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A Brief Review and Role of Local Field Correction Functions in Condensed Matter Physics

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The importance of various local field correction functions (LFCFs) in condensed matter physics that have been proposed thus far from diverse literature surveys is reported in the current article. Total 40 different forms of LFCFs have been identified in the literature so far. Each LFCF's essential parameters are supplied along with a brief summary. Our main objective is to emphasize the different local field corrections that have been published in the literature since 1957 and provide the scientific community with complete reference information.

Keywords: Compressibility sum rule; homogeneous electron gas; local field correction functions (LFCFs); diffusion Monte Carlo (DMC) method; dielectric screening theory.

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Introduction

In condensed matter physics, the dielectric screening plays an important role in the evaluation of self-consistent potential due to the screening of the electron gas. Such screening affects in elimination of the long-range Coulomb field of the ion [1-20].

Bardeen [21] in the study of the electron-phonon interaction first of all utilizes the self-consistent method of screening by the electrons in the Hartree approximation. The dielectric function is particularly useful in such approximation where it leads to the potential that enters in one electron Schrödinger equation. If exchange and correlation effect is included in the screening (i.e. Hartree-Fock approximation) then it enters as a non-local (energy dependent) potential and the problem becomes more difficult.

While, the exchange and correlation interactions have been investigated extensively for the free electron gas using many body perturbation theories. As noted above the Hartree approximation neglects any direct electron-electron interactions [2, 3]. In particular, the neglect of the requirement of the Pauli exclusion principle for antisymmetric wave functions is corrected in the Hartree-Fock approximation which gives an extra exchange term in the energy. The correlation effects arise from the Coulomb repulsion between electrons, leading to the concept of a ‘correlation hole’ around each electron, which excludes other electrons. As in the case of screening there have been a number of calculation schemes proposed [2, 3, 22-67] to introduce such exchange and correlation effects of local field corrections into the potential via a modified dielectric function [2, 3, 22-67].

Looking to the advantages of screening and their local

field corrections in the literature, there are large number of local field corrections functions are proposed by various authors in the literature [2, 3, 22-67] and reported in the present article. Also, their natures are plotted via $f(q) \rightarrow q$ graph and their limiting values at $q \rightarrow 0$ and $q \rightarrow \infty$ are also reported in Table 1.

I. Dielectric Screening Theory

In general, no one has yet determined the precise homogeneous gas dielectric function. Instead, a number of researchers have found approximations to the answers. Some of these have been discovered to be particularly effective due to their clarity or correctness. They have been given their inventors' names. These are their lists [11]:

- Thomas-Fermi,
- Lindhard or Random Phase Approximation (RPA),
- Hubbard, and,
- Singwi-Sjölander.

A degenerate Fermi gas's dielectric function, $\varepsilon(q)$, is typically expressed as

$$\varepsilon(q) = 1 + \frac{q_s^2}{q^2}. \quad (1)$$

Through $q_s^2 = 4\pi e^2 N(E)$ is the screening length.

Here, $N(E)$ is the density of state per energy E and specified by

$$N(E) = \frac{2\Omega_0}{(2\pi)^3} \int \frac{dS_k}{\text{grad}_k E(k)} \quad (2)$$

Table 1.

Long wave length and Short wave length limits of LFCFs.

Sr. No.	Name of Screening Functions	Year	$\lim_{q \rightarrow 0} f(q)$	$\lim_{q \rightarrow \infty} f(q)$
1	Hubbard (HB)	1957	0	0.5
2	Hubbard-Sham (HS)	1957	0	0.5
3	Hubbard-Sham-Geldart-Vosko (HSGV)	1957	0	0.5
4	Sham (SM)	1965	0	0.5
5	Kohn-Sham (KS)	1965	0	∞
6	Geldart-Vosko (GV)	1966	0	0.5
7	Hartree (HT)	1967	-	-
8	Harrison (HR)	1967	0	0.5
9	Kleinmann (KM)	1968	0	∞
10	Ashcroft (AS)	1968	0	0.5
11	Singwi-Tosi-Sjölander-Land (STSL)	1968	0	0.5
12	Kleinmann-Langreth (KL)	1968	0	∞
13	Shaw-Pynn (SP)	1969	0	0.5
14	Singwi-Sjölander-Tosi-Land (SSTL)	1970	0	A
15	Shaw (SH)	1970	0	0.5
16	Toigo-Woodruff (TW)	1970	0	0.762
17	King-Cutler (KC)	1971	0	0.5
18	Overhouser (OV)	1971	0	0.898
19	Mahanti-Das (MD)	1971	0	∞
20	Vashishta-Singwi (VS)	1972	0	A
21	Jain-Jain (JJ)	1973	0	A
22	Pathak-Vashishta (PV)	1973	$\frac{2}{3}\gamma$	$\frac{2}{3}[1 - g(0)]$
23	Kuglar (KR)	1975	$\frac{3}{20}$	$\frac{1}{3} = 0.3333$
24	Srivastava (SR)	1977	0	0.316
25	Tripathi-Mandal (TM)	1977	0	0.33365
26	Taylor (TY)	1978	0	∞
27	Ichimaru-Utsumi (IU)	1981	0	$1 - g(0)$
28	Alvarellos and Flores (AF)	1984	0.375	$13/30 = 0.4333$
29	Bhatia-Singh (BS)	1985	0	0.5
30	Nagy (NG)	1986	$\frac{q^2}{3C^2}[g(0, n) - 3b]$	$1 - g(0, n)$
31	Farid-Heine-Engle-Robertson (FHER)	1993	0	∞
32	Gold-Calmels (GC)	1993	0	$1 - g(0)$
33	Ortiz and Ballone (OB)	1994	$\gamma_0 \left(\frac{q}{k_F}\right)^2$	$1 - g(0)$
34	Moroni, Ceperley-Senatore (MCS)	1995	$A \left(\frac{q}{k_F}\right)^2$	$C \left(\frac{q}{k_F}\right)^2 + B$
35	Bretonnet-Boulahbak (BB)	1996	$\gamma_0 \left(\frac{q}{k_F}\right)^2$	$1 - g(0)$
36	Sarkar-Sen-Haldar-Roy (SSHR)	1998	0	A
37	Hellal, Gasser-Issolah (HGI)	2003	$\gamma\eta^2$	$1 - g(0)$
38	Sarkar-Haldar-Roy- Sen (SHRS)	2004	$1 - g(0)$	$-g(0)$
39	Dornheim-Vorberger-Groth-Hoffmann-Moldabekov-Bonitz (DVGHMB)	2020	0	$1 - g(0)$
40	Kukkonen-Chen (KC)	2021	$f_+(q) = \left(1 - \frac{\kappa_0}{\kappa}\right)$ $f_-(q) = \left(1 - \frac{\chi_0}{\chi}\right)$	∞

It exhibits a dielectric screening function after being substituted in Eq. (1),

$$\varepsilon(q) = 1 + \left(\frac{8\pi Z}{\Omega_0 q^2}\right) \left(\frac{2}{3} E_F\right)^{-1} \left[0.5 + \frac{4k_F^2 - q^2}{8qk_F} \ln \left|\frac{q+2k_F}{q-2k_F}\right|\right]. \quad (3)$$

In this case, Z is the metal's valence, E_F is the Fermi energy, and k_F is the Fermi momentum. On the basis of the self-consistent treatment of screening, Bardeen [21] constructed this equation, which is a static Hartree dielectric constant. Lindhard [19] has also produced a formula for the dielectric function generated by the random phase approximation (RPA) as,

$$\varepsilon_{RPA}(q) = 1 + \frac{q_s^2}{q^2} = 1 + \left(\frac{\lambda_s}{q^2}\right) \mathcal{F}(q), \quad (4)$$

$$\text{with } \lambda_s = \frac{4k_F}{\pi a_0} \mathcal{F} \text{ and } \mathcal{F}(q) = \left[0.5 + \frac{4k_F^2 - q^2}{8qk_F} \ln \left|\frac{q+2k_F}{q-2k_F}\right|\right].$$

It is noticeable that how equations (3) and (4) are identical. The high electron density zone is the only one where the Lindhard function [16] is valid. Additionally, this idea does not take into account the short-term impacts. Due to its foundation being a sharp fermi surface, the electrons have an unlimited mean-free path. Leavens et al.

[68] have developed a rough generalisation of such a function that takes the finite mean free path impact into account. At slightly higher temperatures, it might be more crucial for liquid metals [11].

Hubbard [23, 24] suggested a self-consistent approach to enhance the RPA value of the energy in their seminal articles, employing a complex diagrammatic technique. In this approach, he has included the exchange hole's contribution to the Hartree-Fock approximation. The modified Hartree dielectric function $\varepsilon^*(q)$ [2, 3] is thus given by

$$\varepsilon^*(q) = 1 + \{\varepsilon_H(q) - 1\}\{1 - f(q)\}. \quad (5)$$

The LFCF, often known as the exchange and correlation function, is $f(q)$. Additionally, the Hartree [2, 3] dielectric function is $\varepsilon_H(q)$. Such a function's mathematical notation is represented as [2,3].

$$\varepsilon_H(q) = 1 + \frac{3\pi e^2 Z}{\Omega_0 Y^2 k_F^2} \left[1 + \frac{4-Y^2}{2Y} \ln \left|\frac{2+Y}{2-Y}\right|\right]; \text{ with } Y = \frac{q}{2k_F}. \quad (6)$$

Levine and Louie [69] postulated that the spatial dielectric function for semiconducting materials is of the type,

$$\varepsilon_{LL}(q) = 1 + \frac{1}{Lq^2} \left[0.5 - \frac{\lambda}{4Y} \left(\tan^{-1} \frac{y_+}{\lambda} + \tan^{-1} \frac{y_-}{\lambda}\right) + \left(\frac{\lambda^2}{16Y^2} + \frac{1}{4Y} - \frac{Y}{16}\right) \ln \left(\frac{\lambda^2 + y_+^2}{\lambda^2 + y_-^2}\right)\right]. \quad (7)$$

with,

$$y_+ = Y(2 + Y),$$

$$y_- = Y(2 - Y),$$

$$L = \sqrt{\frac{\pi}{4k_F}}, \text{ and } \lambda = \frac{2}{\sqrt{3L^2 k_F^2 (\varepsilon_0 - 1)}}.$$

Where, ε_0 signifies the finite dielectric constant of the semiconductor.

