EFFECTIVE INTERACTION AND POLARIZATION
NOTES BY L. G. MOLINARI

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1. The effective interaction

In a many body system the "bare" interaction U^0 between two particles in empty space is "dressed" by polarization insertions. I give here a derivation of the expression of the polarization based on the diagrammatic expansion of the propagator.

The one-particle Green function (propagator) $iG(x,y) = \langle E_0|TS\psi(x)\psi^\dagger(y)|E_0\rangle_\star$ is the sum of all diagrams with a particle being created at y and destroyed at x that do not contain vacuum factors (spin is included in the variable. For the interaction each variable has a spin pair). The first-order rainbow diagram is

$$\frac{i}{\hbar}\int dx_1 dx_2 G^0(x,x_1)G^0(x_1,x_2^+)G^0(x_2,y)U^0(x_1,x_2)$$

If we select the diagrams of $G(x,y)$ with fixed configuration of three bare propagators, the sum of such diagrams defines the effective interaction $U(x_1,x_2)$:

$$\frac{i}{\hbar}\int dx_1 dx_2 G^0(x,x_1)G^0(x_1,x_2)G^0(x_2,y)U(x_1,x_2)$$

The zero-order term of $U(x_1,x_2)$ is $U^0(x_1,x_2)$. The next ones arise in diagrams of second and higher orders of $G(x,y)$, and necessarily contain two U^0 lines as follows:

$$\frac{i}{\hbar}\int dx_1 dx_2 dy_1 dy_2\; G^0(x,x_1)G^0(x_1,x_2)G^0(x_2,y)\left[U^0(x_1,y_1)\Pi(y_1,y_2)U^0(y_2,x_2)\right]$$

$\Pi(y_1,y_2)$ is the polarization, that sums all possible insertions among the two factors U^0. Therefore, the effective potential is:

$$U(x_1,x_2) = U^0(x_1,x_2) + \int dy_1 dy_2 U^0(x_1,y_1)\Pi(y_1,y_2)U^0(y_2,x_2) \tag{1}$$

The expression for Π is now derived by considering the diagrams associated to contractions of $G(x,y)$ that maintain the product of three bare propagators. Accordingly, we write the expansion of S from second order, where only $V(t_1)$ and $V(t_2)$ are specified in second quantization[1] and the contractions $\psi(x)$ with $\psi^\dagger(x_1)$, $\psi(x_1)$ with $\psi^\dagger(x_2)$ and $\psi(x_2)$ with $\psi^\dagger(y)$ are frozen:

$$\frac{1}{i}\sum_{N=2}^{\infty}\frac{1}{(i\hbar)^N}\int dx_1 dx_2 dy_1 dy_2 U^0(x_1,y_1)U^0(y_2,x_2)\int_{-\infty}^{+\infty}dt_2' \ldots \int_{-\infty}^{+\infty}dt_{N-1}' \times$$
$$\langle T\psi^\dagger(x_1)\psi^\dagger(y_1)\psi(y_1)\psi(x_1)V(t_2')\ldots V(t_{N-1}')\psi^\dagger(x_2)\psi^\dagger(y_2)\psi(y_2)\psi(x_2)\psi(x)\psi^\dagger(y)\rangle_{\star C}$$

The star means that we avoid diagrams with vacuum factors; C means making only contractions linking x_1 to x_2.

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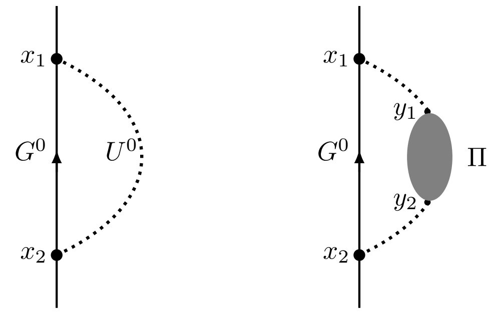
[1]Note the absence of factors $k!2^k$, as we consider topologically different diagrams.



1st diagram with bare interaction and with polarization insertions.

