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New general scheme for improving accuracy in implementing self-consistent iterative calculations: illustration in the STLS theory

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Abstract

By imposing the Pauli's exclusion principle and other known exact relations at each stage in the self-consistent iteration scheme due to Singwi, Tosi, Land, and Sjölander (STLS), we propose an algorithm to obtain accurate results for the static structure factor and other related physical quantities in electron liquids. Its actual implementation is illustrated in the spin fully polarized homogeneous electron liquid. We suggest the usefulness of our idea in improving accuracy in other iteration schemes as well.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

A comprehensive understanding of the many-body effect in the homogeneous electron gas is indispensable not only for clarifying the physical properties in simple metals but also for constructing a useful exchange–correlation potential in the Kohn–Sham density functional theory [1], but it is hampered by the complication that different series of terms in the perturbation expansion dominate in three different ranges: for describing the long-range correlation we have to sum all the ring terms, culminating in the RPA [2], while for the short range we must include the electron–electron ladder terms. In order to respect the Pauli's exclusion principle, these terms should be complemented by proper account of the exchange contribution, which becomes important in the medium range.

A conventional idea to overcome this complication is to modify the RPA by introducing the concept of a local-field correction $G(q)$ with an expectation that it will take due care of short- and medium-range effects, but it is not an easy task to obtain a good, if not the best, form for $G(q)$.

Four decades ago, Singwi, Tosi, Land, and Sjölander (STLS) [3] proposed a powerful self-consistent iteration loop to determine $G(q)$ in conjunction with the static structure factor $S(q)$, starting with the information on the polarization

function in the RPA $\Pi_0(q, \omega)$. This STLS scheme provides reasonably good results for both $G(q)$ and $S(q)$. From the latter quantity, in particular, we can obtain the correlation energy ε_c , which agrees very well with the result given by quantum Monte Carlo (QMC) simulations [4, 5] in the whole metallic-density region. Even in recent years, there are many successful applications of this scheme to various systems [6–10].

In spite of all these merits, this STLS is not a scheme for obtaining rigorous results, as signaled by the fact that several exact relations are violated. For example, the obtained $G(q)$ does not satisfy the compressibility sum rule. The Pauli's exclusion principle is not properly incorporated, as observed by the result that the parallel-spin pair distribution function $g_{\uparrow\uparrow}(\mathbf{r})$ (the Fourier transform of the parallel-spin static structure factor $S_{\uparrow\uparrow}(q)$) does not vanish in the limit of $|\mathbf{r}| \rightarrow 0$. Actually, for small $|\mathbf{r}|$, $g_{\uparrow\uparrow}(\mathbf{r})$ shows a very unphysical behavior of $g_{\uparrow\uparrow}(\mathbf{r}) < 0$ even for high electron densities.

In the past, there have been many attempts to amend these insufficient points in the STLS framework. Among others, Vashishta and Singwi [11] and Utsumi and Ichimaru [12] tried to modify the expression for $G(q)$ so as to satisfy the compressibility sum rule as well as the non-negativity

condition $g_{\uparrow\uparrow}(\mathbf{r}) \geq 0$. Unfortunately, their results for the correlation energy became much worse than those in the original STLS scheme.

In this paper, we propose an amendment to the STLS scheme from a totally new point of view. Namely, we do not intend to modify the original expression for $G(\mathbf{q})$ but revise the self-consistent loop itself by adding new procedures to the loop in order to impose all the known exact relations. This new idea of amending self-consistent iterative calculations is rather general and therefore we hope that it will find useful applications in other self-consistent iterative schemes.