The model band topologies make it clear that all of the d-sub bands are occupied and that the Fermi level only crosses the s-band, according to Singh and Prakash [70]. Therefore, the two forms of transition from the unoccupied s-band to the vacant s-band and from the occupied d-sub bands to empty s-bands, are what induce

the electron to rearrange in response to the displacement of ions caused by lattice vibrations. In light of this, the dielectric function is provided by

$$\varepsilon(p) = 1 - \varepsilon_{ss}(p) - \varepsilon_{ds}(p). \quad (8)$$

Where, $\varepsilon_{ss}(p)$ and $\varepsilon_{ds}(p)$ are $-8\pi/p^2$ times the polarizability functions rise from the intraband and interband transitions, respectively. And $p = q + G$ where q is the phonon wavevector and G the reciprocal-lattice vector, respectively. The mathematical notations for $\varepsilon_{ss}(p)$ and $\varepsilon_{ds}(p)$ are narrated by [70]

$$\varepsilon_{ss}(p) = -\frac{2m_s k_{Fs} e^2}{\pi \hbar^2 p^2} \left[1 + \frac{4k_{Fs}^2 - p^2}{4k_{Fs} p} \ln \left|\frac{2k_{Fs} + p}{2k_{Fs} - p}\right|\right], \quad (9)$$

and

$$\varepsilon_{ds}(p) = \frac{32m_s e^2}{\Omega_0 \hbar^2 p^2} \sum_m (-1)^m \left(\int_0^{k_{Fdm}} dk k^2 [F_2(k)]^2 \left\{ \begin{aligned} &D_{0m}^2 D_{0-m}^2 I_0 \\ &+ (D_{1m}^2 D_{-1-m}^2 + D_{-1m}^2 D_{1-m}^2) I_1 \\ &+ (D_{2m}^2 D_{-2-m}^2 + D_{-2m}^2 D_{2-m}^2) I_2 \end{aligned} \right\} \right). \quad (10)$$

Where,

$$m_s = \frac{\hbar^2 k_{Fs}^2}{2E_F},$$

$$k_{Fs} = \left(\frac{3\pi^2 Z_s}{\Omega_0}\right)^{1/3},$$

$$k_{Fdm} = \left(\frac{3\pi^2 Z_{dm}}{\Omega_0}\right)^{1/3}.$$

Where, E_F is the Fermi energy, Z_s the number of s-electrons per atom, Ω_0 the atomic volume and e the electronic charge, respectively. While D_{mm}^2 are the elements of rotation matrix with argument

$(-\gamma', -\beta', -\alpha')$ where α' , β' , and γ' are the Euler's angles, k is electron wave vector.

$$I_0 = \frac{5}{4}(0.5I_{n0} - 3I_{n2} + 4.5I_{n4}),$$

$$I_1 = \frac{15}{4}(-I_{n2} + I_{n4}),$$

$$I_2 = \frac{15}{8}(0.5I_{n0} - I_{n2} + 0.5I_{n4}),$$

here,

$$I_{n0} = -\frac{1}{b} \ln \left| \frac{b-a}{b+a} \right|,$$

$$I_{n2} = -\frac{1}{b} \left[\frac{2a}{b} + \frac{a^2}{b^2} \ln \left| \frac{b-a}{b+a} \right| \right],$$

$$I_{n4} = -\frac{1}{b} \left[\frac{2a}{3b} + \frac{2a^3}{b^3} + \frac{a^4}{b^4} \ln \left| \frac{b-a}{b+a} \right| \right],$$

$$a = k^2(m_s/m_{dm} - 1) - p^2,$$

$$b = 2kp.$$

The radial component of the d-wave function is involved in the function $F_2(k)$, which is defined as

$$F_2(k) = \int_0^\infty j_2(kr) R_d(r) r^2 dr, \quad (11)$$

where $j_2(kr)$ is the spherical Bessel function and the radial part of the d -wave function.

$$f(q) = \left(\frac{9q^2}{32k_F^2} \right) \left[\left(\frac{2}{105} \right) \left\{ 24 \left(\frac{k_F^2}{q^2} \right) + 44 + \left(\frac{q}{k_F} \right)^2 \right\} - \left(\frac{2k_F}{q} \right) \left\{ \left(\frac{8}{305} \right) \left(\frac{k_F}{q} \right)^2 - \frac{4}{15} + \left(\frac{1}{16} \right) \left(\frac{q}{k_F} \right)^2 \right\} \ln \left| \frac{2k_F+q}{2k_F-q} \right| + \left(\frac{q}{k_F} \right)^2 \left\{ \left(\frac{1}{210} \right) \left(\frac{q}{k_F} \right)^2 - \frac{2}{15} \right\} \ln \left| \frac{q^2-4k_F^2}{q^2} \right| \right]. \quad (13)$$

In order to get a self-consistent form, the cycle of equations describing the relationship between $S(q)$, $\varepsilon(q)$, and the pair correlation function $g(r)$ is iteratively solved on a computer.

Similar to this, Toigo and Woodruff [37] used the double-time Green function technique and a momentum-saving decoupling scheme to derive a mathematical formula for the dielectric function of the electron liquid. A similar plan would include applying the f-sum rule to the dielectric function. Consequently, it is expressed as follows:

$$\varepsilon(q, \omega) = 1 + [Q_0(q, \omega)/1 - G(q, \omega)Q_0(q, \omega)]. \quad (14)$$

The Lindhard function in the RPA approximation (polarizability of the free electron gas) is $Q_0(q, \omega)$ [16]. $p_0(q, \omega)$ comprises the exchange and correlation effects left out of the function $Q_0(q, \omega)$, whereas $(q, \omega) = \frac{p_0(q, \omega)}{Q_0(q, \omega)}$. In the case of an electron liquid, $\omega = 0$ transforms the equation above into

$$\varepsilon(q, 0) = 1 + [Q_0(q, 0)/1 - G(q, 0)Q_0(q, 0)]. \quad (15)$$

$$R_d(r) = \sum_i a_i r^2 e^{-\alpha_i r},$$

where, a_i and α_i are the two parameters. Such values are substituted in the equation above to get,

$$F_2(k) = 48k^2 \sum_i \frac{a_i \alpha_i}{(k^2 + \alpha_i^2)^4}.$$

There is no doubt that the compressibility sum rule is satisfied by the dielectric function $\varepsilon(q)$ defined by Geldert and Vosko [26], but the pair correlation function obtained from it has a $-\infty$, producing physically incorrect results. Although the pair correlation function is driven to infinity over the whole range of metallic densities, the dielectric function of Kleinman [28, 29] poses a major problem. The theory presented by Singwi and colleagues [34, 71] complies with both constraints. The dynamical structure factor $S(q)$ was specifically derived by their method from the correlation function, and the expression for the dielectric constant is given by relating $S(q)$ to the $\varepsilon(q)$ derived from the local field corrections for Coulomb and exchange contributions,

$$\varepsilon(q) = 1 + [Q_0(q)/\{1 - f(q)Q_0(q)\}], \quad (12)$$

Here

$$Q_0(q) = \frac{q_s^2}{q^2} = \frac{4k_F}{\pi a_0 q^2} \left[\frac{1}{2} + \frac{4k_F^2 - q^2}{8qk_F} \ln \left| \frac{q+2k_F}{q-2k_F} \right| \right].$$

The algebraically challenging expression for $f(q)$ is

Toigo and Woodruff's [37] tabulation of the values for Green's function $G(q, 0)$ is shown here. Geldert and Taylor [64] used perturbation theory to create a screening constant, confirming the discussion of it offered in [37]. Additionally, Vashishta and Singwi [43] have more precisely expanded the theory of collective motion's [7] applicability to electron screening.

Unfortunately, the literature does not pay much attention to a thorough study of LFCFs. Because they necessitate a thorough handling of electronic many-body effects, an incredibly complex subject, a vast number of distinct approximations exist as a result. The local density functional (LDF) form proposed by Hedin and Lundquist [72] and Taylor [49] is the most straightforward and practical method for considering $f(q)$.

The compressibility sum rule is a useful tool for navigating the extensive local field literature. There are further sum rules connecting the static dielectric function to the correlation energy, the electron-electron pair correlation function, etc., but the compressibility sum rule is by far the most significant, as the LDF theory's enormous success illustrates. Therefore, it has been demonstrated by studying the suggested local fields in the context of sum rules that all $f(q)$ expressions published

prior to 1970 are replaced by more recent work. The remaining methods, such as those proposed by Toigo and Woodruff [37], Vashishta and Singwi [43], Ichimaru and Utsumi [50], and Geldert and Taylor [73], merit further study.

II. Several Forms of LFCFs

Total 40 LFCFs that are listed in the literature are briefly discussed in this section, along with their accurate mathematical notations.

2.1. Hubbard (HB) LFCF (1957)

According to the Hubbard LFCF [23, 24], the exchange contact between parallel spin electrons essentially cancels out half of the direct, or Coulomb, interaction at very small wavelengths. It is noted as follows:

$$f(q) = \frac{0.5q^2}{(q^2 + k_F^2)}. \quad (16)$$

2.2. Hubbard-Sham (HS) LFCF (1957)

The introduction of exchange between electrons with parallel 'spins' results in the Hubbard-Sham [23–25] LFCF. Hubbard-Sham effects are insufficient for low q values. The exchange and correlation function has the following form:

$$f(q) = \frac{0.5q^2}{(q^2 + \xi k_F^2)}. \quad (17)$$

Here, parameter $\xi = \frac{0.916}{[0.458 + 0.01r_S]}$ and r_S is the Wigner-Seitz radius.

2.3. Hubbard-Sham-Geldart-Vosko LFCF (HSGV) (1957)

The parameter ξ in the Hubbard-Sham-Geldart-Vosko [23–26] LFCF is selected in a way that satisfies the compressibility sum rule. This LFCF violates the requirement that the electron pair correlation function $g(r)$ must be positive for all r for tiny r in the range of typically occurring r_S values. It is provided by,

$$f(q) = \frac{0.5q^2}{q^2 + \xi^2}. \quad (18)$$

here, parameter $\xi = \frac{2}{[1 + (\frac{0.153}{\pi a_0 k_F})]}$.

2.4. Sham (SM) LFCF (1965)

Sham [25] changed the Hartree approximation by altering the Coulomb interaction between two electrons using the provided LFCF $f(q)$, which incorporates the Thomas-Fermi local field correction length K_{TF} .

$$f(q) = \frac{0.5q^2}{(q^2 + k_F^2 + K_{TF}^2)} \quad \text{with} \quad K_{TF}^2 = \frac{4k_F}{\pi a_0}. \quad (19)$$

2.5. Kohn-Sham (KS) LFCF (1965)

Approximation techniques for treating an

inhomogeneous system of interacting electrons are created based on the theory of Hohenberg and Kohn [27]. For systems with slowly fluctuating or high densities, these approaches are precise. They result in self-consistent equations that are equivalent to the Hartree and Hartree-Fock equations for the ground state, respectively. These equations provide additional effective potentials for the exchange and correlation parts of the chemical potential of a uniform electron gas. The same approach is used to treat electronic systems operating in magnetic fields and at limited temperatures. The function's expression is written as

$$f(q) = 1 - \frac{D}{D_0} \left(1 - \frac{5Y^2}{6}\right), \quad (20)$$

where

$$\frac{D}{D_0} = \left[1 + \frac{mr_S}{12.07} (1.47 + 0.0625r_S - \ln r_S)\right]^{-1}$$

with $Y = \frac{q}{2k_F}$.

