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.

Kukkonen and Overhauser[1] (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. KO were the first to exploit, to its fullest extent for the case of paramagnetic jellium, the many-body local field methodology introduced by Hubbard to account for vertex corrections.[2] 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 an unpolarized 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.[3] The diagrammatic analysis was then extended to the case of an infinitesimally polarized electron gas by Ng and Singwi.[4] 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.[5,6] This theory found successful application to the study of many-body effects in two-dimensional electronic systems.[7]

A popular alternative approach for calculating the physical properties of the Landau quasiparticles in an electron gas is represented by the total energy method.[8] 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.[9,6] 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. 6 via the pseudo-Hamiltonian method. The self-energy obtained by this procedure proved to be equivalent to that independently derived by Ng and Singwi.[4]

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 multicomponent systems, we derive the screened interaction between two electrons by generalizing the theories of Refs. 1 and 10 to an infinitesimally polarized degenerate multivalley system. Then 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.[11] 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. 6.

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 end we adopt the same formalism utilized in Appendix A of Ref. 6 for obtaining the various response functions. We begin by introducing a spin up electron, represented by a (number) density of Fourier amplitude $\rho_\uparrow$, into the Fermi sea. Let Δn_σ be the linear density fluctuation of spin $\sigma = \pm 1$, set up by the introduction of this electron. Furthermore let $G^v_\pm$ be the generalized many-body multivalley local fields defined in Ref. 6 with the same simplifying approximations holding between the intra and intervalley exchange and correlation related many-body local fields. 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 spin σ in the Fermi sea can be obtained in the following compact form:

$$\phi_{\sigma\uparrow} = v(q)\{(1-G^v_+ - \sigma G^v_-)\rho_\uparrow + [\Delta n_\uparrow + \Delta n_\downarrow](1-G^v_+) - \sigma[\Delta n_\uparrow - \Delta n_\downarrow]G^v_-\}, \quad (1)$$

where it is understood that the potential $\phi_{\sigma\uparrow}$, the density fluctuations, and the many-body local fields G are all functions of both $\vec{q}$ and ω. Furthermore, in obtaining the above expression, explicit account has been taken of the exchange and correlation effects between the perturbing and the spectator electrons. We next recognize that within linear response one can write

$$\Delta n_\sigma = \nu_v \chi_0^\sigma \phi_{\sigma\uparrow}, \tag{2}$$

where χ_0^σ is the spin σ response for a noninteracting electron gas. Then using Eqs. (1) and (2), we obtain the following relationships for the potentials:

$$\phi_{\uparrow\uparrow} = \frac{v(q)[(1-G_+^v-G_-^v)+4v(q)\nu_v\chi_0^\downarrow G_-^v(1-G_+^v)]}{\mathcal{D}^v}\rho_\uparrow \tag{3}$$

and

$$\phi_{\downarrow\uparrow} = \frac{v(q)(1-G_+^v+G_-^v)}{\mathcal{D}^v}\rho_\uparrow, \tag{4}$$

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

$$\mathcal{D}^v \equiv 1 - v(q)(\nu_v\chi_0^\uparrow + \nu_v\chi_0^\downarrow)(1-G_+^v-G_-^v) - 4v^2(q)\nu_v^2\chi_0^\uparrow\chi_0^\downarrow G_-^v(1-G_+^v). \tag{5}$$

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 $G_\pm^v$ 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

$$W_{\sigma\uparrow}\ \ \rho_\uparrow = \phi_{\sigma\uparrow} + v(q)[(G_+^v + \sigma G_-^v)\rho_\uparrow]. \tag{6}$$

For an unpolarized system, based on the isotropy, we have for the spin dependent screened interaction potential the more general expression

$$W_{\vec{\sigma}_1\vec{\sigma}_2} = \frac{W_{\uparrow\uparrow}+W_{\downarrow\uparrow}}{2} + \vec{\sigma}_1\cdot\vec{\sigma}_2\frac{W_{\uparrow\uparrow}-W_{\downarrow\uparrow}}{2}. \tag{7}$$

