Vol. **106** (2004) *ACTA PHYSICA POLONICA A* No. 4

Static Local Field Factor and Ground State Properties of Interacting Electron Gas

A. Sarkar[a], S. Haldar[b], D. Roy[c] and D. Sen[d,*]

[a]Physics Department, Bijay Krishna Girls' College
Howrah-711 101, West Bengal, India
[b]Physics Department, Asansol Engineering College
Asansol-4, West Bengal, India
[c]Department of Physics, Jadavpur University
Calcutta-700032, West Bengal, India
[d]Department of Physics, Barasat Govt. College
Barasat 700124, West Bengal, India

(Received August 20, 2003)

In the most general case, the calculation of the static local field factor $G(q)$ for the unpolarised electron gas requires the knowledge of exchange--correlation energy functionals for both the parallel and antiparallel relative spin orientations of the electron gas system. Accurate density interpolation formulae using the quantum Monte Carlo data of Ceperley–Alder for the correlation energy of electron gas in both the "para" and "ferro" states, respectively, in the given density range are used for the calculation of $G(q)$. Fulfilment of relevant consistency criteria is ensured and the local field factor so obtained renders significant improvement of *ab initio* pseudopotential calculation of effective interaction of Al. The Levin like interpolant of the correlation energy Ceperley–Alder data has been further used to study the ground state properties of the electron gas. It is also noted that a better understanding of the interacting electron gas properties requires a more accurate spin interpolation formula for the correlation energy than the existing ones.

PACS numbers: 71.10.–w, 71.45.Gm

*corresponding author; e-mail: debsen@vsnl.net

1. Introduction

In self consistent dielectric screening theory, the local field factor (LFF) simulates the exchange and correlation effects of the electron gas. LFF has been found to be important in explaining plasmon like collective excitations and recent studies [1] indicate that it may have a significant role in characterizing quasi one--dimensional systems. Vast literature on LFF reflects its importance and in earlier papers [2–5] elaborate discussions on the existing literature have been made. In Ref. [5] Sarkar et al. have also proposed a simple analytic expression for the static LFF, using a very accurate fit of quantum Monte Carlo (QMC) data [6] of electron correlation energy for the entire density range, which satisfies a number of self-consistent criteria. In a recent communication Sarkar et al. [7] have further outlined the extension of the scheme to the evaluation of charge and magnetic response functions of an interacting electron gas. Vosko, Wilk and Nusair [8] have provided the data of correlation energy per electron $e_{\mathrm{C}}(r_s)$ (r_s being the Wigner–Seitz radius in units of Bohr radius) in both "para" (antiparallel) and "ferro" (parallel) states of the electron gas for six different densities from the QMC calculation of Ceperley–Alder using Green's function algorithm [6] and have fitted the data using rational interpolation. The rational interpolation of Ceperley–Alder [6] data by Vosko, Wilk and Nusair [8] and Perdew and Zunger [9] are usually regarded as good standard for local density approximation (LDA) calculations [10]. Perdew and Wang [11] also have considered the analytic representation, removing some problems with the procedure from [8], by employing all of the Ceperley–Alder [6] data and taking into account the data uncertainties. They have also claimed a definite improvement within random phase approximation (RPA) over the form from [8]. Most importantly they provide a single analytical expression with different parameters for $e_{\mathrm{C}}(r_s)$ in both the "para" and "ferro" states and also for the spin stiffness factor (correlation energy contribution only) $\alpha_{\mathrm{C}}(r_s)$ defined as:

$$\alpha_{\mathrm{C}}(r_s) = \left[\frac{\mathrm{d}^2 e_{\mathrm{C}}(r_s,\zeta)}{\mathrm{d}\zeta^2}\right]_{\zeta=0},$$

where $\zeta(r)$ is the spin polarisation function (Eq. (10)). However, Perdew and Wang [11] have also used a rational interpolant for parametrization of the Ceperley–Alder [6] data. Singh et al. [12] have concluded, from their study on the stability of ferromagnetic iron, the inadequacy of the existing density and spin interpolation formulae. Earlier, we have also discussed [5] some problems regarding the density interpolation formula in [8]. In the present work we have used the Levin like interpolant taking into account the entire Ceperley–Alder [6] data set as input. Bhattacharyya et al. [13] have shown that for a number of input points, interpolants obtained with Levin like transforms are usually better compared to the Padé type rational interpolants.

As the Wigner–Seitz radius r_s is increased, the electron gas system may become unstable [14] with respect to the formation of states with charge density wave or spin density wave. The instability may involve either the divergence of charge susceptibility $\chi(q)$ for charge density wave, i.e. the divergence of the corresponding response function or the divergence of the magnetic susceptibility $\chi_{\mathrm{m}}(q)$ for spin density wave. The onset of charge density or spin density wave implies a phase transition to the respective state, which is getting a lot of attention for quite some time. The possibility of having negative static dielectric function ("antiscreening") for a real system in connection with the search of high-temperature superconductors among others like Wigner's crystallization, phonon mode softening, etc. on one hand and the spin-magnetic phase transitions on the other, are the most interesting issues. In the calculation of dielectric response of unpolarised electron gas, the distinction of the effects of parallel and antiparallel electrons on each other is usually ignored, although the functions $G^{\mathrm{F}}(q)$ and $G^{\mathrm{P}}(q)$ are not necessarily the same for an interacting system. The superscripts refer to F for "ferro" (parallel) and P for "para" (antiparallel) relative spin orientations of the electrons producing the effective potential and the electrons experiencing that potential. The general LFF for unpolarised state of an interacting system should, therefore, be written as

$$G(q) = \frac{1}{2}[G^{\mathrm{F}}(q) + G^{\mathrm{P}}(q)]. \tag{1}$$

In the static limit the familiar test charge dielectric function is consequently given by

$$\epsilon(q) = 1 - \frac{v(q)\chi_0(q)}{1 + v(q)G(q)\chi_0(q)}$$

and the charge susceptibility defined as $\chi(q) = [1/\epsilon(q) - 1]/v(q)$, correspondingly expressed as

$$\chi(q) = \frac{\chi_0(q)}{1 - v(q)[1 - G(q)]\chi_0(q)} = \frac{\chi_0(q)}{\tilde{\epsilon}(q)}, \tag{2}$$

where $v(q) = 4\pi e^2/q^2$, $\chi_0(q)$ is the Lindhard (static) response function, $\tilde{\epsilon}(q)$ is the electronic or the Kohn–Sham dielectric function.

