Screened interaction and self-energy in an infinitesimally polarized electron gas via the Kukkonen-Overhauser method

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The screened electron-electron interaction $W_{\sigma,\sigma'}$ and the electron self-energy in an infinitesimally polarized electron gas are derived by extending the approach of Kukkonen and Overhauser. Various quantities in the expression for $W_{\sigma,\sigma'}$ are identified in terms of the relevant response functions of the electron gas. The self-energy is obtained from $W_{\sigma,\sigma'}$ by making use of the GW method which in this case represents a consistent approximation. Contact with previous calculations is made.

71.10.+x, 71.45.Gm, 72.10.Bg, 73.50.Bk

I. INTRODUCTION

Kukkonen and Overhauser (KO) proposed an approximate analytic scheme for calculating the effects of exchange and correlations in an electron gas which accounts for both charge and spin fluctuations. The main merits of the KO method are its simplicity and physical clarity. One of the main results of the KO theory was an expression for the quasiparticle effective interaction for a paramagnetic electron gas. Although this was not initially appreciated, these results were later confirmed for the paramagnetic case, by means of a more complex, less physically transparent, diagrammatic technique by Vignale and Singwi. The diagrammatic analysis was then extended to the case of an infinitesimally polarized electron gas by Ng and Singwi. The situation was eventually clarified by the present authors who derived equivalent results within the framework of a theory of the electron gas based on the concept of quasiparticle pseudo hamiltonian. This theory found successful application to the study of many-body effects in two-dimensional electronic systems.

Even in the simple scenario of the electron gas, electronic correlations can be satisfactorily handled by analytic means only in the high density regime where the random-phase-approximation provides a rigorous approach. Earlier attempts to go beyond this simple scheme at metallic densities involved explicitly including short range exchange and correlation effects corrections in the charge response. In particular, the original contribution by Hubbard, i.e. the introduction of the so called many-body local field, established a useful physical framework within which the description of what amounts in practice to vertex corrections, became possible. KO were the first to exploit this methodology to its fullest extent for the case of paramagnetic jellium.

A popular alternative approach for calculating the physical properties of the Landau quasiparticles in an electron gas is represented by the total energy method. In this approach a key step is represented by the determination of a suitable expression for the electron gas total energy as a functional of the particle occupation numbers. Although the procedure is quite standard and has been in use for quite some time, it was only recently realized that, in order to be able to achieve a correct microscopic theory, it is necessary to carefully keep separate track of the spin up and spin down occupation numbers. Accordingly even when studying the physics of an electron gas in its paramagnetic state, it is necessary, within this framework, to determine the energy of an infinitesimally polarized electron gas. This problem was tackled in Ref. via the pseudo hamiltonian method. The self-energy obtained by this procedure proved to be equivalent to that independently derived by Ng and Singwi.

The purpose of the present paper is to generalize the simple, elegant procedure developed by KO to the case of an infinitesimally polarized electron gas. To obtain a result useful also for multi-component systems, in Sec. II we derive the screened interaction between two electrons by generalizing the theories of Refs. and to an infinitesimally polarized degenerate multi-valley system. In Sec. III the electron self-energy is obtained in a consistent fashion by making use of the lowest order diagram within what is commonly referred to as the GW approximation. We also show that the self-energy obtained following this procedure, although not identical, is very similar to that derived by the present authors in Ref. Lastly, in Sec. IV we present our conclusions.
II. EFFECTIVE INTERACTION