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 $W_{\vec{\sigma}_1\vec{\sigma}_2}$ will automatically account for exchange and (to some extent) correlation effects.[12,13] This can be seen from

$$M_{\alpha,\beta} = \frac{1}{2}\langle\psi_f|W_{\vec{\sigma}_1\vec{\sigma}_2}(\vec{r}_1-\vec{r}_2,\omega)|\psi_i\rangle = W_{\alpha\beta}(\vec{q},\omega) - \delta_{\alpha,\beta}W_{\alpha\alpha}(\vec{k}_1-\vec{k}_2-\vec{q},\omega) - \delta_{-\alpha,\beta} \times W^T(\vec{k}_1-\vec{k}_2-\vec{q},\omega), \tag{8}$$

where, with obvious notation

$$|\psi_i\rangle \equiv |\vec{k}_1,\alpha;\vec{k}_2,\beta\rangle - |\vec{k}_2,\beta;\vec{k}_1,\alpha\rangle, \tag{9}$$

$$\langle\psi_f| \equiv \langle\vec{k}_1-\vec{q},\alpha;\vec{k}_2+\vec{q},\beta| - \langle\vec{k}_2+\vec{q},\beta;\vec{k}_1-\vec{q},\alpha|, \tag{10}$$

we have defined

$$W^T(\vec{q},\omega) = W_{\uparrow\uparrow}(\vec{q},\omega) - W_{\downarrow\uparrow}(\vec{q},\omega). \tag{11}$$

In Eq. (8), $W_{\vec{\sigma}_1\vec{\sigma}_2}(\vec{r},\omega)$ is the real space Fourier transform of the screened interaction given in Eq. (7). Thus the matrix elements $M_{\sigma\sigma}$ automatically incorporate antisymmetrization effects and quite naturally contain nonlocal contributions.

As for $W_{-\sigma\sigma}$, the correlation effects between two opposite spin Fermi sea electrons are accounted through spin-flip scattering processes with the corresponding screened potential in the transverse (spin-flip) channel being given by

$$W^T = -2\mu_B^{-2}[v(q)G_-^v(\vec{q},\omega)]^2\chi_S(\vec{q},\omega), \tag{12}$$

which is twice the contribution from the longitudinal spin fluctuations.

For an infinitesimally polarized multivalley system, using Eqs. (3)–(6) and the expressions for the charge response χ_C, the spin response χ_S, and the mixed charge-spin response $\chi_{\rm CS}$ derived in Ref. 6, it can be shown that

$$W_{\sigma\sigma}(\vec{q},\omega) = v(q)\{1+v(q)[1-G_+^v(\vec{q},\omega)]^2\chi_C(\vec{q},\omega)\} - \mu_B^{-2}[v(q)G_-^v(\vec{q},\omega)]^2\chi_S(\vec{q},\omega) - 2\sigma v(q)^2 G_-^v(\vec{q},\omega)[1-G_+^v(\vec{q},\omega)]\chi_{\rm CS}(\vec{q},\omega), \tag{13}$$

and that

$$W_{\downarrow\uparrow}(\vec{q},\omega) = v(q)\{1+v(q)[1-G_+^v(\vec{q},\omega)]^2\chi_C(\vec{q},\omega)\} + \mu_B^{-2}[v(q)G_-^v(\vec{q},\omega)]^2\chi_S(\vec{q},\omega). \tag{14}$$

Now, for the infinitesimally polarized case, while the matrix elements $M_{\alpha,\beta}$ are still given by Eq. (8), for W^T *we propose the following natural ansatz* based on the structure of its unpolarized counterpart:

$$W^T = \frac{W_{\uparrow\uparrow}(\vec{q},\omega)+W_{\downarrow\downarrow}(\vec{q},\omega)}{2} - W_{\downarrow\uparrow}(\vec{q},\omega) = -2\mu_B^{-2}[v(q)G_-^v(\vec{q},\omega)]^2\chi_S(\vec{q},\omega). \tag{15}$$