2. Original STLS loop

In terms of $\Pi_0(\mathbf{q}, \omega)$ and the local-field correction between spin- σ and spin- σ' electrons $G_{\sigma\sigma'}(\mathbf{q})$, the density–density response function $\chi_+(\mathbf{q}, \omega)$ and the spin–density response function $\chi_-(\mathbf{q}, \omega)$ are, respectively, expressed as

$$\chi_{\pm}(\mathbf{q}, \omega) = -\frac{\Pi_0(\mathbf{q}, \omega)}{1 + f_{\pm}(\mathbf{q})\Pi_0(\mathbf{q}, \omega)}, \quad (1)$$

where $f_{\pm}(\mathbf{q})$ are defined as $f_+(\mathbf{q}) = [1 - G_+(\mathbf{q})]V(\mathbf{q})$ and $f_-(\mathbf{q}) = -G_-(\mathbf{q})V(\mathbf{q})$, with $V(\mathbf{q}) = 4\pi e^2/q^2$ the bare Coulomb interaction and $G_{\pm}(\mathbf{q}) \equiv G_{\uparrow\uparrow}(\mathbf{q}) \pm G_{\uparrow\downarrow}(\mathbf{q})$ [13].

In the STLS theory [3], $G_{\pm}(\mathbf{q})$ is connected with the static structure factor $S_{\pm}(\mathbf{q}) (\equiv S_{\uparrow\uparrow}(\mathbf{q}) \pm S_{\uparrow\downarrow}(\mathbf{q}))$ through

$$G_{\pm}(\mathbf{q}) = \frac{1}{n\Omega_t} \sum_{\mathbf{q}' \neq \mathbf{0}, -\mathbf{q}} \frac{\mathbf{q} \cdot \mathbf{q}'}{q'^2} [S_{\pm}(\mathbf{q} + \mathbf{q}') - 1], \quad (2)$$

where n is the electron density and Ω_t represents the total volume of the system. This relation was deduced from consideration of the equation of motion for density operators. On the other hand, by using equation (1) or the fluctuation-dissipation theorem, $S_{\pm}(\mathbf{q})$ is related to $G_{\pm}(\mathbf{q})$ through

$$S_{\pm}(\mathbf{q}) = \frac{1}{n\Omega_t\pi} \int_0^{\infty} d\omega \frac{\Pi_0(\mathbf{q}, i\omega)}{1 + f_{\pm}(\mathbf{q})\Pi_0(\mathbf{q}, i\omega)}. \quad (3)$$

In this way, $G(\mathbf{q})$ and $S(\mathbf{q})$ are made directly interconnected in the STLS framework, composing a self-consistent loop, as schematically represented in figure 1(a), where $G_{\pm}(\mathbf{q})$ and $S_{\pm}(\mathbf{q})$ are, respectively, expressed symbolically as $G = \mathcal{F}_1[S]$ and $S = \mathcal{F}_2[G]$, indicating mutual functional relations.

3. Extension of the STLS loop

Suppose we know better functionals, $\tilde{\mathcal{F}}_1$ and $\tilde{\mathcal{F}}_2$, that provide better local-field correction $\tilde{G}(\mathbf{q})$ and static structure factor $\tilde{S}(\mathbf{q})$, amounting to $\tilde{G} = \tilde{\mathcal{F}}_1[\tilde{S}]$ and $\tilde{S} = \tilde{\mathcal{F}}_2[\tilde{G}]$. In reality, however, we know the concrete functional forms only for \mathcal{F}_1 and \mathcal{F}_2 . Taking this fact into account, we shall rewrite the functional relations as

$$\tilde{G} = \tilde{\mathcal{F}}_1[\tilde{S}] = \mathcal{F}_1[\tilde{S}] + (\tilde{\mathcal{F}}_1[\tilde{S}] - \mathcal{F}_1[\tilde{S}]) \equiv G + \delta G, \quad (4)$$

$$\tilde{S} = \tilde{\mathcal{F}}_2[\tilde{G}] = \mathcal{F}_2[\tilde{G}] + (\tilde{\mathcal{F}}_2[\tilde{G}] - \mathcal{F}_2[\tilde{G}]) \equiv S + \delta S. \quad (5)$$