In the case of spin-magnetic response the distinction becomes more crucial because the induced effective magnetic field is approximately proportional to the difference between the two functions $G^{\mathrm{F}}(q)$ and $G^{\mathrm{P}}(q)$ and the relevant local field factor $\bar{G}(q)$ for the magnetic response becomes of the form [15]:

$$\bar{G}(q) = \frac{1}{2}[G^{\mathrm{F}}(q) - G^{\mathrm{P}}(q)]. \tag{3}$$

Using the formalism of Singwi et al. [16], the magnetic susceptibility of unpolarised electron gas is approximately given by

$$\chi_{\mathrm{m}}(q) = \frac{-{\mu_{\mathrm{e}}}^2 \chi_0(q)}{1 + v(q)\bar{G}(q)\chi_0(q)} \tag{4}$$

with μ_{e} as the magnetic moment of an electron. Most of the earlier works including the recent ones [3, 5, 17] dealt with the calculation of $G^{\mathrm{P}}(q)$. We also note that our result for $G^{\mathrm{P}}(q)$ agrees closely with the fixed-node diffusion QMC calculations by Bowen et al. [18] and Moroni et al. [19] (cf. also Table III). In this paper we intend to present a reliable calculation of $G(q)$ and $\bar{G}(q)$ which are found to yield some new interesting results. Only, Richardson and Ashcroft [4] have provided a calculation for the equivalent pair of quantities "$G_{s,a}(q)$" for $r_s = 2$ a.u..

Evaluation of $G(q)$ requires the knowledge of exchange-correlation (XC) energy density functional $e_{\mathrm{XC}}[n]$ and its derivative for both the "para" and "ferro" states of the electron gas. This is achieved to good accuracy through a new fit of Ceperley–Alder [6] data, discussed earlier [5]. Following our earlier communications [5, 7], the same set of criteria is used for the derivation of LFF $G^{\mathrm{F}}(q)$ for spin parallel state of the electron gas. $G^{\mathrm{F}}(q)$ must satisfy: (i) exact compressibility sum rule in the low q limit, (ii) positivity of pair correlation function with the fulfilment of Kimball's [15] criterion of the large q limit and (iii) reproduce the XC energy/particle of the spin parallel state of the electron gas under LDA. The mathematical expressions for the above outlined criteria for the derivation of a reliable LFF are discussed in our earlier work [5], starting from the self-consistency condition (the low q limit) of $G(q)$ as given by

$$\lim_{q\to 0}[-v(q)G(q)] = \langle \frac{\mathrm{d}^2}{\mathrm{d}n^2}(n e_{\mathrm{XC}}[n])\rangle,$$

where $e_{\mathrm{XC}}[n]$ is the XC energy functional per particle, n $(= n(r))$ is the ground state density of the interacting system.

2. Formalism

Local density approximation has been very successful in describing the ground state energy and the response function of unpolarised electron gas. In LDA, the ground state energy density functional of an inhomogeneous electron gas is obtained from the corresponding ground state energy density of a fictitious homogeneous electron gas by replacing its constant density n_0 (say) with the local density $n(r)$ of the actual system [10]:

$$e^{\mathrm{LDA}}(n(r)) = e^{\mathrm{hom}}(n_0)_{n_0\to n(r)}.$$

The LFF $G^{\mathrm{F}}(q)$ in the case of "ferro" (spin parallel) state, obtained in the present work, is expressed by a three-parameter expression as follows:

$$G^{\mathrm{F}}(q) = A^{\mathrm{F}}\left\{1 - \left[1 + \left(\frac{q}{k_{\mathrm{F}}}\right)^4 B^{\mathrm{F}}\right]\exp\left[-\left(\frac{q}{k_{\mathrm{F}}}\right)^2 C^{\mathrm{F}}\right]\right\}, \tag{5}$$

where A^{F}, B^{F}, and C^{F} are functions of density (r_s) and k_{F} is the Fermi wave

vector. A^{F} and C^{F} are determined from the two limiting behaviours of $G^{\mathrm{F}}(q)$. The compressibility sum rule (criterion (i)) is satisfied in the present calculation only approximately. Neglecting the term involving the spin stiffness factor, we write

$$\lim_{q\to 0} G^{\mathrm{F}}(q) = \gamma_0^{\mathrm{F}}(r_s)\left(\frac{q}{k_{\mathrm{F}}}\right)^2$$

with

$$\gamma_0^{\mathrm{F}}(r_s) = \frac{1}{4} - \frac{\pi\alpha}{24} r_{\mathrm{s}}^5 \frac{\mathrm{d}}{\mathrm{d}r_s}[r_s^{-2}\frac{\mathrm{d}}{\mathrm{d}r_s} e_{\mathrm{C}}^{\mathrm{F}}(r_s)], \tag{6}$$

where $\alpha = (4/9\pi)^{1/3}$ and $e_{\mathrm{C}}^{\mathrm{F}}(r_s)$ is the electron correlation energy for the "ferro" state. The term involving the spin stiffness factor in compressibility sum rule offers a higher order correction and is necessary to guarantee the consistency of Eq. (14) (to be followed) with respect to Eq. (4) which the present formulation lacks. But, with the existing spin interpolation formulae for the correlation energy functional, the calculation of the spin stiffness factor is not very reliable. The necessary correction term is also not so important in the context of the calculation of the static local field factor and will be considered elsewhere.