The frozen contractions $iG^0(x,x_1)$, $iG^0(x_1,x_2)$, $iG^0(x_2,y)$ are specified:

$$\frac{1}{i}\frac{i^3}{(i\hbar)^2}\int dx_1dx_2G^0(x,x_1)G^0(x_1,x_2)G^0(x_2,y)\int dy_1dy_NU^0(x_1,y_1)U^0(y_2,x_2)$$
$$\times\sum_{k=0}^{\infty}\frac{1}{(i\hbar)^k}\int dt_1...dt_k\langle T\psi^\dagger(y_1)\psi(y_1)V(t_1)...V(t_k)\psi^\dagger(y_2)\psi(y_2)\rangle_{\star C}$$
$$=\frac{i}{\hbar}\int dx_1dx_2G^0(x,x_1)G^0(x_1,x_2)G^0(x_2,y)$$
$$\times\left[\frac{1}{i\hbar}\int dy_1dy_2U^0(x_1,y_1)U^0(x_2,y_2)\langle E_0|TS\psi^\dagger(y_1)\psi(y_1)\psi^\dagger(y_2)\psi(y_2)|E_0\rangle_{\star C}\right]$$

We leave the interaction picture:

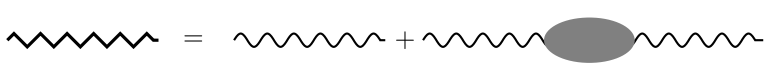
$$\langle E_0|TS\psi^\dagger(y_1)\psi(y_1)\psi^\dagger(y_2)\psi(y_2)|E_0\rangle_{\star C}=\langle E|T\psi^\dagger(y_1)\psi(y_1)\psi^\dagger(y_2)\psi(y_2)|E\rangle_C$$

The unwanted contractions are those that factor (disconnect) into a function of y_1 and a function of y_2[2].

$$\langle E|T\psi^\dagger_\mu(x)\psi_{\mu'}(x)\psi^\dagger_\nu(y)\psi_{\nu'}(y)|E\rangle_C=\langle E|T\delta[\psi^\dagger_\mu(x)\psi_{\mu'}(x)]\,\delta[\psi^\dagger_\nu(y)\psi_{\nu'}(y)]|E\rangle \tag{2}$$

We now write the expression of the effective potential (1) in full detail:

$$U_{\mu\mu',\nu\nu'}(x_1,x_2)=U^0_{\mu\mu',\nu\nu'}(x_1,x_2)+\sum_{\rho\rho'\sigma\sigma'}\int dy_1dy_2\;U^0_{\mu\mu',\rho\rho'}(x_1,y_1)$$
$$\times\Pi_{\rho\rho',\sigma\sigma'}(y_1,y_2)U^0_{\sigma\sigma',\nu\nu'}(y_2,x_2) \tag{3}$$



$$\boxed{\Pi_{\rho\rho',\sigma\sigma'}(x,y)=\frac{1}{i\hbar}\langle E|T\psi^\dagger_\rho(x^+)\psi_{\rho'}(x)\psi^\dagger_\sigma(y^+)\psi_{\sigma'}(y)|E\rangle_C} \tag{4}$$

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[2] A 2-point correlator can be decomposed into connected and disconnected parts:

$$\langle E|TA(x)B(y)|E\rangle=\langle E|TA(x)B(y)|E\rangle_C+\langle E|A(x)|E\rangle\langle E|B(y)|E\rangle$$

By defining $\delta A(x)\equiv A(x)-\langle E|A(x)|E\rangle$, the connected correlator is

$$\langle E|TA(x)B(y)|E\rangle_C=\langle E|T\delta A(x)\delta B(y)|E\rangle$$

The polarization $\Pi_{\rho\rho',\sigma\sigma'}(x,y)$ is the sum of all topologically distinct connected diagrams where a particle is being created with spin ρ and one destroyed with spin ρ' at the space-time point x and another pair of similar events occurs at y.

Because of time-ordering, the polarization is symmetric: $\Pi_{\rho\rho',\sigma\sigma'}(x,y) = \Pi_{\sigma\sigma'\rho\rho'}(y,x)$. The symmetry implies that *the exchange symmetry of the bare interaction U^0 is inherited by the effective potential*:

$$U_{\mu\mu',\nu\nu'}(x,y) = U_{\nu\nu',\mu\mu'}(y,x) \tag{5}$$

If the bare interaction does not modify the spin of the particles, i.e. $U^0_{\mu\mu'\nu\nu'}(x,y) = \delta_{\mu\mu'}\delta_{\nu\nu'}U^0(x,y)$, then the same property holds for the effective interaction: $U_{\mu\mu'\nu\nu'}(x,y) = \delta_{\mu\mu'}\delta_{\nu\nu'}U(x,y)$.
In this case, equation (3) is:

$$U(x_1,x_2) = U^0(x_1,x_2) + \sum_{\rho\sigma}\int dy_1 dy_2 U^0(x_1,y_1)\Pi(y_1,y_2)U^0(y_2,x_2) \tag{6}$$

$$\boxed{\Pi(x,y) = \sum_{\mu\nu}\Pi_{\mu\mu,\nu\nu}(x,y) = \frac{1}{i\hbar}\langle E|T\delta n(x)\delta n(y)|E\rangle} \tag{7}$$

$\Pi(x,y)$ is the scalar polarization.

