$

$$P(q) = -i2(2\pi)^{-4} \int d^4k \, \exp(i\delta k_0) G(k)\, \Gamma(k,q)\, G(k-q) \tag{1d}$$

$$\Gamma(k,q) = \sum_{n=0}^{\infty} f_n(G,W) \tag{1e}$$

where G and G^0 are the exact and the non-interacting Green function respectively, Σ the self-energy, W the screened interaction, P the polarization propagator, Γ the vertex function, and $v_q\,(= 4\pi e^2/q^2)$ the Coulomb interaction. The quantity f_n is a known functional of G and W of order n in W (see for instance Hedin and Lundqvist 1969). The first two functionals are $f_0 = 1$ and $f_1 = i(2\pi)^{-4}\int d^4k' G(k-k')\, G(k-k'-q)\, W(k')$. Thus

$$\Gamma_N(k,q) = \sum_{n=0}^{N} f_n(G,W), \qquad N = 0, 1, 2\ldots$$

defines a set of coupled integral equations with a corresponding set of Green functions $G_1(k)$, $G_2(k)\ldots$ as solution. Figure 1 shows the diagrams involved in a diagrammatic representation of the first two integral equations.
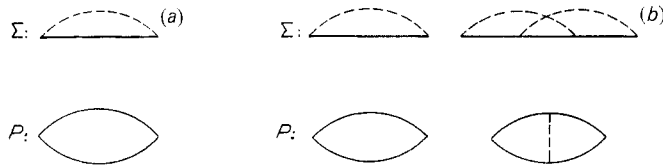

Figure 1. Self-energy and polarization diagrams involved in the first (*a*) and the second (*b*) integral equations. Full line: Green function; broken line: screened interaction.

In practice these equations are too complicated to solve even in lowest order in the screened interaction. In order to simplify the problem a model of the electron gas is introduced in which $P(q)$ is given as an *a priori* parametrization. This reduces the coupled equations to (1a), (1b) and (1e). The implicit assumption is that the detailed structure of the dielectric function will not influence the basic features of the Green function.

2.2. Plasmon model of an electron gas

The 'plasmon model' of an electron gas is defined by equations (1a), (1b) and (1e) together with the plasmon-pole parametrization.

$[\epsilon(q)]^{-1} = 1 + \omega_p^2/(\omega^2 - \omega_q^2)$, where ω_p $(= (4\pi n e^2/m)^{1/2})$ is the plasmon frequency and ω_q remains to be chosen (Lundqvist 1967a, b). It is expected that the qualitative features will be insensitive to the precise choice of ω_q and that the replacement of the plasmon-pole parametrization by RPA parametrization will not change the qualitative results (Lundqvist 1967a, b).

In the following, two simple ω_q expressions will be used:

$${}^1\omega_q = [q^4/(\omega_p^0)^2 + 4q^2/(3(\omega_p^0)^2) + 1]^{1/2}\omega_p \qquad \text{(Lundqvist 1967)}$$

$${}^2\omega_q = [q^4/(\omega_p^0)^2 + 2q^2/\omega_p^0 + 1]^{1/2}\omega_p = (1 + q^2/\omega_p^0)\omega_p \qquad \text{(Hedin } et\ al\ 1971),$$

where $\omega_p^0 = \omega_p/E_F$, and q is given in units of k_F. ${}^1\omega_q$ and ${}^2\omega_q$ may be regarded as interpolations of the static RPA result between the limits $q \to 0$ and $q \to \infty$.

2.3. Effective Hamiltonian related to plasmon model of an electron gas

Considering a plasmon model for the electron gas, it is noticed (Lundqvist 1967a, b) that if the interaction is split into two parts

$$W(q) = v_1 + v_2 = v_q + v_q([\epsilon(q)]^{-1} - 1), \qquad (2)$$

the second part may be given as an effective electron–electron interaction, presuming a boson field coupling to the electrons $v_2 = g_q^2 B(q)$, where

$$B(q) = 2\omega_q/(\omega^2 - (\omega_q - i\delta)^2)$$

is a boson propagator and $g_q = (\omega_p^2 v_q/2\omega_q)^{1/2}$ is the coupling constant.

This suggests that a model defined by the effective Hamiltonian

$$H_{\text{eff}} = \sum_k \epsilon_k c_k^+ c_k + \sum_q \omega_q b_q^+ b_q + \sum_{kq} g_q c_{k+q}^+ c_k (b_q + b_{-q}^+),$$

where $c_k^+ (b_q^+)$ is the electron (boson) creation operator, would be adequate in connection with the electron gas (Lundqvist 1967a, b, Overhauser 1971). The H_{eff} model may be viewed as representing a subset of the total set of diagrams describing the plasmon model.

