Vertex correction calculations for an electron gas

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Abstract. A straightforward attempt to estimate the influence of the first vertex correction for a homogeneous electron gas is made. The approximation scheme is also tested on a solvable model of a core electron coupled to an electron gas.

1. Introduction

In order to calculate properties of an electron gas Hedin (1965, see also Hedin and Lundqvist 1969) applied a method based on the expansion of the self-energy in a screened interaction. The same approach was used by Hedin *et al* (1967) and Lundqvist (1967a, b) to investigate the single-particle spectrum of an interacting homogeneous electron gas. A characteristic structure in the single-particle spectral weight function was reported, originating in the singular Coulomb potential and the plasmon pole of the effective interaction. These calculations were based essentially on the first-order self-energy diagram. Some aspects of the self-energy method were discussed by Blomberg and Bergersen (1972) and Bergersen *et al* (1973).

The present paper describes an attempt to make a straightforward extension of the self-energy expansion to second order in the screened interaction. This is referred to as including the first vertex correction. A test of the expansion is also included by applying it to a solvable model, namely that of a core electron coupled to an electron gas.

2. Computational procedure

The investigation concerns the extraction of information from a complicated set of coupled integral equations (see eg Hedin and Lundqvist 1969):

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

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

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

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

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

Here G and G^0 are the exact and the free fermion Green functions 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. The first two functionals are $f_0 = 1$ and

$$f_1 = i\hbar(2\pi)^{-4} \int d^4 k' \, H(k - k') \, G(k - k' - q) \, W(k). \tag{2}$$

One systematic approximation scheme for solving the equations (1) consists in taking

$$\Gamma = \Gamma_N(k, q) \equiv \sum_{n=0}^{N} f_n(G, W)$$

for $N = 0, 1, 2$ etc. The equations are conveniently represented by diagrams (Kadanoff and Baym 1962, Hedin 1965, Hedin and Lundqvist 1969). Figure 1 illustrates polarization propagator and self-energy diagrams for the two lowest-order approximations
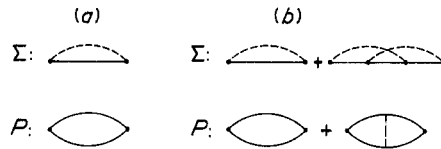

Figure 1. Polarization and self-energy diagrams involved in the first (a) and second (b) integral equations. Full line: Green function; broken line: screened interaction.
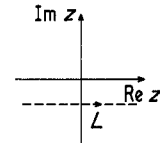
Figure 2. Integration contour.

$(N = 0$ and 1 respectively). The present paper deals with the second approximation $(N = 1)$. In order to facilitate the treatment additional approximations are introduced, similar to those used by Lundqvist (1967 a, b).

(i) The function $W(q)$ is replaced by an explicitly given function defined by introducing a plasmon-pole approximation for the dielectric function $\epsilon(q)$ (Lundqvist 1967a, b, Overhauser 1971):

$$W(q) = v_q/\epsilon(q) \tag{3a}$$

$$\epsilon^{-1}(q) = 1 + \left[(\omega - \phi(k) + i\delta)^{-1} - (\omega + \phi(k) - i\delta)^{-1} \right] \omega_P^2 [2\phi(k)]^{-1} \tag{3b}$$

$$\phi(k) = \omega_p + E(k) \qquad E(k) = \hbar^2 k^2 (2m)^{-1} \tag{3c}$$

where ω_p is the plasmon energy.

(ii) A fully self-consistent solution of the remaining equations:

$$G(k) = G^0(k) + G^0(k) \Sigma(k) G(k) \tag{4a}$$

$$\Sigma(k) = i\hbar(2\pi)^{-4} \int d^4 q \exp(-i\delta q_0) \, G(k - q) \, \Gamma_1(k, q) W(q) \tag{4b}$$

seems outside present-day computational possibilities. Instead an 'ansatz' is introduced into equation (4b) (Hedin 1965, Lundqvist 1967a, b):

$$G^a(\mathbf{k}, \omega) = G^0(\mathbf{k}, \omega - \Delta) = \left[\omega - E(k) - \Delta + i\delta \, \text{sign}(|\mathbf{k}| - k_F) \right]^{-1} \tag{5}$$

which by means of equation (4a) gives the solution (the superscript c stands for calculated):

$$G^c(\boldsymbol{k}, \omega, \Delta) = [\omega - E(k) - \Sigma^0(\boldsymbol{k}, \omega - \Delta)]^{-1}.$$

The superscript 0 on a quantity indicates that it has been calculated using the free fermion Green function. The constant Δ is determined so as to ensure that G^c and G^a have the 'quasi-particle-pole' at the same energy, $E(k_F) + \Delta$, for $k = k_F$. Consequently, $\Delta = \Sigma^0(k_F, E(k_F))$.