The first step in the KO procedure consists in obtaining a suitable expression for the total effective potential felt by any given electron of the liquid as a result of the introduction of a perturbing electron. To this purpose we introduce a spin up electron, represented by a (number) density of Fourier amplitude $\rho_\uparrow$, into the Fermi sea. Let $\Delta n_\sigma$ be the linear density fluctuation of spin $\sigma = \pm 1$, set up by the introduction of this electron, and let $G^{\sigma\sigma'}_{x(c),\text{intra(inter)}}$ be the appropriate generalized many-body local fields. Here the subscripts $x$ and $c$ refer respectively to exchange and correlation, while the labels $\text{intra}$ and $\text{inter}$ refer respectively to intra-valley and inter-valley processes. Then, on assuming that the density fluctuations in all the valleys are the same, and by following the standard linear response analysis, a complete expression for the potential felt by a spectator electron of opposite spin (down in this case) in the Fermi sea can be written as:

$$\phi_{\downarrow\uparrow} = v(q)\left\{[\rho_\uparrow + \Delta n_\uparrow + \Delta n_\downarrow] - \left[G_{x,\text{intra}}^{\uparrow\downarrow} + G_{c,\text{intra}}^{\uparrow\downarrow}\right]ight. + (\nu_\sigma - 1)G_{c,\text{inter}}^{\uparrow\downarrow} \left[\frac{2\Delta n_\downarrow}{\nu_\sigma}\right] - \left[G_{c,\text{intra}}^{\downarrow\uparrow} + G_{c,\text{inter}}^{\downarrow\uparrow}(\nu_\sigma - 1)\right] \frac{2\rho_\uparrow + 2\Delta n_\uparrow}{\nu_\sigma}\right\},$$

where it is understood that the potential $\phi_{\downarrow\uparrow}$, the density fluctuations, and the many-body local fields $G$ are all functions of both $\mathbf{q}$ and $\omega$. We immediately notice that, while the first term in this expression represents the Hartree term, the remaining contributions stem from exchange and correlation effects.

The potential felt by a spin up electron is obtained in a similar way. One finds:

$$\phi_{\uparrow\downarrow} = v(q)\left\{[\rho_\downarrow + \Delta n_\downarrow + \Delta n_\uparrow] - \left[G_{x,\text{intra}}^{\downarrow\uparrow} + G_{c,\text{intra}}^{\downarrow\uparrow}\right]ight. + (\nu_\sigma - 1)G_{c,\text{inter}}^{\downarrow\uparrow} \left[\frac{2\Delta n_\uparrow}{\nu_\sigma}\right] - \left[G_{c,\text{intra}}^{\uparrow\downarrow} + G_{c,\text{inter}}^{\uparrow\downarrow}(\nu_\sigma - 1)\right] \frac{2\rho_\downarrow + 2\Delta n_\downarrow}{\nu_\sigma}\right\},$$

where, in this case, explicit account has been taken of the extra exchange contribution arising from the fact that the perturbing and the spectator electrons have the same spin.

These expressions can be simplified as follows. As in Ref. [3], for the infinitsimally polarized case one can assume the following relations:

$$G_{x,\text{intra}}^{\uparrow\downarrow} = G_{x,\text{intra}}^{\downarrow\uparrow},$$

and

$$G_{c,\text{intra(inter)}}^{\uparrow\downarrow,\downarrow\uparrow} = G_{c,\text{intra(inter)}}^{\downarrow\uparrow,\uparrow\downarrow} \quad \text{(1)}$$

which, strictly speaking, are valid (by symmetry) for an unpolarized electron gas. Moreover, if upon scattering the electrons retain their valleys we also have:

$$G_{c,\text{inter}}^{\uparrow\downarrow} = G_{c,\text{inter}}^{\downarrow\uparrow} = G_{c,\text{intra}}^{\downarrow\uparrow} \quad \text{(2)}$$

Then, on defining the single valley local fields $G_\pm$ as

$$G_\pm \equiv G_{x,\text{intra}}^{\uparrow\downarrow} + G_{c,\text{inter}}^{\uparrow\downarrow} \pm G_{c,\text{intra}}^{\downarrow\uparrow},$$

and the multi-valley local fields $G'_\pm$ as

$$G'_{\pm{-}} = G_\pm - G_{-{-}} + \frac{G_-}{\nu_\sigma},$$

the potential felt by an electron with spin $\sigma$ can be cast in the following compact form:

