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LETTER TO THE EDITOR

Asymptotic behaviour of a dynamic local field: is the order of the $k \to \infty$ and $\omega \to \infty$ limits interchangeable in an interacting many-body system?

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Abstract. The wavevector- and frequency-dependent susceptibility $\chi_k(\omega)$ in many-body theory is customarily expressed in terms of a dynamic local field term $G_k(\omega)$. For $k \to \infty$ there are certain asymptotic forms for $G_k(\omega)$ due to Shaw and to Niklasson. It is shown that they represent the two different orders of the $k \to \infty$ and $\omega \to \infty$ limits. The validity of our result is tested in an exactly solvable physical system.

The dynamic susceptibility $\chi_k(\omega)$, where $\boldsymbol{k}$ and ω are, respectively, wavevector and frequency, is an essential theoretical quantity for describing the dynamic behaviour of both classical and quantum many-body systems. It links theory to experiment through its imaginary part, Im $\chi_k(\omega)$, which is directly proportional to an inelastic scattering cross section. It is a response function in linear response theory, and is thus important for theoretical analysis. No one has been able to obtain an exact general expression or solution for it in the case of an interacting system in a strong-coupling regime.

For an electron gas it is nowadays customary to express the density–density response function in terms of another many-body quantity known as a dynamic local field term $G_k(\omega)$ defined with respect to an ideal system as

$$\chi_k(\omega) = \chi_k^0(\omega)/\{1 - v_k[1 - G_k(\omega)]\chi_k^0(\omega)\} \tag{1}$$

where $\chi_k^0(\omega)$ is the dynamic susceptibility for an ideal system, v_k is the Fourier transform of the Coulomb interaction. Note that $G_k(\omega) = 0$ gives an RPA form which is approximately valid in a weak coupling regime, e.g., high densities. Hence, $G_k(\omega) \neq 0$ implies that a system is in a non-weak or strong coupling regime. The local field term was originally introduced phenomenologically to take into account short-range correlations absent in mean-field theory. In recent years, much interest has centred on finding a proper form for $G_k(\omega)$, beginning with the pioneering work of Singwi *et al* [2].

Any approximate form for $G_k(\omega)$ is subject to self-consistency checks through the dynamic susceptibility. That is, frequency moments obtained with (1) must agree with those based only on static properties [1, 3]. This agreement is not easily obtained in strong coupling regimes, e.g., low densities. As a result, to date there are still unresolved controversies and confusion concerning a proper form for $G_k(\omega)$ [4–6].

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Some years ago, an asymptotic form for $G_k(\omega)$ was derived [7]. Assuming that $G_k(\omega) = G_k$ for all ω, it was shown that

$$G_{k\to\infty} = 1 - g(0) \tag{2}$$

where $g(r)$ is the pair correlation function. Shaw's relation [7] is regarded as approximate at best because of his use of a generalised RPA form of $G_k(\omega)$. Subsequently, a different result was derived [8]:

$$\lim_{k\to\infty} G_k(\omega) = s_D[1 - g(0)] \tag{3}$$

where $s_D = (D-1)/D$, where D denotes spatial dimensions. Niklasson's relation [8] is generally regarded as asymptotically exact. In fact, the work [8] is based on a kind of perturbation which appears to become exact as $\boldsymbol{k} \to \infty$ or $\omega \to \infty$ or both.

These two relations [7, 8] are the only definitive statements that can be made about $G_k(\omega)$. Important as they are, to our knowledge they have not been tested experimentally or theoretically. A closer examination of [8] shows that one can also conclude

$$\lim_{k\to\infty} \lim_{\omega\to\infty} G_k(\omega) = s_D[1 - g(0)]. \tag{4}$$

Since (3) is also valid as $\omega \to \infty$, one has

$$\lim_{\omega\to\infty} \lim_{k\to\infty} G_k(\omega) = \lim_{k\to\infty} \lim_{\omega\to\infty} G_k(\omega) \tag{5}$$

i.e., the order of the two limiting processes is interchangeable. In the absence of an exact solution, this interchangeability of order may possibly provide a way of testing the validity of the relation [8]. It is clearly a simpler test, although not sufficient by itself. Generally, the question of interchangeability of the order of limits of physical quantities is an interesting one. In an ideal system or possibly in an interacting system in a weak-coupling regime, one may perhaps expect interchangeability. But whether the interchangeability should prevail even in a strong-coupling regime, as suggested by [8], appears yet to be established.