Following Kimball [15] the second criterion involving large q limit leads, for frequency independent LFF, to the following conditions:

$$g^{\mathrm{F}}(0) = 1 - G^{\mathrm{F}}(\infty), \qquad g^{\mathrm{P}}(0) = 1 - G^{\mathrm{P}}(\infty).$$

The pair correlation function between electrons $g(r)$ is the average of the two functions for parallel and antiparallel spins, i.e.,

$$g(r) = \frac{1}{2}[g^{\mathrm{F}}(r) + g^{\mathrm{P}}(r)].$$

According to Pauli exclusion principle $g^{\mathrm{F}}(0) = 0$, which implies $G^{\mathrm{F}}(\infty) = 1$ and $G^{\mathrm{P}}(\infty) = 1 - 2g(0)$. Finally we get,

$$\lim_{q\to\infty} G(q) = 1 - g(0),$$

and

$$\lim_{q\to\infty} \bar{G}(q) = -g(0).$$

Thus both the response functions, $\chi(q)$ and $-\chi_{\mathrm{m}}(q)/\mu_{\mathrm{e}}^2$ to be precise, approach the same $q \to \infty$ asymptotic limit indicating that the short range correlation of an interacting electron gas is dominated by the Coulomb interaction [15].

Incorporating aspects of dynamical theory, several authors [3, 4, 19] have argued, following Holas [20] that the large-q limit of LFF should be diverging ($\sim q^2$). If the Lindhard function is not corrected for the exact occupation number of the interacting system, the local field factors diverge for large-q, producing

an incorrect large-q limit for the effective electron–electron interaction. However, strictly within the static theory, we use the Kimball relation and Lein et al. [21] have inferred only a small error in Corradini et al. [22] static calculation compared to the static limit of the frequency dependent "dynamical" LFF calculation of Richardson and Ashcroft [4].

The short range correlation $g(0)(\equiv\ g(0,r_s))$ is obtained from the ladder diagrammatic calculation of Yasuhara [23] as $g^{\mathrm{P}}(0) = (z/I_1(z))^2/8$, $I_1(z)$ being the modified Bessel function of the first kind and of first order, with $z = 4(\alpha r_s/\pi)^{1/2}$. Using the two limiting behaviours of $G^{\mathrm{F}}(q)$, we finally get $A^{\mathrm{F}} = 1$ and $C^{\mathrm{F}} = \gamma_0^{\mathrm{F}}(r_s)$. The value of $B^{\mathrm{F}}(r_s)$ is obtained following criterion (iii) and its r_s dependence can be expressed as:

$$B^{\mathrm{F}}(r_s) = a + br_s + cr_s^2 + dr_s \ln r_s + er_s^2 \ln r_s, \tag{7}$$

where

$$a = 0.27120697, \qquad b = 0.023367297, \qquad c = 0.0004025675,$$

$$d = -0.0067372145, \qquad e = -6.3667962 \times 10^{-5}.$$

Using the entire set of QMC data of Ceperley–Alder [6] for the electron correlation energy a very accurate fit, valid over the entire density range, is obtained for the ferromagnetic state by Levin like interpolant as:

$$e_{\mathrm{C}}^{\mathrm{F}}(r_s) = -\frac{1 + a_1 r_s + a_2 r_s^2 + a_3 r_s^3 + a_4 r_s^4}{b_0 + b_1 r_s + b_2 r_s^2 + b_3 r_s^3 + b_4 r_s^4 + b_5 r_s^5}[\ \mathrm{mRyd}], \tag{8}$$

where

$$a_1 = 0.24979381, \qquad a_2 = 0.042193510, \qquad a_3 = 0.00273095,$$

$$a_4 = 0.00003620, \qquad b_0 = 0.01258694, \qquad b_1 = 0.00723687,$$

$$b_2 = 0.00165158, \qquad b_3 = 0.00017853, \qquad b_4 = 7.9656334 \times 10^{-6},$$

$$b_5 = 6.47520896 \times 10^{-8}.$$

It may be noted that, though we have ten parameters in Eq. (8), not all of them are independent. Only six of them are independent and the rest are nonlinearly related to these six independent parameters. The details of the method may be found in our previous work [5] and the papers cited therein. This new expression for the correlation energy satisfies the usual low density limit $\sim r_s^{-1}$ but disobeys the logarithmic large density behaviour of RPA calculation.

Gori-Giorgi et al. [24] have observed that the parallel spin contribution of the unpolarised system should be different from that for the fully polarised state unlike the estimates from both [8] and [11], which use a simple rescaling of correlation of fully polarised gas. We too have neglected this error in our calculation and yet, meaningful results are obtained in the present study.

The study of real many electron system requires the energy functionals in terms of both the density and the spin polarisation function $\zeta(r)$ (of Eq. (10)). The LDA prescription can be extended to partially spin polarised state of electron gas in the spin density functional approach by expressing the energy functional in terms of the spin polarisation function in addition to the density variable ($n(r)$) given by, respectively:

$$n(r) = n_+(r) + n_-(r), \tag{9}$$

where $n_\pm(r)$ are the densities of the spin-up and spin-down states, respectively, and

$$\zeta(r) = \frac{n_+(r) - n_-(r)}{n(r)} \tag{10}$$

describing the degree of local magnetisation. The spin densities are readily given by

$$n_\pm(r) = \frac{1}{2}(1 \pm \zeta)n(r).$$

Following Barth–Hedin [25] and Gunnarsson–Lundqvist [26] it is well known that the kinetic (Hartree) and exchange energy (per particle) of a partially polarised electron gas may be expressed through an interpolation between the paramagnetic ($\zeta = 0$) and the ferromagnetic ($\zeta = \pm 1$) limits as in Hartree–Fock approximation:

$$e_i(r_s, \zeta) = e_i^{\mathrm{P}}(r_s) + [e_i^{\mathrm{F}}(r_s) - e_i^{\mathrm{P}}(r_s)]f_i(\zeta) = e_i^{\mathrm{P}}(r_s) + \Delta e_i(r_s, \zeta) \tag{11}$$

where i stands for either kinetic (K) or exchange (X) and the spin-interpolation functions $f_i(\zeta)$, respectively,

$$f_{\mathrm{K}}(\zeta) = \frac{[(1+\zeta)^{\frac{5}{3}} + (1-\zeta)^{\frac{5}{3}} - 2]}{[2(2^{\frac{2}{3}} - 1)]}$$

and

$$f_{\mathrm{X}}(\zeta) = \frac{[(1+\zeta)^{\frac{4}{3}} + (1-\zeta)^{\frac{4}{3}} - 2]}{[2(2^{\frac{1}{3}} - 1)]} \tag{12}$$

ensure exact ζ dependence of the kinetic and exchange energies. In the para- and ferromagnetic limits, they have the following forms:

$$e_{\mathrm{K}}^{\mathrm{P}}(r_s) = \frac{2.21}{r_s^2}, \qquad e_{\mathrm{K}}^{\mathrm{F}}(r_s) = 2^{\frac{2}{3}} e_{\mathrm{K}}^{\mathrm{P}}(r_s)$$

and

$$e_{\mathrm{X}}^{\mathrm{P}}(r_s) = -\frac{0.916}{r_s}, \qquad e_{\mathrm{X}}^{\mathrm{F}}(r_s) = 2^{\frac{1}{3}} e_{\mathrm{X}}^{\mathrm{P}}(r_s).$$

