Interacting electron gas — ground state energy

§1: Hartree - Fock approximation energy

$$H = H_0 + H_{int} = \sum_{k\sigma} \frac{\hbar^2 k^2}{2m} C^+_{k\sigma} C_{k\sigma} + \frac{1}{2V} \sum_q{}' v(q) \left(\rho^+_q \rho_q - N \right)$$

$$\rho_q = \sum_{k\sigma} C^+_{k-q\,\sigma} C_{k\sigma} , \quad \rho_{-q} = \rho^+_q = \sum_{k\sigma} C^+_{k\sigma} C_{k-q,\sigma}$$

$$v(q) = \frac{4\pi e^2}{q^2} , \quad V(r) = \frac{1}{V} \sum_q e^{i\vec{q}\cdot\vec{r}} v(q)$$

HF approximation assumes a determinant wavefunction with filled Fermi surfaces. We have derived before that

$$\frac{1}{N} E_0(HFA) = \frac{3}{5} \frac{\hbar^2 k_F^2}{2m} - \frac{3e^2}{4\pi} k_F \quad \text{where } k_F^3 = 3\pi^2 N/V = 3\pi^2 \rho$$

if use the dimensionless parameter r_s defined through $\rho \frac{4\pi}{3} (r_s a_0)^3 = 1$

with $a_0 = \frac{\hbar^2}{me^2}$, we have $k_F = \left(\frac{9\pi}{4}\right)^{1/3} \frac{1}{r_s a_0}$, we express

$$\frac{1}{N} E_0(HFA) = \left[\frac{3}{10} \left(\frac{9\pi}{4}\right)^{2/3} \frac{1}{r_s^2} - \frac{3}{2\pi} \left(\frac{9\pi}{4}\right)^{1/3} \frac{1}{r_s} \right] \frac{e^2}{2a_0}$$

$$= \left(\frac{2.21}{r_s^2} - \frac{0.916}{r_s} \right) R_y , \quad \text{where } R_y = \frac{e^2}{2a_0} = 13.6\,eV.$$

§2 Dielectric-function

Response function: consider a many-body system with an external perturbation $H_e(t)$. The Schrödinger Eq reads (at $t \to -\infty$, $H_e(t) \to 0$).

$$i\hbar \frac{\partial}{\partial t} \psi = H\psi + H_e(t)\psi, \quad \longrightarrow \text{change to interaction picture}$$

$$\psi(t) = e^{-\frac{i}{\hbar}Ht} \varphi(t) \quad \rightarrow \quad i\hbar \frac{\partial}{\partial t} \varphi(t) = H_e'(t)\varphi$$

$$H_e'(t) = e^{\frac{i}{\hbar}Ht} \, H_e(t) \, e^{-\frac{i}{\hbar}Ht}$$

The time evolution:

$$\varphi(t) = \Phi_0 + \frac{1}{i\hbar}\int_{-\infty}^{t} H_e'(t')\varphi(t')\,dt', \qquad \boxed{|\Phi_0\rangle \text{ is ground state of } H}$$

$\xrightarrow{\text{linear order}}$

$$\varphi(t) = \left[1 + \frac{1}{i\hbar}\int_{-\infty}^{t} H_e'(t')\,dt'\right]\Phi_0$$

operator evolution $\quad A(t) = e^{\frac{i}{\hbar}Ht} \, A \, e^{-\frac{i}{\hbar}Ht}$

$$\Rightarrow \quad \bar{A} = \langle \varphi(t)|A(t)|\varphi(t)\rangle = \langle \Phi_0|A(t)|\Phi_0\rangle + \frac{1}{i\hbar}\int_{-\infty}^{t} \langle \Phi_0|[A(t), H_e'(t')]\,|\Phi_0\rangle\, dt'$$

$|\Phi_0\rangle$ is an eigenstate of $H \Rightarrow \langle \Phi_0|A(t)|\Phi_0\rangle = \langle \Phi_0|A|\Phi_0\rangle$

$\Rightarrow$ the response

$$\Delta A = \bar{A}(t) - \bar{A}(t\to-\infty) = \frac{1}{i\hbar}\int_{-\infty}^{+\infty} dt'\, \Theta(t-t')\langle \Phi_0|[A(t), H_e'(t')]|\Phi_0\rangle$$

