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Collective phenomena in a quasi-classical electron fluid within the interpolational self-consistent method of moments

S. A. Syzganbayeva[1(a)], J. Ara[2], A. Askaruly[1], A. B. Ashikbayeva[1], I. M. Tkachenko[3,1] and Y. V. Arkhipov[1]

[1] *Al-Farabi Kazakh National University - al-Farabi ave., 71, 050040, Almaty, Kazakhstan*
[2] *Instituto de Tecnología Química, Universitat Politècnica de València-Consejo Superior de Investigaciones Cientificas Camino de Vera s/n, 46022, Valencia, Spain*
[3] *Departament de Matemàtica Aplicada, Universitat Polièchica de València - Camino de Vera s/n, 46022 Valencia, Spain*

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Abstract – Collective processes in a quasi-classical electron gas are investigated within the framework of the interpolational self-consistent method of moments, which makes it possible to express the dispersion and decrement of plasma waves, and the dynamic structural factor of the system exclusively in terms of its static structural factor so that five sum rules are satisfied automatically. Different models are used of the static structure factor; the stability and robustness of the results of the moment approach taking into account the accuracy of these models is confirmed and tested by comparison to the alternative molecular dynamics simulation data.

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Introduction. – Recently, one observes a growing interest in the study of warm dense matter, an exotic state at the boundary between condensed matter and plasmas. The gas of interacting electrons, enclosed in a homogeneous positive background, is the basic theoretical model of such a system. Despite its apparent simplicity, it offers many interesting effects, such as collective excitations and the Wigner crystallization at lower densities. Interest in such a system arose at least due to its detection in astrophysical objects [1] and its creation in the context of the inertial confinement fusion caused by laser pulses [2].

The uniform electron gas (UEG) can be created in a laboratory [3], and many encouraging theoretical results have been achieved in recent years [4,5]. On the other hand, there have been productive attempts to describe the dynamical characteristics of model plasmas using various numerical modelling techniques [6,7]. Significant progress has been achieved lately using the *ab initio* path-integral Monte Carlo simulation method, see [8,9] and references therein. However, due to the long-range interactions, thermal excitations, quantum degeneracy, and the Coulomb scattering, scarce attention has been paid to the dynamical properties of UEG from the theoretical point of view.

(a) E-mail: syzganbaeva.saule1@gmail.com (corresponding author)

It is significant that dense warm electron gas is characterized by the values of the coupling

$$\Gamma = \frac{\beta e^2}{a} \tag{1}$$

and degeneracy

$$\theta = \frac{k_B T}{\mathrm{E}_F} = 2\left(\frac{4}{9\pi}\right)^{\frac{2}{3}} \frac{r_s}{\Gamma} \tag{2}$$

parameters varying around unity, so that standard perturbative methods are not applicable for its description.

In the previous equations $a = (3/4\pi n)^{1/3}$ is the Wigner-Seitz radius, n is the density of electrons, $\beta = 1/k_B T$ is the inverse temperature in energy units, E_F is the Fermi energy of the electrons, r_S is the Brueckner parameter.

Important information about the nature of the electron gas can be extracted from the system dielectric function and its dynamic structural factor. For ideal plasmas the coupling parameter $\Gamma \ll 1$, *i.e.*, at low densities and/or sufficiently high temperatures, the random-phase approximation (RPA) [10] gives reliable results for the dielectric function, since the kinetic energy is dominant. In contrast, for electron densities corresponding to those of the conduction band in real metals, the average kinetic and potential energies of the electrons are of the same order of magnitude, and the plasma is moderately coupled so that $\Gamma \sim 1$.

Under these conditions, RPA gradually becomes inapplicable since exchange and correlational corrections to RPA cannot be accurately calculated, although several approximate expressions of the dielectric function have been proposed [11,12]. This is why an analytical description of the dynamical properties of dense quasi-classical Coulomb systems within an alternative non-perturbative mathematical approach is proposed that can automatically take into account the converging sum rules.