In analogy with the core-electron case below it is noticed that if G is restricted to hole propagation then the plasmon model and the H_{eff} model are equivalent provided ϵ_k is defined as the Hartree–Fock type energy

$$\epsilon_k = E(k) + i(2\pi)^{-4} \int d^4q \exp(-i\delta q_0) G(k - q)v_q.$$

2.4. Plasmon model of a core electron

A model of a core electron coupled to an electron gas is obtained by regarding the core electron as a probe particle in the electron gas. The free core-electron Green function is given by

$$G_{\text{core}}^0(\omega) = (\omega - E_0 - i\delta)^{-1},$$

where the constant E_0' is the excitation energy of a core electron in absence of the electron gas. Substituting $G^0_{core}(\omega)$ for $G^0(k)$ in equations (1*a*), (1*b*) and (1*e*) will thus switch the description of an electron gas to a description of a core electron coupled to an electron gas.

2.5. Effective Hamiltonian related to the plasmon model of a core electron

The effective Hamiltonian in case of a core electron is

$$H_{eff} = Ec^+c + \sum_q \omega_q b_q^+ b_q + \sum_q g_q c^+ c(b_q + b_{-q}^+).$$

For the core-electron case there exists a precise connection between the solution defined by a plasmon model and the solution defined by the corresponding effective Hamiltonian. Starting with (1*b*) and $W(q) = v_1 + v_2$ (equation 2) it is noticed that v_1 contributes only in the first self-energy diagram (figure 1*a*) yielding a constant (which is infinite if, as here, the extension in space of the core-electron wavefunction is neglected) (Hedin *et al* 1971). This constant may be taken into account by renormalizing the excitation energy for the free core-electron to E. This means that, as far as properties relative to the renormalized excitation energy E are concerned, the plasmon model and the H_{eff} model are equivalent.

2.6. S-model

A particularly simple model of a core electron is obtained by further replacing ω_q^{-1} with a step function $({}^S\omega_q)^{-1} = \omega_p^{-1}\theta(q_c - q)$, where the cut-off parameter q_c is determined by

$$q_c = \int_0^{q_c} dq = \int_0^\infty \frac{\omega_p^2}{\omega_q^2} dq$$

(compare figure 2). From this definition of q_c it follows that the energy shift parameter

$$D \equiv \sum_q g_q^2/\omega_q = \tfrac{1}{2} \sum_q v_q \, \omega_p^2/\omega_q^2$$

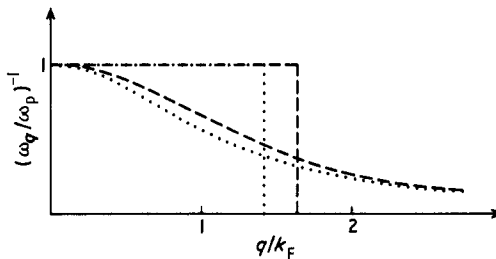(see §4.3) is the same as for the corresponding plasmon model.

Figure 2. The function ω_q^{-1} of the plasmon model and the corresponding step-function $({}^S\omega_q)^{-1}$ of the S-model. Broken line: the function $({}^1\omega_q/\omega_p)^{-1}$ and the corresponding step function $({}^S\omega_q/\omega_p)^{-1}$, $r_s = 4$. Dotted line: the function $({}^2\omega_q/\omega_p)^{-1}$ and the corresponding step function $({}^S\omega_q/\omega_p)^{-1}$, $r_s = 4$.

3. Approximation methods

3.1. General aspects

In this section the function $G(k)$ given by the coupled set of equations (1a), (1b) and (1e) is considered. The equations are schematically written as

$$G(k) = G^0(k) + G^0(k)\Sigma(k)G(k) \tag{3a}$$

$$\Sigma(k) = \Sigma(k; G). \tag{3b}$$

These equations yield a sequence of dressed Green functions $G_N = G_1, G_2 \ldots G_N \ldots$ where N refers to the vertex Γ_{N-1}. The required G is then formally the limit of this sequence (G_∞).

An alternative approach is to expand in terms of bare diagrams. This may be described as an iteration of equations (3). An approximation of G is obtained by choosing a finite set of bare diagrams, usually all diagrams up to a certain order in the interaction.

3.2. Partial renormalization of energy

Let $h(k)$ be an arbitrary function; then the equations

$$G(k) = G^0(\boldsymbol{k}, \omega - h(k)) + G^0(\boldsymbol{k}, \omega - h(k))\{\Sigma(k) - h(k)\}G(k)$$

$$\Sigma(k) = \Sigma(k; G)$$

have the solution

$$G(k) = \{\omega - E(\boldsymbol{k}) - \Sigma(\boldsymbol{k})\}^{-1}.$$

Thus the formal solution $G(k)$ is independent of $h(k)$.

The arbitrary function $h(k)$ may be chosen in a way which makes $G^0(\boldsymbol{k}, \omega - h(k))$ approximate $G(k)$ as well as possible (some $G(k)$ features presumed). This means that $G^0(\boldsymbol{k}, \omega - h(k))\{\Sigma(k) - h(k)\}G(k)$ is as 'small' as possible. It is expected that the equations obtained this way will be optimized in the sense of their ability of yielding approximate solutions to G. An extreme case is of course $h(k) = \Sigma(k)$.