Consider the perturbation

$$H_e(t) = \frac{1}{V}\sum_q \rho(-q,t)\, V_{ex}(q,t)$$

$$\delta\rho(q,t) = -\frac{i}{\hbar}\int_{-\infty}^{+\infty} dt'\, \Theta(t-t')\, \frac{1}{V} \langle \Phi_0 | [\rho(q t)\ \rho(-q t')] | \Phi_0 \rangle\, V_{ex}(q t')$$

$$= -\int_{-\infty}^{+\infty} dt'\ \chi_{ret}(q, t-t')\, V_{ex}(q, t')$$

→ Fourier ~~trans~~form $\Rightarrow$ $\boxed{\delta\rho(q,\omega) = -\chi_{ret}(q,\omega)\, V_{ex}(q,\omega)}$

where $\chi_{ret}(q,\omega) = \frac{1}{V}\frac{i}{\hbar}\int_{-\infty}^{+\infty} dt\ e^{i(\omega+i\eta)t} \langle \Phi_0 | [\rho(q t)\ \rho(-q, 0)] | \Phi_0 \rangle$

From poisson equation: $-\nabla^2 V_{ind} = 4\pi e^2 \delta\rho(q,\omega) \Rightarrow V_{ind}(q,\omega) = \frac{4\pi e^2}{q^2}\delta\rho(q,\omega)$

$$V_{tot} = V_{ex} + V_{ind} = V_{ex} + \frac{4\pi e^2}{q^2}\delta\rho(q,\omega) = \frac{1}{\epsilon} V_{ex}$$

$$\Rightarrow \boxed{\frac{1}{\epsilon(q,\omega)} = 1 - \chi_{ret}(q,\omega)\cdot\frac{4\pi e^2}{q^2}}$$

Now we use Lehman Representation

$$\chi_{ret}(q,\omega) = \frac{i}{V\hbar}\int_{-\infty}^{+\infty} dt\ \underset{\Theta(t)}{e^{i(\omega+i\eta)t}} \Big\{ \langle \Phi_0 | e^{iHt} \rho(q) e^{-iHt} | m \rangle \langle m | \rho(-q) | \Phi_0 \rangle - \langle \Phi_0 | \rho(-q) | m \rangle \langle m | e^{iHt} \rho(q) e^{-iHt} | \Phi_0 \rangle \Big\}$$

$$= \frac{1}{V}\sum_m \frac{i}{\hbar}\int_{-\infty}^{+\infty} dt\ \Theta(t) \Big[e^{i(\omega+i\eta)t + \frac{(E_0-E_m)t}{\hbar}} \langle \Phi_0 | \rho(q) | m \rangle \langle m | \rho(-q) | \Phi_0 \rangle - e^{i(\omega+i\eta + \frac{(E_m-E_0)}{\hbar})t} \langle \Phi_0 | \rho(-q) | m \rangle \langle m | \rho(q) | \Phi_0 \rangle \Big]$$

$$= \frac{1}{V}\Big[\sum_m \frac{-1}{\hbar\omega + E_0 - E_m + i\eta} \langle \Phi_0 | \rho(q) | m \rangle \langle m | \rho(-q) | \Phi_0 \rangle$$

$$+ \sum_m \frac{1}{\hbar\omega + E_m - E_0 + i\eta} \langle \Phi_0 | \rho(-q) | m \rangle \langle m | \rho(q) | \Phi_0 \rangle \Big]$$

$$\boxed{\chi_{ret}(q,\omega) = \frac{1}{V}\sum_m |\langle m|\rho(q)|0\rangle|^2 \left[\frac{1}{\hbar\omega - \hbar\omega_{m,0} + i\eta} - \frac{1}{\hbar\omega + \hbar\omega_{m,0} + i\eta} \right]}$$

we used $|\langle m|\rho_{-q}|0\rangle| = |\langle m|\rho_q|0\rangle|$ for isotropic systems.

and $|0\rangle$ for ground state

$$\Rightarrow \boxed{\frac{1}{\epsilon(q,\omega)} = 1 - \frac{4\pi e^2}{q^2 V}\sum_n |\langle n|\rho_q|0\rangle|^2 \left(\frac{1}{\hbar\omega + \hbar\omega_{n,0} + i\eta} - \frac{1}{\hbar\omega - \hbar\omega_{n,0} + i\eta} \right)}$$

Check dimensin: $|\langle n|\rho_q|0\rangle|$ is dimensinless

Take imaginary part

$$\mathrm{Im}\frac{1}{\varepsilon(q,\omega)} = \pi\, v(q)\frac{1}{\hbar V}\sum_n |\langle n|\rho_q|0\rangle|^2 [\delta(\omega+\omega_{n,0}) - \delta(\omega-\omega_{n,0})]$$