The moment approach is based on solving the Hamburger problem of the theory of moments [13]. Power moments of the dynamic structural factor in a classical fluid are actually sum rules that must be satisfied at arbitrary values of the above coupling and degeneracy parameters corresponding to the classical statistics conditions. The essence of the moment approach is that the moments can be calculated independently from the static structural factor (SSF) or the radial distribution function (RDF), and with an appropriate choice of the Nevanlinna parameter function, which possesses certain mathematical properties, the values of the dynamic structure factor (DSF) can be reconstructed, see [14] and references therein. Reducing the calculation of the DSF to the knowledge of static characteristics (SSF or RDF) only means, in our opinion, the self-consistency of the moment approach. In previous works, in particular in [15], we emphasized that the reliability of the proposed approach in relation to the accuracy of the employed data on the static structural factor required further study. In 2020 we showed that the moment approach in classical one-component plasmas is robust with respect to the precision of the input static data. It remains to be seen whether it is true in a quasi-classical or partly degenerate electron gas or other Fermi systems of charged particles. Here the "classical" stability is confirmed by comparison with alternative quasi-classical molecular-dynamics data of [16], where the exchange and other quantum effects were indirectly reflected through a specific pseudopotential. Such an approach is presumably unable to reproduce consequences of purely quantum characteristics of a Fermi system correctly directly described by the quantum Monte Carlo method [8]. Simulations in [16] were carried out at $\theta = 50$ so that from the point of view of statistics, the system modelled there can be approximately treated as a classical one. Application of the self-consistent method of moments to the description of the dynamical properties of a quantum UEG is beyond the scope of the present work. Here we wish to confirm the robustness of the moment approach in quasi-classical systems of charged particles. In other words, we want to demonstrate that to describe in a satisfactory way the dynamical properties of quasi-classical one-component plasmas in a wide range of variation of the coupling parameter Γ, it is sufficient to abandon not only the laborious method of hyper-netted chains modified by the bridge function, but even avoid cumbersome adjustments of these data given in the papers [17] and [18]. To this end, we employ a simple interpolation [19] of the results of numerical modeling of the static structural factor. We will show that the accuracy of these data is sufficient to obtain quite satisfactory results with respect to the UEG dynamical properties, especially concerning the characteristics of the collective modes in this model Coulomb system. A limited sensitivity of the dynamic properties, in particular, of the dispersion relations in classical one-component plasmas, was demonstrated previously in the long-wavelength regime within the quasi-localized charge approximation (QLCA) and its modifications/simplifications, please, see refs. [20–22].

Interpolational self-consistent method of moments. – The knowledge of the dynamic structure factor $S(q,\omega)$ permits to describe both electrodynamical and dynamical characteristics of the plasma. Due to the classical form of the fluctuation-dissipation theorem, DSF is directly related to the inverse dielectric function (IDF) of the system, $\varepsilon^{-1}(k,\omega)$,

$$-\frac{\operatorname{Im}\varepsilon^{-1}(k,\omega)}{\omega} = \frac{(2\pi e)^2\beta}{k^2}S(k,\omega). \tag{3}$$

On the other hand, within the framework of the method of moments, using Nevanlinna's theorem, the inverse dielectric (response or Nevanlinna) function

$$\varepsilon^{-1}(k,z) = 1 + \frac{\omega_p^2(z+Q)}{z\left(z^2-\omega_2^2(k)\right)+Q\left(z^2-\omega_1^2(k)\right)} \tag{4}$$

can be expressed in terms of the non-phenomenological Nevanlinna parameter function, $Q(k,z)$, which we approximate here, like in [23] and many other publications, by its static value $Q(k,0) = ih_0(k)$. On the assumption that DSF has an extremum at the zero frequency, the positive parameter $h_0(k)$ was expressed in [23] in terms of the characteristic frequencies $\omega_1(k)$ and $\omega_2(k)$:

$$h_0(k) = \frac{\omega_2^2(k)}{\sqrt{2}\omega_1(k)}. \tag{5}$$

The squares of the latter static characteristics are defined by the ratios of the DSF moments:

$$\omega_1^2(k) = \frac{C_2(k)}{C_0(k)}, \quad \omega_2^2(k) = \frac{C_4(k)}{C_2(k)}, \tag{6}$$

$$C_v(k) = (1/n)\int_{-\infty}^{\infty}\omega^v S(k,\omega)\mathrm{d}\omega, v = 0,2,4. \tag{7}$$