The application of this approximation scheme to the present problem means a considerable simplification; the remaining difficulty consists in computing the self-energy using the 'ansatz' G^a. The first self-energy diagram (figure 1a) can then readily be evaluated while the second self-energy diagram (figure 1b) can be reduced to a five-dimensional integral after performing the frequency integrations and a trivial angular integration. The evaluation of the five-dimensional integral is complicated by (a) singularities in the integrand, (b) step functions in the integrand and (c) a high dimensionality of the integral.

After the frequency integrations have been performed it is convenient to work with advanced rather than causal functions. The first difficulty was then essentially circumvented by subtracting a small finite imaginary part $i\epsilon$ from the frequency, that is, calculating $\Sigma_A^0(k, \omega - i\epsilon)$ (the subscript A denotes the advanced function). The use of a finite $i\epsilon$ corresponds to a Lorentzian weighting over the frequency, since for any function that is analytic and bounded in the lower half-plane one has

$$f(\omega - i\epsilon) = \int_{-\infty}^{\infty} d\omega' f(\omega') \pi^{-1} \epsilon [(\omega - \omega')^2 + \epsilon^2]^{-1}. \tag{6}$$

Equation (6) follows directly by expanding the denominator in partial fractions and applying Cauchy's integral theorem. Subsequently the self-energy $\Sigma_A^0(\boldsymbol{k}, \omega - i\epsilon)$ was computed with a Monte Carlo integration method. The spectral function was obtained by the relation $A(\boldsymbol{k}, \omega) = \pi^{-1} \operatorname{Im} G_A^c(\boldsymbol{k}, \omega)$. It should be noticed that the use of a finite $i\epsilon$ also gives rise to a Lorentzian weighting of the spectral function derived.

3. Analyticity

The analyticity of the calculated advanced Green function G_A^c was investigated using the following theorem. Let $f(z)$ be a function that is analytic below a certain horizontal line, L, in the lower half-plane and such that $\lim_{|z| \to \infty} \operatorname{Re}(zf(z)) \to 1$, then $(1/\pi)\int_L \operatorname{Im} f(z) \, dz = 1$ (figure 2). Since the condition $\lim_{|z| \to \infty} \operatorname{Re}(zG_A^c(z)) \to 1$ always is fulfilled, then $\int_L A(k, \omega) \, d\omega = 1$, if G_A^c is analytic below the line L.

The spectral function $A(k, z)$ along various lines parallel to the real axis in the lower half-plane is given in figure 3 (for $r_s = 5$, $k = 0.6k_F$). From the sum-rule values $S = \int_L A(k, \omega) \, d\omega$ it is seen that G_A^c has a pole between $\operatorname{Im} z = -0.35\omega_p$ and $\operatorname{Im} z = -0.51\omega_p$. Thus, for this k value, the calculated Green function has not the correct analyticity. This result seems to be representative for k values outside a narrow range around $k = k_F$. A comparison between the spectral functions derived for selected k values ($k = 0.6$, 1.0 and $1.4k_F$; $\epsilon = 0.09\omega_p$) and those obtained from a similar calculation based on the first integral equation ($N = 0$) is shown in figure 4. The negative parts of the spectral functions are due to the incorrect analytic properties of the approximate Green functions. They also cause the large differences between the results obtained from the first and the

second integral equation. Thus, for example, the full-drawn curve in figure 4(*a*) resembles the curve in figure 3(*c*) (for which the sum rule is fulfilled) more than the curves in figures 3(*a*) and 3(*b*).

The results are representative for r_s values corresponding to metallic densities (r_s values as low as $r_s = 0.5$ have been checked).