↙ sum rule

$$\int_0^\infty d\omega\, \mathrm{Im}\frac{1}{\varepsilon(q,\omega)} = -\pi\, v(q)\frac{1}{\hbar V}\sum_n \langle n|\rho_q|0\rangle\langle 0|\rho_{-q}|n\rangle$$

$$= -\frac{\pi v(q)}{\hbar V}\langle 0|\rho_q^+\rho_q|0\rangle$$

$$\Rightarrow \boxed{\langle 0|H_{int}|0\rangle = \frac{1}{2V}{\sum_q}' \langle 0|v(q)\rho_q^+\rho_q|0\rangle - Nv(q)] = -\left[{\sum_q}' \frac{\hbar}{2\pi}\int_0^\infty d\omega\, \mathrm{Im}\left[\frac{1}{\varepsilon(q,\omega)}\right] + \frac{1}{2}v(q)N\right]}$$

3. Feynman-Hellman theorem

Consider Hamiltonian containing parameter λ, denoted $H(\lambda)$, then the eigenvalue $E_n(\lambda)$ for the n-th eigenstate satisfies

$$\frac{\partial E_n(\lambda)}{\partial \lambda} = \langle \psi_n(\lambda) | \frac{\partial H}{\partial \lambda} | \psi_n(\lambda) \rangle ,$$ where the wavefunction $|\psi_n(\lambda)\rangle$

is normalized, and $E_n(\lambda) = \langle \psi_n(\lambda) | H | \psi_n(\lambda) \rangle$. — Please prove it.

Consider $H(\lambda) = H_0 + \lambda H_{int}$, then $H(0) = H_0$ and $H(1) = H_0 + H_{int}$.

Then $$E_G = E_0(\lambda=0) + \int_0^1 d\lambda \, \langle \psi_0(\lambda) | \frac{\partial H(\lambda)}{\partial \lambda} | \psi_0(\lambda) \rangle$$

$$\boxed{E_G = E_0(\lambda=0) + \int_0^1 \frac{d\lambda}{\lambda} \langle \psi_0(\lambda) | \lambda H_{int} | \psi_0(\lambda) \rangle .}$$

The first term is the kinetic energy of the ground state of the free system. We use this trick because the kinetic energy on the true ground state is difficult to direct calculate. We define ε_λ as the dielectric function for the ground state for $H(\lambda)$. Then

$$\langle \psi_0(\lambda) | \lambda H_{int} | \psi_0(\lambda) \rangle = -\sum_q{}' \left[\frac{\hbar}{2\pi} \int_0^\infty d\omega \, \mathrm{Im}\left[\frac{1}{\varepsilon_\lambda(q\omega)} \right] + \frac{\lambda}{2} v(q) N \right]$$

$$\Rightarrow \boxed{E_G = \frac{3}{5} N E_F - \sum_q{}' \left\{ \frac{\hbar}{2\pi} \int_0^\infty d\omega \int_0^1 \frac{d\lambda}{\lambda} \mathrm{Im}\left[\frac{1}{\varepsilon_\lambda(q\omega)} \right] + \frac{\lambda}{2} v(q) N \right\}}$$

where $$\frac{\hbar}{\pi} \int_0^\infty d\omega \, \mathrm{Im}\left[\frac{1}{\varepsilon_\lambda(q,\omega)} \right] = -\lambda v(q) \langle \psi_0(\lambda) | \rho_q^\dagger \rho_q | \psi_0(\lambda) \rangle$$

§4: Hartree - Fock Approximation

The HFA does not change the ground state wavefunction, $|\psi_0(\lambda=0)\rangle$, but directly does 1st order perturbation theory based on $|\psi_0(\lambda=0)\rangle$, i.e

$$\frac{1}{\epsilon_{HFA}(q\omega)} = 1 - v(q)\, \chi^0_{ret}(q,\omega),$$ where $\chi^0_{ret}(q,\omega)$ is

the Lindhardt response function. $\chi^0_{ret}(q,\omega)$ is the retarded response function for the free system: it's Lehman reespresentation

$$\chi^0_{ret}(q\omega) = \frac{1}{V}\sum \left|\langle \psi_m(\lambda=0)|\rho(q)|\psi_0(\lambda=0)\rangle\right|^2 \left[\frac{1}{\hbar\omega - \hbar\omega^0_{m,0} + i\eta} - \frac{1}{\hbar\omega + \hbar\omega^0_{m0} + i\eta}\right]$$