The zero moment is obviously equal to the static structure factor (SSF), $C_0(k) = S(k)$, whereas the second moment is the f-sum rule:

$$C_2(k) = \omega_p^2\left(\frac{k^2}{k_D^2}\right), \tag{8}$$

where $\omega_p = \sqrt{4\pi ne^2/m}$ is the plasma frequency, $k_D = \sqrt{4\pi ne^2\beta}$ is the inverse Debye screening radius. The fourth moment in a classical one-component system has only three contributions:

$$C_4(k) = \omega_p^2\left(1+\frac{3k^2}{k_D^2}+U(k)\right), \tag{9}$$

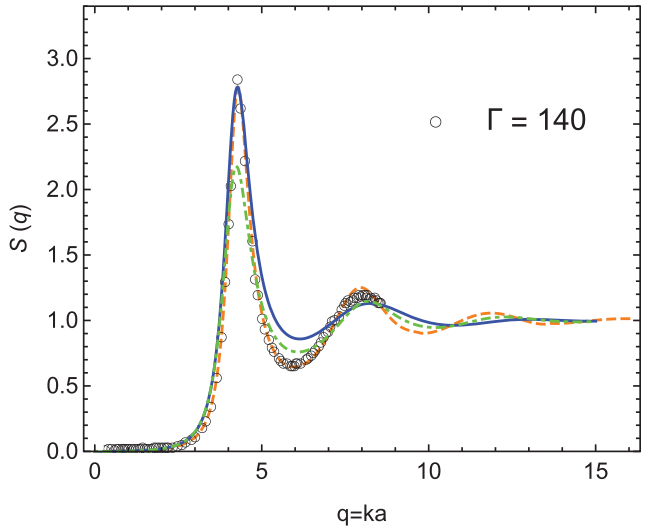

Fig. 1: The UEG static structure factor for $\Gamma = 140$. The blue (solid) line corresponds to the interpolation of [19], green (dot-dashed) and orange (dashed) lines represent the results of HNC [15] and of the modified HNC (MHNC) [24] approximations, respectively, while the circles are the results of the molecular-dynamics simulations [18].

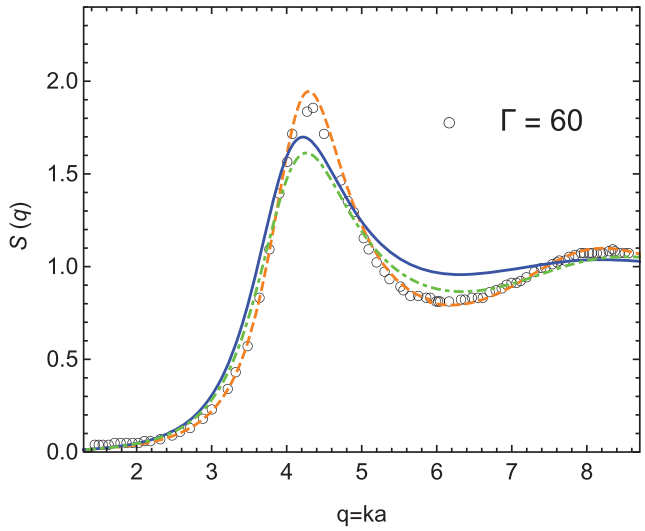

Fig. 2: As in fig. 1 but for $\Gamma = 60$.