2.6. Geldart-Vosko LFCF (GV) (1966)

The many-body perturbation theory is used to examine the Geldart-Vosko [26] LFCF of an interacting electron gas at high metallic densities. The study is based on a fundamental relationship between the system's compressibility and the local field correction constant, also known as the zero-frequency small wave-vector LFCF. A connected set of integral equations for the propagator, the self-energy, the vertex function, and the LFCF is used to explore the basic problem of selecting a self-consistent set of graphs for computing the LFCF. On the basis of these findings, a modification of Hubbard's [23, 24] form of the LFCF is proposed. It's indicated by

$$f(q) = \frac{0.5q^2}{q^2 + \xi k_F^2}, \quad (21)$$

where, parameter $\xi = \frac{2}{[1 + 0.153(\frac{K_{TF}^2}{4k_F^2})]}$ and $K_{TF}^2 = \frac{4k_F}{\pi a_0}$.

2.7. Hartree (HT) LFCF (1967)

It is a popular LFCF that is employed by the majority of researchers in all areas pertaining to metals. The Hartree [2, 3] dielectric function $\epsilon_H(q)$, discovered for the first time by Lindhard [19], is derived from the first-order perturbation and corresponds to those solid-state physics approximations, namely the Hartree model, which ignore interaction and electron correlation; for example, one can write

$$f(q) = 0. \quad (22)$$

According to equation (17), as $q \rightarrow 0$ at long wavelength limit $\epsilon(q) \rightarrow \frac{4me^2 k_F}{\pi \hbar^2 q^2}$ or $\epsilon(q) \rightarrow \infty$, and at short wavelength limit i.e. $q \rightarrow \infty$, $\epsilon(q) \rightarrow 1 + \frac{16me^2 k_F^2}{3\pi \hbar^2 q^2}$ or $\epsilon(q) \rightarrow 1$. There is a tiny logarithmic singularity at $q = 2k_F$. Additionally, this singularity may have a notable impact on qualities that depend on the dielectric function's

Fourier transform.

2.8. Harrison (HR) LFCF (1967)

At long wavelengths, Harrison [2, 3] has discovered that the form factors are unaffected by the LFCF and continue to be the same as in the Hartree computations. In this limit, the exchange potential is not insignificant, but the direct potential has adjusted itself so that the sum of the two is nearly equal to the Hartree potential. The LFCFs do not significantly change form factors or electrical characteristics at short wavelengths. It is provided by

$$f(q) = \frac{0.5q^2}{(q^2 + \frac{4}{3}k_F^2)}. \quad (23)$$

2.9. Kleinmann (KM) LFCF (1968)

Kleinmann [28, 29] obtains the dynamic dielectric constants suited to electrons and to the test charge using self-consistent field approaches. This alters with the inclusion of the screened Hartree-Fock exchange. The formula for it is

$$f(q) = \frac{1}{4} \left(\frac{q^2}{q^2 + \xi k_F^2} + \frac{q^2}{\xi k_F^2} \right), \quad (24)$$

where, parameter $\xi = \frac{2}{[1 + (\frac{0.153}{\pi a_0 k_F})]}$.

The Coulomb contributions are less than the exchange contributions for high wave vectors (in the static limit), and the electronic dielectric constant decreases to less than

one. Additionally, he develops screened exchange potentials that are linearly dependent on the charge density $\rho(r)$, which appears to be more accurate for energy-band computations than the Slater $n^{1/3}(r)$ approximation.

2.10. Ashcroft (AS) LFCF (1968)

The non-local screening by the electron gas and spin-orbit coupling have both been added to Ashcroft's [30] theory of the model pseudopotential, with the latter consequence being far more significant. The variations in the matrix elements that arise in most metals are negligible, but simulations show that the effect of spin-orbit coupling is to enhance resistivity, which is further amplified by non-local field correction. Its mathematical formulation is provided by

$$f(q) = \frac{Y^2}{2} (Y^2 + \beta_{AS})^{-1}, \quad (25)$$

with, parameter $\beta_{AS} = \frac{1}{2} (1 + 0.0152\lambda)^{-1}$, $\lambda = \frac{1}{\pi k_F}$.

2.11. Singwi-Tosi-Sjölander-Land (STSL) LFCF (1968)

Singwi et al.'s improved version of the dielectric function [31] explicitly and roughly includes the short-range correlations resulting from both the Coulomb and exchange effects. Consequently, the following method can be used to determine dielectric function in a self-consistent manner:

$$f(q) = \frac{9}{32} X^2 \left\{ \frac{2}{105} \left(\frac{24}{X^2} + 44 + X^2 \right) - \frac{2}{X} \left(\frac{8}{35X^2} - \frac{4}{15} + \frac{X^2}{6} \right) \ln \left| \frac{X+2}{X-2} \right| \right. \\ \left. + X^2 \left(\frac{X^2}{210} - \frac{2}{15} \right) \ln \left| 1 - \frac{4}{X^2} \right| \right\}. \quad (26)$$

where, $X = \frac{q}{k_F}$.

2.12. Kleinmann-Langreth (KL) LFCF (1968)

It is demonstrated that the approximation created by Kleinmann [28, 29] and Langreth [32] is erroneous overall but performs admirably in a huge static q-limit. An approximate integral equation for the local field corrections of the electron gas is solved using the variational principle. It is demonstrated that the equation for the dielectric constant can be solved using the simplest trial functions and that this solution is accurate in both the limits of small and large momentum transfer. The variational calculation's dielectric constant is used to construct an equation for the ground-state energy and is written as

$$f(q) = \frac{1}{4} \left[\frac{q^2}{(q^2 + k_F^2 + k_S^2)} + \frac{q^2}{(k_F^2 + k_S^2)} \right], \quad (27)$$

where, $k_S^2 = \frac{2k_F}{\pi a_0}$.

2.13. Shaw-Pynn (SP) LFCF (SP) (1969)

The LFCF mentioned above was developed by Shaw and Pynn [33] and is more appropriate than Hubbard's form [19]. The notation reads as follows:

$$f(q) = \frac{1}{2} \left[1 - \exp \left(-\frac{q^2}{\beta k_F^2} \right) \right] + \frac{\gamma q^2}{k_F^3} \exp \left(-\frac{\alpha q^2}{\gamma k_F^2} \right). \quad (28)$$

Where $\beta=0$ for the Kohn-Sham approximation, $\gamma=0$, but the optimal values are $\beta=2$, $\gamma = 0.0123$, $\alpha = 0.0538$. Here, the first term depicts the energy of exchange, and the second term, the energy of correlation.

2.14. Singwi-Sjölander-Tosi-Land (SSTL) LFCF (1970)

The local field correction of the coulomb potential entering the local field is the consequence of the pair correlation function being adjusted to the external field, according to Singwi and colleagues [34]. The density correlation function and the dielectric function in the metallic density range have been evaluated using self-consistent numerical methods, and they are provided as

$$f(q) = A \left[1 - \exp \left(-B \frac{q^2}{k_F^2} \right) \right], \quad (29)$$

where, $A = 1.0630 - 0.153k_F$ and $B = -0.2736 + 0.61k_F^{1/5}$.

2.15. Shaw (SH) LFCF (1970)

Shaw [35, 36] has given two standards for

determining if a LFCF $f(q)$ is appropriate: (1) the degree to which $f(q)$ (the pair correlation function) is physically valid and (2) self-consistent.

Shaw [35, 36] has proposed the above LFCF $f(q)$ based on the aforementioned criteria.

It is represented mathematically as follows:

$$f(q) = \frac{1}{2} \left[1 - \exp \left(-\frac{q^2}{\xi k_F^2} \right) \right], \quad (30)$$

here, parameter $\xi = \frac{2}{1+0.0254r_s}$.

Second expression was also proposed by Shaw [35, 36]

$$f(q) = 1 - \exp(-0.535Y^2) \quad \text{with } Y = \frac{q}{k_F} \quad (31)$$

2.16. Toigo-Woodruff (TW) LFCF (1970)

A novel method for computing the frequency and wave-vector-dependent dielectric response function has been described by Toigo-Woodruff [37]. The dielectric function is based on decoupling and using a moment-conserving technique to solve the equations of motion for the charge-density operators' Green's function. This technique yields an expression for the dielectric function in the static limit ($\omega \rightarrow 0$), which depends on $f(q)$, for which numerical values are derived and tabulated for small, moderate, and high values of q . This expression is shown in Table 2 below.

2.17. King-Cutler (KC) LFCF (KC) (1971)

By extrapolating between the short and long wavelength constraints, King and Cutler [38–40] have developed the LFCF $f(q)$. They discovered that the correlation was negligible in comparison to the exchange interaction and hence disregarded the correlation's impact. It is spelled as

$$f(q) = \frac{0.5q^2}{q^2 + 2k_F^2}. \quad (32)$$

2.18. Overhouser (OV) LFCF (1971)

The condensed theory of electron correlation in metals was presented by Overhouser [41]. Here, a model that enables computing the correlation effect of interacting electrons is devised. The plasma frequency $\omega(q)$ is determined by requiring the model to have a valid electron-gas dielectric function, as stated above, and the interaction coefficient is determined by satisfying the f-sum rule. Additionally, the q -dependence of the exchange

and correlation contributions to the one-electron energy $E(q)$ is almost the reverse. It is expressed in textual form as

$$f(q) = \frac{0.275X^2}{(1+2.5X^2+0.09375X^4)^{\frac{1}{2}}}, \quad (33)$$

where, $X = \frac{q}{k_F}$.

