Dynamical mean-field theories and velocity-average approximation

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We compare two dynamical mean-field theories for the calculation of the dielectric response function $\epsilon(\mathbf{k}\omega)$ of a strongly coupled Coulomb liquid. The two approximations share the feature that they express the correlational part of the linear response function in terms of the quadratic response function. We point out that even though the two approaches, the velocity-average approximation of Golden and Kalman [Phys. Rev. A **19**, 2112 (1979)] and the universal mean-field approximation of Tao and Kalman [Phys. Rev. A **43**, 973 (1990)], start from entirely different premises, they lead to the same result as to how the linear and quadratic response functions are related. On the other hand, they ultimately differ from each other in the way they break up the quadratic response function in order to achieve self-consistency.

The determination of the wave-number- and frequency-dependent dielectric function, $\epsilon(\mathbf{k},\omega)$, is one of the central problems in the study of strongly correlated Coulomb systems. In this Brief Report we focus on the one-component plasma (OCP)—identical charges dispersed in an inert neutralizing background only, with the coupling parameter $\Gamma=e^2\beta/a$, in which $a=(3n/4\pi)^{1/3}$ is the Wigner-Seitz radius and β the inverse temperature: our interest is primarily in strongly coupled ($\Gamma>1$) systems. We note, however, that the degenerate electron gas, with the coupling parameter $r_s=a/a_0$ where a_0 is the Bohr radius, presents a very similar problem in the domain $r_s>1$. [The equivalence between Γ and r_s can be established by observing that both of them are of the order of the (potential energy per particle)/(kinetic energy per particle); on this basis $\Gamma\rightarrow 1.36r_s$.] In what follows we present the formalism anchored in the classical theory—similar considerations would apply though to the calculation of $\epsilon(\mathbf{k}\omega)$ for a degenerate electron gas. The main difference between the classical and quantum formalism, in the language of this paper, appears in Eq. (8) below: The present classical relationship would be replaced for the degenerate electron gas by a similar, but more complex, relationship between the two response functions involved.

In the absence of any systematic procedure for strong coupling, various approximation methods have been proposed for the calculation of $\epsilon(\mathbf{k}\omega)$, both for classical systems and for the degenerate electron gas.[1,2] One possible avenue consists of exploiting the relationship between the linear and quadratic response functions.[1(d),2,3] Two approaches[2,3] have been proposed for introducing the quadratic response function as an intermediary in the calculation of the dielectric response function. The two approaches, referred to as the velocity-average approximation (VAA) and the universal mean-field theory (UMFT), start from entirely different premises, as described below, and the formulations of the resulting approximation schemes are also different. Nevertheless, a more careful analysis reveals a profound *a posteriori* similarity between the VAA and the UMFT. Any approximation scheme that seeks to establish a self-consistency condition and algorithm for the calculation of $\epsilon(\mathbf{k}\omega)$ via the quadratic response function consists, necessarily, of two stages. In the first stage one establishes an approximate relationship that expresses the linear response function as a functional of the quadratic one; in the second stage a further approximation is sought to find a decomposition of the quadratic response function in terms of linear responses. The combination of the results of the two stages of the approximation scheme leads to the desired self-consistency criterion for $\epsilon(\mathbf{k}\omega)$. It is the purpose of this Brief Report to establish the claimed similarity between the VAA and UMFT. More precisely, we demonstrate that the first stages of the two derivations, though seemingly different, run on parallel tracks and lead to identical results; next, we identify the essential difference that appears in the second stages of the approximations. This clarification helps one to formulate a self-consistency condition for $\epsilon(\mathbf{k}\omega)$ in a compact and physically transparent form.

First we show that, cast in the appropriate language of the response function of the second kind (or "double response function") defined below, there is a common starting point for both approximations. It has been recognized that the dynamical, frequency-dependent correlations[4] play a crucial part in obtaining the correct behavior of $\epsilon(\mathbf{k}\omega)$. In the dynamical mean-field theories (DMFT) a frequency-dependent mean field is introduced (explicitly or implicitly), leading to $\epsilon(\mathbf{k}\omega)$ being expressed in terms of $\epsilon_0(\mathbf{k}\omega)$, the random-phase-approximation (RPA) dielectric response function. In general, $\epsilon(\mathbf{k}\omega)$ is related to the density response function $\chi(\mathbf{k}\omega)$ by