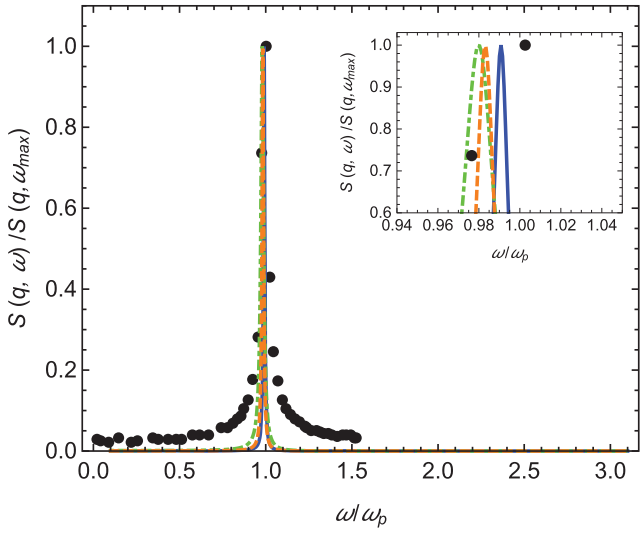

Fig. 3: The dynamic structure factor normalized to its maximum value at $\Gamma = 100$, $\theta = 50$, $q = ka = 0.619$, obtained within the present approach using different SSF data: the green (dot-dashed) line corresponds to the results of HNC [15], the blue (solid) line corresponds to the interpolation formalism of [19], and the orange (dashed) line to the modified HNC (MHNC) [24], in comparison with the modelling data [16] (circles).

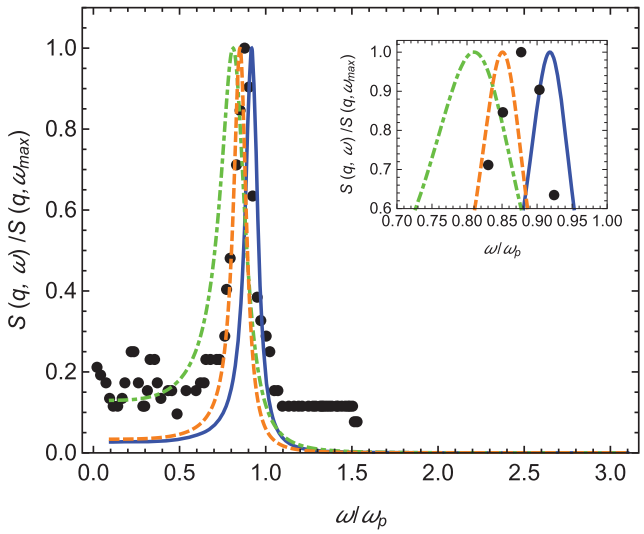

Fig. 4: As in fig. 3, but for $q = ka = 1.856$.

where

$$U(k) = \frac{1}{4\pi^2 n}\int_0^\infty [S(p) - 1]\, f(p;k)\, p^2 \mathrm{d}p, \qquad (10)$$

is due to the interparticle correlations with

$$f(p;k) = \frac{5}{6} - \frac{p^2}{2k^2} + \left(\frac{p^3}{4k^3} - \frac{p}{2k} + \frac{k}{4p}\right)\ln\left|\frac{k+p}{k-p}\right|, \qquad (11)$$

being the angular-averaging factor, while the second contribution in (10) is the kinetic one. The precision of the SSF data influences the level of quantitative agreement of our results with the DSF simulation data. Here we analyze the influence on our results of three different approaches to the calculation of plasma SSFs $S(k)$ in (10), including both theoretical (the hyper-netted chain approximation (HNC)) [15], the modified HNC (MHNC) [24] and those based on the fitting of precalculated data [19]. In what follows we present graphical material which demonstrates that except for the higher wave number values, little discrepancy is observed for the plasma dynamic characteristics calculated with the SSF data obtained within these approaches. This stability supports the idea of the robustness of the present model. In fig. 1 and fig. 2 various model SSF graphs are displayed in comparison to the simulation data of [16].

