MASTER'S DEGREE IN PHYSICS
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Introduction to Many Body Theory

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HOMEWORK 4

Exercise 4.1

As first step we show that the $(a), (c), (d), (e)$ first order contributions to the proper polarization (1) are vanishing.

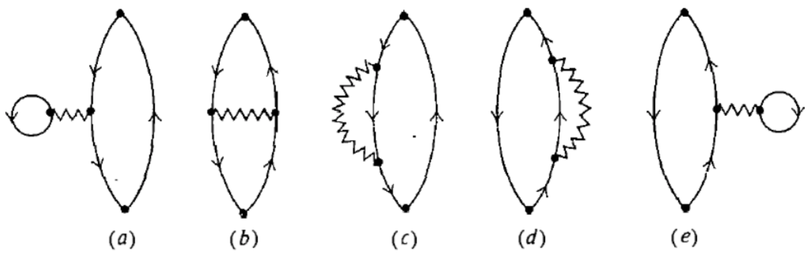

Figure 1: All first-order contributions to proper polarization.

We continue with the evaluation of the (b) term in 1 with the aim of computing the (b) first order contribution to the correlation energy E_2^b. In figure 2 the diagram is written in momentum space

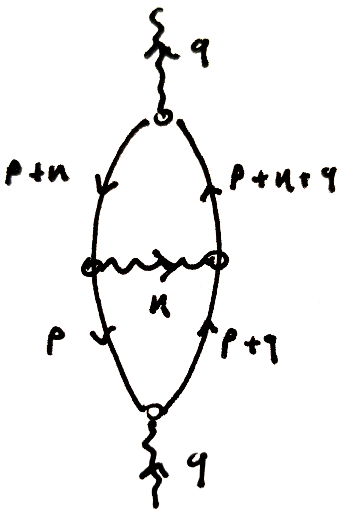

Figure 2: (b) contribution to proper polarization.

with the momentum conserved at each node; the spin part is omitted since it's easily proven that its contraction gives a $2s + 1 \overset{s=1/2}{\rightarrow} 2$ factor; this is due to the fact that each non interacting GF is diagonal in spin space and the interaction is spin-independent. The analytic expression associated to the diagram in (2) is:

UP* EXPRESSION AS GGGUG

that can be written explicitly knowing the expression of the GF for free fermions in momentum space as:

$$\int \frac{\mathrm{d}^4 q}{(2\pi)^4} U(q)\Pi^*(q) = -\frac{2(4\pi e)^2}{(2\pi)^{12}}\left(\frac{i}{\hbar}\right)^2 \int \mathrm{d}^4 q\, \mathrm{d}^4 p\, \mathrm{d}^4 k\, \frac{1}{q^2 k^2}\left[\frac{\Theta(|\vec{\mathbf{p}}+\vec{\mathbf{q}}|-k_F)}{p^0+q^0-\omega_{\vec{\mathbf{p}}+\vec{\mathbf{q}}}+i\eta}+\frac{\Theta(k_F-|\vec{\mathbf{p}}+\vec{\mathbf{q}}|)}{p^0+q^0-\omega_{\vec{\mathbf{p}}+\vec{\mathbf{q}}}-i\eta}\right]\times$$
$$\times\left[\frac{\Theta\left(\left|\vec{\mathbf{p}}+\vec{\mathbf{k}}+\vec{\mathbf{q}}\right|-k_F\right)}{p^0+q^0+k^0-\omega_{\vec{\mathbf{p}}+\vec{\mathbf{k}}+\vec{\mathbf{q}}}+i\eta}+\frac{\Theta\left(k_F-\left|\vec{\mathbf{p}}+\vec{\mathbf{k}}+\vec{\mathbf{q}}\right|\right)}{p^0+q^0+k^0-\omega_{\vec{\mathbf{p}}+\vec{\mathbf{k}}+\vec{\mathbf{q}}}-i\eta}\right]\times$$
$$\times\left[\frac{\Theta\left(\left|\vec{\mathbf{p}}+\vec{\mathbf{k}}\right|-k_F\right)}{p^0+k^0-\omega_{\vec{\mathbf{p}}+\vec{\mathbf{k}}}+i\eta}+\frac{\Theta\left(k_F-\left|\vec{\mathbf{p}}+\vec{\mathbf{k}}\right|\right)}{p^0+k^0-\omega_{\vec{\mathbf{p}}+\vec{\mathbf{k}}}-i\eta}\right]\times$$
$$\times\left[\frac{\Theta(|\vec{\mathbf{p}}|-k_F)}{p^0-\omega_{\vec{\mathbf{p}}}+i\eta}+\frac{\Theta(k_F-|\vec{\mathbf{p}}|)}{p^0-\omega_{\vec{\mathbf{p}}}-i\eta}\right]. \tag{1}$$