$$\epsilon(\mathbf{k}\omega)=1-\phi(k)\chi(\mathbf{k}\omega)\ , \tag{1}$$

where $\phi(k)=4\pi e^2/k^2$ is the Fourier transform of the

Coulomb potential. In the RPA

$$\epsilon_0(\mathbf{k}\omega)=1-\phi(k)\chi_0(\mathbf{k}\omega) \tag{2}$$

and $\chi_0(\mathbf{k}\omega)$ is the density response of the noninteracting gas. The DMFT of Refs. 2 and 3 relate $\chi(\mathbf{k}\omega)$ to $\chi_0(\mathbf{k}\omega)$ either through[3]

$$\chi(\mathbf{k}\omega)=\frac{\chi_0(\mathbf{k}\omega)}{\Theta(\mathbf{k}\omega)},\quad \Theta(\mathbf{k}\omega)=1+\phi(k)G(\mathbf{k}\omega)\chi_0(\mathbf{k}\omega)\ , \tag{3}$$

or through[2]

$$\chi(\mathbf{k}\omega)=\chi_0(\mathbf{k}\omega)[1+v(\mathbf{k}\omega)] \tag{4}$$

by introducing the dynamical mean field $G(\mathbf{k}\omega)$ or the dynamical coupling function $v(\mathbf{k}\omega)$. The difference between (3) and (4) is only notational, but the calculational procedures leading to $v(\mathbf{k}\omega)$ and $G(\mathbf{k}\omega)$ in Refs. 2 and 3, respectively, are quite different.

Both of the approaches of Refs. 2 and 3 for the determination of $v(\mathbf{k}\omega)$ or $G(\mathbf{k}\omega)$ for the classical OCP introduce the quadratic density response function $\chi(\mathbf{k}_1\omega_1;\mathbf{k}_2\omega_2)$ (where $\mathbf{k}=\mathbf{k}_1+\mathbf{k}_2$, $\omega=\omega_1+\omega_2$) and the response function of the second kind (or "double response function") $\Xi(\mathbf{k}_1,\mathbf{k}_2;\omega)$. These response functions are defined as follows:

$$\langle\bar{n}(\mathbf{k}\omega)\rangle^{(1)}=\chi(\mathbf{k}\omega)\Phi(\mathbf{k}\omega)=\hat{\chi}(\mathbf{k}\omega)\hat{\Phi}(\mathbf{k}\omega)\ ,$$

$$\hat{\chi}(\mathbf{k}\omega)=\frac{\chi(\mathbf{k}\omega)}{\epsilon(\mathbf{k}\omega)}\ , \tag{5}$$

$$\begin{aligned}\langle\bar{n}(\mathbf{k}\omega)\rangle^{(2)}&=\frac{1}{2\pi V}\sum_{\mathbf{k}_1}\int d\omega_1\chi(\mathbf{k}_1\omega_1;\mathbf{k}_2\omega_2)\\&\quad\times\Phi(\mathbf{k}_1\omega_1)\Phi(\mathbf{k}_2\omega_2)\\&=\frac{1}{2\pi V}\sum_{\mathbf{k}_1}\int d\omega\hat{\chi}(\mathbf{k}_1\omega_1;\mathbf{k}_2\omega_2)\\&\quad\times\hat{\Phi}(\mathbf{k}_1\omega_1)\hat{\Phi}(\mathbf{k}_2\omega_2)\ ,\end{aligned}$$

$$\hat{\chi}(\mathbf{k}_1\omega_1;\mathbf{k}_2\omega_2)=\frac{\chi(\mathbf{k}_1\omega;\mathbf{k}_2\omega_2)}{\epsilon(\mathbf{k}_1\omega_1)\epsilon(\mathbf{k}_2\omega_2)\epsilon(\mathbf{k}\omega)}\ , \tag{6}$$

$$\begin{aligned}\langle\bar{n}(\mathbf{k}_1)\bar{n}(\mathbf{k}_2)\rangle^{(1)}(\omega)&=\Xi(\mathbf{k}_1,\mathbf{k}_2;\omega)\Phi(\mathbf{k}\omega)\\&=\hat{\Xi}(\mathbf{k}_1,\mathbf{k}_2;\omega)\hat{\Phi}(\mathbf{k}\omega)\ ,\end{aligned}$$

$$\hat{\Xi}(\mathbf{k}_1,\mathbf{k}_2;\omega)=\frac{\Xi(\mathbf{k}_1,\mathbf{k}_2;\omega)}{\epsilon(\mathbf{k}\omega)},\quad \mathbf{k}=\mathbf{k}_1+\mathbf{k}_2,\ \omega=\omega_1+\omega_2\ . \tag{7}$$