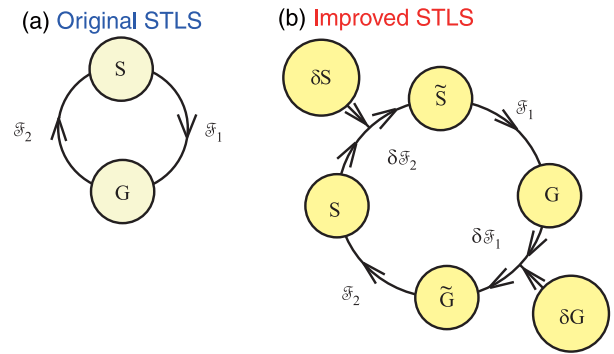


Figure 1. (a) Self-consistent loop in the original STLS theory; (b) self-consistent loop in the present theory.

Then we can regard δG as a functional of G , because we can derive the following relation: $\delta G = (\tilde{\mathcal{F}}_1 - \mathcal{F}_1)[\tilde{S}] = (\tilde{\mathcal{F}}_1 - \mathcal{F}_1)\mathcal{F}_1^{-1}[G] \equiv \delta\mathcal{F}_1[G]$. Similarly, we can write δS as $\delta S = (\tilde{\mathcal{F}}_2 - \mathcal{F}_2)[\tilde{G}] = (\tilde{\mathcal{F}}_2 - \mathcal{F}_2)\mathcal{F}_2^{-1}[S] \equiv \delta\mathcal{F}_2[S]$ and thus we end up obtaining an extended version of the self-consistent loop as $\tilde{S} \rightarrow G \rightarrow \delta G \rightarrow \tilde{G} (= G + \delta G) \rightarrow S \rightarrow \delta S \rightarrow \tilde{S} (= S + \delta S)$, which is also shown schematically in figure 1(b).

4. Trial functional form

Since they are basically at our disposal, we shall choose the actual functional forms for $\delta\mathcal{F}_1$ and $\delta\mathcal{F}_2$ so as to satisfy all the known exact relations for the local-field correction and the static structure factor.

To be more specific, let us consider $\delta G(\mathbf{q})$ first. The relevant relation to determine this quantity is the compressibility sum rule, which dictates that the correct local-field correction $\tilde{G}(\mathbf{q})$ should behave in the long-wavelength limit as [14]

$$\tilde{G}(\mathbf{q}) \xrightarrow{q \rightarrow 0} \gamma_0 \left(\frac{q}{p_F} \right)^2, \quad (6)$$

$$\text{with } \gamma_0 = \frac{1}{4} - \frac{\pi\alpha}{24} \left(r_s^3 \frac{d^2 \epsilon_c}{dr_s^2} - 2r_s^2 \frac{d\epsilon_c}{dr_s} \right),$$

where p_F is the Fermi momentum, r_s is the conventional nondimensional density parameter, and $\alpha = (4/9\pi)^{1/3} \approx 0.521$. The result of $G(\mathbf{q})$ obtained by using the operator \mathcal{F}_1 , however, does not satisfy this relation [3, 11], although it still behaves quadratically as $G(\mathbf{q}) \rightarrow \gamma_0^G (q/p_F)^2$ in this limit. Thus we can impose the compressibility sum rule by setting

$$\delta G(\mathbf{q}) = \delta\mathcal{F}_1[G] = \delta\gamma_0[G] \frac{(q/p_F)^2}{1 + (q/p_F)^4}, \quad (7)$$

with $\delta\gamma_0[G] = \gamma_0 - \gamma_0^G$.