For the correlation energy, the spin dependence is rather involved and cannot be expressed correctly in a similar closed analytical form using a simple interpolation function $f_i(\zeta)$. However, following [8], we can always write

$$e_{\mathrm{C}}(r_s,\zeta) = e_{\mathrm{C}}^{\mathrm{P}}(r_s) + \Delta e_{\mathrm{C}}(r_s,\zeta). \tag{13}$$

Vosko, Wilk and Nusair [8] have pointed out the inadequacy of the use of Barth–Hedin [25] spin interpolation formula

$$\Delta e_{\mathrm{C}}(r_s,\zeta) = [e_{\mathrm{C}}^{\mathrm{F}}(r_s) - e_{\mathrm{C}}^{\mathrm{P}}(r_s)] f_{\mathrm{C}}(\zeta)$$

with $f_{\mathrm{C}}(\zeta) = f_{\mathrm{X}}(\zeta)$, by most researchers doing spin density functional calculations. Both made Padé type spin interpolations from [8] and [11] scaled in terms of RPA ζ-variation of the correlation energy. Unfortunately, more accurate QMC data are available only for $\zeta = 0$ and $\zeta = 1$, the spin interpolation in beyond-RPA calculation therefore, has to adopt some approximations. In the present calculation we use the prescription [8]

$$\Delta e_{\mathrm{C}}(r_s,\zeta) = \frac{e_{\mathrm{C}}^{\mathrm{F}}(r_s) - e_{\mathrm{C}}^{\mathrm{P}}(r_s)}{[e_{\mathrm{C}}^{\mathrm{F}}(r_s) - e_{\mathrm{C}}^{\mathrm{P}}(r_s)]^{\mathrm{RPA}}} \Delta e_{\mathrm{C}}^{\mathrm{R}}\mathrm{PA}(r_s,\zeta).$$

Noting that, for small ζ, $\Delta e_{\mathrm{C}}(r_s,\zeta)$ can be accurately approximated by the first non-vanishing term of the Taylor series:

$$\Delta e_{\mathrm{C}}(r_s,\zeta) \simeq \frac{1}{2}\alpha_{\mathrm{C}}(r_s)\zeta^2,$$

the spin stiffness factor can be accordingly scaled in terms of the corresponding RPA values:

$$\alpha_{\mathrm{C}}(r_s) = \frac{e_{\mathrm{C}}^{\mathrm{F}}(r_s) - e_{\mathrm{C}}^{\mathrm{P}}(r_s)}{[e_{\mathrm{C}}^{\mathrm{F}}(r_s) - e_{\mathrm{C}}^{\mathrm{P}}(r_s)]^{\mathrm{RPA}}} \alpha_{\mathrm{C}}^{\mathrm{RPA}}(r_s).$$

Using Eqs. (11), (12), and (13), the total ground state energy of the spin polarised system may be estimated.

3. Results and discussions

Table I compares the density interpolation of Ceperley–Alder [6] data for the correlation energy at various r_s from 0.5 a.u. to 100 a.u. of the present calculation with the results in [11]. It may be noted that both the calculations from [11] and [8] produce almost identical values for the correlation energy. The present calculation which uses all the six Ceperley–Alder [6] data as input shows small differences with the values in [11] within the interpolation range. However, large differences are observed with their (and [8] also) results for high densities ($r_s < 2$ a.u.) in the extrapolated region for the ferro state. In order to compare the functional derivative of the correlation energy in the two calculations we first study (Fig. 1) the variation of $\beta(r_s)$, the relative strength of XC potential compared to exchange

TABLE I

Correlation energy (fitted value) in mRyd for different r_s values.

r_s (a.u.)	Different calculations	$-e_{\mathrm{C}}^{\mathrm{P}}(r_s)$	$-e_{\mathrm{C}}^{\mathrm{F}}(r_s)$
	present	154.38	68.25
0.5	[11]	153.24	80.38
	present	122.11	59.77
1.0	[11]	119.55	63.25
	present	90.20	48.00
2.0	[11]	89.52	47.82
	present	73.85	40.37
3.0	[11]	73.88	39.82
	present	63.56	35.08
4.0	[11]	63.73	34.68
	present	56.30	31.20
5.0	[11]	56.43	30.89
	present	50.80	28.23
6.0	[11]	50.85	28.03
	present	44.55	24.88
7.5	[11]	44.51	24.77
	present	37.22	21.00
10.0	[11]	37.14	20.96
	present	28.29	16.34
15.0	[11]	28.29	16.33
	present	22.99	13.55
20.0	[11]	23.06	13.55
	present	16.98	10.27
30.0	[11]	17.03	10.27
	present	11.40	7.09
50.0	[11]	11.38	7.09
	present	8.17	5.21
75.0	[11]	8.15	5.21
	present	6.38	4.15
100.0	[11]	6.38	4.14

only potential as a function of density (r_s). The expression for $\beta(r_s)$ is given by

$$\beta(r_s) = \frac{v_{\mathrm{XC}}(r_s)}{v_{\mathrm{X}}(r_s)},$$

where $v_{\mathrm{XC}}(r_s)$ is the XC potential defined as the functional derivative of the energy term:

$$v_{\mathrm{XC}}(r_s) = \frac{\partial[n e_{\mathrm{XC}}(r_s)]}{\partial n} = e_{\mathrm{XC}}(r_s) + n\frac{\partial e_{\mathrm{XC}}(r_s)}{\partial n}$$

and $v_{\mathrm{X}}(r_s)$ is the exchange potential of the electron gas. Very similar results are obtained in the two calculations which show (Fig. 1) appreciable differences with earlier calculation by Hedin et al. [27].