The superscripts indicate the perturbation order in the external perturbation; $\hat{\Phi}$ and Φ are the external and total potentials (potential energies)—the latter includes the induced potential generated by the particles: $\Phi=\hat{\Phi}+\Phi^{\text{ind}}$— and $\bar{n}(\mathbf{k}\omega)=n(\mathbf{k}\omega)-n\delta_{\mathbf{k}}\delta(\omega)$ is the density fluctuation around its equilibrium n value.

An important relationship derived from the quadratic fluctuation-dissipation theorem[5,6] links[3,7,8] $\hat{\Xi}(\mathbf{k}_1,\mathbf{k}_2;\omega)$ to $\hat{\chi}(\mathbf{k}_1\omega_1;\mathbf{k}_2\omega_2)$:

$$\begin{aligned}\hat{\Xi}(\mathbf{k}_1,\mathbf{k}_2;\omega)=-\frac{2}{\beta}\int d\mu\,\delta_-(\mu)[&\hat{\chi}(\mathbf{k}_1\mu;\mathbf{k}_2\omega-\mu)\\&+\hat{\chi}(\mathbf{k}_1\omega-\mu;\mathbf{k}_2\mu)]\ ,\end{aligned} \tag{8}$$

where, as usual,

$$\delta_-(\mu)=\lim_{o\to 0}\frac{i}{2\pi}\frac{1}{\mu-io}\ .$$

This is the common starting ground for the development of the approximation schemes.

The first approximation scheme, referred to above as the VAA, was proposed by Golden, Kalman, and Silevitch[9] and worked out in detail by Golden and Kalman.[2] The scheme is based on replacing the perturbed two-body function $G^{(1)}(\mathbf{x}_1,\mathbf{v}_1;\mathbf{x}_2,\mathbf{v}_2)$ in the first Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) equation by its velocity average

$$\bar{G}^{(1)}(\mathbf{x}_1,\mathbf{x}_2)=\int d^3v_1\int d^3v_2 G^{(1)}(\mathbf{x}_1,\mathbf{v}_1;\mathbf{x}_2,\mathbf{v}_2)\ .$$

As a result, $\chi(\mathbf{k}\omega)$ becomes expressible in terms of the density-density correlations, or, equivalently, in terms of the double density response function $\Xi(\mathbf{k}_1,\mathbf{k}_2;\omega)$. Using $v(\mathbf{k}\omega)$ as defined in Eq. (4), one obtains the central relationship of the VAA,

$$v(\mathbf{k}\omega)=\frac{1}{nV}\sum_{\mathbf{q}}\frac{\mathbf{k}\cdot\mathbf{q}}{k^2}\phi(q)\Xi(\mathbf{k},\mathbf{k}-\mathbf{q};\omega)\ . \tag{9}$$

The second approximation scheme referred to as the UMFT was proposed quite recently by Tao and Kalman.[3] This latter approach focuses on the moment equation obtainable from the first BBGKY equation. To obtain closure of the chain of equations, one adopts the assumption that all response functions can be generated from their noninteracting-gas values by the same universal mean field (UMF); thus response functions related to physical quantities other than the density [e.g., $\lambda(\mathbf{k}\omega)$] are expressed through the same factor $1/\Theta$ as $\chi(\mathbf{k}\omega)$:

$$\lambda(\mathbf{k}\omega)=\frac{\lambda_0(\mathbf{k}\omega)}{\Theta(\mathbf{k}\omega)}\ . \tag{10}$$

The resulting closed set of equations provides

$$\frac{G(\mathbf{k}\omega)\chi_0(\mathbf{k}\omega)}{\Theta(\mathbf{k}\omega)}=-\frac{1}{nV}\sum_{\mathbf{q}}\frac{\mathbf{k}\cdot\mathbf{q}}{q^2}\Xi(\mathbf{k},\mathbf{k}-\mathbf{q};\omega)\ . \tag{11}$$

It is now a matter of simple algebra to realize that (9) and (11) are completely equivalent.