2.19. Mahanti-Das (MD) LFCF (1971)

By screening the bare Coulomb potential with the Thomas-Fermi model of the dielectric function and applying a specific local approximation, Mahanti and Das [42] created the LFCF $f(q)$. Although the Thomas-Fermi model left the local field correction parameter ξ as an open parameter to be calculated from experimental values, it provided the value of the parameter as a function of r_s (electron sphere radius). The importance of the exchange core polarisation effect and the exchange-enhancement impact of the susceptibility caused by electron-electron contact are clearly characterised using the Mahanti-Das dielectric function [42]. It is demonstrated that one can reach an overall agreement with experiment by taking into account these effects in addition to the relativistic corrections to the spin density for heavier alkali metals. Its expression is described as

$$f(q) = \frac{1}{2} \left\{ \frac{q^2}{k_F^2(\xi^2+1)} + \frac{q^2}{q^2+k_F^2(\xi^2+1)} \right\}, \quad (34)$$

where, $\xi = \frac{2}{1+0.026r_s}$.

2.20. Vashishta-Singwi (VS) LFCF (1972)

At metallic concentrations, electron correlations have been changed by Vashishta and Singwi [43]. The modification entails incorporating the pair correlation function into an external weak field via the equilibrium pair correlation function's density derivative. The local-field correction fulfilling the compressibility sum rule is given a new expression as a result, which is stated as

$$f(q) = A \left[1 - \exp \left(-B \frac{q^2}{k_F^2} \right) \right]. \quad (35)$$

Where, $A = 0.4666 + 0.3735k_F^{-\frac{2}{3}}$ and $B = -0.0085 + 0.3318k_F^{\frac{1}{5}}$.

Table 2.

Numerical Values of Toigo-Woodruff LFCF.

q	$f(q)$	q	$f(q)$	q	$f(q)$	q	$f(q)$	q	$f(q)$
0.1	0.00251	1.1	0.25231	2.1	0.74824	3.1	0.72873	5	0.74886
0.2	0.01001	1.2	0.3046	2.2	0.73439	3.2	0.73037	6	0.753
0.3	0.02257	1.3	0.42162	2.3	0.72756	3.3	0.73199	7	0.75547
0.4	0.04021	1.4	0.48534	2.4	0.72416	3.4	0.73355	8	0.75705
0.5	0.06296	1.5	0.55147	2.5	0.72275	3.5	0.73503	2x10 ³	0.76213
0.6	0.09081	1.6	0.61871	2.6	0.72309	3.6	0.73644		
0.7	0.12374	1.7	0.68493	2.7	0.72309	3.7	0.73776		
0.8	0.16171	1.8	0.74631	2.8	0.72418	3.8	0.739		
0.9	0.20461	1.9	0.79435	2.9	0.72558	3.9	0.74016		
1.0	0.25231	2.0	0.78999	3.0	0.7271	4.0	0.74124		

2.21. Jain-Jain (JJ) LFCF (1973)

On the basis of the ideas of Singwi et al. [31] and utilising new details on $g(0)$ from the partial-wave phase-shift analysis, Jain and Jain [44] present a phenomenological definition for the local field correction term $f(\mathbf{q})$. Such a shape almost exactly satisfies the compressibility sum rule, and the current plan results in positivity of $g(r)$ at $r \approx 0$ for every r_s from 1 to 6. Such a function's mathematical expression is as follows:

$$f(q) = A[1 - \exp(-Bq^2) - q^2 \exp(-Cq^2) + \delta(q)]. \quad (36)$$

Where, the constants are

$$\delta(q) = 0.75q^2 \exp(-10q^2),$$

$$A = 0.9395 \text{ or } A = 1 - g(0),$$

$$B = 0.6068.$$

$$C = 4.5541.$$

Here, $g(0) \approx \frac{32}{(8+3r_s)^2}$ and lies in the range of $0 < g(0) < 0.5$.

2.22. Pathak-Vashishta (PV) LFCF (1973)

An equation for the local-field correction has been provided by Pathak and Vashishta [45]. It is derived by using the third frequency moment of the spectrum function of the electron-density response function with the self-consistent method of Singwi et al. [34]. This local field is connected to the imaginary portion of the dielectric function by the fluctuation-dissipation theorem and is a functional of the structure factor $S(q)$. Its mathematical equivalent is

$$f(q) = -\frac{3}{4} \int_0^\infty dq q^2 (S(q) - 1) \left\{ \frac{5}{6} - \frac{k_F^2}{2q^2} + \frac{(k_F^2 - q^2)^2}{4k_F q^3} \ln \left| \frac{k_F + q}{k_F - q} \right| \right\}. \quad (37)$$

2.23. Kuglar (KR) LFCF (1975)

The wave-vector and frequency-dependent dielectric function of an electron gas, $\epsilon(\mathbf{k}, \omega)$, has been proposed by Kuglar [46] and is described in terms of Lindhard's function. Additionally, he has developed a sophisticated local field correction, denoted by the notation $G(\mathbf{k}, \omega)$, that encompasses all of the impacts of dynamic exchange and correlation in the system.

$$f(q) = -\frac{3}{16} \left\{ \frac{32}{63Y^2} - \frac{608}{943} - \frac{142}{315} Y^2 - \frac{2}{315} Y^4 + \frac{Y^4}{35} \left(2 - \frac{Y^2}{18} \right) \ln \left| 1 - \frac{4}{Y^2} \right| + \frac{1}{Y} \left(-\frac{32}{63Y^2} + \frac{24}{35} \right) - \frac{2}{5} Y^2 + \frac{1}{6} Y^4 \ln \left| \frac{Y+2}{Y-2} \right| \right\} \text{ with } Y = \frac{q}{k_F} \quad (38)$$

2.24. Srivastava (SR) LFCF (1977)

Srivastava [47] presented the exponential form of the LFCF, which takes into account the effects of exchange and correlation on conduction electrons, which are taken into account independently by employing distinct dielectric local field corrections in various characteristics.

$$f(q) = \frac{1}{2} \left[1 - \exp \left(-\frac{q^2}{(q^2 + \xi k_F^2)} \right) \right]. \quad (39)$$

$$\text{Where, } \xi = \frac{2}{\left[1 + \frac{3(1-2\lambda^2)}{5+6\lambda^2} \right]}, \lambda^2 = (\pi a_0 k_F)^{-1}.$$

2.25. Tripathi-Mandal (TM) LFCF (1977)

By using effective mean field theory to solve the equation of motion for the double-time retarded commutator of the classical density fluctuation operators, Tripathi and Mandal [48] were able to get the density response function. Additionally, it is discovered that the local field correction's notation is similar to that obtained by Pathak and Vashishta [43]. For small, intermediate, and large values of q , the numerical values of the LFCF are calculated and tabulated and are displayed in Table 3.

2.26. Taylor (TY) LFCF (1978)

Taylor's [49] LFCF complies with the compressibility sum rule. A straightforward and practical analytic form of the static electron gas dielectric function is constructed using this LFCF, $f(\mathbf{q})$. A straightforward formula for the static electron gas dielectric function that takes exchange and correlation effects into account produces estimated physical parameters with remarkably high levels of accuracy and has excellent formal support. The notation reads as follows:

$$f(q) = \frac{q^2 \left(1 + \frac{0.1534}{\pi k_F} \right)}{4k_F^2}. \quad (40)$$

2.27. Ichimaru-Utsumi (IU) LFCF (1981)

A formula that fits the compressibility sum rule and the short-range correlation microscopic computations has been put out by Ichimaru and Utsumi [50] for the dielectric LFCF of the degenerate electron liquid. The equation of continuity, long-time relaxation behaviour, static and dynamic local-field correlations, and frequency-moment sum rules are some of the physical criteria that are satisfied by the longitudinal dielectric response function for a strongly coupled plasma. It is symbolised by

$$f(q) = AX^4 + BX^2 + C + \left\{ \left[AX^4 + \left(B + \frac{8}{3} A \right) X^2 - C \right] \frac{(4-X^2)}{4X} \ln \left| \frac{2+X}{2-X} \right| \right\}. \quad (41)$$

where, $X = \frac{q}{k_F}$. While A, B and C are the r_s dependent

parameters given by the expressions

Table 4.

Numerical Values of Alvarelos-Flores LFCF.

q	$f(q)$	q	$f(q)$	q	$f(q)$	q	$f(q)$	q	$f(q)$
0.1	0.00376	1.1	0.44053	1.9	0.82237	2.6	0.53185	20.0	0.43451
0.2	0.01510	1.2	0.51311	1.95	0.79455	2.7	0.52170	30.0	0.43386
0.3	0.03411	1.3	0.58591	2.0	0.73579	2.8	0.51322	40.0	0.43363
0.4	0.06084	1.4	0.65647	2.05	0.67897	2.9	0.50602	50.0	0.43352
0.5	0.09524	1.5	0.72166	2.1	0.64777	3.0	0.49984		
0.6	0.13713	1.6	0.77749	2.15	0.62494	4.0	0.46662		
0.7	0.18617	1.7	0.81862	2.2	0.60693	5.0	0.45365		
0.8	0.24187	1.75	0.83148	2.3	0.57970	6.0	0.44710		
0.9	0.30351	1.8	0.83760	2.4	0.55970	8.0	0.44331		
1.0	0.37014	1.85	0.83536	2.5	0.54423	10.0	0.43813		

$$A = 0.029 \quad (0 \leq r_s \leq 15),$$

$$B = \left(\frac{9}{16}\right)\gamma_0 - \left(\frac{3}{64}\right)\{1 - g(0)\} - \left(\frac{16}{15}\right)A,$$

$$C = \left(-\frac{3}{4}\right)\gamma_0 + \left(\frac{9}{16}\right)\{1 - g(0)\} - \left(\frac{16}{15}\right)A,$$

$$\gamma_0 = 0.25 - \left(\frac{\pi}{24}\right)\left(\frac{4}{9\pi}\right)^{1/3} r_s^5 \frac{d}{dr_s} \left(r_s^{-2} \frac{d}{dr_s} \{E_c(r_s)\} \right),$$

$$g(0) = \frac{1}{8} \left(\frac{Z}{I_1(Z)} \right).$$

Here, the correlation energy is indicated by $E_c(r_s)$, and $I_1(Z)$ is the first order modified Bessel's function.

$$r_s \frac{d}{dr_s} \{E_c(r_s)\} = b_0 \left(\frac{1+b_1x}{1+b_1x+b_2x^2+b_3x^3} \right); x = \sqrt{r_s}.$$

With $b_0 = 0.0621814$, $b_1 = 9.81379$, $b_2 = 2.8224$ and $b_3 = 0.736411$.

2.28. Alvarelos-Flores (AF) LFCF (1984)

By using a new approach, Alvarelos and Flores [51] have presented a local field effect in both the static and dynamic limits. In essence, it is an expansion of Slater's treatment method for exchange and correlation effects in

an electron liquid, which falls short of several other approaches described in the literature. They acquire static $f(q)$ and contrast their pair correlation function and correlation energy results with those obtained using alternative techniques. They noticed that their method gives reasonable agreement with more complex methods for metallic densities and is suitable for high densities. The key benefit of the suggested static local field correction, $f(q)$, is that it turns out to be a universal function of q/k_F (k_F is the Fermi wavelength), which is an easy expression to employ in calculating metallic characteristics. Table 4 tabulates the numerical values of the function $f(q)$.