It is reasonable to assume that $G(k)$ has a quasiparticle pole for all $\boldsymbol{k}$ at a complex energy $E(\boldsymbol{k}) + \Delta(\boldsymbol{k})$ determined by the Dyson equation $E(\boldsymbol{k}) + \Delta(\boldsymbol{k}) = E(\boldsymbol{k}) + \Sigma(\boldsymbol{k}, E(\boldsymbol{k}) + \Delta(\boldsymbol{k}))$. This *a priori* knowledge of $G(k)$ may be used by setting $h(k) = \Delta(\boldsymbol{k})$. The function $\Delta(\boldsymbol{k})$ is determined by the consistency requirement that any approximate $G(k)$ obtained from the corresponding optimized equations should have a quasiparticle pole at $E(\boldsymbol{k}) + \Delta(\boldsymbol{k})$. As will be seen below, this consistency requirement presumes that an analytic continuation of the self-energy from the real axis to the complex energy of the quasiparticle can be made. This may be avoided by further assuming that the quasiparticle pole is close to the real axis in the sense that $G \sim (\omega - E(\boldsymbol{k}) - \Delta(\boldsymbol{k}))^{-1}$ for $\omega \simeq E(\boldsymbol{k}) + \text{Re}\Delta(\boldsymbol{k})$ and using this as a simplified consistency requirement.

3.3. Feasible approximation methods

The starting point for further approximations is the pair of equations

$$G(k) = G^0(\boldsymbol{k}, \omega - \Delta(\boldsymbol{k})) + G^0(\boldsymbol{k}, \omega - \Delta(\boldsymbol{k}))\{\Sigma(k) - \Delta(\boldsymbol{k})\}G(k) \tag{4a}$$

$$\Sigma(k) = \Sigma(\boldsymbol{k}, \omega; G) \tag{4b}$$

together with the consistency requirement for $\Delta(\boldsymbol{k})$.

3.3.1. Approximated Dyson equation (AD method). One commonly used method (Hedin 1965) is based on the idea of dressed diagrams. By setting $\Delta(k) = \Delta$ where Δ is a real constant, and making the approximation $\Sigma(k; G) \simeq \Sigma(k; G_\Delta^0)$ where $G_\Delta^0(k, \omega) = G^0(k, \omega - \Delta)$, a sequence of approximately dressed Green functions $\{G_N^{AD}\}$ is obtained explicitly given by

$$G^{AD}(k) = \{\omega - E(k) - \Sigma(k, \omega; G_\Delta^0)\}^{-1} \tag{5a}$$

$$\Delta = \Sigma(k_F, E(k_F) + \Delta; G_\Delta^0) = \Sigma^0(k_F, E(k_F)). \tag{5b}$$

In the last equation the notation $\Sigma^0(k, \omega) \equiv \Sigma(k, \omega; G^0)$ is used. Δ has been determined by imposing the consistency requirement for $k = k_F$ (Δ is real since the imaginary part of the self-energy $\Sigma^0(k_F, E(k_F))$ vanishes). In the following this will be referred to as the AD method.

Alternatively, the consistency requirement could be imposed on each k separately. Two cases with a constant Δ may be distinguished. Provided that Δ is real, then equation (5b) will become $\Delta = \Sigma^0(k, E(k))$. If a real constant Δ does not fulfil the consistency requirement, then a modification to a complex constant Δ is needed.

A more general treatment requires a k-dependent $\Delta(k)$ in order to fulfil for all k-values simultaneously the consistency requirement:

$$G_\Delta^0(k, \omega) = G^0(k, \omega - \Delta(k)) \tag{6a}$$

$$\Delta(k) = \Sigma(k, E(k) + \Delta(k); G_\Delta^0). \tag{6b}$$

Equations 6 define a self-consistent $\Delta(k)$. Such a calculation seems feasible for a plasmon model of the electron gas at least in lowest order and using the simplified consistency requirement (see end of § 3.2).

3.3.2. Consistent iterative method (cit). Another procedure, essentially equivalent to the one recently proposed by Bergersen *et al* (1973), consists in iteration of equation (4). An iteration to first and second order may be carried out as described below in some detail, while extensions to higher orders may be inferred by analogy. The order in the interaction is determined from the effective self-energy $\Sigma - \Delta$, thus formally $\Sigma - \Delta = \sum_{n=1}^\infty ({}^n\Sigma - \Delta_n)$ where ${}^n\Sigma$ and Δ_n are of nth order in the interaction and the effective self-energy is a functional of G_Δ^0.

The first order in the interaction gives

$$G^1(k) = G_{\Delta_1}^0(k) + G_{\Delta_1}^0(k)\{{}^1\Sigma(k; G_{\Delta_1}^0) - \Delta_1(k)\}G_{\Delta_1}^0(k) \tag{7a}$$

$$\Delta_1(k) = {}^1\Sigma(k, E(k) + \Delta_1(k); G_{\Delta_1}^0) \tag{7b}$$

$$G_{\Delta_1}^0(k) = G^0(k, \omega - \Delta_1(k)) \tag{7c}$$

where ${}^1\Sigma$ is the diagram in figure 1a and $\Delta_1(k)$ has to be determined self-consistently from equations (7b) and (7c). Making the further approximation $\Delta(k) = \Delta$, where Δ is a real constant, changes equation (7b) to $\Delta = \Sigma^0(k, E(k))$. Notice that for $k = k_F$ this is identical with the consistency requirement for G_1^{AD} in the AD method.