An exact formal expression for $G_k(\omega)$ can be derived by the method of recurrence relations [9, 10], from which one can deduce its asymptotic forms. Let our many-body system be defined by its energy $\mathcal{H} = \mathcal{H}_0 + \mathcal{V}$, where $\mathcal{H}_0$ denotes the kinetic energy and $\mathcal{V}$ the Coulomb interaction energy. Let the dynamic variable be the density fluctuation operator ρ_k, such that $(1/v)\langle\rho_{k=0}\rangle = n$, where n is the number density, v is the volume and the brackets denote an ensemble average. Then the time evolution of ρ_k may be given an orthogonal expansion

$$\rho_k(t) = \sum_{\nu=0}^{d-1} a_\nu(t) f_\nu \tag{6}$$

where $\{f_\nu\}$ is a set of basis vectors which span the d-dimensional Hilbert space $\mathcal{S}$ such that $(f_\nu, f_\mu) = 0$ if $\nu \neq \mu$, the inner product meaning the Kubo scalar product (KSP) [9], and the $a_\nu(t)$ are real functions of time. We shall denote the norm of f_ν as $\|f_\nu\| \equiv (f_\nu, f_\nu)$. If $\mathcal{S}$ is realised by the KSP, there are recurrence relations for the f_ν and a_ν, which are functions solely of $\Delta_\nu \equiv \|f_\nu\|/\|f_{\nu-1}\|$. The dependence of $\boldsymbol{k}$ in the f_ν and a_ν is suppressed.

If one chooses $f_0 = \rho_k$, the time-dependent response function† $\tilde{\chi}_k(t) \equiv \chi_k(t)/\chi_k = \Delta_1 a_1(t)$. Let $a_\nu(z) = \mathcal{F}[a_\nu(t)]$ where $\mathcal{F}$ is the Laplace transform operator. Then by the recurrence relation [9]

$$\tilde{\chi}_k(z) = \Delta_1 a_1(z) = 1 - z a_0(z). \tag{7}$$

Define

$$G_k(z) = G_k + H_k(z) \tag{8}$$

such that $G_k = G_k(z = 0)$, i.e., $H_k(z = 0) = 0$, $z = \mathrm{i}\omega$. Then taking the zero-frequency limit of (1), we obtain

$$G_k = 1 + v_k^{-1}(1/\chi_k - 1/\chi_k^0) = 1 - (\Delta_1 - \Delta_1^0)/v_k\|f_1\| = 1 - \Delta_1^0\eta_1(k)/\omega_\mathrm{p}^2 \tag{9}$$

where $\eta_1(k) = \Delta_1/\Delta_1^0 - 1$ and $\omega_p^2 = v_k\|f_1\|$, $\|f_1\| = \|f_1\|^0 = nk^2/m$, where m is the mass. The superscript 0 denotes an ideal quantity, i.e., obtained with $\mathcal{H}_0$. Next using (8) we put (7) into the form of (1), with $z = \mathrm{i}\omega$, to obtain

$$H_k(z) = -(z/v_k\|f_1\|)[1/b_1(z) - 1/b_1^0(z)] \tag{10}$$

where [11]

$$b_1(z) \equiv a_1(z)/a_0(z) = 1/\{z + \Delta_2/[z + \Delta_3/(z + \ldots)]\}. \tag{11}$$

Using (8)–(11), one can obtain asymptotic forms of $G_k(z)$. We first look at the $z \to \infty$ behaviour. For $z \to \infty$, (11) can be expressed as

$$1/b_1(z) = z + \Delta_2/z - \Delta_2\Delta_3/z^3 + \mathrm{O}(z^{-5}). \tag{12}$$

Hence,

$$H_k(z) = -\Delta_2^0\eta_2(\boldsymbol{k})/\omega_\mathrm{p}^2 + \mathrm{O}(z^{-2}) \tag{13}$$

where $\eta_2(\boldsymbol{k}) = \Delta_2/\Delta_2^0 - 1$. Thus, there is a frequency-independent contribution $H_k(\infty) \neq 0$, depending on $\boldsymbol{k}$. This is different from the $z \to 0$ limit where $H_k(0) = 0$‡.