In determining the functional form for δS , it is important to consider the correct asymptotic behavior of $\tilde{S}(\mathbf{q})$ in the limit of $q \rightarrow \infty$. Since it is closely connected with the cusp condition on the spin-dependent pair distribution function $g_{\sigma\sigma'}(\mathbf{r})$ [15], the behavior is written in terms of $g_{\sigma\sigma'}(\mathbf{r})$ as

$$\tilde{S}_{\uparrow\downarrow}(\mathbf{q}) \xrightarrow{q \rightarrow \infty} -\frac{4}{3} \left(\frac{\alpha r_s}{\pi} \right) \left(\frac{p_F}{q} \right)^4 g_{\uparrow\downarrow}(0) + \dots, \quad (8)$$

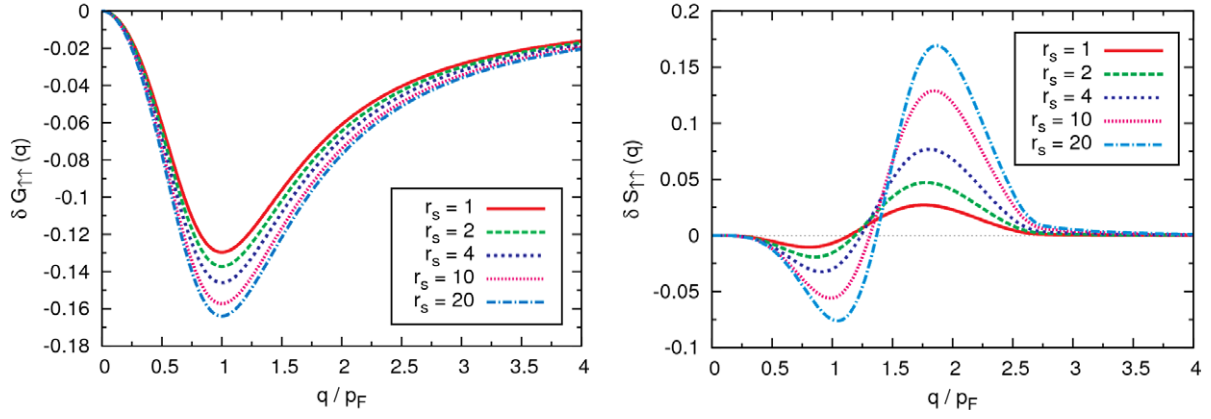


Figure 2. Left, $\delta G_{\uparrow\uparrow}(q)$, and right, $\delta S_{\uparrow\uparrow}(q)$, in the spin fully polarized electron liquid at $r_s = 1, 2, 4, 10,$ and 20 as a function of q/p_F .

$$\begin{aligned} \tilde{S}_{\uparrow\uparrow}(q) &\xrightarrow{q \rightarrow \infty} -\frac{4}{3} \left(\frac{\alpha r_s}{\pi} \right) \left(\frac{p_F}{q} \right)^4 g_{\uparrow\uparrow}(0) \\ &+ 4 \left(\frac{\alpha r_s}{\pi} \right) \left(\frac{p_F}{q} \right)^6 \frac{d^2 g_{\uparrow\uparrow}(r)}{d(p_F r)^2} \Big|_{r=0} + \dots \end{aligned} \quad (9)$$

These equations indicate that, while $\tilde{S}_{\uparrow\downarrow}(q) \propto q^{-4}$ for large q , $\tilde{S}_{\uparrow\uparrow}(q) \propto q^{-6}$ because of $g_{\uparrow\uparrow}(0) = 0$. From its very nature, however, the operator \mathcal{F}_2 necessarily provides $S_{\uparrow\uparrow}(q)$ that behaves as q^{-4} for large q , violating the Pauli's exclusion principle. This violation should be rectified by choosing δS so as to satisfy

$$g_{\uparrow\uparrow}(0) = 1 + \frac{2}{N} \sum_{q \neq 0} [\tilde{S}_{\uparrow\uparrow}(q) - 1] = 0. \quad (10)$$

Another important condition to determine δS comes from consideration of the correlation energy, which reads

$$\frac{1}{N} \sum_{q \neq 0} V(q) [\tilde{S}_+(q) - S^{\text{HF}}(q)] = 2\varepsilon_c + r_s \frac{d\varepsilon_c}{dr_s}, \quad (11)$$

where $S^{\text{HF}}(q)$ is the static structure factor in the Hartree–Fock approximation, given as

$$S^{\text{HF}}(q) = \frac{1}{n\Omega_i\pi} \int_0^\infty d\omega \Pi_0(q, i\omega). \quad (12)$$

If we employ the QMC data on $\varepsilon_c(r_s)$ [5] in the right-hand side of equation (11), the correlation energy obtained through our $\tilde{S}_+(q)$ reproduces $\varepsilon_c(r_s)$ itself, assuring not only self-consistency of our scheme but also its accuracy.