2.29. Bhatia-Singh (BS) LFCF (1985)

The exchange and correlation function proposed by Sham [25] has been updated by Bhatia and Singh [52] by including the second half of the Thomas-Fermi screening length term in the calculation $f(q)$. The exchange and correlation potentials must be equivalent to those for a uniform electron gas at that density at very low wavelengths. It is spelled as

$$f(q) = \frac{0.5q^2}{(q^2 + k_F^2 + \frac{1}{2}K_{TF}^2)}. \quad (42)$$

$$\text{Where, } K_{TF}^2 = \frac{4k_F}{\pi a_0}.$$

Table 3.

Numerical Values of Tripathi-Mandal LFCF

q	$f(q)$	q	$f(q)$	q	$f(q)$	q	$f(q)$	q	$f(q)$
0.1	0.00248	1.6	0.99096	2.09	0.88639	3.5	0.40636	14.0	0.33704
0.2	0.00995	1.7	1.20813	2.1	0.8625	3.6	0.40126	15.0	0.33657
0.3	0.02255	1.8	1.47685	2.2	0.70973	3.7	0.39672	16.0	0.33619
0.4	0.04048	1.9	1.79698	2.3	0.62802	3.8	0.39265	16.0	0.33587
0.5	0.06407	1.95	1.94114	2.4	0.57537	3.9	0.38898	17.0	0.33661
0.6	0.09372	1.99	1.96407	2.5	0.53814	4.0	0.38566	18.0	0.33539
0.7	0.13003	2.0	1.8992	2.6	0.51025	5.0	0.36454	19.0	0.3352
0.8	0.17371	2.01	1.75113	2.7	0.48852	6.0	0.35427	20.0	0.33456
0.9	0.22572	2.02	1.32512	2.8	0.47109	7.0	0.34842	25.0	0.33422
1.0	0.28727	2.03	1.20682	2.9	0.45681	8.0	0.34476	30.0	0.33379
1.1	0.35994	2.04	1.12736	3	0.44489	9.0	0.3423	45.0	0.33371
1.2	0.44576	2.05	1.06708	3.1	0.43479	10.0	0.34058	50.0	0.33365
1.3	0.54745	2.06	1.01855	3.2	0.42614	11.0	0.33931	90.0	0.33704
1.4	0.66862	2.07	0.97803	3.3	0.41866	12.0	0.33836		
1.5	0.8142	2.08	0.94335	3.4	0.41212	13.0	0.33762		

2.30. Nagy (NG) LFCF (1986)

Most current Nagy's static LFCF [53] is specified by,

$$f(q) = 1 - g(0, n) + \frac{cb}{c^2 + q^2} - \frac{g(0, n)}{q} \tan^{-1}\left(\frac{q}{c}\right). \quad (43)$$

Here, $g(r, n)$ is the density dependent pair-correlation function supposed to having analytical form

$$g(r, n) = 1 + (a + br)\exp(-cr).$$

From the analysis of the s -wave Schrödinger equation in the $r \rightarrow 0_+$ limit it is identified that

$$\frac{d}{dr} [\ln g(r, n)]_{r=0} = 1.$$

It gives a precise formulation for $g(r, n)$ with $r = 0$.

$$g(0, n) = \frac{1}{2} \left[\frac{1 + 2\exp(-0.6r_s)}{1 + \exp(-0.6r_s) + 2r_s} \right],$$

with,

$$a = g(0, n) - 1,$$

$$b = g(0, n)(1 + c) - c,$$

$$c = \left(\frac{R}{2}\right)^{0.5} \left[1 + \left(\frac{-2A}{\{2R\}^{1.5}} - 1 \right)^{0.5} \right],$$

$$R = \left\{ \left(\frac{A}{4}\right)^2 + \left[\left(\frac{A}{4}\right)^4 - \left(\frac{B}{3}\right)^3 \right]^{0.5} \right\}^{1/3} + \left\{ \left(\frac{A}{4}\right)^2 - \left[\left(\frac{A}{4}\right)^4 - \left(\frac{B}{3}\right)^3 \right]^{0.5} \right\}^{1/3},$$

$$A = -\frac{24}{r_s^3} [1 - g(0, n)],$$

$$B = \frac{18}{r_s^3} g(0, n).$$

2.31. Farid-Heine-Engle-Robertson (FHER) LFCF (1993)

An improved and extremely precise formulation for $f(q, \omega \rightarrow 0)$ is given by Farid et al. in [54]. According to the precise frequency moments of the density-density correlation function, this expression satisfies the exact asymptotic results for the short- and long-wavelength limitations. Although this $f(q, 0)$ and the $f(q)$ of the IU-function [50] share some similarities, they are fundamentally different. Farid *et al.* [54] also present a model for this function, along with some very accurate interpolation expressions for a number of the coefficients both in this and $f(q, 0)$. This is because $f(q, 0)$ involves momentum moments of the momentum distribution function of the interacting electron gas. Consequently, it is symbolised by

$$f(q) = (AX^4 + BX^2 + C) + \left\{ [(AX^4 + DX^2 - C) \frac{(4-X^2)}{4X}] \ln \left[\frac{2+X}{2-X} \right] \right\}, \quad (44)$$

where, $X = \frac{q}{k_F}$. While A, B, C and D are the r_s dependent parameters specified by the following expressions

$$A = \left(\frac{63}{64}\right) a_0 - \left(\frac{15}{4096}\right) \{b_0^A - 2(b_0^B + b_0^C)\} - 16b_{-2},$$

$$B = \left(\frac{9}{16}\right) \gamma_0 + \left(\frac{7}{16}\right) b_{-2} - \left(\frac{3}{64}\right) b_0 - \left(\frac{16}{15}\right) A,$$

$$C = \left(-\frac{3}{4}\right) \gamma_0 + \left(\frac{3}{4}\right) b_{-2} - \left(\frac{9}{16}\right) b_0 - \left(\frac{16}{5}\right) A,$$

$$D = \left(\frac{9}{16}\right) \gamma_0 - \left(\frac{9}{16}\right) b_{-2} - \left(\frac{3}{64}\right) b_0 + \left(\frac{8}{5}\right) A,$$

$$\gamma_0 = 0.25 - \left(\frac{\pi}{24}\right) \left(\frac{4}{9\pi}\right)^{1/3} r_s^5 \frac{d}{dr_s} \left(r_s^{-2} \frac{d}{dr_s} \{E_C(r_s)\} \right),$$

$$b_0 = b_0^A + b_0^B + b_0^C,$$

$$b_0^A = \frac{2}{3} [1 - g(0)],$$

$$b_0^B = \frac{48E_F^2}{35\omega_p^2} \delta_4,$$

$$b_0^C = -\frac{16E_F^2}{25\omega_p^2} [2\delta_2 + \delta_2^2],$$

$$b_{-2} = \frac{4E_F^2}{5\omega_p^2} \delta_2,$$

$$\frac{E_F^2}{\omega_p^2} = \frac{1}{12\lambda^4 r_s},$$

$$\lambda \rightarrow \alpha = \left(\frac{4}{9\pi}\right)^{1/3} = 0.52106,$$

$$a_0 = 0.029 \quad (0 \leq r_s \leq 15),$$

$$\delta_2 = \frac{\sum_{j=1}^6 \xi_j x^j}{x^4 + \sum_{j=0}^3 \rho_j x^j} \quad \text{with } x = r_s^{1/2},$$

$$\xi_1 = -2.2963827 \times 10^{-3},$$

$$\xi_2 = 5.6991691 \times 10^{-2},$$

$$\xi_3 = -0.8533622,$$

$$\xi_4 = -8.7736539,$$

$$\xi_5 = 0.7881997,$$

$$\xi_6 = -1.2707788 \times 10^{-2},$$

$$\rho_0 = -79.9684540,$$

$$\rho_1 = -140.5268938,$$

$$\rho_2 = -35.2575566,$$

$$\rho_3 = -10.6331769,$$

$$\frac{\delta_4}{\delta_2} = \frac{\sum_{j=0}^8 \varphi_j x^j}{x^6 + \sum_{j=0}^5 \varrho_j x^j},$$

$$\varphi_0 = 23.0118890,$$

$$\varphi_1 = -64.8378723,$$

$$\varphi_2 = 63.5105927,$$

$$\varphi_3 = -13.9457829,$$

$$\varphi_4 = -12.6252782,$$

$$\varphi_5 = 13.8524989,$$

$$\varphi_6 = -5.2740937,$$

$$\varphi_7 = 1.0156885,$$

$$\varphi_8 = -1.1039532 \times 10^{-2},$$

$$\varrho_0 = 9.5753544,$$

$$\varrho_1 = -32.9770151,$$

$$\varrho_2 = 48.2528870,$$

$$\varrho_3 = -38.7189788,$$

$$\varrho_4 = 20.5595956,$$

$$\varrho_5 = -6.3066750,$$

$$Z = 4 \left(\frac{\alpha r_s}{\pi} \right)^{1/2} = 4\lambda^{1/2},$$

$$\lambda = \frac{\alpha r_s}{\pi},$$

$$g(0) = \frac{1}{8} \left(\frac{Z}{I_1(Z)} \right)^2.$$

Here, $I_1(Z)$ is the Bessel's function of first kind and first order.

3.32. Gold-Calmels (GC) LFCF (1993)

With the aid of the sum-rule variant of Singwi et al.'s [34] self-consistent technique, Gold and Calmels [55] suggested the local field correction for the two-

dimensional and three-dimensional electron gas. They reported their findings within the $0.001 < r_s < 100$ tolerance. They compute the LFCF using an analytical expression for the static structure factor that represents a generalised Feynman-Bijl spectrum. Such a function's mathematical expression is provided by

$$f(q) = r_s^{\frac{3}{4}} \left(\frac{0.846Y^2}{2.188C_{13}(r_s) + Y^2 C_{23}(r_s)} \right). \quad (45)$$

Where, $C_{13}(r_s) = 1.0956r_s^{\frac{1}{4}}$ and $C_{23}(r_s) = 1.6911r_s^{\frac{3}{4}}$.

In his extended papers, Gold [56, 57] has modified and discussed this function for two-dimensional and three-dimensional electron gases.