$$\phi_{\sigma\uparrow} = v(q)\left\{(1 - G^\sigma_- - \sigma G^\sigma_+)\rho_\uparrow + [\Delta n_\uparrow + \Delta n_\downarrow] (1 - G^\sigma_+) \right. - \left[\Delta n_\downarrow - \Delta n_\uparrow] G^\sigma_- \right\}.$$
We next recognize that within linear response one can write:

$$\Delta n_\sigma = v_\sigma \chi_0^\sigma \phi_{\sigma \uparrow},$$

where $\chi_0^\sigma$ is the spin $\sigma$ response for a non interacting electron gas and can be expressed as follows:

$$\chi_0^\sigma(q, \omega) \equiv \sum_{\vec{p}} \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi i} g^\sigma(\vec{p}, \epsilon) g^\sigma(\vec{p} + \vec{q}, \epsilon + \omega).$$

In this expression $g^\sigma(\vec{p}, \omega)$ is the bare one electron Green’s function given by

$$g^\sigma(\vec{p}, \omega) \equiv \frac{n_p^\sigma}{\omega - \epsilon_p - i\eta} + \frac{1 - n_p^\sigma}{\omega - \epsilon_p + i\eta},$$

with $n_p^\sigma$ being the exact occupation number. Then using Eqs. (8) and (9), we obtain the following relationships for the potentials:

$$\phi_{\uparrow \uparrow} = \frac{v(q) \left[ (1 - G_{\uparrow}^u - G_{\uparrow}^d) + 4v(q)\nu_\sigma \chi_0^\downarrow G_{\downarrow}^\uparrow (1 - G_{\uparrow}^u) \right]}{\mathcal{D}^u} \rho_{\uparrow},$$

and

$$\phi_{\downarrow \uparrow} = \frac{v(q)(1 - G_{\uparrow}^u + G_{\uparrow}^d)}{\mathcal{D}^u} \rho_{\uparrow},$$

with $\mathcal{D}^u$ defined as follows:

$$\mathcal{D}^u \equiv 1 - v(q) \left( \nu_\sigma \chi_0^\downarrow + \nu_\sigma \chi_0^\uparrow \right) \left( 1 - G_{\downarrow}^u - G_{\downarrow}^d \right) - 4v^2(q)\nu_\sigma^2 \chi_0^\uparrow \chi_0^\downarrow G_{\downarrow}^\uparrow (1 - G_{\uparrow}^u).$$

At this point, in order to obtain the screened electron-electron interaction from the effective potentials $\phi_{\sigma \uparrow}$ in the KO method one argues as follows. To correctly describe the physics of the problem, several different contributions stemming from exchange and correlation effects have been approximately accounted for through the local fields $G_{\uparrow}^\alpha$ in the formulas for $\phi_{\sigma \uparrow}$. A physically satisfactory expression for the electron-electron screened interaction $W_{\sigma \uparrow}$ between two electrons can then be obtained by simply subtracting from such expressions the terms accounting for the explicit exchange and correlation contributions between the spectator and the perturbing electron. Accordingly following KO we write:

$$W_{\sigma \uparrow} \rho_{\uparrow} = \phi_{\sigma \uparrow} + v(q) \left[ ( G_{\uparrow}^u + \sigma G_{\uparrow}^d ) \rho_{\uparrow} \right].$$

More generally, based on the isotropy of the unpolarized system, we have for the spin dependent screened interaction potential:

$$W_{\sigma_1 \sigma_2} = \frac{W_{\uparrow \uparrow} + W_{\downarrow \uparrow} + \sigma_1 \cdot \sigma_2 W_{\uparrow \uparrow} - W_{\downarrow \downarrow}}{2}.$$

