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CORRELATION ENERGY OF A HIGH-DENSITY ELECTRON GAS

SREĆKO KILIĆ, TULLIO PERSI* and KARMEN RIVIER**

Faculty of Natural Sciences and Arts, University of Split, 58 000 Split, Croatia
**Department of Civil Engineering, University of Rijeka, 51 000 Rijeka, Croatia*
*** Department of Electrical Engineering, University of Split, 58 000 Split, Croatia*

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The Brillouin-Wigner-Feenberg perturbation theory has been applied to a many-body fermion system, an electron gas at high density. The correlation energy has been calculated. An approximative expression of the term fr_s, is also derived. In our approximation, the calculated value of the constant f is equal to 0.8184.

1. *Introduction*

Rayleigh-Schrödinger (RS) perturbation theory has been successfully applied to many-body quantum problems [1,2]. For a relatively long period, the Brillouin-Wigner (BW) perturbation method has been considered unappropriate for treatment of these problems.

In a series of papers [3-6], it was shown how the BW relations can be transformed into the Feenberg perturbative formulae [7-9] and employed in quantum many-body theory; this approach in many-body theory is sometimes called Brillouin-Wigner-Feenberg perturbation (BWF) theory.

The correlation energy of an electron gas at high density is calculated using the BWF energy expression. It is assumed that the Hamiltonian of N identical fermions in the volume Ω can be written in the form

$$H = H_0 + V \tag{1}$$

and that the eigenstates and eigenvalues of the unperturbed Hamiltonian H_0 are known

$$H_0|\varphi_n >= \varepsilon_n|\varphi_n > . \tag{2}$$

In the BW procedure the solution of the equation

$$H|\Psi >= E|\Psi > \tag{3}$$

for energy is given by

$$E = \varepsilon_l + V_{ll} + \sum_{n(\neq l)} \frac{|V_{ln}|^2}{E - \varepsilon_n} + \sum_{nn'(\neq l)} \frac{V_{ln}V_{nn'}V_{n'l}}{(E - \varepsilon_n)(E - \varepsilon_{n'})}$$

$$+ \sum_{\substack{nn'n'' \\ (\neq l)}} \frac{V_{ln}V_{nn'}V_{n'n''}V_{n''l}}{(E - \varepsilon_n)(E - \varepsilon_{n'})(E - \varepsilon_{n''})} + \ldots , \tag{4}$$

where

$$V_{ij} =< \varphi_i|V|\varphi_j > . \tag{5}$$

This equation is solved by successive iterations.

Studying the BW expression (4) regarding dependence on N, Ljolje [3] showed that it could be improved if an infinite number of terms from higher order were put in the second order term. Indeed, if one picks out the term $n^{'} = n$ from the third order, $n = n^{''} = n^{'}$ from the fourth order, and so on, and collects them with the second order term, one finds

$$\sum_{n(\neq l)} \frac{|V_{ln}|^2}{E - \varepsilon_n - V_{nn}}.$$

The same can be done for the higher terms. Finally, repeating the procedure, BW energy formula is transformed into the Feenberg equation

$$E = \varepsilon_l + V_{ll} + \sum_{n}^{\odot} \frac{V_{ln}V_{nl}}{E - E_n^F} + \sum_{nn'}^{\odot} \frac{V_{ln}V_{nn'}V_{n'l}}{(E - E_n^F)(E - E_{nn'}^F)} +$$

$$+\sum_{nn'n''}^{\odot}\frac{V_{ln}V_{nn'}V_{n'n''}V_{n''l}}{(E-E_n^F)(E-E_{nn'}^F)(E-E_{nn'n''}^F)}+\ldots, \tag{6}$$

where

$$E_n^F=\varepsilon_n+V_{nn}+\sum_{n'\neq ln}\frac{V_{nn'}V_{n'n}}{E-E_{nn'}^F}+\sum_{\substack{n'\neq ln\\ n''\neq lnn'}}\frac{V_{nn'}V_{n'n''}V_{n''n}}{(E-E_{nn'}^F)(E-E_{nn'n''}^F)}$$