Further specification of δS can be done only on the trial and error basis. At the present time, we have arrived at the following trial functional form for δS :

$$\begin{aligned} \delta S(q) &= \delta \mathcal{F}_2[S] \\ &= A [S^{\text{RPA}}(q) - S(q)] \left[\{S^{\text{HF}}(q)\}^3 - \{S^{\text{HF}}(q/q_c)\}^5 \right] \\ &+ [S^{\text{HF}}(q) - S(q)] \left[B \{S^{\text{HF}}(q)\}^3 + (1 - B) \right. \\ &\left. \times \{S^{\text{HF}}(q/q_c)\}^5 \right], \end{aligned} \quad (13)$$

where the parameter q_c plays the role of a large- q cutoff and is taken as $1.1 p_F$, and $S^{\text{RPA}}(q)$ is defined as

$$S^{\text{RPA}}(q) = \frac{1}{n\Omega_i\pi} \int_0^\infty d\omega \frac{\Pi_0(q, i\omega)}{1 + V(q)\Pi_0(q, i\omega)}. \quad (14)$$

This form of $\delta S(q)$ cancels the q^{-4} -term in $S(q)$ for large q to make $\tilde{S}(q)$ decay as q^{-6} or faster, removing the problem of the STLS scheme for large q . On the other hand, the first term including the factor $S^{\text{RPA}}(q) - S(q)$ stands for the correction to the result in the RPA at small q , and the second term including the factor $S^{\text{HF}}(q) - S(q)$ takes care of the correction to the exchange processes. In this way, we have imposed that $\tilde{S}(q)$ should behave in accordance with the known exact behaviors in both long- and short-wavelength regions. The poorly known medium-range behavior is reasonably determined by choosing the coefficients A and B in equation (13) to satisfy equations (10) and (11).

5. Spin fully polarized electron gas

We have applied the above framework to the spin fully polarized electron liquid, primarily because this is the system which is most seriously affected by the violation of the Pauli's exclusion principle.

In figure 2, the obtained results of $\delta G_{\uparrow\uparrow}(q)$ and $\delta S_{\uparrow\uparrow}(q)$ are shown as a function of q for several values of r_s . With the increase of r_s , the overall features of these quantities do not change at all but are only amplified. It should be noted that even at $r_s = 1$ (high-density case) both $\delta G_{\uparrow\uparrow}(q)$ and $\delta S_{\uparrow\uparrow}(q)$ are not small, suggesting that the results in the original STLS scheme are not very accurate even at this high density and that the agreement of the STLS data with the QMC ones on ε_c must be only fortuitous. It should also be noted that $\delta S_{\uparrow\uparrow}(q)$ exhibits an interesting nonmonotonic behavior as a function of q : it has a minimum around $q \sim p_F$ and a maximum around $q \sim 2p_F$. The minimum indicates that the correct $\tilde{S}_{\uparrow\uparrow}(q)$ must be closer to $S^{\text{RPA}}(q)$ than $S_{\uparrow\uparrow}(q)$ in the STLS in this long-wavelength region, while in the region of shorter wavelengths the effect of $S^{\text{HF}}(q)$ or the exchange effect is much enhanced over the result in the STLS.