The second order in the interaction gives

$$G^2 = (G^0 + G^0\{\Sigma[G^1] - \Delta\}G^1)_{\text{2nd order}}$$

$$= (G^0 + G^0\{{}^1\Sigma[G^0 + G^0({}^1\Sigma[G^0] - \Delta_1)G^0] + {}^2\Sigma[G^0] - \Delta_1 - \Delta_2\}$$

$$\times \{G^0 + G^0({}^1\Sigma[G^0] - \Delta_1)G^0\})_{\text{2nd order}} = G^0 + G^0\zeta G^0 \tag{8a}$$

$$\xi = {}^1\Sigma[G^0] - \Delta_1 - \Delta_2 + ({}^1\Sigma[G^0] - \Delta_1)^2 G^0 + {}^1\Sigma[G^0({}^1\Sigma[G^0] - \Delta_1)G^0] + {}^2\Sigma[G^0] \quad (8b)$$

where G^0 stands for $G^0_{\Delta_1+\Delta_2}$, ${}^2\Sigma$ is the second diagram in figure 1b and $\Delta_1(k)$ and $\Delta_2(k)$ are determined self-consistently by the conditions

$$\xi(k, E(k) + \Delta_1(k) + \Delta_2(k); G^0_{\Delta_1+\Delta_2}) = 0 \quad (9a)$$

$$G^0_{\Delta_1+\Delta_2}(k, \omega) = G^0(k, \omega - \Delta_1(k) - \Delta_2(k)) \quad (9b)$$

$$\Delta_1(k) = {}^1\Sigma(k, E(k) + \Delta_1(k) + \Delta_2(k); G^0_{\Delta_1+\Delta_2}) \quad (9c)$$

where equation (9c) comes from (7b) by replacing $G^0_{\Delta_1}$ by $G^0_{\Delta_1+\Delta_2}$; the effective self-energy $\Sigma - \Delta$ being regarded as a functional of G^0_Δ. In this way Δ_1 will cancel the first-order and Δ_2 the second-order terms in $\xi(k, E(k) + \Delta(k); G^0)$ as must be. Notice that the full self-consistent CIT method in nth order gives the quasiparticle properties correctly to nth order in the interaction.

Simplifying to the case $\Delta(k) = \Delta$, where Δ is a real constant, changes (9) to explicit equations for Δ_1 and Δ_2,

$$\Delta_1 = {}^1\Sigma^0(k, E(k))$$

$$\Delta_2 = {}^1\Sigma(k, E(k); G^0\{{}^1\Sigma(; G^0) - \Delta_1\}G^0) + {}^2\Sigma(k, E(k); G^0)$$

and

$$G^0 = G^0(k, \omega).$$

This last second-order scheme is feasible for a plasmon model of an electron gas.

Since any self-energy diagram $\Sigma(k, \omega; G)$, regarded as a functional of G, is holomorphic on the proper parts of the complex ω plane provided the Green function G and the interaction W have proper spectral resolutions, it follows that an approximate Green function obtained from an iteration of equations (4) will be holomorphic on the proper parts of the complex ω plane. The sum rule

$$\int_{-\infty}^{\infty} A(\omega)\mathrm{d}\omega = \frac{1}{\pi} \int_{-\infty}^{\infty} \mathrm{Im}\,(G_A)\mathrm{d}\omega = 1$$

will be fulfilled since

$$\int_{-\infty}^{\infty} G_A(\omega)\mathrm{d}\omega = \int_{-\infty}^{\infty} G_A^0(\omega - \Delta)\mathrm{d}\omega + \int_{-\infty}^{\infty} G_A^0(\omega - \Delta)\{\Sigma_A - \Delta\}G_A^0(\omega - \Delta)\mathrm{d}\omega = \mathrm{i}\pi,$$

which is realized by closing the contour in the lower half-plane; only the first term on the right-hand side contributes on the semicircle at infinity. The advanced function G_A is defined as $G_A(\omega) = G(\omega)\theta(\mu - \omega) + G^*(\omega^*)\theta(\mu - \omega)$ where μ is the Fermi energy $(\mu = E(k_F) + \mathrm{Re}\,\Delta(k_F))$.