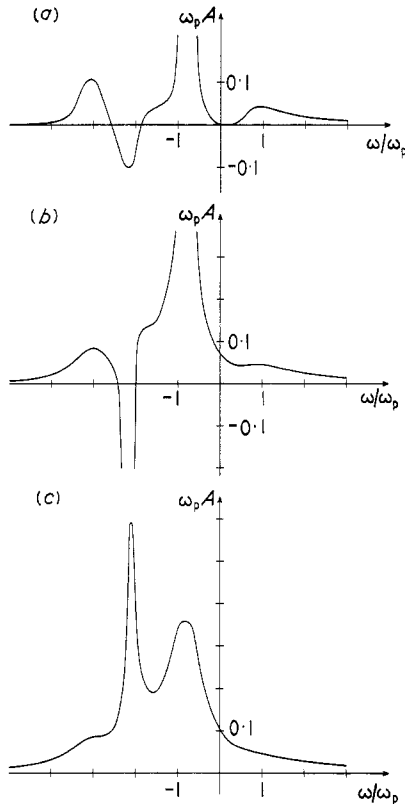The position of the quasi-particle peak obtained from the calculations based on the

Figure 3. Spectral functions obtained along different lines L for $r_s = 5$ and $k = 0.6\,k_F$. S is the estimated area below the respective curve. (*a*) L: Im $z = -0.09\omega_p$, $S = 0.67$. (*b*) L: Im $z = -0.35\omega_p$, $S = 0.68$. (*c*) L: Im $z = -0.51\omega_p$, $S = 1.00$.

two first integral equations coincide. This is, as far as the calculations give a relevant estimate of the property in question, in agreement with the assumption that the influence of the first vertex correction is small (Hedin and Lundqvist 1969, pp 81–2).

4. The core-electron case

In order to investigate further the origin of the anomalous features the same 'ansatz' approach was applied to a model (Lundqvist 1969) consisting of a core electron coupled to an electron gas. The model has the advantage of being exactly solvable and, further, after applying the 'ansatz', the equations corresponding to (4*a*) and (4*b*) may be treated
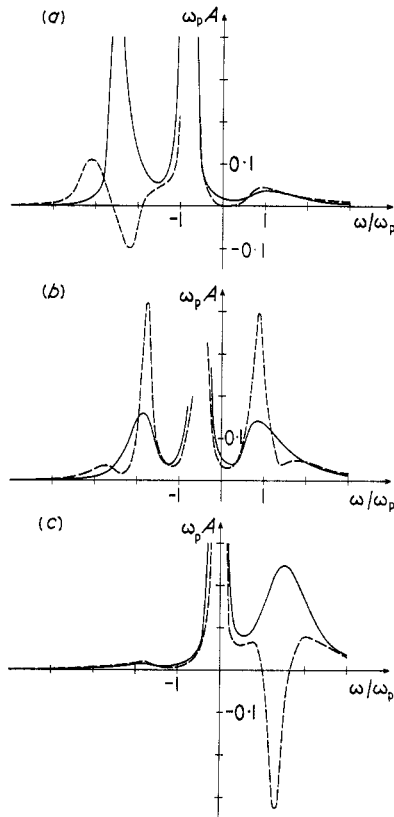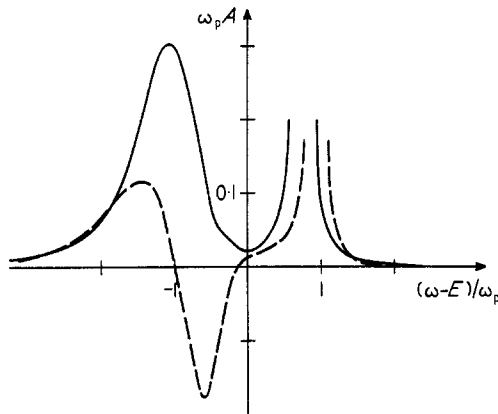
Figure 4. Comparison between spectral functions obtained from the first (full curve) and the second (broken curve) integral equation for $r_s = 5$ and $\epsilon = 0.09\omega_p$. (a) $k = 0.6k_F$. (b) $k = k_1$. (c) $k = 1.4k_F$.