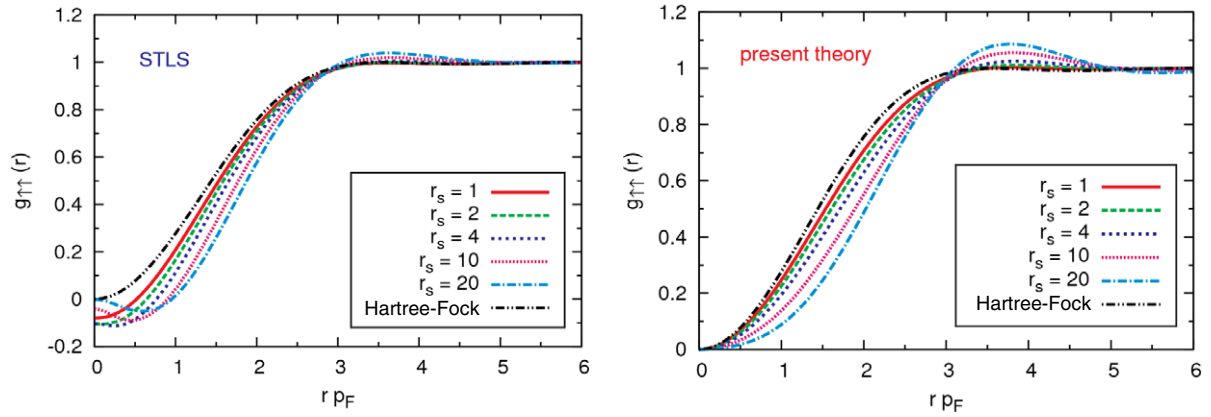


Figure 3. Parallel-spin pair distribution function $g_{\uparrow\uparrow}(r)$ in the spin fully polarized electron liquid at $r_s = 1, 2, 4, 10,$ and 20 . Our result (right) is compared with that in the original STLS (left).

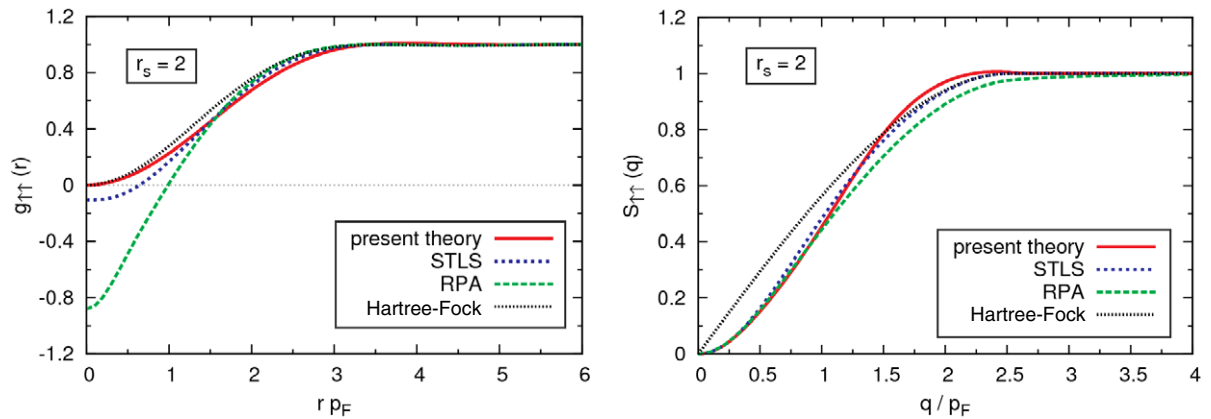


Figure 4. Left: parallel-spin pair distribution function $g_{\uparrow\uparrow}(r)$ in the spin fully polarized electron liquid at $r_s = 2$. Right: parallel-spin static structure factor $S_{\uparrow\uparrow}(q)$ as a function of q/p_F . Our result (red line) is compared with those in the STLS (blue line), the RPA (green line), and the Hartree-Fock (black line).