The evaluation of this integral starts from the temporal component k^0 relative to the four-vector k. Observing the expression we note that some of the products involved in the k^0 integration present both poles on the same side (above or below) of the k^0 complex plane; this means that the integral on the real variable k^0 can be extended to an integration on the complex plane that does not include any pole and is therefore vanishing. For this reason we can rearrange the previous expression keeping only the non vanishing terms:

$$= -\frac{2(4\pi e)^2}{(2\pi)^{12}}\left(\frac{i}{\hbar}\right)^2 \int \mathrm{d}^4 q\, \mathrm{d}^4 p\, \mathrm{d}^4 k \frac{1}{q^2 k^2}\left[\frac{\Theta(|\vec{\mathbf{p}}+\vec{\mathbf{q}}|-k_F)}{p^0+q^0-\omega_{\vec{\mathbf{p}}+\vec{\mathbf{q}}}+i\eta}+\frac{\Theta(k_F-|\vec{\mathbf{p}}+\vec{\mathbf{q}}|)}{p^0+q^0-\omega_{\vec{\mathbf{p}}+\vec{\mathbf{q}}}-i\eta}\right]\times$$
$$\times\left[\frac{\Theta(|\vec{\mathbf{p}}|-k_F)}{p^0-\omega_{\vec{\mathbf{p}}}+i\eta}+\frac{\Theta(k_F-|\vec{\mathbf{p}}|)}{p^0-\omega_{\vec{\mathbf{p}}}-i\eta}\right]\times$$
$$\times\left[\frac{\Theta\left(k_F-\left|\vec{\mathbf{p}}+\vec{\mathbf{k}}\right|\right)\Theta\left(\left|\vec{\mathbf{p}}+\vec{\mathbf{k}}+\vec{\mathbf{q}}\right|-k_F\right)}{\left(p^0+k^0-\omega_{\vec{\mathbf{p}}+\vec{\mathbf{k}}}-i\eta\right)\left(p^0+q^0+k^0-\omega_{\vec{\mathbf{p}}+\vec{\mathbf{k}}+\vec{\mathbf{q}}}+i\eta\right)}+\right.$$
$$\left.+\frac{\Theta\left(\left|\vec{\mathbf{p}}+\vec{\mathbf{k}}\right|-k_F\right)\Theta\left(k_F-\left|\vec{\mathbf{p}}+\vec{\mathbf{k}}+\vec{\mathbf{q}}\right|\right)}{\left(p^0+k^0-\omega_{\vec{\mathbf{p}}+\vec{\mathbf{k}}}+i\eta\right)\left(p^0+q^0+k^0-\omega_{\vec{\mathbf{p}}+\vec{\mathbf{k}}+\vec{\mathbf{q}}}-i\eta\right)}\right]. \tag{2}$$

The integral over k^0 can be evaluated computing the residues at $\bar{q}^0_a = p^0+\omega_{\vec{\mathbf{p}}+\vec{\mathbf{k}}}+i\eta$ for the first term and at $\bar{q}^0_b = p^0+\omega_{\vec{\mathbf{p}}+\vec{\mathbf{k}}}-i\eta$ for the second one, obtaining:

$$= -\frac{2(4\pi e)^2}{(2\pi)^{12}}\left(\frac{i}{\hbar}\right)^2 \int \mathrm{d}^4 q\, \mathrm{d}^4 p\, \mathrm{d}^4 k \frac{1}{q^2 k^2}\left[\frac{\Theta(|\vec{\mathbf{p}}+\vec{\mathbf{q}}|-k_F)}{p^0+q^0-\omega_{\vec{\mathbf{p}}+\vec{\mathbf{q}}}+i\eta}+\frac{\Theta(k_F-|\vec{\mathbf{p}}+\vec{\mathbf{q}}|)}{p^0+q^0-\omega_{\vec{\mathbf{p}}+\vec{\mathbf{q}}}-i\eta}\right]\times$$
$$\times\left[\frac{\Theta(|\vec{\mathbf{p}}|-k_F)}{p^0-\omega_{\vec{\mathbf{p}}}+i\eta}+\frac{\Theta(k_F-|\vec{\mathbf{p}}|)}{p^0-\omega_{\vec{\mathbf{p}}}-i\eta}\right]\times$$
$$\times\left[\frac{\Theta\left(k_F-\left|\vec{\mathbf{p}}+\vec{\mathbf{k}}\right|\right)\Theta\left(\left|\vec{\mathbf{p}}+\vec{\mathbf{k}}+\vec{\mathbf{q}}\right|-k_F\right)}{p^0+q^0+\omega_{\vec{\mathbf{p}}+\vec{\mathbf{k}}}-\omega_{\vec{\mathbf{p}}+\vec{\mathbf{k}}+\vec{\mathbf{q}}}+i\eta}-\right.$$
$$\left.-\frac{\Theta\left(\left|\vec{\mathbf{p}}+\vec{\mathbf{k}}\right|-k_F\right)\Theta\left(k_F-\left|\vec{\mathbf{p}}+\vec{\mathbf{k}}+\vec{\mathbf{q}}\right|\right)}{p^0+q^0+\omega_{\vec{\mathbf{p}}+\vec{\mathbf{k}}}-\omega_{\vec{\mathbf{p}}+\vec{\mathbf{k}}+\vec{\mathbf{q}}}-i\eta}\right]. \tag{3}$$

An analogous procedure helps us to compute the integration over the p^0 temporal component; in this case the expression to evaluate is:

$$
\begin{aligned}
= -\frac{2(4\pi e)^2}{(2\pi)^{12}}\left(\frac{i}{\hbar}\right)^2 \int \mathrm{d}^4 q\, \mathrm{d}^4 p\, \mathrm{d}^4 k \frac{1}{q^2 k^2} & \left[\frac{\Theta(|\vec{\mathbf{p}}+\vec{\mathbf{q}}|-k_F)\Theta(k_F-|\vec{\mathbf{p}}|)}{(p^0+q^0-\omega_{\vec{\mathbf{p}}+\vec{\mathbf{q}}}+i\eta)(p^0-\omega_{\vec{\mathbf{p}}}-i\eta)}\right. \\
& \left. + \frac{\Theta(k_F-|\vec{\mathbf{p}}+\vec{\mathbf{q}}|)\Theta(|\vec{\mathbf{p}}|-k_F)}{(p^0+q^0-\omega_{\vec{\mathbf{p}}+\vec{\mathbf{q}}}-i\eta)(p^0-\omega_{\vec{\mathbf{p}}}+i\eta)}\right] \times \\
& \times \left[\frac{\Theta\Big(k_F-\left|\vec{\mathbf{p}}+\vec{\mathbf{k}}\right|\Big)\Theta\Big(\left|\vec{\mathbf{p}}+\vec{\mathbf{k}}+\vec{\mathbf{q}}\right|-k_F\Big)}{p^0+q^0+\omega_{\vec{\mathbf{p}}+\vec{\mathbf{k}}}-\omega_{\vec{\mathbf{p}}+\vec{\mathbf{k}}+\vec{\mathbf{q}}}+i\eta}+\right. \\
& \left. + \frac{\Theta\Big(\left|\vec{\mathbf{p}}+\vec{\mathbf{k}}\right|-k_F\Big)\Theta\Big(k_F-\left|\vec{\mathbf{p}}+\vec{\mathbf{k}}+\vec{\mathbf{q}}\right|\Big)}{p^0+q^0+\omega_{\vec{\mathbf{p}}+\vec{\mathbf{k}}}-\omega_{\vec{\mathbf{p}}+\vec{\mathbf{k}}+\vec{\mathbf{q}}}-i\eta}\right].
\end{aligned}
\tag{4}
$$

and the poles to compute the residues are located respectively at $p_a^0 = \omega_{\vec{\mathbf{p}}} + i\eta$ and at $p_b^0 = \omega_{\vec{\mathbf{p}}} - i\eta$. The result is the following:

GF POST P0 EVALUATION

The last integration is over the q^0 temporal part:

GF PRE Q0 EVALUATION

and the concerned poles are $q_a^0 = \omega_{\vec{\mathbf{p}}+\vec{\mathbf{q}}} - \omega_{\vec{\mathbf{p}}} - i\eta$ and $q_b^0 = \omega_{\vec{\mathbf{p}}+\vec{\mathbf{q}}} - \omega_{\vec{\mathbf{p}}} + i\eta$:

GF POST Q0 EVALUATION

Note that we removed the complex $i\eta$ terms since the temporal part has been completely evaluated. Now we proceed with a change of variables in order to exploit the symmetry of the expression and simplify one of the addends; the change

CHANGE OF VARIABLES 1 (5)

applied to the second addend modifies the numerator to:

MODIFIED NUMERATOR (6)

which allows us to write the integral as:

ONE TERM GF

On the other hand, the denominator can also be written more explicitly as:

DENOMINATOR REWRITTEN

A scaling of the variables by a k_F^{-1} factor brings in front an overall $k_F^3 factor$; simplifying some factors one gets:

FINAL EXPR FOR UP*

The second order (b) energy contribution differs from the expression we computed for a $i\hbar V/2/(2\pi^4)$ factor; gathering all the factors together we get:

FACTOR COMPUTATION

and therefore the expression for the second order contribution to the correlation energy is

FINAL FORMULA (7)

as we wanted to prove.

Exercise 7.1

For a generic one particle operator $\widehat{O}$ the grand canonical ensemble average is defined as

$$\langle\widehat{O}\rangle = \mathrm{Tr}\Big\{\widehat{\rho}_G\widehat{O}\Big\} = \int \mathrm{d}^3\vec{\mathbf{x}} \lim_{\vec{\mathbf{x}}'\to\vec{\mathbf{x}}} \mathrm{Tr}\Big\{\widehat{\rho}_G\widehat{\psi}^\dagger_\alpha(\vec{\mathbf{x}}')\,O_{\alpha\beta}(\vec{\mathbf{x}})\widehat{\psi}_\beta(\vec{\mathbf{x}})\Big\} = \int \mathrm{d}^3\vec{\mathbf{x}} \lim_{\vec{\mathbf{x}}'\to\vec{\mathbf{x}}} O_{\alpha\beta}\,\mathrm{Tr}\left\{\frac{e^{-\beta\widehat{K}}}{Z_G}\widehat{\psi}^\dagger_\alpha(\vec{\mathbf{x}}')\,\widehat{\psi}_\beta(\vec{\mathbf{x}})\right\} \tag{8}$$

where $O_{\alpha\beta}(\vec{\mathbf{x}})$ is the first quantized form of the operator $\widehat{O}$, $\widehat{\rho}_G = \exp\Big\{-\beta\widehat{K}\Big\}/Z_G$ is the statistic operator and $\widehat{K} = \widehat{H} - \mu\widehat{N}$ is the grand canonical Hamiltonian. In analogy it is possible to define an ensemble average for a two particle operator in second quantization which, in the specific case of the interparticle potential $\widehat{V}(\vec{\mathbf{x}} - \vec{\mathbf{x}}')$ is written as:

$$\langle\widehat{V}\rangle = \mathrm{Tr}\Big\{\widehat{\rho}_G\widehat{V}\Big\} = \int \mathrm{d}^3\vec{\mathbf{x}}_1\,\mathrm{d}^3\vec{\mathbf{x}}_2 \lim_{\substack{\vec{\mathbf{x}}_1'\to\vec{\mathbf{x}}_1\\ \vec{\mathbf{x}}_2'\to\vec{\mathbf{x}}_2}} V_{\substack{\mu\mu'\\ \lambda\lambda'}}(\vec{\mathbf{x}}_1 - \vec{\mathbf{x}}_2)\,\mathrm{Tr}\left\{\frac{e^{-\beta\widehat{K}}}{Z_G}\widehat{\psi}^\dagger_{\lambda'}(\vec{\mathbf{x}}_1')\widehat{\psi}^\dagger_{\mu'}(\vec{\mathbf{x}}_2')\widehat{\psi}_\mu(\vec{\mathbf{x}}_2)\widehat{\psi}_\lambda(\vec{\mathbf{x}}_1)\right\} \tag{9}$$