analytically. They differ technically from the electron-gas calculations in that the free fermion Green function for the core electron is $G^0(\omega) = (\omega - E - i\epsilon)^{-1}$ the constant E representing the core-electron energy. The following expression for the self-energy was found. substituting $G^0(\omega)$ for $G(\omega)$ in equation (4b):

$$\Sigma^0(\omega)/\omega_p = C_1(2 - x)^{-1}[1 - (1 - x)^{-1/2}] + C_2[\![i\pi 2(x + 2)^{-3}(x + 1)^{-1}$$

$$+ i\pi 2(x + 2)^{-3} + \pi(x + 2)^{-2}(x + 1)^{-3/2} - \pi(x + 2)^{-2}(x + 1)^{-1/2}$$

$$+ 4i(x + 2)^{-2}(x + 1)^{-1} + \{4(x + 2)^{-3}[-(x + 1)]^{-1/2}\cdot$$

$$+ (x + 2)^{-1}(x + 1)^{-1}[-(x + 1)]^{-1/2}\}\ln\{(2i[-(x + 1)]^{1/2} - x - 2)/$$

$$(2i[-(x + 1)]^{1/2} + x + 2)\}]\!]. \tag{7}$$

$$C_1 = \alpha r_s(E_F/\omega_p)^{1/2} \qquad C_2 = iC_1^2/2\pi$$

$$\omega_p/E_F = (16\alpha r_s/3\pi)^{1/2} \qquad \alpha = (4/9\pi)^{1/3} = 0.521 \qquad x = (-\omega + E - 2\omega_p + i\epsilon)/\omega_p.$$

The square root is taken with the branch cut along the positive real axis.

Figure 5. Comparison between core-electron spectral functions obtained from the first (full curve) and the second (broken curve) integral equations for $r_s = 4$ and $\epsilon = 0{\cdot}05\omega_p$.

In figure 5 the results obtained from the first and second integral equation are compared. The resemblance between the anomalous features obtained by applying the approximated second integral equation to the electron gas for $k = 0{\cdot}6k_F$ (figure 4) and to the core electron is noticeable.

The core-electron case in the $N^* = 1$ approximation was also evaluated using an 'ansatz' ^1G. Here ^1G is a Green function obtained from the first integral equation ($N = 0$), that is from equations (4a) and (4b) substituting Γ_0 for Γ_1 and applying the original 'ansatz' approach. It is seen in figure 6 that this calculation does not lead to anomalous features, but the results are still far from the exact solution. At present it seems hardly feasible to apply some corresponding 'ansatz' to the case of the electron gas.
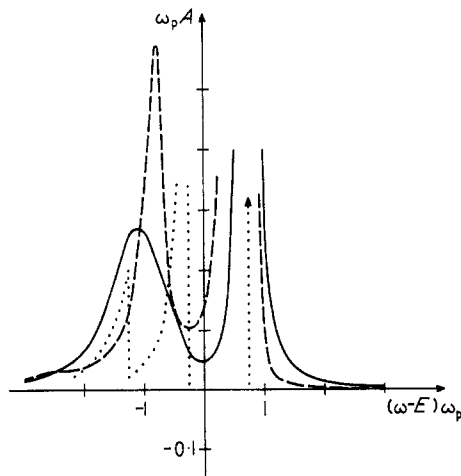
Figure 6. Comparison between core-electron spectral functions obtained from the first integral equation (full curve), the second integral equation using 'ansatz' ^1G (broken curve), and the exact solution (dotted curve) for $r_s = 4$ and $\epsilon = 0{\cdot}1\omega_p$. For the exact solution the quasi-particle peak is a δ-function. (The curve for the exact solution is taken from Hedin *et al* 1971.)

5. Conclusions

It is found that a straightforward extension of the self-energy method as described in the present paper to second order in the screened interaction gives little direct information on the structure of the satellite regions. Presumably the approach is to some extent an over-simplification which, for $N \geqslant 1$, leads to anomalous negative parts in the spectral weight function (or, equivalently, incorrect analytic properties of the Green functions obtained). This indicates that the detailed structure of the satellite regions (eg the existence of the 'plasmaron' satellite) as derived previously from first-order calculations ($N = 0$) (Lundqvist 1967a, b) is not genuine. The satellite structure might rather resemble that found in the core-electron case. Another aspect that should be considered is that the coupled integral equations (1) with $\Gamma = \Gamma_1$ do not necessarily have a solution with correct analyticity.

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