In order to show how well the Fermi hole is described, together with the Pauli's exclusion principle, namely, $g_{\uparrow\uparrow}(0) = 0$, we plot the results for $g_{\uparrow\uparrow}(r)$ as a function of r in both the original STLS scheme and our theory for several values of r_s in figure 3. Here again, the STLS fails to produce a physically reasonable description of the Fermi hole even at high electron density ($r_s = 1$), but our theory yields perfectly reasonable results even at very low density ($r_s = 20$). We add a comment on the fact that at $r_s = 20$ the STLS happens to give $g_{\uparrow\uparrow}(0) \approx 0$, but this does not mean that the STLS scheme works better in this low-density region, because the correlation energy obtained in the STLS deviates very much from the QMC result in this large- r_s region. Of course, our results for ε_c always reproduce the QMC data.

Finally, let us make a more detailed comparison of our theory with others at the typical metallic density or $r_s = 2$. In figure 4, the results for both $g_{\uparrow\uparrow}(r)$ and $S_{\uparrow\uparrow}(q)$ are shown. As is well known, the RPA incorporates the Coulomb correlation effect too much in the short-range region, resulting that $g_{\uparrow\uparrow}(r)$ becomes much lower than zero in this region. This feature is corrected to a large extent in the STLS scheme by adopting the screened interaction $[1 - G(q)]V(q)$ rather than the bare one in the RPA, but still it is not enough, as seen by the fact

that $g_{\uparrow\uparrow}(r) \approx -0.10$ for small r . A further correction is made in our theory by considering the correct asymptotic behavior of $\tilde{S}_{\uparrow\uparrow}(q)$ for large q to give very reasonable $g_{\uparrow\uparrow}(r)$. For the long-range part or in the small- q region, on the other hand, it is seen that our $\tilde{S}_{\uparrow\uparrow}(q)$ is almost identical to $S^{\text{RPA}}(q)$, which is needed to obtain the rigorous result for ε_c , even though $\tilde{S}_{\uparrow\uparrow}(q)$ becomes much larger than that in the STLS for large q . In this way, we can properly account for the many-body effect in the electron liquids in all ranges.

6. New general scheme

So far, we have explained our new idea about how to improve on the STLS self-consistent scheme. As might be easily anticipated, this idea can be applied to more general self-consistent iterative loops, for which we shall make a brief explanation below.

A general self-consistent loop may be symbolically shown in figure 5; physical quantities, A_1, A_2, \dots , are determined simultaneously through a self-consistent iterative loop defined by using mutual relations among them, $A_1 = \mathcal{F}_1\{A_j\}$, $A_2 = \mathcal{F}_2\{A_j\}, \dots$