$$+\cdot\ \cdot\ \cdot\ ,$$

$$E_{nn'}^F=\varepsilon_{n'}+V_{n'n'}+\sum_{n''\neq lnn'}\frac{V_{n'n''}V_{n''n'}}{E-E_{nn'n''}^F}+\ldots$$

$$\vdots \tag{7}$$

Mark $\odot$ means that all summation indices are mutually different. In Ref. 6, the second quantization procedure has been applied to Feenberg relation (6) and the following approximative relation for the ground state energy has been obtained

$$E=\varepsilon_0+V_{00}+E_r+E_{ex}^{(2)}. \tag{8}$$

The zero and the first order terms have the usual form

$$\varepsilon_0=\sum_{\substack{ks\\<k_f}}e_{ks}=\sum_{\substack{ks\\<k_f}}\frac{\hbar^2k^2}{2m}=N\frac{3}{5}e_{k_f}, \tag{9}$$

and

$$V_{00}=\frac{1}{2\Omega}\sum_{\substack{t_1t_2\\<k_f}}\sum_{s_1s_2}(V_0-V_{t_1-t_2}\delta_{s_1s_2}), \tag{10}$$

The generalized ring energy is given by

$$E_r=\frac{\Omega}{16\pi^3}\int\mathrm{d}\vec{g}\,\frac{g}{2\pi}\int\limits_{-\infty}^{+\infty}\mathrm{d}u\sum_{n=2}^{\infty}\frac{s^n}{n}\left(-\frac{m}{\hbar^2}\right)^{n-1}\left[\frac{V_gQ_g(u)}{8\pi^3}\right]^n$$

$$= \frac{\hbar^2\Omega}{16\pi^3 m}\int \mathrm{d}\vec{g}\,\frac{g}{2\pi}\int\limits_{-\infty}^{+\infty}\mathrm{d}u\left\{\ln\left[1+\frac{V_g Q_g(u)ms}{8\pi^3\hbar^2}\right]-\frac{V_g Q_g(u)ms}{8\pi^3\hbar^2}\right\}, \tag{11}$$

where

$$Q_g(u) = \int \mathrm{d}\vec{k}\int\limits_{-\infty}^{+\infty}\mathrm{d}t e^{-D|t|+\mathrm{i}gut}, \quad k<k_f,\ \ |\vec{k}+\vec{g}|>k_f. \tag{12}$$

$$D \equiv D^{(1)} = D^{(0)} + \frac{m}{8\pi^3\hbar^2}\sum_{s\sigma'}\delta_{s\sigma'}\int\limits_{\substack{k_p<k_f\\ |\vec{k}+\vec{g}|>k_f}}\mathrm{d}\vec{p}\,(V_{\vec{p}+\vec{k}}-V_{\vec{p}+\vec{k}+\vec{g}}), \tag{13}$$

$D^{(0)} = (g^2/2) + \vec{k}\vec{g}$ represents pure Gell-Mann–Brueckner (G-MB) denominator [10] and s denotes the number of spin possibilities (for electron it is 2). Finally, the exchange part of the second order energy term is

$$E_{ex}^{(2)} = -\frac{2}{\Omega^2}\sum_{\substack{k_1k_2q\\ k_1,k_2<k_f\\ |\vec{k}_1+\vec{q}|,|\vec{k}_2-\vec{q}|>k_f}}\ \sum_{\substack{\sigma_1\sigma_2\\ \sigma_1'\sigma_2'}}\frac{V_{\vec{q}}V_{\vec{k}_1-\vec{k}_2+\vec{q}}\delta_{\sigma_1\sigma_1'}\delta_{\sigma_2\sigma_2'}\delta_{\sigma_2\sigma_1'}\delta_{\sigma_1\sigma_2'}}{E-E_n^F}. \tag{14}$$