Hence, putting together we have

$$G_k(z \to \infty) = G_k + H_k(\infty) = 1 - [\Delta_1^0\eta_1(\boldsymbol{k}) + \Delta_2^0\eta_2(\boldsymbol{k})]/\omega_\mathrm{p}^2. \tag{14}$$

Now Δ_ν^0 and Δ_ν, $\nu = 1, 2$ are static quantities, i.e., density–density correlation functions in the ideal and non-ideal systems; hence, they are calculable from $\mathcal{H}_0$ and $\mathcal{H}$, respectively. In particular, one can obtain them from the third frequency moment [12]§

$$\begin{aligned}\langle\omega^3(\boldsymbol{k})\rangle &= \langle[\rho_k, [\mathcal{H}, [\mathcal{H}, [\mathcal{H}, \rho_{-k}] \ldots]\rangle = \|f_1\|(\Delta_1 + \Delta_2) \\ &= (nk^2/m)[\hbar^2\omega_k^2 + 12T\omega_k/D + \omega_\mathrm{p}^2(1 - I_k)]\end{aligned} \tag{15}$$

† In the conventional theory, $\chi_k(\omega)$ is defined such that $\chi_k(\omega = 0) = \chi_k < 0$. In the recurrence relations method, it is non-negative since $\chi_k = \|\rho_k\|$, being a norm or a length. Hence, there is an overall minus sign difference between the two approaches. The normalised quantity $\tilde{\chi}_k(\omega) = \chi_k(\omega)/\chi_k$ is, however, independent of any given convention. Equation (1) is defined for the conventional theory.

‡ It is by no means obvious that $H_k(z)$ given by (10) should necessarily give $H_k(z = 0) = 0$ as assumed in (8). In fact, if d is an *odd* integer, $H_k(0) \neq 0$ and $G_k(0) = G_k + H_k(0)$. If, however, d is infinite (as we shall assume here), $H_k(0) = 0$. For most physical problems, $d = \infty$.

§ The first line of equation (15) follows from $\langle\omega^3(\boldsymbol{k})\rangle = -(1/\pi)\int_{-\infty}^{\infty} \mathrm{d}\omega\, \omega^3 \,\mathrm{Im}\, \chi_k(\omega) = \|f_1\|(\Delta_1 + \Delta_2)$. See [11]. The classical solution is obtained by taking $\hbar = 0$ in the second line of (15). See also [13].

where $\omega_k = k^2/2m$, T is the average kinetic energy per particle in the non-ideal system, and

$$I_k = N^{-1} \sum_{q\neq 0,k} [(\boldsymbol{k}\cdot\boldsymbol{q})^2/k^2q^2][S(\boldsymbol{q}) - S(\boldsymbol{q}-\boldsymbol{k})] \tag{16}$$

where $S(\boldsymbol{k})$ is the static structure factor and N is the number of particles. One can write an analogous expression for the ideal system. Hence,

$$\Delta_1^0 \eta_1(k)/\omega_p^2 = 1 - G_k \tag{17}$$

$$\Delta_2^0 \eta_2(k)/\omega_p^2 = \delta\tilde{T}_k + G_k - I_k \tag{18}$$

where $\delta\tilde{T}_k = 12\omega_k \delta T/D\omega_p^2$, $\delta T = T - T^0$. Substitution of (17) and (18) in (14) and setting $z = \mathrm{i}\omega$ yields

$$G_k(\omega \to \infty) = I_k - \delta\tilde{T}_k + \mathrm{O}(\omega^{-2}). \tag{19}$$

Hence,

$$\lim_{k\to\infty} \lim_{\omega\to\infty} G_k(\omega) = I_{k\to\infty} - \delta\tilde{T}_{k\to\infty}. \tag{20}$$

Now from (16)

$$I_{k\to\infty} = s_D[1 - g(0)]. \tag{21}$$

Thus, one can recover the relation (3) [8] if $\delta\tilde{T}_k = 0$ as in classical systems [6].