Now it is possible to connect the previous definition to the one of the two particle temperature Green function:

$$\mathcal{G}_{\alpha\beta;\gamma\delta}(\vec{\mathbf{x}}_1\tau_1, \vec{\mathbf{x}}_2\tau_2; \vec{\mathbf{x}}_1'\tau_1', \vec{\mathbf{x}}_2{}'\tau_2') = \mathrm{Tr}\Big\{\widehat{\rho}_G T\Big[\widehat{\psi}_\alpha(\vec{\mathbf{x}}_1\tau_1)\widehat{\psi}_\beta(\vec{\mathbf{x}}_2\tau_2)\widehat{\psi}^\dagger_\delta(\vec{\mathbf{x}}_2'\tau_2')\widehat{\psi}^\dagger_\gamma(\vec{\mathbf{x}}_1'\tau_1')\Big]\Big\} \tag{10}$$

by proving that the trace in expression (9) is equal to

$$\lim_{\substack{\tau_1'\to\tau_1^+\\ \tau_2'\to\tau_2^+}} \mathrm{Tr}\left\{\frac{e^{-\beta\widehat{K}}}{Z_G}\widehat{\psi}^\dagger_{\lambda'}(\vec{\mathbf{x}}_1'\tau_1')\widehat{\psi}^\dagger_{\mu'}(\vec{\mathbf{x}}_2'\tau_2')\widehat{\psi}_\mu(\vec{\mathbf{x}}_2\tau_2)\widehat{\psi}_\lambda(\vec{\mathbf{x}}_1\tau_1)\right\} \tag{11}$$

where the dime dependence of the fields is given by the modified Heisenberg picture

$$\widehat{\psi}_\lambda(\vec{\mathbf{x}}\tau) = e^{\widehat{K}\tau/\hbar}\widehat{\psi}_\lambda(\vec{\mathbf{x}})e^{-\widehat{K}\tau/\hbar} \tag{12}$$

in which we denote the grand canonical Hamiltonian with $\widehat{K}$ as before and the time with τ. To prove this statement we write the explicit dependence on the time of the fields:

$$\lim_{\substack{\tau_1'\to\tau_1^+\\ \tau_2'\to\tau_2^+}} \mathrm{Tr}\left\{\frac{e^{-\beta\widehat{K}}}{Z_G}e^{\widehat{K}\tau_1'/\hbar}Ae^{-\widehat{K}\tau_1'/\hbar}e^{\widehat{K}\tau_2'/\hbar}B\cancel{e^{-\widehat{K}\tau_2'/\hbar}e^{\widehat{K}\tau_2/\hbar}}Ce^{-\widehat{K}\tau_2/\hbar}e^{\widehat{K}\tau_1/\hbar}De^{-\widehat{K}\tau_1/\hbar}\right\} \tag{13}$$

where we denoted the space-dependent fields with the letters A, B, C, D for brevity. We see that in the limit $\tau_1' \to \tau_1; \tau_2' \to \tau_2$ the highlighted factor cancels out. Using the cyclic property of the trace and the fact that the statistic operator and the time evolution operator commute, we can cancel out another time evolution operator product:

$$\lim_{\substack{\tau_1'\to\tau_1^+\\ \tau_2'\to\tau_2^+}} \mathrm{Tr}\left\{\frac{e^{-\beta\widehat{K}}}{Z_G}\cancel{e^{-\widehat{K}\tau_1/\hbar}e^{\widehat{K}\tau_1'/\hbar}}Ae^{-\widehat{K}\tau_1'/\hbar}e^{\widehat{K}\tau_2'/\hbar}BCe^{-\widehat{K}\tau_2/\hbar}e^{\widehat{K}\tau_1/\hbar}D\right\} \tag{14}$$