2.33. Ortiz-Ballone (OB) LFCF (1994)

Density functional theory has been proposed by the authors [58] as a means of describing exchange and correlation in inhomogeneous systems. The density range

$$f_{\mu,\nu} \left(\frac{q}{k_F} \right) = 1 + \left[A_{\mu,\nu} + B_{\mu,\nu} \left(\frac{q}{k_F} \right) + C_{\mu,\nu} \left(\frac{q}{k_F} \right)^2 + D_{\mu,\nu} \left(\frac{q}{k_F} \right)^3 + E_{\mu,\nu} \left(\frac{q}{k_F} \right)^4 + F_{\mu,\nu} \left(\frac{q}{k_F} \right)^5 \right] \exp \left(-\eta_{\mu,\nu} \left(\frac{q}{k_F} \right)^2 \right). \quad (46)$$

Where the spin is indicated by the symbols μ and ν . The coefficients A, B, C, D, E, F and η , on the other hand, rely on r_s and the corresponding values of the μ and ν spins. These parameters are calculated using the relationships listed below.

$$\begin{aligned} A_{++} &= -1, \\ A_{+-} &= -0.0005r_s^3 + 0.0201r_s^2 - 0.24172r_s - 0.1039, \\ B_{++} &= 0, \\ B_{+-} &= 0.011r_s^3 - 0.1879r_s^2 + 0.7794r_s + 0.0714, \\ C_{++} &= -0.0019r_s^3 + 0.0396r_s^2 - 0.2872r_s + 1.3061, \\ C_{+-} &= -0.0162r_s^3 + 0.2564r_s^2 - 0.8082r_s - 0.0419, \\ D_{++} &= 0.0036r_s^3 - 0.0738r_s^2 + 0.4972r_s - 1.3074, \\ D_{+-} &= 0.0102r_s^3 + 0.1315r_s^2 - 0.4486r_s + 0.6049, \\ E_{++} &= -0.0019r_s^3 + 0.0382r_s^2 - 0.2438r_s + 0.5104, \\ E_{+-} &= -0.018r_s^3 + 0.0278r_s^2 - 0.0683r_s - 0.0171, \\ F_{++} &= 0.0003r_s^3 - 0.0062r_s^2 + 0.0373r_s - 0.0698, \\ F_{+-} &= 0.0001r_s^3 - 0.0021r_s^2 + 0.0047r_s + 0.0018, \\ \eta_{++} &= -0.0009r_s^3 + 0.0215r_s^2 - 0.1552r_s + 0.5155, \\ \eta_{+-} &= -0.0059r_s^3 + 0.0896r_s^2 - 0.31r_s + 0.3491. \end{aligned}$$

The best-fit parameters for the VMC radial distribution functions are used to fit these parameters. The spin-polarised systems are denoted by the ‘++’ sign, while the spin-unpolarized systems are denoted by the ‘+’ sign. The following method is used to determine the $f(q)$.

$$f(q) = \frac{1}{2} [f_{++}(q) + f_{+-}(q)]. \quad (47)$$

2.34. Moroni-Ceperley-Senatore (MCS) LFCF (1995)

The density-density static response of the electron gas at absolute zero and in the metallic domain has been assessed by the authors [59] using a diffusion Monte Carlo method. With a crossover about $2k_F$, the computed local

$0.8 \leq r_s \leq 10$, which is the most relevant for density functional computations, has been fitted using the analytical form developed by the authors, which is closely linked to Ichimaru and Utsumi [50]. They use variational Monte Carlo (VMC) and fixed-node diffusion Monte Carlo methods to analyse the three-dimensional uniform electron gas in the Fermi liquid domain. Here, the VMC approach is used to analyse the spin dependency energy. In a rhombic dodecahedron cell (fcc Wigner-Seitz cell) with periodic boundary conditions (PBCs), they have considered $N = N_\downarrow + N_\uparrow$ electrons. The number of spin-up (-down) electrons in the cell is $N_{\uparrow(\downarrow)}$. Despite the modest drawback of having to impose the PBCs during the simulation, this cell's almost spherical shape is preferable because it more closely resembles the isotropic environment of the fluid phase than the ordinary cubic cell. By using sum rules and approximative relations, the authors have fitted $g(r)$ to a straightforward analytical expression that looks like this:

field factor $f(q)$ smoothly interpolates between the asymptotic small and big q behaviour. The local density approximation to density functional theory for $q \leq 2k_F$ accurately reproduces its almost asymptotic behaviour. Such a function's basic formula is

$$f(q) = \left(\left[(A - C)^{-n} + \left(\frac{q^2}{Bk_F^2} \right)^n \right]^{-1/n} + C \right) \left(\frac{q}{k_F} \right)^2. \quad (48)$$

With $n \cong 8$ for $r_s = 2$ and $r_s = 5$ and $n \cong 4$ for $r_s = 10$. The constants used in current formulation is calculated by

$$A(r_s) = \frac{1}{4} + \frac{(-d\mu_C/dn_0)}{(4\pi e^2/k_F^2)} = -0.033773726 \text{ with } \mu_C \text{ is}$$

the correlation contribution to the chemical potential of the uniform electron gas. It is consuming value near by $-\frac{1}{3\pi^2}$.

$$B(r_s) = \frac{(1+a_1x+a_2x^3)}{(3+b_1x+b_2x^3)}. \quad (49)$$

Here, $x = \sqrt{r_s}$ and $a_1 = 2.15$, $a_2 = 0.435$, $b_1 = 1.57$ and $b_2 = 0.409$.

$C(r_s) = \frac{\pi}{2e^2k_F} \left[\frac{-d(r_s\epsilon_C)}{dr_s} \right] = 0.071033081$ with ϵ_C the correlation energy per particle.

2.35. Bretonnet-Boulahbak (BB) LFCF (1996)

Bretonnet and Boulahbak [60] have proposed a semi-analytical form of the LFCF $f(q)$ for the uniform electron gas in the density range $0 < r_s < 10$, which faithfully reproduces the most recent diffusion Monte Carlo results of Ortiz and Ballone [58]. This is in accordance with the

scheme of Singwi *et al.* [34]. The formula for $f(q)$ is as follows:

$$f(q) = 1 - g(0) - e^{-z} \sum_{\mu=0}^6 C_{\mu} {}_1F_1\left(1 - \frac{\mu}{2}, \frac{3}{2}; z\right). \quad (50)$$

Where,

$$\begin{aligned} z &= \frac{1}{4} \left(\frac{9\pi}{4}\right)^{2/3} \frac{\eta^2}{a}, \\ \gamma &= -0.103756, \\ \beta_1 &= 0.56371, \\ \beta_2 &= 0.27358, \\ A_p &= 0.031091, \\ B_p &= -0.046644, \\ C_p &= -0.00419, \\ D_p &= -0.00983, \\ C_0 &= \frac{B}{2} \sqrt{\pi/a}, \\ C_1 &= \frac{C-aA}{a}, \\ C_2 &= \frac{3D-2aB}{4} \sqrt{\pi/a^3}, \\ C_3 &= \frac{2E-aC}{a^2}, \\ C_4 &= \frac{3}{8} (5F - 2aD) \sqrt{\pi/a^5}, \\ C_5 &= \frac{2E}{a^2}, \\ C_6 &= \frac{15}{8} F \sqrt{\pi/a^5}, \\ \gamma_0 &= \frac{1}{4} - \left(\frac{\pi\alpha}{12}\right) \left(\frac{4}{9\pi}\right)^{1/3} r_s^5 \frac{d}{dr_s} \left(r_s^{-2} \frac{d}{dr_s} \{E_C(r_s)\}\right), \\ g(0) &= \frac{1}{8} \left(\frac{Z}{I_1(Z)}\right)^2, \\ \alpha &= \left(\frac{4}{9\pi}\right)^{1/3}. \end{aligned}$$

Here, $I_1(Z)$ is the first order modified Bessel's function and ${}_1F_1\left(1 - \frac{\mu}{2}, \frac{3}{2}; z\right)$ the degenerate hypergeometric function, respectively. While, $E_C(r_s)$ is the correlation energy and signified by

$$E_C(r_s) = \begin{cases} \frac{\gamma}{1+\beta_1\sqrt{r_s}+\beta_2r_s} & \text{if } r_s > 1 \\ A_p \ln r_s + B_p + C_p r_s \ln r_s + D_p r_s & \text{if } r_s < 1 \end{cases}. \quad (51)$$

Where, the coefficients A, B, C, D, E, F and a are depended on r_s and on the related values of the spins. They are calculated through subsequent expressions.

$$\begin{aligned} A_{++} &= -1, \\ A_{+-} &= -0.021r_s^3 + 0.0469r_s^2 - 0.3403r_s - 0.1597, \\ B_{++} &= 0, \\ B_{+-} &= 0.0065r_s^3 - 0.1001r_s^2 + 0.3194r_s + 0.3189, \\ C_{++} &= -0.0031r_s^3 + 0.0539r_s^2 - 0.3084r_s + 0.1281, \\ C_{+-} &= -0.0061r_s^3 + 0.0432r_s^2 + 0.2077r_s - 0.4261, \\ D_{++} &= -0.001r_s^3 + 0.007r_s^2 + 0.0016r_s + 0.1896, \\ D_{+-} &= 0.0002r_s^3 + 0.0233r_s^2 - 0.3383r_s + 0.3161, \\ E_{++} &= 0.003r_s^3 - 0.0392r_s^2 + 0.1837r_s - 0.0577, \\ E_{+-} &= -0.0002r_s^3 - 0.018r_s^2 + 0.1291r_s - 0.1052, \\ F_{++} &= -0.0008r_s^3 + 0.0107r_s^2 - 0.0515r_s - 0.0045, \\ F_{+-} &= -0.00008r_s^3 + 0.0028r_s^2 - 0.0153r_s + 0.0122, \\ a_{++} &= 0.0007r_s^3 - 0.0094r_s^2 + 0.0444r_s + 0.4823, \\ a_{+-} &= -0.0002r_s^3 + 0.0006r_s^2 + 0.0397r_s + 0.2161. \end{aligned}$$

The best-fit parameters for the VMC radial

distribution functions are used to fit these parameters. The spin-polarised systems are denoted by the '+' sign, while the spin-unpolarized systems are denoted by the '-' sign. The following method is used to determine the $f(q)$.

$$f(q) = \frac{1}{2} [f_{++}(q) + f_{+-}(q)]. \quad (52)$$

2.36. Sarkar-Sen-Haldar-Roy (SSHR) LFCF (1998)

The LFCF proposed by Sarkar *et al.* [61] is developed in the same way as the IU-function [50], obeying the compressibility sum rule. But like Srivastava's LFCF [47], it has an exponential form.

$$f(q) = A\{1 - [1 + BX^4] \exp(-CX^2)\}. \quad (53)$$

where, $X = \frac{q}{k_F}$. While A, B and C are the r_s dependent parameters assumed by the expressions,

$$g(0) = \frac{1}{8} \left(\frac{Z}{I_1(Z)}\right)^2.$$

With,

$$\begin{aligned} a &= 0.0301412, \\ b &= -0.0084724176, \\ c &= 0.0016291083, \\ d &= -0.2386599, \\ e &= 0.027960609. \end{aligned}$$

Constants A and C are determined from the limiting values of $f(q)$.

$$A = \lim_{q \rightarrow 0} f(q) = 1 - g(0),$$

and C is found using the relation

$$\lim_{q \rightarrow 0} f(q) = AC \left(\frac{q}{k_F}\right),$$

$$\therefore \gamma_0 = AC,$$

$$\therefore C = \frac{\gamma_0}{1-g(0)} \text{ with,}$$

$$\gamma_0 = 0.25 - \left(\frac{\pi}{24}\right) \left(\frac{4}{9\pi}\right)^{1/3} r_s^5 \frac{d}{dr_s} \left(r_s^{-2} \frac{d}{dr_s} \{E_C(r_s)\}\right).$$

Here, $I_1(Z)$ is the first kind and first order Bessel's function.