It is crucial to appreciate here that, although the exchange and correlation contributions to the effective potential between the spectator and the perturbing electron have been explicitly removed, the resulting scattering matrix elements $M_{\alpha \beta}$ between two antisymmetrized states of the interaction potential $W_{\sigma_1 \sigma_2}$ will automatically account for exchange and (to some extent) correlation effects. This can be seen from:

$$M_{\alpha \beta} = \frac{1}{2} \langle \psi_f | W_{\sigma_1 \sigma_2} ( \vec{r}_1 - \vec{r}_2, \omega ) | \psi_i \rangle$$

$$= W_{\alpha \beta} (\vec{q}, \omega) - \delta_{\alpha \beta} W_{\alpha \alpha} (\vec{k}_1 - \vec{k}_2 - \vec{q}, \omega)$$

$$- \delta_{-\alpha \beta} W_T (\vec{k}_1 - \vec{k}_2 - \vec{q}, \omega),$$

where, with obvious notation:

$$| \psi_i \rangle \equiv | \vec{k}_1, \alpha; \vec{k}_2, \beta \rangle - | \vec{k}_2, \beta; \vec{k}_1, \alpha \rangle.$$
and the mixed charge-spin responses \( \chi_{M} \) the matrix elements \( W \) in Eq. (17), the only undefined term in Eq. (26) is the transverse many-body local field \( G_{T}^{\nu} \) for which we will assume the relationship:

\[
G_{T}^{\nu} = \frac{1}{2\nu} \left[ G_{x,\text{intra}}^{\uparrow\downarrow} + G_{c,\text{intra}}^{\uparrow\downarrow} + G_{x,\text{intra}}^{\downarrow\uparrow} + G_{c,\text{intra}}^{\downarrow\uparrow} \right].
\]

Here it must be pointed out that with the approximations made in Eqs. (3) and (4), \( G_{T}^{\nu} \) coincides with the longitudinal field \( G_{L}^{\nu} \).
Using Eqs. (12)-(15) and Eqs. (23)-(25) it can finally be shown that

\[
W_{\sigma\sigma}(\vec{q}, \omega) = v(q) \left\{ 1 + v(q) \left[ 1 - G^v_+(\vec{q}, \omega) \right]^2 \chi_C(\vec{q}, \omega) \right\}
- \mu_B^{-2} \left[ v(q)G^v_+(\vec{q}, \omega) \right]^2 \chi_S(\vec{q}, \omega)
- 2\sigma v(q)^2G^v_-(\vec{q}, \omega) \left[ 1 - G^v_+(\vec{q}, \omega) \right] \chi_{CS}(\vec{q}, \omega),
\]

and that

\[
W_{\vec{q}(\vec{q}, \omega)} = v(q) \left\{ 1 + v(q) \left[ 1 - G^v_+(\vec{q}, \omega) \right]^2 \chi_C(\vec{q}, \omega) \right\}
+ \mu_B^{-2} \left[ v(q)G^v_-(\vec{q}, \omega) \right]^2 \chi_S(\vec{q}, \omega).
\]

### III. SELF-ENERGY

The screened interaction \( W_{\sigma\sigma}(\vec{q}, \omega) \) given in Eqs. (29) and (30) is similar to the effective screened interaction \( V_{\sigma\sigma}(\vec{q}, \omega, \omega) \) derived by the present authors (see Eq. (31) of Ref. 1). In fact, if in \( V_{\sigma\sigma}(\vec{q}, \omega, \omega) \) the real response functions are replaced by the full complex responses and the complex conjugate many-body local fields that are pre-factors to the response functions are replaced by their complex counterparts, one gets exactly \( W_{\sigma\sigma}(\vec{q}, \omega) - v(q) \). As argued in Ref. 1, the effective screened interaction \( V_{\sigma\sigma}(\vec{q}, \omega, \omega) \) should be used for calculations carried out up to first order only. This conclusion is supported by the results of the elegant analysis carried out by Takada in Ref. 16.