2. Correlation energy

For an electron gas, placed in a uniform distributed positive background, chosen to ensure that the electron system is neutral, one obtains

$$\varepsilon_0 = N\frac{e^2}{2a_0}\frac{1}{r_s^2}\frac{3}{5}\left(\frac{9\pi}{4}\right)^{2/3}, \tag{15}$$

$$V_{00} = -N\frac{e^2}{2a_0}\frac{1}{r_s}\frac{3}{2\pi}\left(\frac{9\pi}{4}\right)^{1/3}, \tag{16}$$

where $V_t = 4\pi e^2/t^2$, $a_0 = \hbar/me^2$, $r_s = r_0/a_0$, $k_f = (9\pi/4)^{1/3}(1/r_s a_0)$ and r_0 is the radius of a sphere of a volume equal to the volume per particle.

The generalized ring energy is given by

$$E_r = N\frac{e^2}{2a_0}J_R(r_s), \tag{17}$$

where

$$J_R(r_s) = \frac{1}{r_s^2} C_1 J(r_s), \quad C_1 = \frac{3}{4\pi}\left(\frac{9\pi}{4}\right)^{2/3},$$

$$J(r_s) = \int\limits_0^\infty \mathrm{d}q\, q^3 \int\limits_{-\infty}^{+\infty} \mathrm{d}\omega \{\ln[1 + L(q,\omega)] - L(q,\omega)\}, \tag{18}$$

and

$$L(q,\omega) = C_2 \frac{1}{q^2} r_s \begin{cases} I_a(r_s), & q \le 2 \\ I_b(r_s), & q \ge 2 \end{cases}, \quad C_2 = \frac{2}{\pi}\left(\frac{4}{9\pi}\right)^{1/3} s.$$

The functions I_a and I_b are given by

$$I_a = \int\limits_0^{\sqrt{1-(g/2)^2}} r\mathrm{d}r \int\limits_{-q+\sqrt{1-r^2}}^{\sqrt{1-r^2}} F_1(q,\omega,r,z)\mathrm{d}z +$$

$$+ \int\limits_{\sqrt{1-(g/2)^2}}^{1} r\mathrm{d}r \int\limits_{-\sqrt{1-r^2}}^{\sqrt{1-r^2}} F_1(q,\omega,r,z)\mathrm{d}z, \tag{19}$$

$$I_b = \int\limits_0^1 \kappa^2 \mathrm{d}\kappa \int\limits_0^\pi F_2(q,\omega,\kappa,\vartheta)\sin\vartheta \mathrm{d}\vartheta, \tag{20}$$

where

$$F_1 = \frac{\tilde{d}_0 + Cr_s d_1(\alpha,\beta)}{(\tilde{d}_0 + Cr_s d_1(\alpha,\beta))^2 + q^2\omega^2}, \tag{21}$$

$$F_2 = \frac{\overline{d_0} + Cr_s d_1(\kappa,\lambda)}{(\overline{d_0} + Cr_s d_1(\kappa,\lambda))^2 + q^2\omega^2}, \tag{22}$$

$$\tilde{d}_0 = \frac{q^2}{2} + qz, \;\; \overline{d_0} = \frac{q^2}{2} + \kappa q\cos\vartheta, \;\; \alpha = \sqrt{r^2+z^2},$$

$$\beta = \sqrt{r^2 + z^2 + q^2 + 2qz}, \quad \lambda = \sqrt{\kappa + q^2 + 2\kappa q \cos\vartheta},$$

$$d_0(\kappa) = \frac{q^2}{2} + \vec{\kappa}\vec{q}$$

$$d_1(x,y) = \frac{1}{x}(1-x^2)\ln\frac{1+x}{1-x} - \frac{1}{y}(1-y^2)\ln\frac{1+y}{-1+y}, \tag{23}$$

$$\vec{\kappa} = \frac{\vec{k}}{k_f}, \quad \vec{q} = \frac{\vec{g}}{k_f}, \quad C = (18\pi^4)^{-1/3}, \quad V_g = V_q/k_f^2.$$