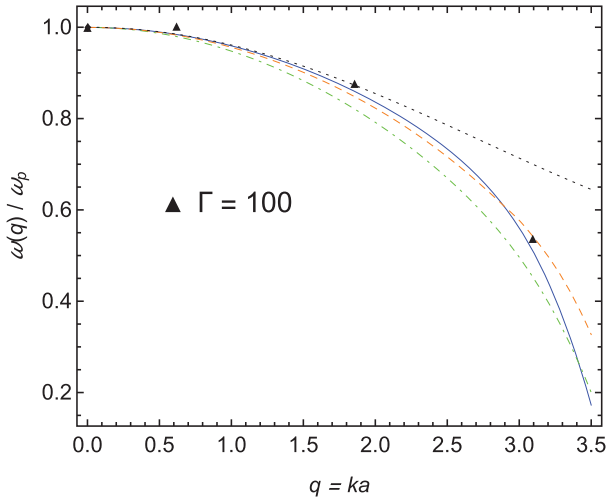

Fig. 5: Dispersion of plasma waves (15) within the framework of the self-consistent method of moments with the SSF data taken from the interpolation formalism [19] (blue solid line), found in the HNC [15] (green dot-dashed line) and MHNC [24] (orange dashed line) approximations and the results obtained using eq. (10) from ref. [20] with the parameter R estimated as $R \sim 1.09545$ [20] (black dotted line), in comparison to the modelling data taken as the DSF maxima positions [25] (triangles).

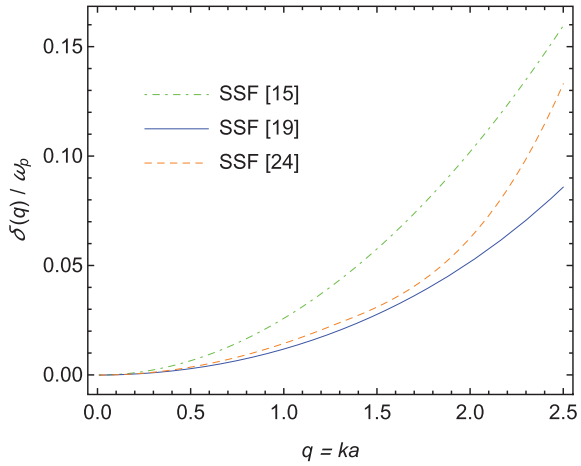

Fig. 6: The plasma wave decrement (15) calculated within the present approach for $\Gamma = 100$.

Dynamic structure factor (DSF). – Within the moment approach, we can construct DSF using the Nevanlinna formula [14,26,27]:

$$S(k,z) = -n\frac{E_3(\omega;k) + Q(k,\omega)E_2(\omega;k)}{D_3(\omega;k) + Q(k,\omega)D_2(\omega;k)}. \qquad (12)$$

Here the polynomials $D_j(z;k), j = 0,1,2,3$ are orthogonal with the weight $S(k,z)$, and the corresponding conjugate polynomials $E_j(z;k), j = 0,1,2,3$, are determined as

$$E_j(z;k) = \int_{-\infty}^{\infty} \frac{D_j(\omega;k) - D_j(z;k)}{\omega - z} S(k,\omega)\mathrm{d}\omega. \qquad (13)$$

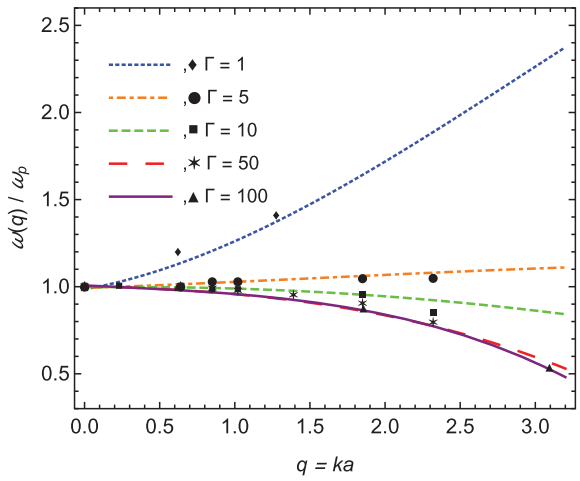

Fig. 7: Plots of the dispersion of plasma waves obtained from (A.1) in comparison with numerical simulation data [25].