2. Proper polarization

The polarization diagrams may be reordered as

$$\Pi = \Pi^\star + \Pi^1 + \Pi^2 \dots$$

where $\Pi^\star$ is the sum of *proper* or *irreducible* polarization diagrams, i.e. diagrams that cannot be disconnected into two polarisation diagrams by removal of a single U^0 line. Π^1 is the sum of polarization diagrams that may be disconnected (into polarization diagrams) in a unique way, i.e. there is just one line U^0 whose removal disconnects the diagram into two proper ones ($\Pi^1 = \Pi^\star U^0\Pi^\star$), and so on. Therefore:

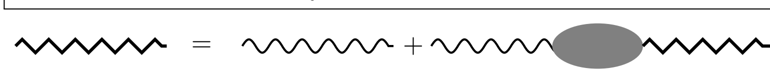
$$\begin{aligned}\Pi =&\Pi^\star + \Pi^\star U^0\Pi^\star + \Pi^\star U^0\Pi^\star U^0\Pi^\star + \dots\\ =&\Pi^\star + \Pi^\star U^0(\Pi^\star + \Pi^\star U^0\Pi^\star + \dots)\\ =&\Pi^\star + \Pi^\star U^0\Pi.\end{aligned}$$

In the same way one obtains $\Pi = \Pi^\star + \Pi U^0\Pi^\star$. These are the Dyson's equations for the polarization Π, in terms of the proper polarization. One of them is:

$$\boxed{\Pi(x_1,x_2) = \Pi^\star(x_1,x_2) + \int dx_3x_4\ \Pi^\star(x_1,x_3)U^0(x_3,x_4)\Pi(x_4,x_2)} \tag{8}$$

As a consequence, one obtains a Dyson equation for the effective interaction in terms of the proper polarization:

$$\boxed{U(x_1,x_2) = U^0(x_1,x_2) + \int dx_3dx_4\ U^0(x_1,x_3)\Pi^\star(x_3,x_4)U(x_4,x_2)} \tag{9}$$



Exercise 2.1. *Show that* $U(1,2) = U^0(1,2) + \int d3\,d4\,U(1,3)\Pi^\star(3,4)U^0(4,2)$ *and* $\int d3\ U^0(1,3)\Pi(3,2) = \int d3\ U(1,3)\Pi^\star(3,2)$.

Exercise 2.2. *Show that* $\int d1\, \Pi(1,2) = 0$. *Does this imply* $\int d1\, \Pi^*(1,2) = 0$*?*

In analogy with electrostatics, let us set:

$$U(1,2) = \int d3\; \epsilon^{-1}(1,3) U^0(3,2) \tag{10}$$

where ϵ^{-1} is the functional inverse the *generalized dielectric function* $\epsilon(1,2)$: $\int d2 \epsilon^{-1}(1,2)\epsilon(2,3) = \delta(1,3)$. Comparison with Ex.2.1 shows that

$$\epsilon^{-1}(1,2) = \delta(1,2) + \int d3\, U(1,3)\Pi^\star(3,2)$$

Then: $\epsilon(1,2) = \delta(1,2) - \int d3d4\, \epsilon(1,3)U(3,4)\Pi^\star(4,2)$ so that

$$\boxed{\epsilon(1,2) = \delta(1,2) - \int d3 U^0(1,3)\Pi^\star(3,2)} \tag{11}$$

3. Space-time translation invariance

If U^0 and Π are space-time translation-invariant, then U and $\Pi^\star$ are invariant. It is convenient to expand them in $k = (\mathbf{k}, \omega)$ space: $f(x - x') = \int \frac{d^4k}{(2\pi)^4} e^{ik(x-x')} f(k)$, $kx = \mathbf{k}\cdot\mathbf{x} - \omega t$.
The Dyson equations become algebraic (matrix equations in spin variables):

$$U(k) = U^0(k) + U^0(k)\Pi^\star(k)U(k)$$
$$\Pi(k) = \Pi^\star(k) + \Pi^\star(k)U^0(k)\Pi(k)$$