The screened interaction $W_{\sigma\sigma'}(\vec{q},\omega)$ given in Eqs. (13) and (14) is similar to the effective screened interaction $V_{\sigma,\sigma'}(\vec{q},\omega,\omega,\omega)$ derived by the present authors [see Eq. (31) of Ref. 6]. In fact, if in $V_{\sigma,\sigma'}(\vec{q},\omega,\omega,\omega)$ the real response functions are replaced by the full complex responses and the complex conjugate many-body local fields that are prefactors 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. 6, the effective screened interaction $V_{\sigma,\sigma'}(\vec{q},\omega,\omega,\omega)$ 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. 14. To evaluate higher order terms would in this case not only lead to better results but would in fact be erroneous. It is then quite rea-

sonable to evaluate the quasiparticle self-energy to first order in the screened interaction from the expression

$$\Sigma^{\sigma}(\vec{p},\omega)=-\sum_{\vec{q}}\int_{-\infty}^{\infty}\frac{d\epsilon}{2\pi i}\{W_{\sigma\sigma}g^{\sigma}(\vec{p}-\vec{q},\omega-\epsilon)+W_{\sigma}^{T}g^{-\sigma}(\vec{p}-\vec{q},\omega-\epsilon)\},\tag{16}$$

where $W_{\sigma\sigma}$ is given by Eq. (13) and W_{σ}^{T} is defined as follows:

$$W_{\sigma}^{T}(\vec{q},\omega)\equiv-4\mu_{B}^{-2}[v(q)G_{-}^{Tv}(\vec{q},\omega)]^{2}\chi^{T\sigma}(\vec{q},\omega),\tag{17}$$

with $\chi^{T\sigma}$ being the transverse spin response defined in Ref. 6. In the above equation for $\Sigma^{\sigma}(\vec{p},\omega)$ it is understood that $W_{\sigma\sigma}$ and W_{σ}^{T} are defined in terms of time ordered response functions and many-body local fields. Furthermore, the above expression for W_{σ}^{T} has been obtained from Eq. (15) 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. 6, the present authors derived the following expression for the self-energy of an infinitesimally polarized Fermi gas

$$\Sigma^{\sigma}(\vec{p},\epsilon_{\vec{p}}^{\sigma})=-\sum_{\vec{q}}\left\{n_{\vec{p}-\vec{q}}^{\sigma}\mathrm{Re}[v(q)+D_{1}(\vec{q},\epsilon_{\vec{p}}^{\sigma}-\epsilon_{\vec{p}-\vec{q}}^{\sigma})]+n_{\vec{p}-\vec{q}}^{-\sigma}\mathrm{Re}[D_{2}(\vec{q},\epsilon_{\vec{p}}^{\sigma}-\epsilon_{\vec{p}-\vec{q}}^{\sigma})]-P\int_{0}^{\infty}\frac{d\omega}{\pi}\left[\frac{\mathrm{Im}[D_{1}(\vec{q},\omega)]}{\omega-\epsilon_{\vec{p}}^{\sigma}+\epsilon_{\vec{p}-\vec{q}}^{\sigma}}+\frac{\mathrm{Im}[D_{2}(\vec{q},\omega)]}{\omega-\epsilon_{\vec{p}}^{\sigma}+\epsilon_{\vec{p}-\vec{q}}^{-\sigma}}\right]\right\},\tag{18}$$

where

$$D_{1}(\vec{q},\epsilon)\equiv v(q)^{2}[|1-G_{+}^{v}|^{2}\chi_{C}(\vec{q},\epsilon)-\mu_{B}^{-2}|G_{-}^{v}|^{2}\chi_{S}(\vec{q},\epsilon)-2\sigma\,\mathrm{Re}[G_{-}^{v}(1-G_{+}^{v\star})]\chi_{\mathrm{CS}}(\vec{q},\epsilon)]\tag{19}$$

and

$$D_{2}(\vec{q},\epsilon)\equiv-4\mu_{B}^{-2}v(q)^{2}|G_{-}^{Tv}|^{2}\chi^{T\sigma}(\vec{q},\epsilon),\tag{20}$$

with the local fields $G_{\pm}$ being functions of $\vec{q}$ and $\epsilon_{\vec{p}}^{\sigma}-\epsilon_{\vec{p}-\vec{q}}^{\sigma}$ while G_{-}^{T} being a function of $\epsilon_{\vec{p}}^{\sigma}-\epsilon_{\vec{p}-\vec{q}}^{-\sigma}$.