Further progress can be reached by eliminating Ξ with the aid of Eq. (8):

$$\phi(k)\frac{G(\mathbf{k}\omega)\chi_0(\mathbf{k}\omega)}{\Theta(\mathbf{k}\omega)}=-v(\mathbf{k}\omega)=\frac{2}{nV\beta}\sum_{\mathbf{q}}\frac{\mathbf{k}\cdot\mathbf{q}}{k^2}\phi(q)\int d\mu\,\delta_-(\mu)\left[\frac{\chi(\mathbf{k}-\mathbf{q}\mu;\mathbf{q}\omega-\mu)}{\epsilon(\mathbf{k}-\mathbf{q}\mu)\epsilon(\mathbf{q}\omega-\mu)}+\frac{\chi(\mathbf{k}-\mathbf{q}\omega-\mu;\mathbf{q}\mu)}{\epsilon(\mathbf{k}-\mathbf{q}\omega-\mu)\epsilon(\mathbf{q}\mu)}\right]\ . \tag{12}$$

This relationship can now be identified as the primary product of the VAA, whether applied directly, as in Ref. 2, or implicitly, as in Ref. 3. Thus, rather unexpectedly, one arrives at the conclusion that the DMFT based on the VAA and that based on the UMF scheme proposed in Ref. 3, although predicated on seemingly quite different approximations, are, in terms of their final product, identical: both lead to the same functional relationship between $\chi(\mathbf{k}\omega)$ and $\Xi(\mathbf{k},\mathbf{k}-\mathbf{q};\omega)$.

We note that the result (12) possesses two important features: first, it satisfies the ω^{-4} (third frequency moment) high-frequency sum rule; second, it is exact in the static ($\omega=0$) limit.[3]

Equation (12) is basically the form in which the intermediate stage of the calculations was reported in Refs. 2 and 3. Having converged to this point, the two works deviate from each other in the way they seek to reduce Eq. (12) to a self-consistency criterion for $v(\mathbf{k}\omega)$ or $G(\mathbf{k}\omega)$. In Ref. 2 a decomposition of $\chi(\mathbf{k}_1\omega_1;\mathbf{k}_2\omega_2)$ into the product $\chi(\mathbf{k}_1\omega_1)\chi(\mathbf{k}_2\omega)$ is postulated. The justification for such a procedure is the observation that a similar structure prevails in relation to $\chi_0(\mathbf{k}_1\omega_1;\mathbf{k}_2\omega_2)$ and $\chi_0(\mathbf{k}_1\omega_1)\chi(\mathbf{k}_2\omega_2)$ in a certain $(k\omega)$ domain. The resulting self-consistency criterion (with the additional simplifying condition $k/\omega\to 0$) is

$$v(\mathbf{k}\omega)=-\frac{1}{\omega^2}\frac{1}{m\beta n}\frac{1}{V}\sum_{\mathbf{q}}\left[\tfrac{3}{5}k^2\phi^2(q)\int d\mu\,\delta_-(\mu)\frac{\chi(\mathbf{k}-\mathbf{q}\mu)\chi(\mathbf{q}\omega-\mu)}{\epsilon(\mathbf{k}-\mathbf{q}\mu)\epsilon(\mathbf{q}\omega-\mu)}+\frac{(\mathbf{k}\cdot\mathbf{q})^2}{k^2}\phi(q)\left[\frac{\chi(\mathbf{k}-\mathbf{q}0)}{\epsilon(\mathbf{k}-\mathbf{q}0)}-\frac{\chi(\mathbf{q}0)}{\epsilon(\mathbf{q}0)}\right]\right]. \tag{13}$$

In contrast, in Ref. 3 one approximates $\chi(\mathbf{k}_1\omega_1;\mathbf{k}_2\omega_2)$ by again involving the idea of a universal mean field:

$$\chi(\mathbf{k}_1\omega_1;\mathbf{k}_2\omega_2)=\frac{\chi_0(\mathbf{k}_1\omega_1;\mathbf{k}_2\omega_2)}{\Theta(\mathbf{k}\omega)\Theta(\mathbf{k}_1\omega_1)\Theta(\mathbf{k}_2\omega_2)}\,. \tag{14}$$

Equation (14) can actually be derived on the basis of the same mean-field assumption that has led to (3).[10] It should be noted, however, that while (3) does not actually restrict $\chi(\mathbf{k}\omega)$ as long as $G(\mathbf{k}\omega)$ is unspecified, the ansatz (14) represents a rather severe limitation on the structure of $\chi(\mathbf{k}_1\omega_1;\mathbf{k}_2\omega_2)$, no matter what $G(\mathbf{k}\omega)$ is.