For the exchange energy one obtains

$$E_{ex}^{(2)} = N\frac{e^2}{2a_0}\varepsilon^{(2)}, \tag{24}$$

where

$$\varepsilon^{(2)} = \frac{3}{2^4\pi^5}\int \mathrm{d}q \int\limits_{\substack{\kappa_1,\kappa_2<1 \\ |\vec{\kappa}_1+\vec{q}|,|\vec{\kappa}_2+\vec{q}|>1}} \mathrm{d}\kappa_1 \int \mathrm{d}\vec{\kappa}_2 \frac{1}{q^2}\frac{1}{(\vec{q}+\vec{\kappa}_1+\vec{\kappa}_2)^2}\frac{1}{F_3(\vec{q},\vec{\kappa}_1,\vec{\kappa}_2)}, \tag{25}$$

and

$$F_3 = d_0(\kappa_1) + d_0(\kappa_2) + Cr_s[d_1(\kappa_1,|\vec{\kappa}_1+\vec{q}|) + d_1(\kappa_2,|\vec{\kappa}_2+\vec{q}|)]. \tag{26}$$

The nine–dimensional integral (25) can be transformed into a five–dimensional one:

$$\varepsilon^{(2)} = \frac{3}{\pi}\int_0^1 \kappa_1^2 \mathrm{d}\kappa_1 \int_0^1 \kappa_2^2 \mathrm{d}\kappa_2 \int_0^\pi \sin\vartheta_1 \mathrm{d}\vartheta_1 \int_0^\pi \sin\vartheta_2 \mathrm{d}\vartheta_2 \cdot$$

$$\cdot \int_{q_1}^{\infty} \mathrm{d}q \frac{1}{\sqrt{f_1^2 - f_2^2}}\frac{1}{F_3(\vec{q},\vec{\kappa}_1,\vec{\kappa}_2)}, \tag{27}$$

where

$$f_1 = \kappa_1^2 + \kappa_2^2 + q^2 + 2q(\kappa_1\cos\vartheta_1 + \kappa_2\cos\vartheta_2) + 2\kappa_1\kappa_2\cos\vartheta_1\cos\vartheta_2, \tag{28}$$

$$f_2 = 2\kappa_1\kappa_2 \sin\vartheta_1 \sin\vartheta_2, \tag{29}$$

$$q_l = \mathrm{Max}(q_{l_1}, q_{l_2}), \tag{30}$$

and

$$q_{l_i} = \sqrt{1-\kappa_i^2\sin^2\vartheta_i} - \kappa_i\cos\vartheta_i. \tag{31}$$

Two four-dimensional integrals in Eq. (18) and a five-dimensional integral in Eq. (27) were calculated numerically. We used Gaussian quadrature. The sum of the results is the correlation energy. It is presented in Table 1 (second column). The corresponding G-MB and Pines energies are also given in Table 1. Some values of the exchange energy are given in the fifth column of the Table 1.

TABLE 1.

Comparison of results of calculations of correlation energies; the value of r_s is in a_0 and energies are in rydbergs *(*Ry= 2.18×10^{-18} J*).*

r_s	ε_c	$\varepsilon_{\text{G-MB}}$	$\varepsilon_{\text{Pines}}$	$\varepsilon^{(2)}$
1	-0.1095	-0.096	-0.158	
0.1	-0.240	-0.2392	–0.3012	0.0470
0.01	-0.3809	-0.3824	-0.4444	0.0484
0.001	-0.5238	-0.5257	-0.5877	0.0486