To evaluate higher order terms would in this case not only not lead to better results but would in fact be erroneous. It is then quite reasonable to evaluate the quasiparticle self-energy to first order in the screened interaction from the expression:

\[
\Sigma^\sigma(\vec{p}, \omega) = -\sum_q \int_{-\infty}^\infty \frac{d\epsilon}{2\pi i} \left\{ W_{\sigma\sigma}g^\sigma(\vec{p} - \vec{q}, \omega - \epsilon) + W^T_{\sigma}g^{-\sigma}(\vec{p} - \vec{q}, \omega - \epsilon) \right\},
\]

where \( W_{\sigma\sigma} \) is given by Eq. (29) and \( W^T_{\sigma} \) is defined as follows:

\[
W^T_{\sigma}(\vec{q}, \omega) \equiv -4\mu_B^{-2} \left[ v(q)G^T_{\sigma}(\vec{q}, \omega) \right]^2 \chi^{T\sigma}(\vec{q}, \omega).
\]

In the above equation for \( \Sigma^\sigma(\vec{p}, \omega) \) it is understood that \( W_{\sigma\sigma} \) and \( W^T_{\sigma} \) are defined in terms of time ordered response functions and many-body local fields. Furthermore, the above expression for \( W^T_{\sigma} \) has been obtained from Eq. (21) after noting that in the transverse channel we expect the screened interaction potential to be determined by the transverse spin susceptibility.

Earlier on, in Ref. 3, the present authors derived the following expression for the self-energy of an infinitesimally polarized Fermi gas:

\[
\Sigma^\sigma(\vec{p}, \epsilon^\sigma_{\vec{p}}) = -\sum_q \left\{ n^\sigma_{\vec{p} - \vec{q}} \text{Re} \left[ v(q) + D_1(\vec{q}, \epsilon^\sigma_{\vec{p}} - \epsilon^\sigma_{\vec{p} - \vec{q}}) \right] 
+ n^{-\sigma}_{\vec{p} - \vec{q}} \text{Re} \left[ D_2(\vec{q}, \epsilon^\sigma_{\vec{p}} - \epsilon^{-\sigma}_{\vec{p} - \vec{q}}) \right] 
- \frac{P}{\pi} \int_0^\infty d\omega \left\{ \frac{1}{\omega - \epsilon^\sigma_{\vec{p}} + \epsilon^\sigma_{\vec{p} - \vec{q}}} + \frac{1}{\omega - \epsilon^{-\sigma}_{\vec{p}} + \epsilon^{-\sigma}_{\vec{p} - \vec{q}}} \right\},
\]

where

\[
D_1(\vec{q}, \epsilon) \equiv v(q)^2 \left[ 1 - G^v_+(\vec{q}, \epsilon) - \mu_B^{-2} \left| G^v_+(\vec{q}, \epsilon) \right|^2 \chi_S(\vec{q}, \epsilon) - 2\sigma Re(G^v_+(1 - G^v_+))\chi_{CS}(\vec{q}, \epsilon) \right],
\]

and

\[
D_2(\vec{q}, \epsilon) \equiv -4\mu_B^{-2} v(q)^2 \left| G^T_{\sigma}(\vec{q}, \epsilon) \right|^2 \chi^{T\sigma}(\vec{q}, \epsilon),
\]
with the local fields $G_{\pm}$ being functions of $\vec{q}$ and $\epsilon_{\sigma}^2 - \epsilon_{\sigma - q}^2$ while $G^T$ being a function of $\epsilon_{\sigma}^2 - \epsilon_{\sigma - q}^2$.

The expression for the self-energy given in Eq. (33) can be rearranged, as will be shown below, to give the following expression similar to that of Eq. (31) derived above:

$$\Sigma^\sigma(\vec{p}, \omega) = -\sum_{\vec{q}} \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi i} \left[ (v(q) + D_1(\vec{q}, \epsilon)) g^\sigma(\vec{p} - \vec{q}, \omega - \epsilon) + D_2(\vec{q}, \epsilon) g^{-\sigma}(\vec{p} - \vec{q}, \omega - \epsilon) \right].$$

(36)

Now, if in Eq. (36) the complex conjugate local fields are replaced by complex local fields and the frequencies of the local fields that are pre-factors to the response functions are replaced by those of the response functions, we then get exactly the self-energy given by Eq. (31). We further note that the expression for the self-energy as given by Eq. (31) is identical to the result of Ref. [3].