These states are for non-interacting systems.

repeat the same process, we arrive at

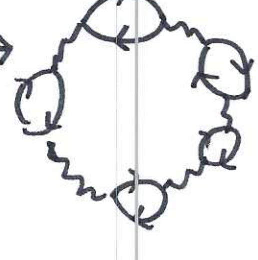
$$\int_0^\infty d\omega\, I_m \frac{1}{\epsilon_{HFA}(q\omega)} = -\frac{\pi v(q)}{\hbar V} \langle \psi_0(\lambda=0)|\rho^+(q)\rho(q)|\psi_0(\lambda=0)\rangle,$$

— this is precisely the spirit of HFA. $\rightarrow$

§5 RPA

$$\frac{1}{\varepsilon^{RPA}_\lambda(k,\omega)} = 1 + \sum_{n=1}^{\infty} [-\lambda v(q)\, \chi^0_{ret}(q,\omega)] = \frac{1}{1 + \lambda v(q)\, \chi^0_{ret}(q,\omega)}$$

where $$\chi^0_{ret}(q,\omega) = \frac{-2}{\hbar V}\sum_k \frac{n_k - n_{k+q}}{\omega - \omega_{kq} + i\eta}.$$ $\rightarrow$

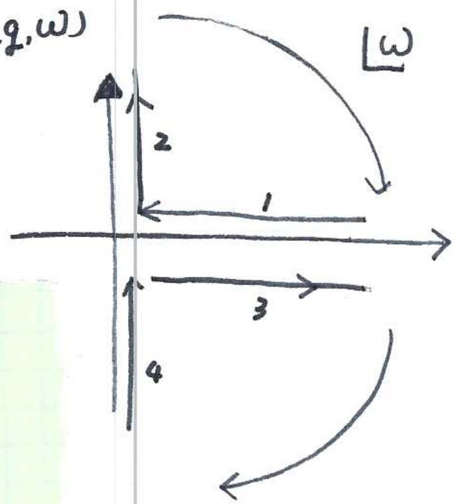


The RPA result

$$-\frac{\hbar}{2\pi}\sum_q{}' \int_0^1 \frac{d\lambda}{\lambda}\int_0^{+\infty} d\omega\ \mathrm{Im}\left[\frac{1}{\varepsilon_\lambda^{RPA}(k,\omega)}\right] = -\frac{\hbar}{2\pi}\sum_q{}'\int_0^1 d\lambda \int_0^{\infty} \mathrm{Im}\,\frac{-v(q)\chi^0_{ret}(q\,\omega)}{1+\lambda v(q)\chi^0_{ret}}$$

we use $\mathrm{Im}\left[\frac{1}{\varepsilon_\lambda^{RPA}}\right] = \mathrm{Im}\left[\frac{1}{\varepsilon_\lambda^{RPA}} - 1\right] = \frac{-\lambda v(q)\chi^0}{1+\lambda v(q)\chi^0}$.

Define function $B(q,\omega) \equiv \dfrac{-v(q)\chi^0_{ret}(q,\omega)}{1+\lambda v(q)\chi^0_{ret}(q,\omega)}$



$B(q,\omega+i\eta)$ is analytic on the upper-half plane

$B(q\,\omega_{-i\eta})$ is analytic on the lower-half plane

In the upper-half plane, we have

$$\int_{+\infty}^{0} d\omega\ B(q,\omega+i\eta) + i\int_0^{+\infty} d\nu\ B(q,i\nu) = 0$$

In the lower-half plane, we have

$$\int_0^{+\infty} d\omega\ B(q,\omega-i\eta) + i\int_{-\infty}^{0} d\nu\ B(q,i\nu) = 0$$

$$\Rightarrow i\int_{-\infty}^{+\infty} d\nu\ B(q,i\nu) = -\int_0^{+\infty} d\omega\ B(q,\omega-i\eta) - \int_{+\infty}^{0} d\omega\ B(q,\omega+i\eta)$$

$$= \int_0^{+\infty} d\omega\ \left(B(q,\omega+i\eta) - B(q,\omega-i\eta)\right) = 2i\int_0^{+\infty} d\omega\ \mathrm{Im}\,B(q,\omega+i\eta)$$

$$\Rightarrow \boxed{\int_0^{+\infty} d\omega\ \mathrm{Im}\,B(q,\omega+i\eta) = \frac{1}{2}\int_{-\infty}^{+\infty} d\nu\ B(q,i\nu)}$$