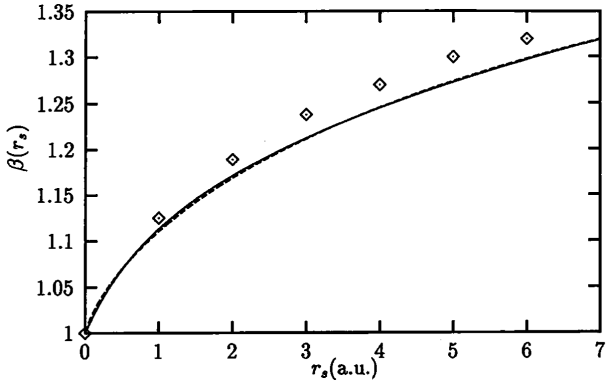

Fig. 1. Variation of $\beta(r_s)$ with (r_s) for $\zeta = 0$. Present calculation (solid curve) is compared with the Perdew and Wang [11] (dashed) curve. Diamonds are from Ref. [27].

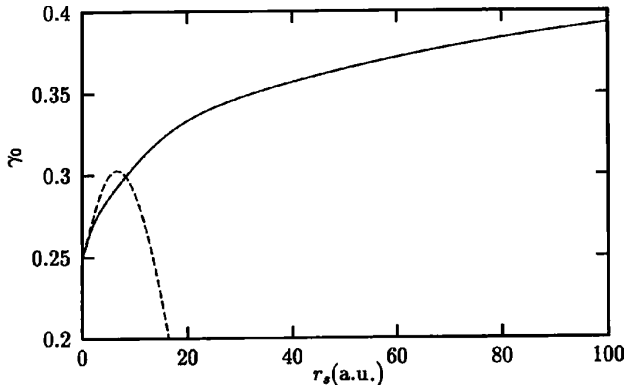

Fig. 2. Comparison of $\gamma_0(r_s)$ vs. r_s curves. The present calculation is shown by solid curve where as the dashed curve is due to Perdew and Wang [11] calculation.

Large difference between the Levin like method and the Padé type density interpolation shows up in the calculation of γ_0 (involving second functional derivative of the correlation energy) which appears in the compressibility sum rule. Figure 2 depicts the variation of $\gamma_0(r_s)$ with r_s over the entire density range, and shows a wide difference of the present calculation with that of Ref. [11]. Table II shows that our results also agree closely with more recent calculations of Ortiz

and Ballone [28]. We also compare the $g(0)$ values of Yasuhara used in our calculation with those of Ref. [28] and of Zhu and Overhauser [29]. Here also we have closer agreement with Ref. [28], whereas calculations of Ref. [29] differ for large r_s. The present calculations also appear to produce reasonable $g(r)$ values (over the relevant density range) which will be discussed elsewhere.

TABLE II

Comparison of calculated values of $\gamma_0^{\mathrm{P}}(r_s)$ and $g(0)$ for different r_s values with results of Ref. [28] and of Ref. [29].

r_s in a.u.	Different calculations	$\gamma_0(r_s)$	$g(0)$
1.0	present	0.2607	0.2662
	[28]	0.2567	0.2724
	[29]	–	0.2644
3.0	present	0.2765	0.0878
	[28]	0.2722	0.0922
	[29]	–	0.1107
5.0	present	0.2887	0.0333
	[28]	0.2850	0.0232
	[29]	–	0.0605
10.0	present	0.3102	0.0042
	[28]	0.3079	0.0024
	[29]	–	0.0220

Figure 3 shows the variation of the total ground state energy $e(r_s, \zeta)$ with r_s over the entire range of density, for $\zeta = 0$ and $\zeta = 1$. It is observed that an interacting electron gas system shows a transition from paramagnetic to ferromagnetic state at $r_s = 83.7$ a.u..

It is generally regarded [8] that for metallic ferromagnets $|\zeta| \leq 0.15$ and reported estimates [30] indicate that a partially polarised electron fluid is stable in the range 2 a.u. $< r_s <$ 84 a.u.. However, a consistent prediction regarding the stability of partially polarised fluid in agreement with the present knowledge is lacking with almost all the existing spin interpolation formulae for the correlation energy. This anomaly is inherent also with the RPA data particularly of Ref. [11], for which they claim a better accuracy. Recently, Ortiz et al. [31] have made an important progress in the study of ferromagnetic transition with their new QMC data set.

It may be further noted that the calculation of $\beta^{\pm}(r_s, \zeta)$, where

$$\beta^{\pm}(r_s, \zeta) = \frac{v_{\mathrm{XC}}^{\pm}(r_s, \zeta)}{v_{\mathrm{X}}(r_s, \zeta = 0)}$$

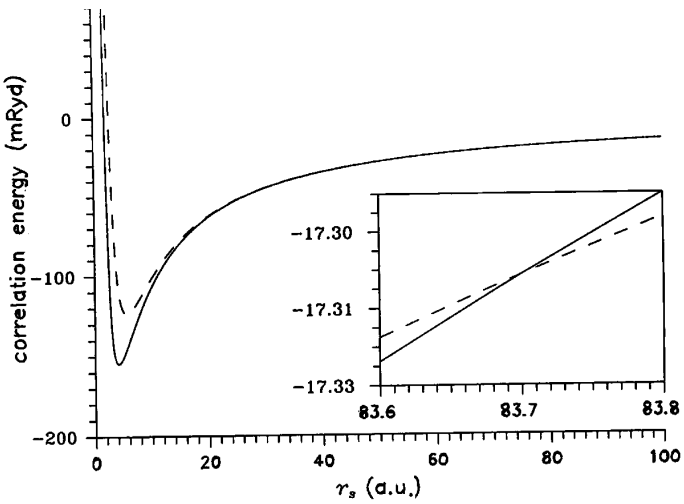

Fig. 3. Total ground state energy $e(r_s, 0)$ (solid curve) and $e(r_s, 1)$ (dashed curve) as a function of r_s. The inset shows the para ($\zeta = 0$) – ferro ($\zeta = 1$) cross-over clearly.