If spin factors, the solutions are:

$$\boxed{U(k) = \frac{U^0(k)}{1 - U^0(k)\Pi^\star(k)}\,, \qquad \Pi(k) = \frac{\Pi^\star(k)}{1 - U^0(k)\Pi^\star(k)}} \tag{12}$$

For a static interaction $U^0(x, x') = v(\mathbf{x} - \mathbf{x}')\delta(t - t')$, it is $U^0(k) = v(\mathbf{k})$. Then

$$U(\mathbf{k}, \omega) = \frac{v(\mathbf{k})}{\epsilon(\mathbf{k}, \omega)}, \qquad \Pi(\mathbf{k}, \omega) = \frac{\Pi^*(\mathbf{k}, \omega)}{\epsilon(\mathbf{k}, \omega)} \tag{13}$$

$$\boxed{\epsilon(\mathbf{k}, \omega) = 1 - v(\mathbf{k})\Pi^\star(\mathbf{k}, \omega)} \tag{14}$$

$\epsilon(k)$ is the (time ordered) *generalised dielectric function.*
Despite the bare interaction being static, the effective interaction is time-dependent through the dielectric function, which describes the response of the medium. For the Coulomb interaction,

$$U(\mathbf{k}, \omega) = \frac{4\pi e^2}{|\mathbf{k}|^2 - 4\pi e^2 \Pi^\star(\mathbf{k}, \omega)}$$

The long-range Coulomb interaction is modified by the screening produced by the polarized medium.

4. The ring diagram

The zeroth-order term of (4) is evaluated by Wick's theorem (fermions), and corresponds to the ring diagram

$$\Pi^{(0)}(x,y) = -\frac{i}{\hbar}\sum_{\mu\nu} G^{(0)}_{\mu\nu}(x,y)G^{(0)}_{\nu\mu}(y,x) \tag{15}$$

It does not depend on the two-body interaction. The approximation $\Pi^\star = \Pi^{(0)}$, is known as "ring approximation" or "random phase approximation" (R.P.A.). The effective interaction U is the sum of insertions of rings, i.e. particle-hole excitations.

Exercise 4.1. *Evaluate the ring diagram for non-interacting fermions with single-particle spin-independent hamiltonian hw with eigenstates $h|a\rangle = \hbar\,\omega_a|a\rangle$:*

$$\Pi^{(0)}(\mathbf{x},\mathbf{x}',\omega) = \frac{1}{\hbar}\sum_{\mu\mu'}\sum_{ab}\langle \mathbf{x}\mu|a\rangle\langle a|\mathbf{x}'\mu'\rangle\langle \mathbf{x}'\mu'|b\rangle\langle b|\mathbf{x}\mu\rangle$$
$$\times\left[\frac{\theta(\omega_a-\omega_F)\theta(\omega_F-\omega_b)}{\omega-(\omega_a-\omega_b)+i\eta} - \frac{\theta(\omega_F-\omega_a)\theta(\omega_b-\omega_F)}{\omega-(\omega_a-\omega_b)-i\eta}\right] \tag{16}$$

4.1. Ideal Fermi gas.

The ring diagram for the ideal Fermi gas can be computed analytically (Jens Lindhard, 1954). In momentum space:

$$\Pi^{(0)}(q) = -2\frac{i}{\hbar}\int\frac{d^4p}{(2\pi)^4}G^0(p)G^0(q+p)$$

After the integral in the frequency p^0:

$$\Pi^{(0)}(\mathbf{q},\omega) = \frac{2}{\hbar}\int\frac{d\mathbf{p}}{(2\pi)^3}\left[\frac{\theta(k_F-p)\theta(|\mathbf{p}+\mathbf{q}|-k_F)}{\omega-(\omega_{|\mathbf{p}+\mathbf{q}|}-\omega_p)+i\eta} - \frac{\theta(p-k_F)\theta(k_F-|\mathbf{p}+\mathbf{q}|)}{\omega-(\omega_{|\mathbf{p}+\mathbf{q}|}-\omega_p)-i\eta}\right]$$

The real and imaginary parts are extracted with the Plemelj-Sokhotski formula.