We next look at the $k \to \infty$ behaviour of $G_k(\omega)$. Now if $\boldsymbol{k} \to \infty$, one may expect $\Delta_\nu \to \Delta_\nu^0$, since the difference between the two families of norms arises from $\mathcal{V} = \mathcal{H} - \mathcal{H}_0 \sim v_k = \mathrm{O}(\boldsymbol{k}^{-2})$. From (10) we see that this difference essentially determines $H_k(\omega)$, the frequency-dependent part of $G_k(\omega)$. Hence, this quantity may be expressible as, e.g., expansions of $\eta_\nu = \Delta_\nu/\Delta_\nu^0 - 1$, $\nu = 2, 3, \ldots$. We assume that $|\eta_\nu(k\to\infty)| < 1$. To obtain such an expression systematically, we set up a discrete process as follows. In the first order, $\eta_2 = \eta_3 = \ldots = 0$. In the second order, $\eta_2 \neq 0$; $\eta_3 = \eta_4 = \ldots = 0$. In the third order, $\eta_2, \eta_3 \neq 0$; $\eta_4 = \eta_5 = \ldots = 0$, etc†. Retaining only linear terms of the η_ν, we find the following expansions of $H_k(\omega)$ for $\boldsymbol{k} \to \infty$:

$$H_k^{(1)}(\omega) = 0 \tag{24a}$$

$$H_k^{(2)}(\omega) = -Q\eta_2/v_k|\chi_k^0| \tag{24b}$$

$$H_k^{(3)}(\omega) = -Q(\eta_2 - \eta_3)/v_k|\chi_k^0| \tag{24c}$$

$$H_k^{(4)}(\omega) = -Q(\eta_2 - \eta_3 + \eta_4)/v_k|\chi_k^0| \tag{24d}$$

where

$$Q \equiv Q_k(\omega) = 1/\tilde{\chi}_k^0(\omega) + \omega^2/\Delta_1^0 - 1. \tag{25}$$

Each expansion has a common factor $Q/v_k|\chi_k^0|$. We first consider the asymptotic behaviour of Q defined by (25). For $\boldsymbol{k} \to \infty$, one can show that

† There are no truncations in this expansion, i.e., $b_1(z)$ and $b_1^0(z)$ are still infinite continued fractions. For a comparison, see [14].

$\tilde{\chi}_k^0(\omega) \equiv \chi_k^0(\omega)/\chi_k^0 = 1 + \omega^2/k^4 + O(k^{-6})$ and $\Delta_1^0 = k^4(1 + O(k^{-2}))$, where ω and k are expressed in dimensionless units†. Hence, from (25) we have

$$\lim_{k\to\infty} Q_k(\omega) = O(k^{-6}).$$

Also, $v_k|\chi_k^0| = O(k^{-4})$. Hence, the common factor behaves as

$$\lim_{k\to\infty} Q_k(\omega)/v_k|\chi_k^0| = O(k^{-2}). \tag{26}$$

We next examine the η_ν. For $k\to\infty$, one can express them as $\eta_\nu = p_\nu + q_\nu k^{-2} + \ldots$, where p_ν and q_ν are constants depending only on such parameters as r_s. Now, $p_\nu = 0$ if ν is odd. But $p_\nu = p = T/T^0 - 1$ if ν is even. For $1 < r_s < 5, p \simeq 0.04$–$0.3$. See the second reference of [6]. Every $H_k^{(\nu)}(\omega)$ consists of terms each of which thus behaves as $O(k^{-2})$. Hence, every $H_k^{(\nu)}(\omega)$ vanishes asymptotically with k. We may, therefore, conclude that, at this limit, the frequency-dependent part makes no contributions at all, and

$$\lim_{\omega\to\infty}\lim_{k\to\infty} G_k(\omega) = G_{k\to\infty}. \tag{27}$$

A similar argument may be used to arrive at the same conclusion for classical systems. Now for $k\to\infty$, we can use the form of G_k given in [2, 16]‡. Thus,

$$G_{k\to\infty} = \lim_{k\to\infty} N^{-1}\sum_q [1 - S(k-q)](k\cdot q)/q^2 = 1 - g(0). \tag{28}$$

We recover Shaw's relation [7]. It follows since the assumption $G_k(\omega) = G_k$ is valid at the limit $k\to\infty$ [7].