as a function of both r_s and ζ with

$$v_{\mathrm{XC}}^{\pm}(r_s, \zeta) = \frac{\partial[n e_{\mathrm{XC}}(r_s, \zeta)]}{\partial n_{\pm}}$$
$$= e_{\mathrm{XC}}(r_s, \zeta) + n\frac{\partial e_{\mathrm{XC}}(r_s, \zeta)}{\partial n} \pm (1 \mp \zeta)\frac{\partial e_{\mathrm{XC}}(r_s, \zeta)}{\partial \zeta}$$

and $v_{\mathrm{X}}(r_s, \zeta = 0)$, the exchange potential in paramagnetic state of the electron gas, also shows similar variations as obtained by Gunnarsson and Lundqvist [26]. No improvement or further insight can be expected with the present spin interpolation formula. From the present study it is ample clear that a better spin interpolation is essential in making meaningful predictions of ground/excited state properties of interacting electron gas. A fresh calculation with the new QMC data [31] is expected to give a better description and will be discussed elsewhere.

In Table III we compare $G^{\mathrm{P}}(q)$ of the present calculation with the LFF obtained by Bowen et al. [18] and Moroni et al. [19]. A direct comparison with both the QMC calculations is possible only at $r_s = 10$ a.u.. The reasonable agreement clearly indicates that these QMC calculations refer to the determination of $G^{\mathrm{P}}(q)$.

In Fig. 4a we compare the variations of $G(q)$ and $G^{\mathrm{P}}(q)$, at $r_s = 10$ a.u.. $G(q)$ shows a weak peak structure around $q = 1.2k_{\mathrm{F}}$, whereas a peak structure is obtained for $G^{\mathrm{P}}(q)$ near $q = 2k_{\mathrm{F}}$, only beyond metallic density [5]. In contrast, the general LFF $G(q)$ has also a trough around $q = 2.3k_{\mathrm{F}}$. Beyond $5k_{\mathrm{F}}$ both $G(q)$ and $G^{\mathrm{P}}(q)$ reach the respective asymptotic values and in this region the difference between $G(q)$ and $G^{\mathrm{P}}(q)$ decreases with decreasing density. Figure 4b shows $G(q)$ vs. q plot for densities corresponding to $r_s = 2$, 4, and 10 a.u.. At

TABLE III

Comparison of $G^{\mathrm{P}}(q)$ with the electron gas local field factor obtained from fixed-node diffusion QMC simulations (Ref [18]), Ref. [19]) for selected values of q/k_{F}.

q/k_{F}	$G^{\mathrm{P}}(q)$	$G(q)$ [19]	$G(q)$ [18]
1.01	0.31	0.29	0.28
1.08	0.35	0.24	–
1.21	0.44	0.41	–
1.51	0.64	0.67	0.65
1.61	0.71	0.78	0.70
1.81	0.84	0.92	0.71
2.01	0.96	1.13	–
2.15	1.03	1.19	0.95
2.42	1.13	1.32	–
2.51	1.15	–	–
2.69	1.18	1.46	–
3.02	1.20	1.45	–

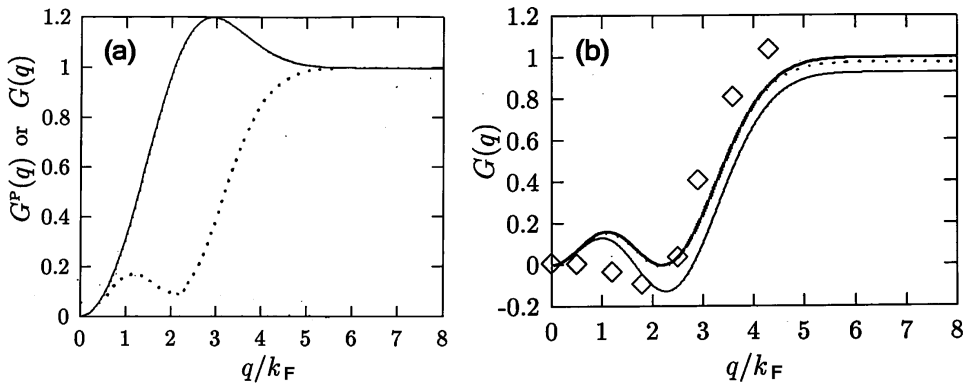

Fig. 4. (a) Comparison of $G(q)$ and $G^{\mathrm{P}}(q)$, plotted against q/k_{F} at $r_s = 10$ a.u. (thin solid curve for $G^{\mathrm{P}}(q)$ and dotted curve for $G(q)$). (b) Variation of $G(q)$ with q/k_{F} for different values of r_s (thin solid curve for $r_s = 2$ a.u., dotted curve for $r_s = 4$ a.u. and thick solid curve for $r_s = 10$ a.u.). Diamonds are for $G_n(q)$ at $r_s = 2$ a.u. from Ref. [4].

$r_s = 2$ a.u., $G(q)$ remains negative for q-value between $1.5k_{\mathrm{F}}$ and $3k_{\mathrm{F}}$. In the low q region, Richardson and Ashcroft's "new" local field factor (static: $\omega = 0$) for $r_s = 2$ a.u. is shown to have very similar features. In a recent *ab initio* pseudopotential study [32] the use of $G(q)$ instead of $G^{\mathrm{P}}(q)$ is found to reproduce the hard-sphere description (Fig. 5) of the effective pair potential of Al, in close

agreement with a recent study [33] based on a large set of *ab initio* data. This result is consistent with the empirical demand from the ionic pair correlation data [32]. The effective interaction is not very sensitive to the values of LFF for $q > 2k_{\mathrm{F}}$. Arguably, it speaks for the reliability of the present $G(q)$ values at least in the low-q region.