The expression for the self-energy given in Eq. (18) can be rearranged, as will be shown below, to give the following expression similar to that of Eq. (16) derived above:

$$\Sigma^{\sigma}(\vec{p},\omega)=-\sum_{\vec{q}}\int_{-\infty}^{\infty}\frac{d\epsilon}{2\pi i}\{[v(q)+D_{1}(\vec{q},\epsilon)]\times g^{\sigma}(\vec{p}-\vec{q},\omega-\epsilon)+D_{2}(\vec{q},\epsilon)\times g^{-\sigma}(\vec{p}-\vec{q},\omega-\epsilon)\}.\tag{21}$$

Now, if in Eq. (21) the complex conjugate local fields are replaced by complex local fields and the frequencies of the local fields that are prefactors to the response functions are replaced by those of the response functions, we then get exactly the self-energy given by Eq. (16). We further note that the expression for the self-energy as given by Eq. (16) is identical to the result of Ref. 4.

We will now rearrange the expression for the self-energy given in Eq. (21) 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:

$$D_{1,2}(\vec{q},\epsilon)=-\int_{0}^{\infty}\frac{dt}{\pi}\left\{\frac{\mathrm{Im}\,D_{1,2}(\vec{q},t)}{\epsilon-t+i\eta}-\frac{\mathrm{Im}\,D_{1,2}(\vec{q},-t)}{\epsilon+t-i\eta}\right\}.\tag{22}$$

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

$$\begin{aligned}
&i\sum_{\vec{q}}\int_{-\infty}^{\infty}\frac{d\epsilon}{2\pi}D_{1,2}(\vec{q},\epsilon)g^{\sigma}(\vec{p}-\vec{q},\omega-\epsilon)\\
&=-\frac{i}{2\pi^{2}}\sum_{\vec{q}}(1-n_{\vec{p}-\vec{q}}^{\sigma})\int_{0}^{\infty}dt[\mathrm{Im}\,D_{1,2}(\vec{q},t)]\int_{-\infty}^{\infty}d\epsilon\frac{1}{[\omega-\epsilon-\epsilon_{\vec{p}-\vec{q}}^{\sigma}+i\eta][\epsilon-t+i\eta]}\\
&\quad+\frac{i}{2\pi^{2}}\sum_{\vec{q}}n_{\vec{p}-\vec{q}}^{\sigma}\int_{0}^{\infty}dt[\mathrm{Im}\,D_{1,2}(\vec{q},-t)]\int_{-\infty}^{\infty}d\epsilon\frac{1}{[\omega-\epsilon-\epsilon_{\vec{p}-\vec{q}}^{\sigma}-i\eta][\epsilon+t-i\eta]}\\
&=\sum_{\vec{q}}n_{\vec{p}-\vec{q}}^{\sigma}\int_{0}^{\infty}\frac{dt}{\pi}\left\{\frac{\mathrm{Im}\,D_{1,2}(\vec{q},t)}{\omega-\epsilon_{\vec{p}-\vec{q}}^{\sigma}-t+i\eta}-\frac{\mathrm{Im}\,D_{1,2}(\vec{q},-t)}{\omega-\epsilon_{\vec{p}-\vec{q}}^{\sigma}+t-i\eta}\right\}-\sum_{\vec{q}}\int_{0}^{\infty}\frac{dt}{\pi}\frac{\mathrm{Im}\,D_{1,2}(\vec{q},t)}{\omega-\epsilon_{\vec{p}-\vec{q}}^{\sigma}-t+i\eta}\\
&=-\sum_{\vec{q}}n_{\vec{p}-\vec{q}}^{\sigma}D_{1,2}(\vec{q},\omega-\epsilon_{\vec{p}-\vec{q}}^{\sigma})-\sum_{\vec{q}}\int_{0}^{\infty}\frac{dt}{\pi}\frac{\mathrm{Im}\,D_{1,2}(\vec{q},t)}{\omega-\epsilon_{\vec{p}-\vec{q}}^{\sigma}-t+i\eta}.
\end{aligned}\tag{23}$$

Finally by noting that

$$\sum_{\vec{q}} \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi i} v(q) g^{\sigma}(\vec{p}-\vec{q}, \omega-\epsilon) = \sum_{\vec{q}} v(q) n^{\sigma}_{\vec{p}-\vec{q}}, \tag{24}$$

we see from Eqs. (23) and (24) that the self-energy given in Eq. (21) is equivalent to the expression in Eq. (18).

We have shown that the Kukkonen-Overhauser approach to derivation of the screened interaction between two electrons in an unpolarized electron liquid can be extended to the case of an infinitesimally polarized system 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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