2.37. Hellal-Gasser-Issolah (HGI) LFCF (2003)

The authors [62] have created semi-analytic expressions of the static local-field correction (LFC) function for the dielectric screening function describing exchange and correlation effects in a homogeneous electron gas using the fixed node diffusion Monte Carlo (DMC) results obtained by Ortiz and Ballone [58]. The prior well-known functions proposed by Vashista and Singwi [43] and Ichimaru and Utsumi [50] were corrected by these expressions, which also addressed several other issues. Additionally, it complies with the 'compressibility sum rule' for an interacting fermion system's physical constraints. Such a model's mathematical formulation is

expressed as

$$f(q) = [1 - Z(\eta)] \sum_n D_n(r_s) Z(\eta)^n, \quad (54)$$

with,

$$Z(\eta) = \frac{1}{2} + \frac{4-\eta^2}{8\eta} \ln \left| \frac{2+\eta}{2-\eta} \right|, \text{ where, } \eta = \frac{q}{k_F}.$$

Such an analytical expression faithfully reproduces the numerical values for metallic densities and the entire q-range fluctuation. Density-dependent coefficients are shown here as $D_n(r_s)$. The condition $G(0) = 0$ is given on the right-hand side of the aforementioned equation. at the short wave limit,

$$\lim_{\eta \rightarrow \infty} f(\eta) = D_0 - D_{-1} + \frac{3D_{-1}}{4} \eta^2 + O\left(\frac{1}{\eta^2}\right). \quad (55)$$

If the local field correction is restricted in this case, the term with coefficient D_{-1} does not show up. As a result, a fitting process is typically used to acquire the

physical information contained in the coefficients $D_n(r_s)$. The three criteria listed below are used to fit such coefficients based on the characteristics of the Lindhard function [16].

$$D_{-1}(r_s) = 0,$$

$D_n(r_s) = \lim_{\eta \rightarrow \infty} G(q)$ (if the local field correction is inadequate)

$$\sum_n D_n(r_s) = 0,$$

and

$$\gamma = -\frac{1}{12} \sum_n n [D_n(r_s) - D_{n-1}(r_s)].$$

The fitting parameter $D_n(r_s)$ is determined by the authors for various r_s values presented for the OB-VS case and the OB-IU case.

For $1 \leq r_s \leq 3$

$$D_0(r_s) = 0.59334 + 0.10489r_s - 0.00491r_s^2 + 1.7400x10^{-4}r_s^3 - 8.95027x10^{-5}r_s^4,$$

$$D_1(r_s) = -0.32951 - 0.21230r_s + 0.00965r_s^2 + 130.44007x10^{-4}r_s^3 - 145.95027x10^{-5}r_s^4,$$

$$D_2(r_s) = 5.30593 + 1.31679r_s + 0.21208r_s^2 - 1684.25993x10^{-4}r_s^3 + 1560.04973x10^{-5}r_s^4,$$

$$D_3(r_s) = -15.07056 - 3.2607089r_s - 1.37773r_s^2 + 7830.9401x10^{-4}r_s^3 - 7529.95027x10^{-5}r_s^4,$$

$$D_4(r_s) = 22.02554 + 4.48947r_s + 2.61918r_s^2 - 13727.75993x10^{-4}r_s^3 + 13490.04973x10^{-5}r_s^4,$$

$$D_5(r_s) = -9.81589 - 2.40712r_s - 1.47717r_s^2 + 7868.54007x10^{-4}r_s^3 - 8063.95027x10^{-5}r_s^4.$$

For $3 \leq r_s \leq 5$

$$D_0(r_s) = 0.64995 + 0.09479r_s - 0.01191r_s^2 + 16.30000x10^{-4}r_s^3 - 0.12052x10^{-5}r_s^4,$$

$$D_1(r_s) = 3.29115 - 2.55653r_s + 0.43412r_s^2 + 6.94645x10^{-4}r_s^3 - 2.39052x10^{-5}r_s^4,$$

$$D_2(r_s) = -24.77987 + 21.24814r_s - 3.78282r_s^2 + 747.24645x10^{-4}r_s^3 + 11.70948x10^{-5}r_s^4,$$

$$D_3(r_s) = 116.18740 - 88.97349r_s + 15.72466r_s^2 - 3562.35355x10^{-4}r_s^3 - 41.95052x10^{-5}r_s^4,$$

$$D_4(r_s) = -211.65547 + 156.15424r_s - 27.61189r_s^2 + 7240.3465x10^{-4}r_s^3 + 63.13948x10^{-5}r_s^4,$$

$$D_5(r_s) = 136.96029 - 97.22916r_s + 17.26022r_s^2 - 4878.08355x10^{-4}r_s^3 - 38.08052x10^{-5}r_s^4.$$

Similarly, for OB-IU case the following fitting equations are used. For $1 \leq r_s \leq 5$

$$D_0(r_s) = 0.57353 + 0.15100r_s - 0.01472r_s^2 - 0.510009x10^{-4}r_s^3 + 1.17066x10^{-5}r_s^4,$$

$$D_1(r_s) = -0.28578 - 0.78691r_s - 0.12015r_s^2 + 71.52999x10^{-4}r_s^3 - 69.12934x10^{-5}r_s^4,$$

$$D_2(r_s) = 12.50176 + 3.83749r_s + 1.11258r_s^2 - 554.48001x10^{-4}r_s^3 + 531.37066x10^{-5}r_s^4,$$

$$D_3(r_s) = -61.25749 - 11.63239r_s - 4.21829r_s^2 + 2035.03999x10^{-4}r_s^3 - 1952.62934x10^{-5}r_s^4,$$

$$D_4(r_s) = 167.31876 + 20.85378r_s + 7.66303r_s^2 - 3744.64001x10^{-4}r_s^3 + 3608.57066x10^{-5}r_s^4,$$

$$D_5(r_s) = -186.10675 - 18.83851r_s - 6.79233r_s^2 + 3367.4799x10^{-4}r_s^3 - 3256.52934x10^{-5}r_s^4,$$

$$D_6(r_S) = 70.45671 + 6.56586r_S + 2.34771r_S^2 - 1173.68001 \times 10^{-4}r_S^3 + 1137.67066 \times 10^{-5}r_S^4.$$

2.38. Sarkar-Haldar-Roy-Sen (SHRS) LFCF (2004)

The authors [57] have proposed the following form of the LFCF in the case of the ‘ferro’ (spin parallel) state based on the precise density interpolation formulae and the quantum Monte Carlo data of Ceperley and Alder [74, 75] for the correlation energy of electron gas in both the ‘para’ and ‘ferro’ states.

$$f(q) = A_F \{1 - [1 + B_F X^4] \exp(-C_F X^2)\}. \quad (56)$$

here, $X = \frac{q}{k_F}$. Whereas A, B and C are the r_S dependent parameters. Factors A and C are obtained from the limiting values of $f(q)$.

$$A = 1,$$

And utilising the relation, C is discovered.

$$C = \gamma_0(r_S) \text{ with,}$$

$$\gamma_0(r_S) = 0.25 - \left(\frac{\pi}{24}\right) \left(\frac{4}{9\pi}\right)^{1/3} r_S^5 \frac{d}{dr_S} \left(r_S^{-2} \frac{d}{dr_S} \{E_C(r_S)\}\right).$$

$$B = a + br_S + cr_S^2 + dr_S \ln r_S + er_S^2 \ln r_S.$$

With,

$$\begin{aligned} a &= 0.27120697, \\ b &= 0.023367297, \\ c &= 0.0004025675, \\ d &= -0.0067372145, \\ e &= -6.3667962 \times 10^{-5}. \end{aligned}$$

And

$$\begin{aligned} E_C(r_S) &= \frac{1+a_1r_S+a_2r_S^2+a_3r_S^3+a_4r_S^4}{b_0+b_1r_S+b_2r_S^2+b_3r_S^3+b_4r_S^4+b_5r_S^5}, \\ a_1 &= 0.24979381, \\ a_2 &= 0.042193510, \\ a_3 &= 0.00273095, \\ a_4 &= 0.00003620, \\ b_0 &= 0.01258694, \\ b_1 &= 0.007263687, \\ b_2 &= 0.00165158, \\ b_3 &= 0.00017853, \\ b_4 &= 7.9656334 \times 10^{-6}, \\ b_5 &= 6.47520896 \times 10^{-8}. \end{aligned}$$

Where, $\alpha = \left(\frac{4}{9\pi}\right)^{1/3}$ and $E_C(r_S)$ is the electron correlation energy for the ‘ferro’ state.

$$g(0) = \frac{1}{8} \left(\frac{z}{I_1(z)}\right)^2.$$

Here, $I_1(Z)$ is the first kind and first order Bessel’s function with $z = 4(\alpha r_S/\pi)^{1/2}$.

2.39. Dornheim-Vorberger-Groth-Hoffmann-Moldabekov-Bonitz (DVGHMB) LFCF (2019-2020)

For the static LFCF of the uniform electron gas, Dornheim and colleagues [64–66] have extensively presented new path integral Monte Carlo (PIMC) results. These results are used to train a fully connected deep neural network with respect to continuous wave-vectors, densities, and temperatures covering the entire warm dense matter regime. This LFCF’s expression is provided by

$$f(q) = A(q)[1 - g(0)] + G_{nn}(q)[1 - A(q)] \quad (57)$$

Where, $G_{nn}(q)$ corresponds to the neutral-net and $A(q)$ is a straightforward activation function [64–67]. Additionally, they have created an analytical parameterization of $g(0)$ using the Spink *et al.* [76] ground state results. They have published this formula using the effective static approximation (ESA), which permits extremely accurate computations of electronic parameters like the interaction energy v , the dynamic structure factor $S(\mathbf{q}, \omega)$ and the static structure factor $S(\mathbf{q})$.