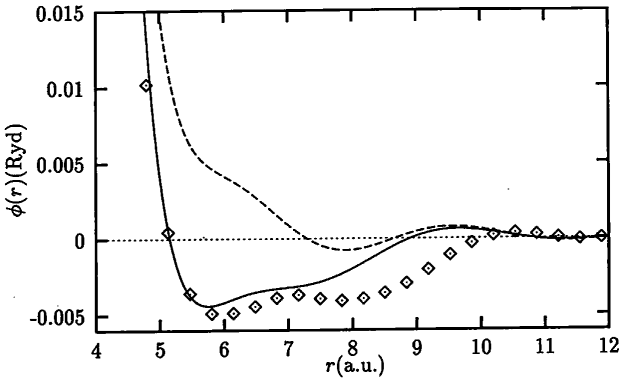

Fig. 5. Comparison of pair potentials $\phi(r)$ of Al calculated using $G(q)$ (solid curve) and $G^{\mathrm{P}}(q)$ (dashed curve). Diamonds are from Ref. [33].

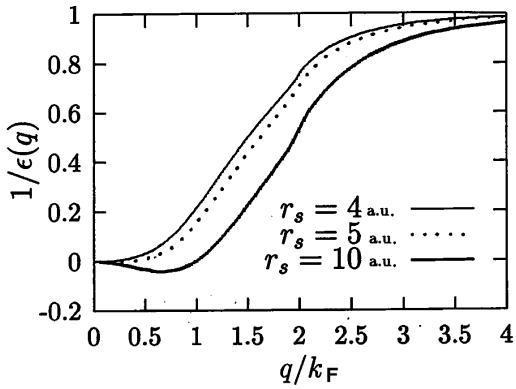

Fig. 6. Screening function $1/\epsilon(q)$ plotted against q/k_{F} for different r_s values.

The screening function $1/\epsilon(q)$, plotted against q for various r_s in Fig. 6, shows that the static dielectric function becomes negative at $r_s \approx 5$ a.u.. The result is in close agreement with the recent ones. The charge- and magnetic-susceptibility enhancements $\chi(q)/\chi_0(q)$ and $-\chi_{\mathrm{m}}(q)/\mu_{\mathrm{e}}^2\chi_0(q)$ (from Eqs. (2) and (4)) plotted against q, at $r_s = 4$ a.u., are shown in Fig. 7. $\chi(q)/\chi_0(q)$ goes to zero as q goes to zero and the value of $-\chi_{\mathrm{m}}(q)/\mu_{\mathrm{e}}^2\chi_0(q)$ at $q = 0$ obtained in the present calculation is 1.07 as compared to 1.65 obtained by Dupree and Geldart [34]. Both the curves come closer as q approaches $2k_{\mathrm{F}}$ and merge beyond $3k_{\mathrm{F}}$.

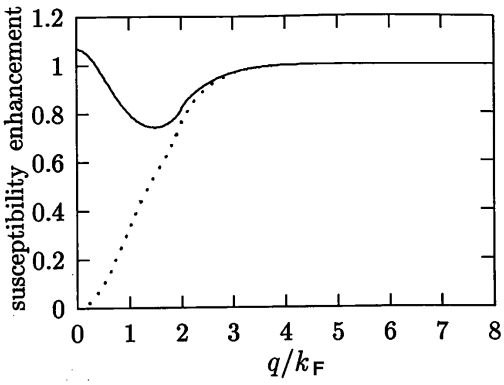

Fig. 7. Variation of charge- and magnetic-susceptibility enhancements $\chi(q)/\chi_0(q)$ (solid curve) and $-\chi_m(q)/\mu_e^2\chi_0(q)$ (dashed curve) with q/k_F at $r_s = 4$ a.u..

TABLE IV

Calculated values of correlational spin stiffness factor in mRyd for different r_s values.

r_s in a.u.	$\alpha_C(r_s)$ (present) in mRyd	$\alpha_C(r_s)$ [11] in mRyd	$\alpha_C(r_s)$ [8] in mRyd
0.5	118.88	100.50	100.10
1.0	90.16	80.64	79.40
2.0	62.94	62.16	60.10
3.0	51.15	52.06	49.80
4.0	44.20	45.26	43.00
5.0	39.47	40.22	38.00
6.0	35.81	36.27	34.20
7.5	31.55	31.70	–
10.0	26.98	26.27	–
15.0	19.68	19.63	–

The numerical values of the fitted QMC spin stiffness factor (correlation only) obtained in the present study at various densities are given in Table IV along with the values from [11] and [8]. The values of $\alpha_C(r_s)$ obtained in the present calculation are higher than the corresponding values from [11] and [8] at high densities.

Assuming the gradient expansion of $e_{XC}(n(r), \zeta(r))$ for small $n(r)$ and $\zeta(r)$ nearly constant, Vosko and Pedrew [35] have the following expression for the magnetic susceptibility enhancements in the long wavelength limit $q = 0$ in terms of the spin stiffness factor:

$$\lim_{q\to 0} \frac{\chi_{\mathrm{m}}(q)}{-\mu_{\mathrm{e}}^2 \chi_0(q)} = \left[1 + \frac{3}{2}\left(\frac{4}{9\pi}\right)^{2/3} r_s^2 \alpha_{\mathrm{XC}}(r_s)\right]^{-1}, \tag{14}$$

where $\alpha_{\mathrm{XC}}(r_s)$ is the spin stiffness factor for the combined XC effect. The divergence of this quantity at $r_s \approx 82$ a.u. indicates spontaneous polarisation from $\zeta = 0$ to $\zeta = 1$. This is consistent with the earlier result obtained from the ground state energy of the system. However, we do not attach much importance on this result obtained with the spin interpolation formula for the correlation energy functional. Moreover, the consistency of Eq. (14) with respect to Eq. (4) is not guaranteed in the present formulation and will be dealt elsewhere.

Finally we summarize the important results of the present study and the conclusion drawn from the comparison with the previous ones. In our study we have used the old QMC data set to compare the present formulation with a number of previous studies using the same QMC data. In most of the existing literatures including the recent attempts [3, 17–19] the spin interaction of the unpolarised system is not considered properly, as no distinction is made between the response of a spin-up electron (say) to the spatial polarisation of the spin-up electrons and that to the spatial polarisation of the spin-down electrons (of the unpolarised electron gas). The spin interaction in the theory of LFF for unpolarised electron gas replaces $G^{\mathrm{P}}(q)$ with $G(q)$.