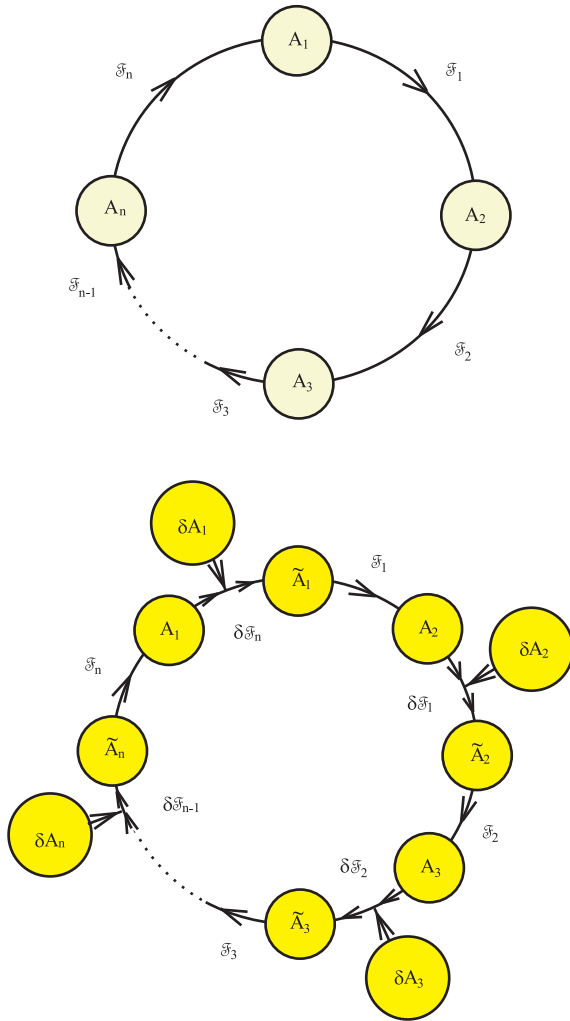


Figure 5. Top: general self-consistent loop. Bottom: new general scheme.

Basically, completion of the iterative loop will provide exact results for the A_j if all the operators \mathcal{F}_j are rigorous and feasible algorithms for them are available. In most actual implementations, however, this is not the case and the resultant A_j are not accurate enough to satisfy some exact relations as symbolically described by $\mathcal{R}_1[A_1] = 0$, $\mathcal{R}_2[A_2] = 0$, \dots , which are either prescribed by some conservation laws or required by consideration of the proper asymptotic behavior of the A_j .

In this situation, we shall revise the operators \mathcal{F}_j into better ones $\tilde{\mathcal{F}}_j$ and consider the difference $\delta\mathcal{F}_j$ between $\tilde{\mathcal{F}}_j$ and \mathcal{F}_j . This difference will be determined so as to satisfy all the existing exact relations $\mathcal{R}_j[A_j] = 0$ and then this will be included in the self-consistent loop.

An improvement on the Kohn–Sham scheme in the density functional theory may be possible through this idea, which will constitute one of the future works along this line of investigations.

7. Conclusion

We have proposed a new scheme to improve on the STLS theory that satisfies all the known exact relations strictly. This

scheme features the inclusion of both $\delta G(\mathbf{q}) (= \delta\mathcal{F}_1[G])$ and $\delta S(\mathbf{q}) (= \delta\mathcal{F}_2[S])$ in the original self-consistent loop, explicitly showing the logic to construct the extended loop.

The actual functional forms for these $\delta\mathcal{F}_1[G]$ and $\delta\mathcal{F}_2[S]$ are not uniquely determined by just imposing these exact relations, and therefore they become somewhat arbitrary, especially in the intermediate region of $|q|$, where there are no known exact relations to impose. In the electron liquid, however, a collection of both extensive and intensive studies on this system over half a century using various many-body techniques including quantum Monte Carlo simulations already suggests to us the correct behavior of $S(\mathbf{q})$ or its Fourier transform $g(\mathbf{r})$ [16]. The results for $S(\mathbf{q})$ and $g(\mathbf{r})$ obtained in this paper are in accord with these suggested ones, indicating that our new scheme properly captures the many-body effect in the electron liquid in all three important ranges, corresponding to rings, ladders, and exchanges.

In the computational aspect, it must be noted that our new scheme requires only the information on the polarization function in the RPA $\Pi_0(\mathbf{q}, \omega)$ as an input for the iteration procedure, just as in the original STLS. In this respect, we retain the feasibility of the original STLS as it is, but our theory goes far beyond it to provide much better results. Incidentally, we note here that we have not determined the ‘function’ forms for $\delta G(\mathbf{q})$ and $\delta S(\mathbf{q})$, only suitable for the electron liquid, but the ‘functional’ forms for $\delta\mathcal{F}_1[G]$ and $\delta\mathcal{F}_2[S]$, indicating that our scheme in just the present form can be applied to systems other than the electron liquid, as long as $\Pi_0(\mathbf{q}, \omega)$ can be obtained by either an analytical or a numerical method.

We have also implied that our idea can be generalized to any self-consistent iterative loops: the numerical procedure of the local-density approximation to the exchange–correlation potential in the Kohn–Sham density functional theory may be improved by our scheme proposed here with the inclusion of a step to rectify the Kohn–Sham potential so as to satisfy correct asymptotic behaviors.

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