4. First-order calculations $(\Gamma = \Gamma_0)$

4.1. Comparison between plasmon model of an electron gas and S-model

Figure 3 shows results from AD calculations with $\Gamma = \Gamma_0$ and $\omega_q = {}^1\omega_q$ for the electron gas $(k = 0)$ and for the S-model. Figure 3(a) compares the spectral weight of the quasiparticle excitation, figure 3(b) the spectral weight of 'plasmaron' excitation (for definition

of plasmaron, see Lundqvist 1967a, b), and figure 3(c) the energy distance between the quasiparticle and the plasmaron excitation. The spectral function for the S-model corresponding to this first-order calculation is completely specified by figure 3. The similarities between the results of the two models support the use of the S-model as a test for diagrammatic expansions. Also notice that figure 3 to some extent illustrates the similarity between a conduction electron at the bottom of the band ($k \simeq 0$)—being rather hole-like in character because of its position in the band—and a core electron coupled to the electron gas.
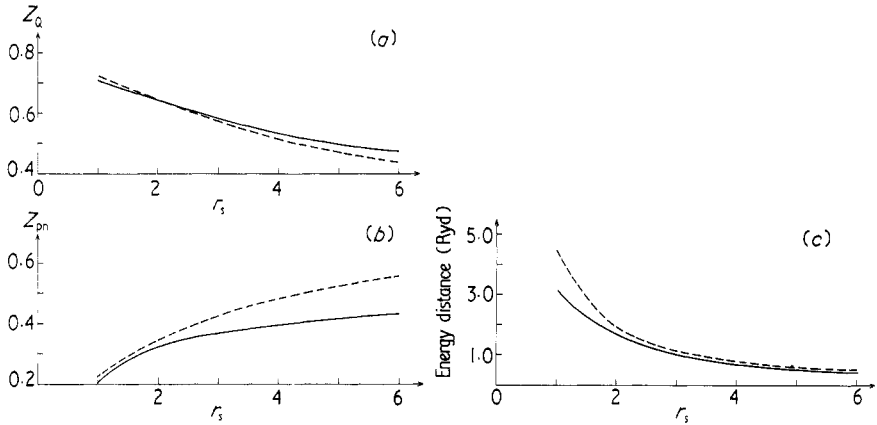
Figure 3. Spectral weight of (a) the quasiparticle obtained in the AD approximation with $\Gamma = \Gamma_0$ and the plasmon dispersion $\omega_q = {}^1\omega_q$ and (b) the 'plasmaron' excitation. Full curve: conduction electron for $k = 0$ (values taken from Lundqvist 1967b); broken curve: core electron in S-model. (c) Distance (in Ryd) between the quasiparticle excitation and the 'plasmaron' excitation for the same two cases as in (a) and (b).

4.2. Plasmon model of electron gas; comparison between different approximations

Figure 4 shows the spectral weight of the quasiparticle Z_Q resulting from an AD calculation for an electron gas (Lundqvist 1967a, b) and from a CIT calculation for an electron gas (Bergersen *et al* 1973). The differences in Z_Q values may almost completely be ascribed to the relation $Z_Q^{AD} = (2 - Z_Q^{CIT})^{-1}$, a relation obtained from equations (5) and (7) for constant Δ and $k = k_F$.

Figure 5 shows the difference between AD and CIT calculations for Z_Q (for $k = k_F$) as a function of r_s with $\omega_q = {}^1\omega_q$ and constant Δ. Also shown in figure 5 are the values taken from Overhauser (1971) which describe a second-order perturbation calculation based on an H_{eff} model of the electron gas (see §2). It is interesting to notice that these values fall just between the AD and CIT values. In figures 4 and 5 $\exp(- \{(Z_Q^{AD})^{-1} - 1\})$ is given as well, constructed in loose analogy with the exact solution of the S-model. (See equations 10 and 11 and make the connection $Z_Q^{AD} \leftrightarrow (1 + D)^{-1}$ and $\exp(-D) \leftrightarrow \exp(- \{(Z_Q^{AD})^{-1} - 1\})$.)
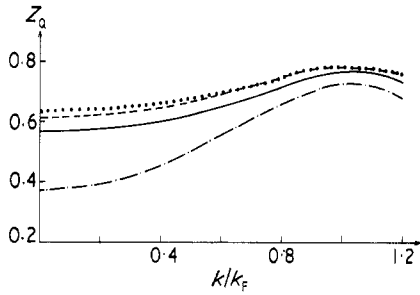
Figure 4. Spectral weight Z_Q as a function of k of a conduction electron corresponding to aluminium ($r_s = 2·07$) from calculations with $\Gamma = \Gamma_0$. Dotted curve: AD results (Z_Q^{AD}) from Lundqvist (1967b); chain curve: CIT-type results (Z_Q^{CIT}) from Bergersen *et al* (1973); broken curve: $(2-Z_Q^{CIT})^{-1}$; full curve: $\exp\{-[(Z_Q^{AD})^{-1} - 1]\}$.
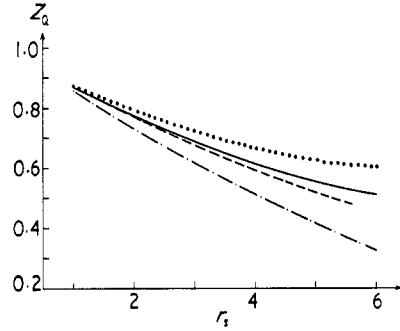
Figure 5. Spectral weight Z_Q of a conduction electron for $k = k_F$ as a function of r_s. Dotted curve: AD calculation, $\Gamma = \Gamma_0$, $\omega_q = {}^1\omega_q$ (from Lundqvist 1967a); chain curve: CIT calculation, $\Gamma = \Gamma_0$, $\omega_q = {}^1\omega_q$ (based on the values of Lundqvist 1967b); broken curve: values based on a H_{eff} model (from Overhauser 1971); full curve: $Z_Q = \exp\{[(Z_Q^{AD})^{-1} -]\}$, where Z_Q^{AD} stands for the Z_Q values of Lundqvist (1967b).