4.2. Real part.

$$\mathrm{Re}\Pi^{(0)}(\mathbf{q},\omega) = \frac{2}{\hbar}⨍\frac{d\mathbf{p}}{(2\pi)^3}\frac{\theta(k_F-p)\theta(|\mathbf{p}+\mathbf{q}|-k_F)-\theta(p-k_F)\theta(k_F-|\mathbf{p}+\mathbf{q}|)}{\omega-(\omega_{|\mathbf{p}+\mathbf{q}|}-\omega_p)}$$

The replacement $\theta(|\mathbf{p}+\mathbf{q}|-k_F) = 1-\theta(k_F-|\mathbf{p}+\mathbf{q}|)$ gives

$$\mathrm{Re}\Pi^{(0)}(\mathbf{q},\omega) = \frac{2}{\hbar}⨍\frac{d\mathbf{p}}{(2\pi)^3}\frac{\theta(k_F-p)-\theta(k_F-|\mathbf{p}+\mathbf{q}|)}{\omega-(\omega_{|\mathbf{p}+\mathbf{q}|}-\omega_p)}$$

The change $\mathbf{p}+\mathbf{q}\to-\mathbf{p}$ gives:

$$\mathrm{Re}\,\Pi^0(\mathbf{q},\omega) = \frac{2}{\hbar}⨍\frac{d\mathbf{p}}{(2\pi)^3}\theta(k_F-p)\left[\frac{1}{\omega-(\omega_{|\mathbf{p}+\mathbf{q}|}-\omega_p)} - \frac{1}{\omega+(\omega_{|\mathbf{p}+\mathbf{q}|}-\omega_p)}\right]$$

The calculations can be carried to the end [1].
The result for $\omega = 0$ is simple and useful:

$$\mathrm{Re}\,\Pi^0(q,0) = -\frac{mk_F}{(\pi\hbar)^2}g\left(\frac{q}{k_F}\right), \qquad g(x) = \frac{1}{2}-\frac{4-x^2}{8x}\log\left|\frac{2-x}{2+x}\right| \tag{17}$$

The function g is plotted in Fig.1. It is $g(0) = 1$, $g'(2)$ divergent, $g(x)\to 0$ for $x\to\infty$

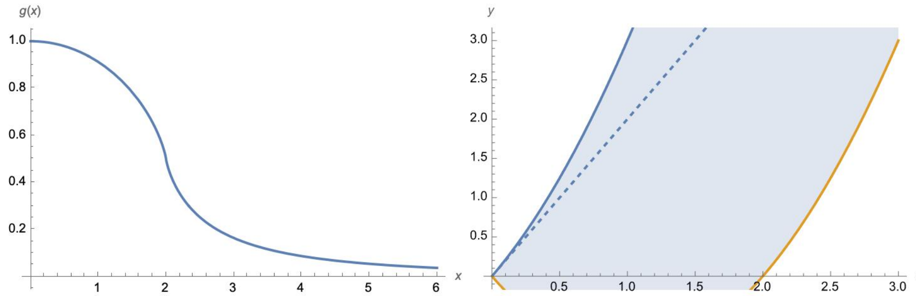


FIGURE 1. Left: the function $g(x)$. Right: the coordinates are $x = q/k_F$ and $y = \omega/\omega_F$. In the shaded region between the curves $y = x^2 \pm 2x$ the imaginary part of $\Pi^{(0)}(q, \omega)$ is non-zero and particle-hole can be produced by exciting the Fermi ground state with a particle of momentum $\hbar q$ and energy $\hbar\omega$. The line $y = 2x$ corresponds to the wave dispersion $\omega = v_F q$. $v < v_F$ produces excitons, while $v > v_F$ produces plasma oscillations.

4.3. **Imaginary part.**

$$\begin{aligned}\operatorname{Im}\Pi^{(0)}(q,\omega) = &-\frac{2\pi}{\hbar}\int\frac{d\mathbf{p}}{(2\pi)^3}\delta(\omega - \omega_{|\mathbf{p}+\mathbf{q}|} + \omega_p)\\ &\times[\theta(k_F - p)\theta(|\mathbf{p}+\mathbf{q}| - k_F) + \theta(p - k_F)\theta(k_F - |\mathbf{p}+\mathbf{q}|)]\end{aligned}$$

The delta and theta functions constrain the region of integration and offer an interpretation: the sum of theta functions implies a particle-hole pair of states, and the delta function appears as a condition of energy conservation. The first term enforces $\omega > 0$, while the second term enforces $\omega < 0$.