We will now rearrange the expression for the self-energy given in Eq. (36) in terms of screened exchange and coulomb hole contributions. It can be verified from Kramers-Kronig relations that $D_{1,2}(\vec{q}, \epsilon)$ can be cast in the following form:

$$D_{1,2}(\vec{q}, \epsilon) = -\int_0^\infty \frac{dt}{\pi} \left\{ \frac{\text{Im}D_{1,2}(\vec{q}, t)}{\epsilon - t + i\eta} - \frac{\text{Im}D_{1,2}(\vec{q}, -t)}{\epsilon + t - i\eta} \right\}.$$  

(37)

Noting that $D_{1,2}(\vec{q}, \epsilon)$ vanishes for large values of $\epsilon$, we readily obtain

$$i \sum_{\vec{q}} \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} D_{1,2}(\vec{q}, \epsilon) g^\sigma(\vec{p} - \vec{q}, \omega - \epsilon)$$

$$= -i \frac{1}{2\pi^2} \sum_{\vec{q}} \left(1 - n_{\vec{p} - \vec{q}}^\sigma\right) \int_0^\infty dt [\text{Im}D_{1,2}(\vec{q}, t)] \int_{-\infty}^{\infty} \frac{d\epsilon}{\omega - \epsilon - e_{\vec{p} - \vec{q}}^\sigma - i\eta} \frac{1}{[\epsilon - t + i\eta]}$$

$$+ i \frac{1}{2\pi^2} \sum_{\vec{q}} n_{\vec{p} - \vec{q}}^\sigma \int_0^\infty dt [\text{Im}D_{1,2}(\vec{q}, -t)] \int_{-\infty}^{\infty} \frac{d\epsilon}{\omega - \epsilon - e_{\vec{p} - \vec{q}}^\sigma - i\eta} \frac{1}{[\epsilon + t - i\eta]}$$

$$= \sum_{\vec{q}} n_{\vec{p} - \vec{q}}^\sigma \int_0^\infty \frac{dt}{\pi} \left\{ \frac{\text{Im}D_{1,2}(\vec{q}, t)}{\omega - e_{\vec{p} - \vec{q}}^\sigma - t + i\eta} - \frac{\text{Im}D_{1,2}(\vec{q}, -t)}{\omega - e_{\vec{p} - \vec{q}}^\sigma + t - i\eta} \right\}$$

$$- \sum_{\vec{q}} \int_0^\infty \frac{dt}{\pi} \frac{\text{Im}D_{1,2}(\vec{q}, t)}{\omega - e_{\vec{p} - \vec{q}}^\sigma - t + i\eta}$$

$$= -\sum_{\vec{q}} n_{\vec{p} - \vec{q}}^\sigma D_{1,2}(\vec{q}, \omega - e_{\vec{p} - \vec{q}}^\sigma) - \sum_{\vec{q}} \int_0^\infty \frac{dt}{\pi} \frac{\text{Im}D_{1,2}(\vec{q}, t)}{\omega - e_{\vec{p} - \vec{q}}^\sigma - t + i\eta}.$$  

(38)

Finally by noting that

$$\sum_{\vec{q}} \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi i} v(q) g^\sigma(\vec{p} - \vec{q}, \omega - \epsilon) = \sum_{\vec{q}} v(q) n_{\vec{p} - \vec{q}}^\sigma.$$  

(39)

we see from Eqs. (38) and (39) that the self-energy given in Eq. (36) is equivalent to the expression in Eq. (33).

**IV. CONCLUSIONS**

We have shown that the Kukkonen-Overhauser approach to derivation of the screened interaction between two electrons in an interacting electron liquid can be extended to the case of an infinitesimally polarized electron gas provided one makes a reasonable ansatz for the spin-flip term. The screened interaction obtained in this approach can be then used to obtain the electron self-energy by means of a GW type of approximation. The self-energy thus obtained is similar to that previously derived by different means by the present authors.

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