Starting from relation (10), it is possible to find an approximative relation for the correlation energy which consist of G-MB term and the next one proportional to r_s. Namely, integrating over t in Eq. (12), one finds an expression in which subintegral function can be expanded. Doing this and keeping the first two terms, we derive

$$Q_q(\omega) = 2k_f\{G(q,\omega) + Cr_sK(q,\omega)\} \tag{32}$$

where

$$G(q,\omega) = \int\limits_{\substack{\kappa<1\\ |\vec\kappa+\vec q|>1}} \mathrm{d}\vec\kappa\, \frac{d_0}{d_0^2+q^2\omega^2}, \tag{33}$$

and

$$K(q,\omega)=\int\limits_{\substack{\kappa<1\\|\vec\kappa+\vec q|>1}}\mathrm{d}\vec\kappa\;\frac{d_1}{d_0^2+q^2\omega^2}\left(1-\frac{2d_0^2}{d_0^2+q^2\omega^2}\right). \tag{34}$$

Square bracket in (10) now becomes

$$[\ \ ]=C_3r_s\{G(q,\omega)+Cr_sK(q,\omega)\} \tag{35}$$

where $C_3=(4/9\pi)^{1/3}s/(\pi q)^2$.

Using the binomial theorem and keeping the two largest terms with respect to $G(q,\omega)$, we find

$$[\ \ ]^n=r_s^nC_3^nG(q,\omega)^n+r_s^nC_3^nG(q,\omega)^{n-1}Cr_sK(q,\omega)n. \tag{36}$$

An approximative expression for generalized ring energy is obtained introducing the above expression in (10) and summing up:

$$E_r=N\frac{e^2}{2a_0}\frac{C_1}{r_s^2}\int\limits_0^\infty q^3\mathrm{d}q\int\limits_{-\infty}^{+\infty}\mathrm{d}\omega\,\{[\ln\left(1+r_sC_3G(q,\omega)\right)$$

$$-r_sC_3G(q,\omega)]-Cr_s^3C_3^2K(q,\omega)G(q,\omega)\}\,. \tag{37}$$

The last term in Eq. (37) is proportional to r_s. It can, therefore, be written as fr_s. After integration and substitution of the constants one obtains $f=0.8184$.

3. Conclusion

As is known [11], in the limit of high densities, $r_s\ll 1$, the correlation energy may be expressed by the following series

$$E_c=N\frac{e^2}{2a_0}\left(c\ln r_s+d+er_s\ln r_s+fr_s+\ldots\right). \tag{38}$$

In this way we find the value of the constant f. This is an approximative value inferred from the special class of processes. Namely, the denominator in the second order term of Eq. (5) includes all processes which begin and vanish through the state $|n>=|1_k,1_h,...;1_{k+q},1_{h-q}>$. In our approximation, which is up to the first order for the denominators, only a class of the above process is included. So we can say that within this approach, we picked up all the processes dealing with "direct and exchange scattering with unexcited particles" (G-MB). Inserting the second order approximation in the denominators of the relation (5) would include other processes.

The ground state energy of a homogeneous electron gas has been studied using different approaches [12-19]. We applied the BWF perturbation method to the high-density electron gas. A systematic numerical analysis of the expression (17) and the corresponding third order term are expected to give an evaluation of the series (38). Our preliminary calculation shows that the series (38) should be convergent for values of r_s, less than one.

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KORELACIJSKA ENERGIJA GUSTOG ELEKTRONSKOG PLINA

SREĆKO KILIĆ, TULLIO PERSI* i KARMEN RIVIER**

Fakultet prirodoslovno-matematičkih znanosti i odgojnih područja, 58 000 Split, Hrvatska
**Građevinski fakultet, 51 000 Rijeka, Hrvatska*
***Fakultet elektrotehnike, strojarstva i brodogradnje, 58 000 Split, Hrvatska*

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U radu je pokazano kako se Brillouin-Wigner-Feenbergov račun smetnje može primijeniti u teoriji elektronskog plina veće gustoće. Određen je aproksimativan izraz za korelacijsku energiju i posebno član linearan u parametru razvoja r_s. Numerička vrijednost konstante proporcionalnosti iznosi $f = 0.8184$.