RPA:

$$E_G = E_G^0 - \sum_q{}' \left\{ \frac{\hbar}{4\pi} \int_0^1 d\lambda \int_{-\infty}^{+\infty} d\nu \, \frac{-v(q)\chi^0(q\, i\nu)}{1+\lambda v(q)\chi^0(q\, i\nu)} + \frac{1}{2} v(q) N \right\}$$

$$= E_G^0 + \sum_q \left\{ \frac{\hbar}{4\pi} \int_{+\infty}^{+\infty} d\nu \, \ln(1+v(q)\chi^0(q, i\nu)) - \frac{1}{2} v(q) N \right\}$$

The difference between RPA and HFA is called the correlation energy at the RPA level

$$\boxed{\mathcal{E}_c^{RPA} = \sum_q \frac{\hbar}{4\pi} \int_{+\infty}^{+\infty} d\nu \left\{ \ln\left(1+v(q)\chi^0(q, i\nu)\right) - v(q)\chi^0(q, i\nu) \right\}}$$

$$\chi^0(q\, i\nu) = -2 \frac{1}{V} \sum_k \frac{n_f(\varepsilon_k) - n_f(\varepsilon_{k+q})}{i\hbar\nu - (\varepsilon_{k+q} - \varepsilon_k)} = 2 \int \frac{d^3k}{(2\pi)^3} \frac{-\delta(\varepsilon_k - \mu)\hbar \vec{v}_F \cdot \vec{q}}{i\hbar\nu - \hbar \vec{v}_F \cdot \vec{q}}$$

$$= N_0 \int \frac{d\Omega}{4\pi} \frac{-\cos\theta}{\frac{i\nu}{v_f q} - \cos\theta} = \frac{N_0}{2} \int_{-1}^{1} d\cos\theta \frac{-\cos\theta}{\frac{i\nu}{v_f q} - \cos\theta}$$

where $N_0 = \frac{2}{(2\pi)^3} \int k^2 dk \int d\Omega \, \delta\left(\frac{\hbar^2 k^2}{2m} - \frac{\hbar^2 k_f^2}{2m}\right) = \frac{2 \cdot 4\pi}{8\pi^3} k_f^2 \Big/ \frac{\hbar^2 k_f}{m} = \frac{m k_f}{\pi^2 \hbar^2}$

define $x = \cos\theta$, $\quad s = \frac{\nu}{v_f q} \Rightarrow \int_{-1}^{1} dx \frac{x}{x - is} = \int_0^1 dx \left[\frac{x}{x-is} + \frac{x}{x+is} \right]$

$$= \int_0^1 dx \frac{2x^2}{x^2+s^2}$$

$$\Rightarrow \boxed{\chi^0(q, i\nu) = N_0 \int_0^1 dx \frac{x^2}{x^2+s^2} = N_0 \left[1 - s \tan^{-1}(1/s)\right]} \leftarrow \text{as } q \to 0.$$

→ dimensinless

$$\chi^0(q, i\nu) = N_0 R(s), \text{ where } s = \frac{\nu}{v_F q} \text{ and } N_0 = \frac{m k_f}{\pi^2 \hbar^2}$$

$$1 + v_q \chi^0(q, i\nu) = 1 + \frac{k_{TF}^2}{q^2} R(s) = 1 + \frac{\lambda_1^2}{x^2} R(s) \quad \text{where } x = q/k_F,$$

$$k_{TF}^2 = 4\pi e^2 N_0 = \frac{4\pi e^2 m k_f}{\pi^2 \hbar^2} = \frac{4 e^2}{\pi \hbar^2} m k_f,$$

$$\lambda_1^2 = k_{TF}^2 / k_F^2 = \frac{4 e^2 m}{\pi \hbar^2 k_f} = \frac{4 m e^2}{\pi \hbar^2} \left(\frac{4}{9\pi}\right)^{1/3} r_s a_0 = \frac{4}{\pi} \left(\frac{4}{9\pi}\right)^{1/3} r_s .$$

$$\mathcal{E}_c = \frac{\hbar V}{4\pi N} \int_0^{+\infty} \frac{d^3\vec{q}}{(2\pi)^3} \int_{-\infty}^{+\infty} d\nu \left\{ \ln\left[1 + v(q)\chi^0(q, i\nu)\right] - v(q)\chi^0(q, i\nu) \right\}$$