The next step is to write down the explicit expression of the trace as a function of a complete set of eigenstates of the grand canonical Hamiltonian such that $\widehat{K}\,|Nj\rangle = E_{Nj}\,|Nj\rangle$; using again the cyclic property of the trace:

$$\lim_{\substack{\tau_1'\to\tau_1^+\\ \tau_2'\to\tau_2^+}} \sum_{Nj} \langle Nj|D\frac{e^{-\beta\widehat{K}}}{Z_G}Ae^{-\widehat{K}\tau_1'/\hbar}e^{\widehat{K}\tau_2'/\hbar}BCe^{-\widehat{K}\tau_2/\hbar}e^{\widehat{K}\tau_1/\hbar}|Nj\rangle \tag{15}$$

$$= \lim_{\substack{\tau_1'\to\tau_1^+\\ \tau_2'\to\tau_2^+}} \sum_{Nj} e^{E_{Nj}\tau_1/\hbar}e^{-E_{Nj}\tau_2/\hbar}\,\langle Nj|D\frac{e^{-\beta\widehat{K}}}{Z_G}Ae^{-\widehat{K}\tau_1'/\hbar}e^{\widehat{K}\tau_2'/\hbar}BC|Nj\rangle \tag{16}$$

$$= \lim_{\substack{\tau_1'\to\tau_1^+\\ \tau_2'\to\tau_2^+}} \sum_{Nj} \cancel{e^{-E_{Nj}\tau_1'/\hbar}e^{E_{Nj}\tau_1/\hbar}}\,\cancel{e^{-E_{Nj}\tau_2/\hbar}e^{E_{Nj}\tau_2'/\hbar}}\,\langle Nj|\frac{e^{-\beta\widehat{K}}}{Z_G}ABCD|Nj\rangle \tag{17}$$

which we can rewrite in the same form as present in (9):

$$(11) = \mathrm{Tr}\left\{\frac{e^{-\beta\widehat{K}}}{Z_G}\widehat{\psi}^{\dagger}_{\lambda'}(\vec{\mathbf{x}}'_1)\widehat{\psi}^{\dagger}_{\mu'}(\vec{\mathbf{x}}'_2)\widehat{\psi}_{\mu}(\vec{\mathbf{x}}_2)\widehat{\psi}_{\lambda}(\vec{\mathbf{x}}_1)\right\} \tag{18}$$

Taking into account the time limit $\tau'_1 \to \tau_1; \tau'_2 \to \tau_2$ in equation (11) the argument of the trace can be rewritten in terms of a time-ordered product:

$$\frac{e^{-\beta\widehat{K}}}{Z_G}\widehat{\psi}^{\dagger}_{\lambda'}(\vec{\mathbf{x}}'_1\tau'_1)\widehat{\psi}^{\dagger}_{\mu'}(\vec{\mathbf{x}}'_2\tau'_2)\widehat{\psi}_{\mu}(\vec{\mathbf{x}}_2\tau_2)\widehat{\psi}_{\lambda}(\vec{\mathbf{x}}_1\tau_1) = \frac{e^{-\beta\widehat{K}}}{Z_G}T\left[\widehat{\psi}_{\lambda}(\vec{\mathbf{x}}_1\tau_1)\widehat{\psi}_{\mu}(\vec{\mathbf{x}}_2\tau_2)\widehat{\psi}^{\dagger}_{\mu'}(\vec{\mathbf{x}}'_2\tau'_2)\widehat{\psi}^{\dagger}_{\lambda'}(\vec{\mathbf{x}}'_1\tau'_1)\right] \tag{19}$$

Therefore, using the definition of the temperature GF (10) we can state that the ensemble average of the interparticle potential is:

$$\langle\widehat{V}\rangle = \mathrm{Tr}\left\{\widehat{\rho}_G\widehat{V}\right\} = \int \mathrm{d}^3\vec{\mathbf{x}}_1\,\mathrm{d}^3\vec{\mathbf{x}}_2\, V_{\substack{\lambda\mu \\ \mu'\lambda'}}(\vec{\mathbf{x}}_1 - \vec{\mathbf{x}}_2)\mathcal{G}_{\substack{\lambda\mu \\ \mu'\lambda'}}(\vec{\mathbf{x}}_1\tau_1, \vec{\mathbf{x}}_2\tau_2; \vec{\mathbf{x}}_1\tau_1^{+}, \vec{\mathbf{x}}_2\tau_2^{+}) \tag{20}$$

as desired.