From (20) and (27) we observe that the order of the two limiting processes is not interchangeable. A system, in a non-weak or strong coupling regime, responds asymmetrically to the order of probes involving very rapid variations in space and time. It does not respond in a free-particle-type manner as some have argued [8].

Our conclusion can be put to a test for one exactly solvable system: a 2D classical single-component plasma gas with a logarithmic potential, i.e., $v_k = 2\pi e^2/k^2$. At $\Gamma \equiv e^2/kT = 2$ (non-weak coupling regime), there is a remarkable result due to Jancovici [17] that $g(r) = 1 - \exp(-r^2)$, hence $S(k) = 1 - \exp(-k^2/4)$, where r and k are given in dimensionless units. For this system at $\Gamma = 2$, it is possible to construct $G_k(\omega)$ which satisfies the third frequency-moment and compressibility sum rules simultaneously [18]. Furthermore, I_k and G_k can be calculated exactly§

$$I_k = \tfrac{1}{2} - (2/k^2)(1 - e^{-k^2/4}) \tag{29}$$

$$G_k = 1 - (k^2/4)(e^{k^2/4} - 1)^{-1}. \tag{30}$$

Recalling that $\delta T = 0$ for a classical system, we obtain from (20) and (27)

$$\lim_{k\to\infty}\lim_{\omega\to\infty} G_k(\omega) = I_{k\to\infty} = \tfrac{1}{2} \tag{31}$$

$$\lim_{\omega\to\infty}\lim_{k\to\infty} G_k(\omega) = G_{k\to\infty} = 1. \tag{32}$$

† With k and ω given in units of k_F and ε_F, respectively, we can express $\chi_k^0(\omega) \equiv \chi(k;\omega)$ as follows: $\chi(k;\omega) = (\frac{1}{2} + \omega/k^2)\chi(k + 2\omega/k) + (\frac{1}{2} - \omega/k^2)\chi(k - 2\omega/k)$, where $\chi(k;0) = \chi(k)$. Now if $k\to\infty$, $|\chi(k)| = (2n/\varepsilon_F)k^{-2} + O(k^{-4})$. See [15]. Hence, for $k\to\infty$, $\chi(k,\omega)/\chi(k) = 1 + \omega^2/k^4 + O(k^{-6})$. Also, $\Delta_1^0 = \|f_1\|^0/\|f_0\|^0 = (nk^2/m)/|\chi_k^0| = \varepsilon_F^2 k^4[1 + O(k^{-2})]$.

‡ A rigorous expression for G_k has been given in terms of the pair and triple correlation functions [16]. See equation (21) of [16], and also see equation (2.71) of [3]. With this expression it is possible to argue that contributions from the triple correlation functions vanish if $k\to\infty$. Then the remainder becomes exactly the form due to [2].

§ (29) has also been obtained [19]. See also [20].

The above results are in exact agreement with the predictions of Niklasson's [8] and Shaw's [7] relations (with $s_D = \frac{1}{2}$ and $g(0) = 0$)†.

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† For $S(k) = 1 - \exp(-k^2/4)$, $k^{-1} = 0$ is an essential singular point. Hence, $S(k)$ may not be expanded in powers of k^{-1}. The well known relation, $g'(0) = 1/(8\pi n) \lim k^4(1 - S(k))$ in 3D, or $1/(2\pi n) \lim k^3(1 - S(k))$ in 2D, is obtained under the assumption that such an expansion is permitted. Hence, this relation does not apply to a 2D one-component classical plasma with a logarithmic potential at $\Gamma = 2$. Since Coulomb interactions are a source of exponential terms, one cannot assume that this relation is applicable to Coulomb systems in general.