4.3. S-model calculations

Energy is expressed in units of ω_p in this section. The exact solution to the S-model is

$$G(\omega) = \sum_{n=0}^{\infty} e^{-D} \frac{D^n}{n!} \frac{1}{\omega - D + n - i\delta} \tag{10}$$

(Langreth 1970), where the energy is measured from the 'non-interacting' energy E or, equivalently in this case, from the mean energy, since

$$\int_{-\infty}^{\infty} \omega A(\omega) d\omega = (\pi)^{-1} \int_{-\infty}^{\infty} \omega \operatorname{Im}(G(\omega)) d\omega = 0$$

for the above $G(\omega)$. The constant D is defined as

$$D \equiv \sum_q g_q^2/\omega_q = \tfrac{1}{2} \sum_q v_q \omega_p^2/\omega_q^2,$$

which for $\omega_q = {}^1\omega_q$ gives

$$D = \alpha r_s \frac{(\omega_p^0)^{1/2}}{[(\omega_p^0)^2 - \tfrac{4}{9}]^{1/2}} \sin\left(\tfrac{1}{2}\tan^{-1}\{\tfrac{1}{2}3[(\omega_p^0)^2 - \tfrac{4}{9}]^{1/2}\}\right).$$

For $\Gamma = \Gamma_0$ three approximate solutions are considered, which are straightforwardly obtained.

(*a*) The exact first-order Green function (that is, solution to equations (1*a*), (1*b*) and (1*e*) with $\Gamma = \Gamma_0$) is given by the recursion relation

$$G_1(\omega) = (\omega - DG_1(\omega + 1))^{-1}$$

and the condition of correct asymptotic behaviour.

(b) The AD approximation

$$G_1^{AD}(\omega) = \frac{1}{1+D} \quad \frac{1}{\omega - D - i\delta} + \frac{D}{1+D} \quad \frac{1}{\omega + 1 - i\delta} \tag{11}$$

(c) The CIT approximation

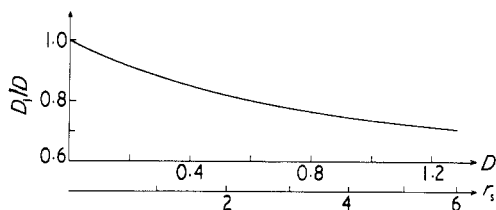$$G_1^{CIT}(\omega) = \frac{1-D}{\omega - D - i\delta} + \frac{D}{\omega - D + 1 - i\delta}. \tag{12}$$

Figure 6. Results in the S-model for D_1/D as a function of D, where D_1 is the core-electron energy as obtained from the first-order solution ($\Gamma = \Gamma_0$), and D is the exact value of the core-electron energy. The AD and the CIT approximations both give the exact core-electron energy for $\Gamma = \Gamma_0$.
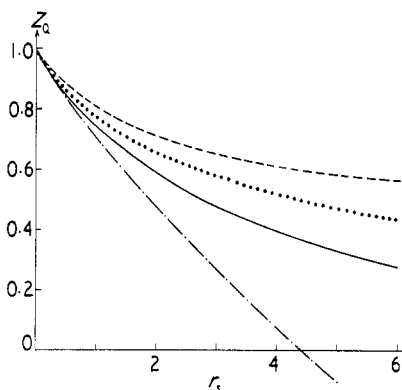
Figure 7. Spectral weight of the core-electron as a function of r_s in the S-model. Full curve: exact solution; broken curve: first-order solution G_1; dotted curve: AD approximation; chain curve: CIT approximation.