define $x = q/k_F \Rightarrow v(q)\chi^0(q, i\nu) = \frac{\lambda_1^2}{x^2} R(s).$

$$\int d^3\vec{q} = \int q^2 dq \cdot 4\pi = 4\pi k_f^3 \int x^2 dx \qquad \int_{-\infty}^{+\infty} d\nu = v_F q \int ds = v_F k_F x \int ds$$

$$\Rightarrow \mathcal{E}_c = \frac{\hbar}{8\pi^3} \frac{v_F k_f^4}{\rho} \lambda_1^4 \int_0^{+\infty} dx \int_{-\infty}^{+\infty} ds \left\{ \frac{x^3}{\lambda_1^4} \ln\left[\left(1 + \frac{\lambda_1^2}{x^2} R(s)\right] - \frac{x}{\lambda_1^2} R(s) \right\}$$

The prefactor $= \frac{\hbar}{8\pi^3} \frac{\hbar k_f}{m} \frac{3\pi^2}{k_f^3} \left(\frac{4e^2}{\pi \hbar^2}\right)^2 m^2 k_f^2 = \frac{6}{\pi^3} \frac{m e^4}{\hbar^2} = \frac{12}{\pi^3} Ry$

The expression $\chi^0(q, i\nu) = N_0 [1 - s \tan^{-1} 1/s]$ is only valid at $q \ll k_F$.

At $q > k_F$, it decays as q^{-2}, or x^{-2}. The ultra-voilet part is convergent, and we only worry the infrared.

at $q > k_F$, $\chi^0(q, i\nu) = N_0 R_x(s) \sim N_0 x^{-2}$,

it cannot be a function of only s.

then $\frac{x^3}{\lambda_1^4} \ln\left(1+\frac{\lambda_1^2}{x^2} R_x(s)\right) - \frac{x}{\lambda_1^2} R_x(s) \approx \frac{1}{x} R_x(s) \sim \frac{1}{x^3} \rightarrow$ Converge quickly

we can set $+\infty \rightarrow 1$, we have

$$\varepsilon_c \simeq \frac{12}{\pi^3} \int_0^1 dx \int_{-\infty}^{+\infty} ds \left\{ \frac{x^3}{\lambda_1^4} \ln\left[1+\frac{\lambda_1^2}{x^2} R(s)\right] - \frac{x}{\lambda_1^2} R(s) \right\}$$

$$= \frac{-12}{\pi^3} \int_{-\infty}^{+\infty} ds \; F[s, \lambda_1^2], \text{ where } F[s, \lambda_1^2] = -\frac{R^2[s]}{4} \left\{ \frac{\ln(1+\lambda_1^2 R(u)) - \lambda_1^2 R(u)}{\lambda_1^4 R^2(s)} - \ln\left(1+\frac{1}{\lambda_1^2 R(s)}\right) \right\}$$

this term $\rightarrow \infty$.

$\lambda_1^2 = \frac{4}{\pi}\left(\frac{4}{9\pi}\right)^{1/3} r_s \ll 1$ in the high density limit

as $r_s \rightarrow 0$

$$F(s, \lambda_1^2) \simeq -\frac{1}{4} R^2(s) \ln r_s + \cdots \text{ (terms not dependent on } r_s)$$

$$\Rightarrow \varepsilon_c \simeq \frac{3}{\pi^3}\left[\int_{-\infty}^{+\infty} ds \; R^2(s)\right] \ln r_s + \text{const not dependent on } r_s$$

$$\int_{-\infty}^{+\infty} ds \; R^2(s) = \int_{-\infty}^{+\infty} ds \int_0^1 dy\, dz \frac{y^2 z^2}{(y^2+s^2)(z^2+s^2)} = \pi \int_0^1 dy \int_0^1 dz \frac{yz}{y+z} = \frac{2\pi}{3}(1-\ln 2)$$

$$\Rightarrow \boxed{\varepsilon_c = \frac{2}{\pi^2}(1-\ln 2) \ln r_s + \text{const} \cdots [Ry]}$$

at $r_s \ll 1$, $\ln r_s$ negative

Correlations save more energy!

More precisely complicate calituations

$$\boxed{\left.\frac{E_G}{N}\right|_{RPA} = \frac{2.21}{r_s^2} - \frac{0.916}{r_s} - 0.094 + 0.0622 \ln r_s + O(r_s \ln r_s) \, [Ry]}$$