Consider a process where a particle-hole pair is created from the unperturbed Fermi ground state by absorbing energy $\hbar\omega$ ($\omega > 0$) and momentum $\hbar\mathbf{q}$. A particle with momentum $\hbar\mathbf{p}$ below the Fermi surface ($p < k_F$) is excited to a state of momentum $\hbar(\mathbf{p}+\mathbf{q})$ above the Fermi surface. The result is a particle-hole state (an exciton) provided that energy conservation is fulfilled (the delta function):

$$\hbar\omega = \hbar\omega_{|\mathbf{p}+\mathbf{q}|} - \hbar\omega_p = \frac{\hbar^2 q^2}{2m} + \frac{\hbar}{m}qp\cos\theta$$

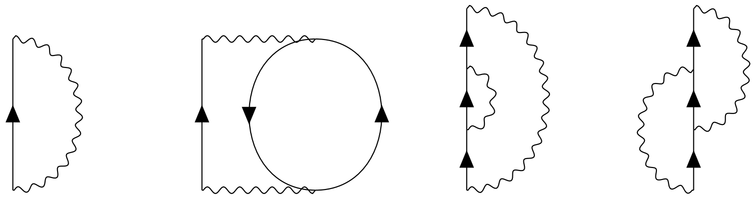
Since $k_F \leq p\cos\theta \leq k_F$, we obtain a region where $\operatorname{Im}\Pi^{(0)} \neq 0$, and the process of exciting a particle-hole pair is possible by energy conservation (see Fig.1):

$$\boxed{\frac{\hbar q^2}{2m} - \frac{\hbar k_F q}{m} \leq \omega \leq \frac{\hbar q^2}{2m} + \frac{\hbar k_F q}{m}} \tag{18}$$

Outside this region the imaginary part of the polarization is zero for $\omega > 0$.

5. THE RANDOM PHASE APPROXIMATION

The first and second order diagrams of the proper self-energy $\Sigma^\star(p)$ of the homogeneous electron gas (HEG):



The second diagram contains the ring diagram and is divergent:

$$\frac{i}{\hbar}\int \frac{d^4q}{(2\pi)^4} G^0(p-q)\frac{(4\pi e^2)^2}{|\mathbf{q}|^4}\Pi^{(0)}(q)$$

The remedy is to sum all the single most divergent diagrams at each order. The summation, including the first order, corresponds to replace the U^0 line of the first diagram with the screened interaction

$$U_{\mathsf{RPA}}(q) = \frac{4\pi e^2}{q^2 - 4\pi e^2 \Pi^{(0)}(q)}$$

Now the perturbative series is convergent up to second order. At third order new divergent diagrams appear.

The ring resummation was introduced by Gell-Mann and Brueckner in the perturbative evaluation of the correlation energy of the HEG [2]. The evaluation is reported in the textbook by Fetter and Walecka [1].

The energy per particle in units e^2/a_0 is the Hartree-Fock term plus the (negative) correlation (for an advanced review see [3])

$$\epsilon_{\mathsf{HEG}} = \left[\frac{3}{10}\frac{\alpha^2}{r_s^2} - \frac{3}{4\pi}\frac{\alpha}{r_s}\right] + \left[\frac{1-\log 2}{\pi^2}\log r_s - 0.07110 + \frac{\log 2}{6} - \frac{3}{4\pi^2}\zeta(3)\right] + \alpha\frac{7\pi^2 - 6 - 72\log 2}{24\pi^3} r_s \log r_s - 0.010 r_s + \dots \tag{19}$$

The $\log r_s$ term arises from the ring summation, the constant in the second bracket is -0.0938417. The $r_s \log r_s$ arises from summation of next most divergent terms of perturbation series.

References

[1] A. L. Fetter and J. D. Walecka, Quantum theory of many-particle systems, McGraw-Hill 1971.

[2] M. Gell-Mann and K. A. Brueckner, *Correlation energy of an electron gas at high density*, Phys. Rev. **106**, (1957) 364.

[3] P. F. Loos and P. M. W. Gill, *The uniform electron gas, WIREs Comput. Mol. Sci.* **6** *(2016), 410–429.* *https://doi.org/10.1002/wcms.1257*.