The self-consistency criterion that now emerges from (14) is

$$G(\mathbf{k}\omega)\chi_0(\mathbf{k}\omega)=\frac{2}{nV\beta}\sum_{\mathbf{q}}\frac{\mathbf{k}\cdot\mathbf{q}}{q^2}\int d\mu\,\delta_-(\mu)\left[\frac{\chi_0(\mathbf{k}-\mathbf{q}\mu;\mathbf{q}\omega-\mu)}{\Delta(\mathbf{k}-\mathbf{q}\mu)\Delta(\mathbf{q}\omega-\mu)}+\frac{\chi_0(\mathbf{q}\mu;\mathbf{k}-\mathbf{q}\omega-\mu)}{\Delta(\mathbf{q}\mu)\Delta(\mathbf{k}-\mathbf{q}\omega-\mu)}\right]$$
$$\Delta(\mathbf{q}\mu)=1+\phi(q)[G(\mathbf{q}\mu)-1]\chi_0(\mathbf{q}\mu)\,. \tag{15}$$

Equations (15) and (13) are now genuinely different: But it bears reemphasizing that this variance is not due to the difference between the VAA of Ref. 2 and the UMF scheme of Ref. 3; it is solely due to the dissimilar character of the two different approximations used to reduce Eq. (12). Even though they are different, (13) and (15) have some common features. First, they become identical in the weak-coupling ($\Gamma\ll 1$) limit; second, both preserve the important property of the parent equation (12), namely, that it satisfies the high-frequency ω^{-4} sum rule; finally, both of them break—albeit differently—the exactness of the parent equation in the static ($\omega=0$) limit. [The approximation (15) breaks the quadratic compressibility sum rule;[11] a systematic improvement of the approximation is, however, possible.[12]]

As to the solution to the integral equation (13), we have some preliminary experience. At the price of rather drastic approximations,[13,14] a reasonable and physically interesting solution, representing $\epsilon(\mathbf{k}\omega)$ over a wide range of k and Γ values, can be found. The integral equation (15), however, is too recent in origin for an actual solution to exist. Nevertheless, it seems that Eq. (15) possesses certain features that make it a better candidate for concrete calculations than Eq. (13), namely the following.

(a) An addition approximation[3,8] which consists of ignoring plasma pole contributions to the μ integral in (15) renders the integral doable, thus reducing the dimensionality of the integral equation.

(b) The static- and low-frequency behavior of Eq. (15)—even though not exact—is more satisfactory[3] than that of Eq. (13).

(c) Comparing the physical foundations of the approximations leading to Eqs. (13) and (15), respectively, one finds the latter more convincing than the former.

(d) In a recent series of papers[14,15] it has been shown that for very strong coupling ($\Gamma\to\Gamma_m$, the crystallization limit of the OCP) the dynamical mean field simplifies to the structure

$$G(\mathbf{k}\omega)\to -D(k)\,, \tag{16}$$

where

$$-\omega_p^2 D(k)=-\frac{\omega_p^2}{nV}\sum_{\mathbf{q}}\frac{(\mathbf{k}\cdot\mathbf{q})^2}{k^2q^2}[S(|\mathbf{k}-\mathbf{q}|)-S(q)]$$

is the ω^{-4} sum-rule coefficient. On the other hand, we know from the calculations of Carini *et al.*[13] that the integral equation (13) has the feature that, for $\Gamma\to\Gamma_m$, $v(\mathbf{k}\omega)\to D(k)$. Then it probably follows that the integral equation (15) in a similar fashion implies Eq. (16), as is desired on physical grounds.

Our conclusions now can be stated as follows. The two

dynamical mean-field theories examined in this Brief Report, i.e., the VAA approximation of Ref. 2 and the UMF approximation of Ref. 3, lead to the same result as to how the linear response function may be expressed in terms of the quadratic density-response function: where the methods presented in Refs. 2 and 3 ultimately differ from each other is in the way they break up $\chi(\mathbf{k}_1\omega_1;\mathbf{k}_2\omega_2)$ into combinations of $\chi(\mathbf{k}_1\omega_1)$ and $\chi(\mathbf{k}_2\omega_2)$: in this respect the approach of Ref. 3 seems to be superior and intuitively more appealing.

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