2.40. Kukkonen-Chen (KC) LFCF (2021)

Kukkonen and Chen [67] used variational diagrammatic quantum Monte Carlo (VDQMC) simulations to present their full spin-dependent LFCFs. In the uniform three-dimensional electron gas, they have discovered a straightforward quadratic formula that quantitatively produces all of the response functions of the electron gas at metallic concentrations of effective electron-electron contact. This LFCF’s notation is represented by

$$f_+(q) = \left(1 - \frac{\kappa_0}{\kappa}\right) \left(\frac{q}{q_{TF}}\right)^2, \text{ with } q_{TF}^2 = \frac{4k_F}{\pi a_0}, \quad (58)$$

$$f_-(q) = \left(1 - \frac{\chi_0}{\chi}\right) \left(\frac{q}{q_{TF}}\right)^2, \text{ with } q_{TF}^2 = \frac{4k_F}{\pi a_0}, \quad (59)$$

here,

$$\frac{\kappa_0}{\kappa} = 1.0025 - 0.1721r_S - 0.0036r_S^2,$$

$$\frac{\chi_0}{\chi} = 0.9825 - 0.1232r_S + 0.0091r_S^2.$$

Both of these local field functions are smooth functions of the wave vector, and the results reveal a little rise over the quadratic between 1.5 and $2k_F$, according to the authors [67].

The LFCFs are important for improving calculations of the electronic structures of the materials, particularly in many-body perturbation theory and time-dependent density functional theory (TDDFT). The study of LFCFs is seeing new trends and development directions as

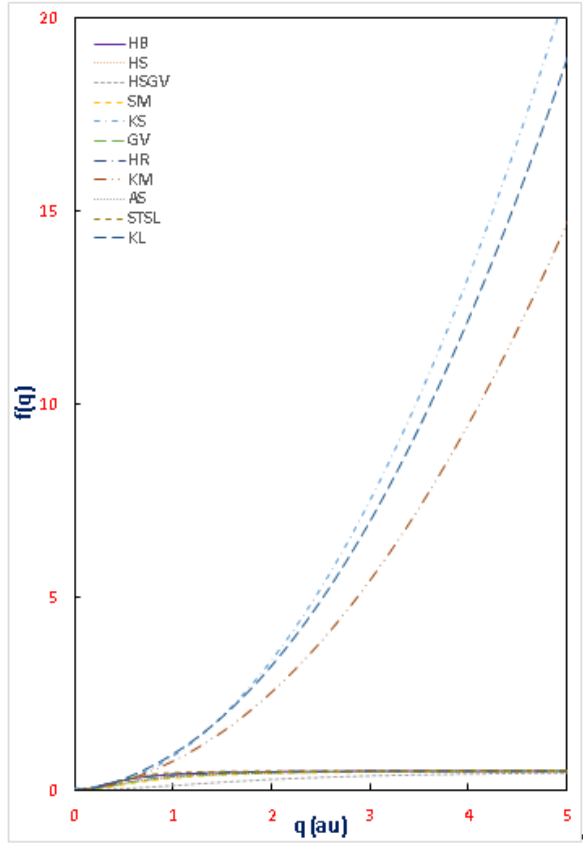


Fig. 1. Comparisons of Various LFCFs-1.

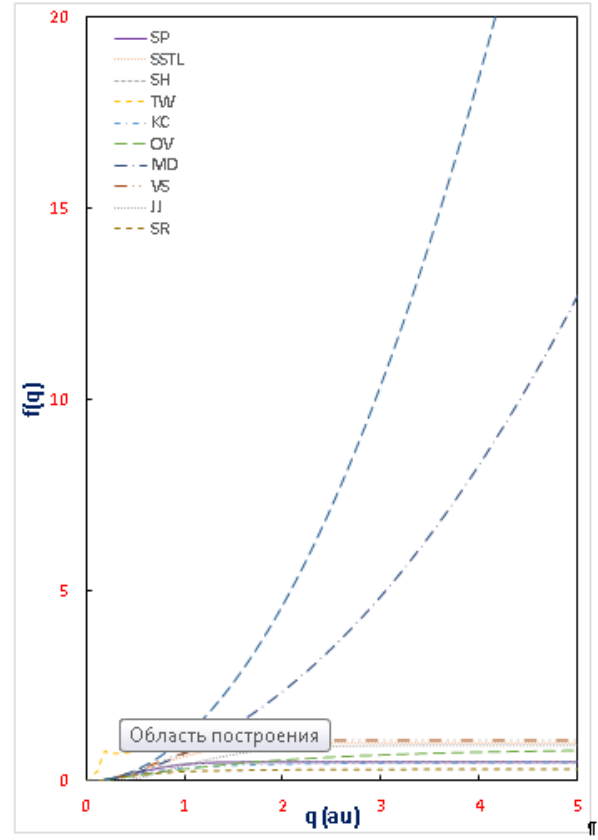


Fig. 2. Comparisons of Various LFCFs-2.

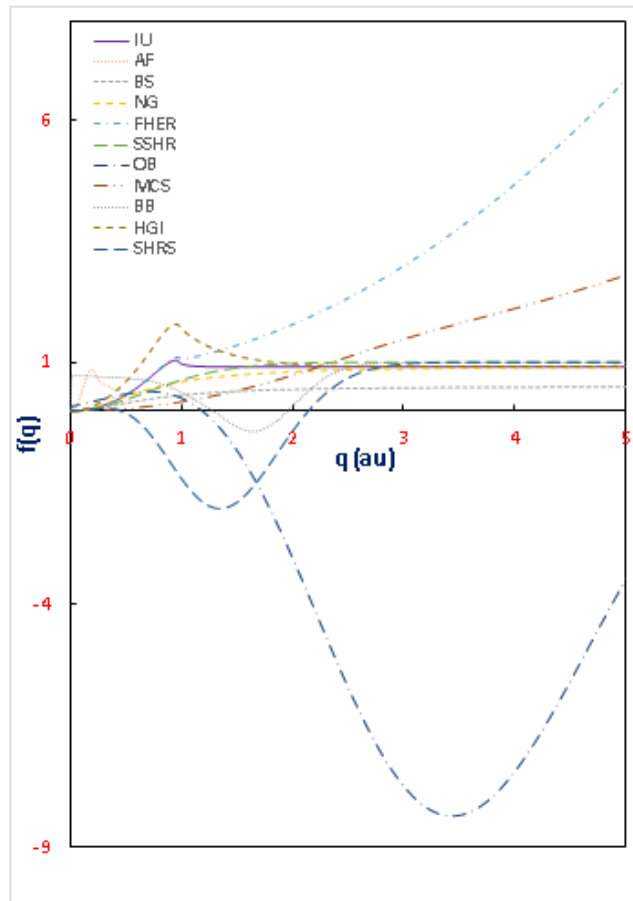


Fig. 3. Comparisons of Various LFCFs-3.

computational materials science progresses. Beyond the Random Phase Approximation (RPA) method, machine learning (ML) can improve the LFCFs by comprehending intricate relationships. Such models that rely on the momentum and the frequency are being created to account for both spatial and temporal dispersion. To improve accuracy without incurring the significant computational costs, material-specific and context-dependent LFCFs are being investigated. One of the main challenges is incorporating precise LFCF treatments into automated DFT and TDDFT pipelines. It is essential to strike a balance between computational efficiency and physical accuracy [77-81].

In order to modify the accuracy of calculated optical spectra, dielectric properties and electron excitations, modern ab initio codes have implemented particular LFCFs with linearly differentiated fields. In order to capture local field effects using the full microscopic dielectric function, LFCFs are incorporated into the GW and Bethe-Salpeter Equation (BSE) modules of VASP, CASTEP, Quantum ESPRESSO, and WIEN2k computational codes. Numerical and theoretical models are both utilized by the Quantum ESPRESSO code to explicitly handle the LFCFs in the dielectric matrix and GW or BSE routines. By taking into consideration the off-diagonal components of the microscopic dielectric matrix in the reciprocal space, the WIEN2k code uses LFCFs into account when computing its optical properties and linear response of the materials. Choosing the right computational tool for precise ab initio predictions requires knowing which models are supported [82-87].

Conclusions

Following some general remarks are to be noted from the present study,

The present study is totally focused on the various

forms of the LFCFs available in the literature.

The graphical nature of all the LFCFs are displayed in Figures 3.1-3.3.

Though it is necessary to examine the stability of various LFCFs against the model pseudopotential before its applications for the comprehensive study of metallic properties.

The long wavelength limit (i.e. $q \rightarrow 0$) and short wavelength limit (i.e. $q \rightarrow \infty$) are tabulated in Table 1 for further comparison.

It is seen that the LFCFs due to KS, KM, KL, MD, T, FHERR and KC give the infinite values at shorter wavelength limit.

While, the SSTL, VS, JJ, IU, NG, SSHR, OB, MCS, BB, HGI and SHRS functions give the constant value depends on r_s at $q \rightarrow \infty$ while TW, OV, SR, AF, KR and TM give 0.762, 0.898, 0.316, 13/30, 0.3333 and 0.33365, respectively.

The remaining LFCFs are having value of 0.5 at $q \rightarrow \infty$ limit.

It is also observed from the Figures 1-3 that, the LFCFs due to TW, IU and FR gives a peak below $q < 2k_F$ which is a notable form in construct with the other functions.

Finally, we conclude from the present article that, it represents a unique documentary data of the LFCFs, which are reported in chronological order. Such type of written information is not available in the literature so far. Hence, the present paper will attend a proper data set on LFCFs for scientific community. Also, the role of LFCF in the condensed matter physics are studied from the present article.

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Короткий огляд та роль корекцій функцій локального поля у фізиці конденсованих систем

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У огляді висвітлюється важливість спектру коригувальних функцій локального поля (LFCFs) у фізиці конденсованих станів, які зустрічаються у різних літературних оглядах. Загалом, у літературі виявлено 40 різних форм LFCFs. Наведено основні параметри кожної функції LFCFs разом із коротким описом. Головна мета – виділити різні корекції локального поля, опубліковані в літературі починаючи з 1957 року та надати науковій спільноті повну довідкову інформацію.

Ключові слова: однорідний електронний газ; корекції функції локального поля (LFCFs); дифузійний метод Монте-Карло (DMC); теорія діелектричного екранування.