Figure 6 compares the position of the quasiparticle pole obtained from various cases, figure 7 the spectral weight of the quasiparticle pole, and figure 8 the spectral functions. An interesting result of the comparisons is that the function $G_1(\omega)$ turns out to be the worst approximation in certain respects. Both $G_1^{AD}(\omega)$ and $G_1^{CIT}(\omega)$ give, for example, the position of the quasiparticle correctly while $G_1(\omega)$ does not (figure 6). Also for the spectral weight of the quasiparticle, $G_1(\omega)$ is worse than $G_1^{AD}(\omega)$ and worse than $G_1^{CIT}(\omega)$ for not too big values of r_s (figure 7). This is surprising since $G_1^{AD}(\omega)$ is an approximation of $G_1(\omega)$. On the other hand it should be realized that G_1^{AD} and G_1^{CIT}, by construction of the approximation method, give the quasiparticle properties correctly to first order (cf § 3.3.2). It is harder to make general statements on the side-band. It is noticed that $G_1^{CIT}(\omega)$ has the first 'satellite' in the correct position while $G_1^{AD}(\omega)$ for small r_s has the first 'satellite' close to the first $G_1(\omega)$ 'satellite'. All three approximations give the correct mean energy ($\int_{-\infty}^{\infty} A(\omega)\omega d\omega = 0$). Apart from this the distribution of spectral weight is rather different in detail. Also notice that G_1^{CIT} gives negative quasi-particle spectral weight for $D > 1$ or equivalently $r_s > 4.5$ (cf equation 12 and figure 7).
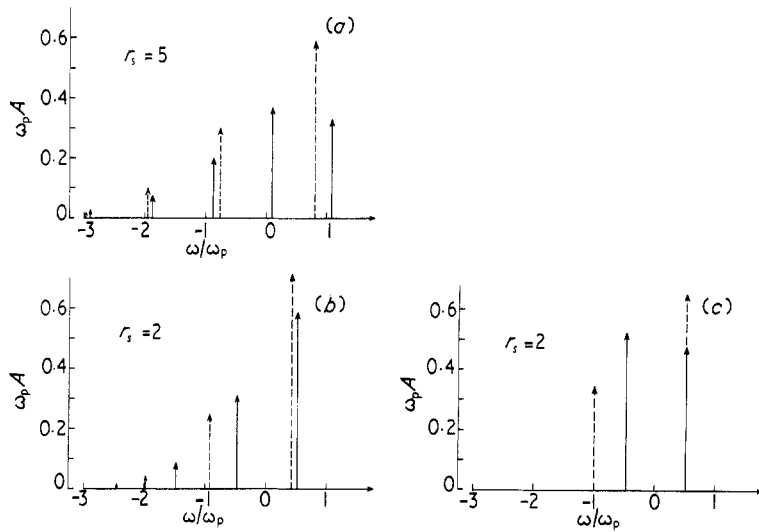
Figure 8. Spectral functions for the core electron in the S-model for (a) $r_s = 5$ and (b) $r_s = 2$—full line: exact solution; broken line: first-order solution ($\Gamma = \Gamma_0$)—and (c) $r_s = 2$, full line: CIT approximation for $\Gamma = \Gamma_0$; broken line: AD approximation for $\Gamma = \Gamma_0$.

5. Second-order calculations ($\Gamma = \Gamma_1$)

5.1. S-model calculations

(a) The exact second-order solution $G_2(\omega)$ is given by

$$G_2(\omega) = (\omega - DG_2(\omega + 1)\{1 + DG_2(\omega + 1)G_2(\omega + 2)\})^{-1} \qquad (13)$$

(which, together with the condition of correct asymptotic behaviour, defines a unique solution) *if* it is *a priori* assumed that $G_2(\omega)$ has the correct analytic properties (that is, is holomorphic in the lower half-plane). In order to check the analytic properties the following theorem is used. Let $f(z)$ be a function that is holomorphic below a certain horizontal line, L, in the lower half-plane and such that $\lim_{|z| \to \infty} \text{Re}(zf(z)) \to 1$, then $(1/\pi)\int_L \text{Im}(f(z))\mathrm{d}z = 1$. Since the condition $\lim_{|z| \to \infty} \text{Re}(zG_2(z)) \to 1$ always is fulfilled, it follows that $\int_L A(\omega)\mathrm{d}\omega = 1$, if $G_2(\omega)$ is analytical below the line L (Minnhagen 1974). Using this criterion it was found that the second-order $G_2(z)$ has incorrect analytic properties.

(b) The AD approximation is given by:

$$G_2^{AD}(\omega) = \left(\omega - \frac{D}{\omega + 1 - D - D^2/2 - \mathrm{i}\delta} \quad \frac{D^2}{(\omega + 1 - D - D^2/2 - \mathrm{i}\delta)^2}\right.$$
$$\left. \times \frac{1}{\omega + 2 - D - D^2/2 - \mathrm{i}\delta}\right)^{-1}.$$

G_2^{AD} has complex roots for all values of r_s except $r_s = 0$ (cf figure 9). Thus G_2^{AD} has incorrect analytic properties (for all $r_s \neq 0$). It seems plausible that the incorrect analytic properties of G_2^{AD} reflects the incorrect analytic properties of G_2.
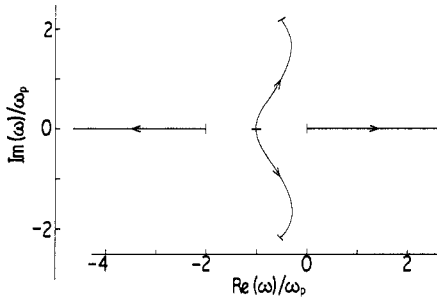
Figure 9. The trajectories traversed by the four poles of the function G_2^{AD} in the complex ω plane with increasing $r_s (0 \to \infty)$.