The reasonable agreement (Table III) between $G^{\mathrm{P}}(q)$ of the present calculation and the LFF obtained by Bowen et al. [18] and Moroni et al. [19] clearly indicates that these QMC calculations refer to the determination of $G^{\mathrm{P}}(q)$. Only Richardson and Ashcroft [4] have provided a calculation for the equivalent pair of quantities "$G_{s,a}(q)$". At $r_s = 2$ a.u., where a direct comparison with Richardson–Ashcroft's "new" local field factor (static: $\omega = 0$) calculations is possible with our present calculation of $G(q)$, close agreement is observed in the low q region. The present paper thus provides a simpler formulation of $G(q)$ through a consistent evaluation of $G^{\mathrm{F}}(q)$ and $G^{\mathrm{P}}(q)$.

The effective interaction of Al is discussed as another encouraging result of application of the present theory of LFF. In the *ab initio* pseudopotential study the use of $G(q)$ instead of $G^{\mathrm{P}}(q)$ is found to reproduce the hard-sphere description (Fig. 5) of the effective pair potential $\phi(r)$ of Al, in close agreement with a recent study [33] based on a large set of *ab initio* data.

With the new QMC data set of Ortiz et al. [31] we hope to derive a better spin interpolation formula and using the present generalised formulation, it is expected to gain a better description of local field factors related to the charge and magnetic response functions, respectively.

References

[1] J.S. Thakur, D. Neilson, *Phys. Rev. B* **56**, 4679 (1997).

[2] S. Ichimaru, *Rev. Mod. Phys.* **54**, 1017 (1982).

[3] B. Farid, V. Heine, G. Engel, I. Robertson, *Phys. Rev. B* **48**, 11602 (1993).

[4] C.F. Richardson, N.W. Ashcroft, *Phys. Rev. B* **50**, 8170 (1994).

[5] A. Sarkar, D. Sen, S. Haldar, D. Roy, *Mod. Phys. Lett. B* **12**, 639 (1998).

[6] D.M. Ceperley, B.J. Alder, *Phys. Rev. Lett.* **45**, 566 (1980).

[7] A. Sarkar, S. Haldar, D. Sen, D. Roy, *Ind. J. Phys. A* **75**, 29 (2001).

[8] S.H. Vosko, L. Wilk, M. Nusair, *Can. J. Phys.* **58**, 1200 (1980).

[9] J.P. Perdew, Y. Zunger, *Phys. Rev. B* **23**, 5048 (1981).

[10] R.M. Dreizler, E.K.U. Gross, in: *Density Functional Theory*, Springer-Verlag, Berlin 1990, p. 76.

[11] J.P. Perdew, Y. Wang, *Phys. Rev. B* **45**, 13244 (1992).

[12] D. Singh, D.P. Clougherty, J.M. MacLaren, R.C. Albers, C.S. Wang, *Phys. Rev. B* **44**, 7701 (1991).

[13] R. Bhattacharyya, D. Roy, S. Bhowmick, *Comp. Phys. Commun. B* **101**, 213 (1997).

[14] O.V. Dolgov, D.A. Kirzhnits, E.G. Maksimov, in: *Superconductivity, Superdiamagnetism, Superfluidity*, Ed. V.L. Ginzburg, Mir Publishers, Moscow 1987, p. 31.

[15] J.C. Kimball, *Phys. Rev. A* **7**, 1648 (1973).

[16] K.S. Singwi, A. Sjölander, M.P. Tosi, R.H. Land, *Phys. Rev. B* **1**, 1044 (1970).

[17] S. Ichimaru, K. Utsumi, *Phys. Rev. B* **24**, 7385 (1981).

[18] C. Bowen, G. Sugiyama, B.J. Alder, *Phys. Rev. B* **50**, 14838 (1994).

[19] S. Moroni, D.M. Ceperley, G. Senatore, *Phys. Rev. Lett.* **75**, 689 (1995); G. Senatore, S. Moroni, D.M. Ceperley, *J. Non-Cryst. Solid* **205**, 851 (1996).

[20] A. Holas, in: *Strongly Coupled Plasma Physics,* Eds. F.J. Rogers, H.E. DeWitt, Plenum, New York 1987, p. 463.

[21] M. Lein, E. Gross, J.P. Perdew, *Phys. Rev. B* **61**, 13431 (2000).

[22] M. Corradini, R. Del Sole, G. Onida, M. Palummo, *Phys. Rev. B* **57**, 14569 (1998).

[23] H. Yasuhara, *Solid. State. Commun.* **11**, 1481 (1972).

[24] P. Gori-Giorgi, F. Sacchetti, G.B. Bachelet, *Phys. Rev. B* **61**, 7353 (2000).

[25] U.V. Barth, L. Hedin, *J. Phys. C* **53**, 1629 (1972).

[26] O. Gunnarsson, B.I. Lundqvist, *Phys. Rev. B* **13**, 4274 (1976).

[27] L. Hedin, B.I. Lundqvist, S. Lundqvist, *Solid. State. Commun.* **9**, 537 (1971).

[28] G. Ortiz, P. Ballone, *Phys. Rev. B* **50**, 1391 (1994).

[29] X. Zhu, A.W. Overhauser, *Phys. Rev. B* **30**, 3158 (1994).

[30] D.M. Ceperley, in: *Monte Carlo Methods in Quantum Physics,* Ed. M.H. Kalos, Reidel, Dordrecht 1984, p. 47.

[31] G. Ortiz, M. Harris, P. Ballone, *Phys. Rev. Lett.* **82**, 5317 (1999).

[32] S. Haldar, A. Sarkar, D. Sen, *Ind. J. Phys. A* **75**, 25 (2001).

[33] Y. Mishin, D. Farkas, M.J. Mehl, D.A. Papaconstantopoulos, *Phys. Rev. B* **59**, 3393 (1999).

[34] R. Dupree, D.J.W. Geldart, *Solid. State. Commun.* **9**, 145 (1971).

[35] S.H. Vosko, J.P. Pedrew, *Can. J. Phys.* **53**, 1385 (1975).