(c) The CIT approximation to second order in the interaction is

$$G_2^{CIT}(\omega) = \frac{1 - D + D^2/2}{\omega - D - i\delta} + \frac{D - D^2}{\omega + 1 - D - i\delta} + \frac{D^2/2}{\omega + 2 - D - i\delta}.$$

It is obvious that this function is holomorphic in the lower half-plane and that $\int_{-\infty}^{\infty} A(\omega)\, d\omega = 1$. This is in accord with the general observation that an iterative procedure (as described in § 3) will preserve the analytic properties at every step. Figure 10 shows a comparison between the exact solution G and the approximate solutions G_2^{AD} and G_2^{CIT} for $r_s = 2$. It is concluded that G_2^{CIT} is a better approximation than G_1^{CIT} and that the CIT method is useful if the coupling constant is not too big. Notice that G_2^{CIT}, in contrast to G_2^{AD}, fulfils the relation $\int_{-\infty}^{\infty} \omega A(\omega)\, d\omega = 0$ which is also fulfilled by the exact solution.
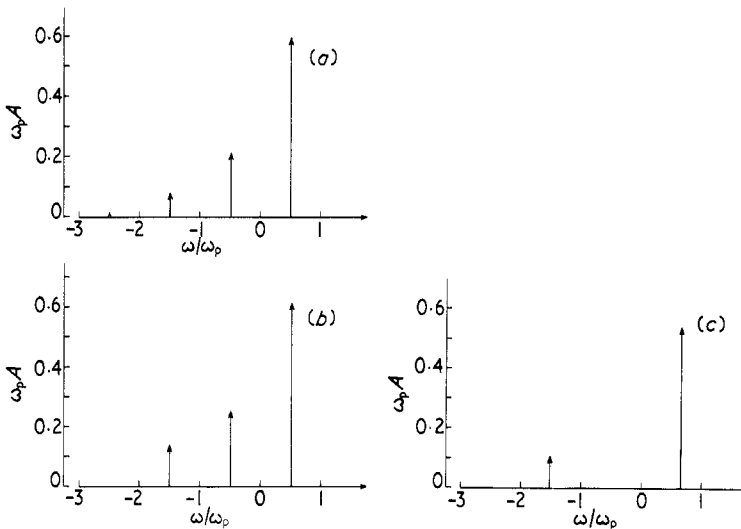

Figure 10. Spectral functions for core electrons in the S-model for $r_s = 2$. (a) exact solution; (b) CIT approximation to second order; (c) AD approximation to second order.

5.2. Comparison between S-model, plasmon model of core electron and plasmon model of electron gas

Figure 11 shows $A(\omega)$ along a horizontal line in the lower half-plane obtained with the AD approximation for $\omega_q = {}^2\omega_q$ and $r_s = 5$ for (a) plasmon model of electron gas for $k = 0$ and $k = 0 \cdot 6(k_F)$; and (b) S-model and plasmon model of core electron. The four curves show a strong resemblance. It has been shown (Minnhagen 1974) that the negative parts of the curves in figure 11 are connected with incorrect analytic properties. By analogy with the S-model, it is plausible that the incorrect analytic properties of G_2^{AD} for the plasmon model of the electron gas and for the core electron also reflects incorrect analytic properties of the corresponding second-order G_2. Thus it is suggested here that the incorrect analytic properties of the second-order G_2 are a general feature for models related to a homogeneous electron gas.
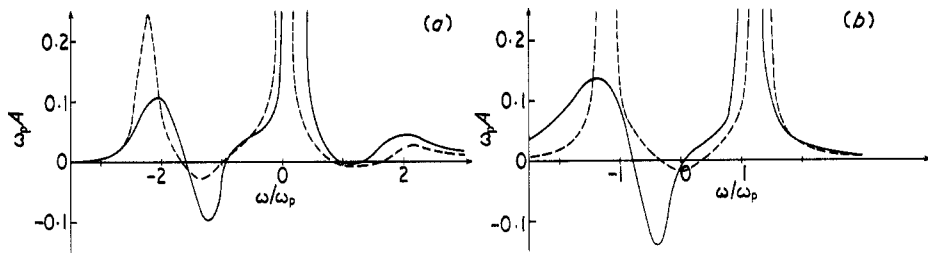

Figure 11. Spectral functions along the line L: $\mathrm{Im}\, z = -0 \cdot 09\omega_p$ for AD approximation; $\omega_q = {}^2\omega_q$, $\Gamma = \Gamma_1$, and $r_s = 2$. (a) full curve: conduction electron with $z = 0 \cdot 6k_F$ (Minnhagen 1974); broken curve: conduction electron with $k = 0$. (b) full curve: plasmon model of core electron; broken curve: S-model of core electron.

6. Conclusions

We have explored the relationships among different models related to an electron gas in order to make plausible the generality of some results obtained explicitly for the S-model. One result found is the incorrect analytic properties of the exact second-order solution G_2. This suggests that expansion in dressed Green functions (in the sense of, for instance, Hedin and Lundqvist 1969) is of limited utility when looking for approximations to the exact spectral weight function. The AD approximation which is based on expansion in dressed Green functions has the same drawback. We have pointed out that an iterative procedure guarantees correct analytic properties and have explicitly described such a method, the CIT method. We have shown that this method gives good results in second order when applied to the S-model and expect that the method is appropriate and of practical use for calculations of electron gas properties.

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