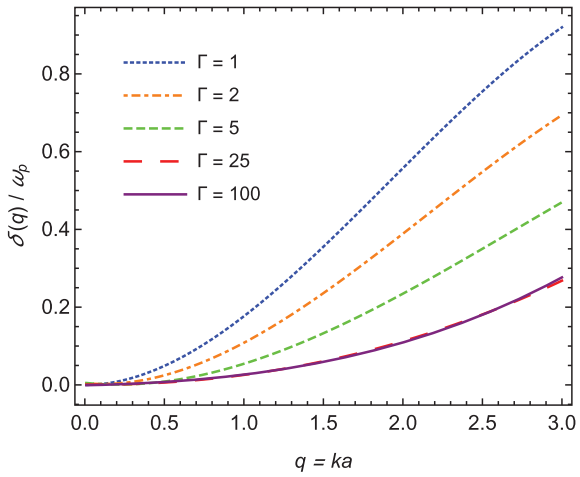

Fig. 8: Plots of the decrement of plasma waves obtained from (A.2).

Moreover, all these polynomials have real coefficients, and their real zeros alternate. The standard Gram-Schmidt procedure with the same weight applied to the basis of the space of polynomials $\{1, z, z^2, \ldots\}$, leads to the following explicit form for these polynomials independent of the DSF:

$$D_0(z;k) = 1, \quad D_1(z;k) = z, \quad D_2(z;k) = z^2 - \omega_1^2(k),$$
$$D_3(z;k) = z^3 - z\omega_2^2(k), \quad E_0(z;k) = 0, \quad E_1(z;k) = C_0(k),$$
$$E_2(z;k) = C_0(k)z,$$
$$E_3(z;k) = C_0(k)\left[z^2 + \omega_1^2(k) - \omega_2^2(k)\right].$$

Therefore, the DSF found from eq. (12) takes the following form [14]:

$$S(k,\omega) = \frac{n}{\pi}\lim_{\eta\downarrow 0}\mathrm{Im}\, S(k,\omega+i\eta) = \frac{n}{\pi}\frac{S(k)\omega_1^2\left(\omega_2^2-\omega_1^2\right)h_0(k)}{\left[\omega\left(\omega^2-\omega_2^2\right)\right]^2 + \left[h_0(k)\right]^2\left(\omega^2-\omega_1^2\right)^2}. \qquad (14)$$

The graphs of the dynamic structure factor calculated within the framework of the interpolational self-consistent method of moments at different values of the coupling parameter $\Gamma = 100$ are presented in fig. 3 and fig. 4 in comparison with the numerical modeling results of [16]. Notice that comparison with these data, as far as we know, has not been carried out earlier.

Dispersion of plasma waves. – One of the advantages of the self-consistent method of moments is that it permits to investigate the properties of collective modes in an electron gas analytically, including, in the five-moment case, even using Cardano's formulas. Precisely, we can solve the cubic dispersion equation stemming from (4) and the approximation (5),

$$z\left(z^2 - \omega_2^2(k)\right) + ih_0(k)\left(z^2 - \omega_1^2(k)\right) = 0. \qquad (15)$$

The real parts of the three solutions of eq. (15) provide the dispersion of the modes, and the imaginary parts give the decrements of the modes. Observe that the Rayleigh mode is located at the zero frequency, and we focus here on the plasma mode, see figs. 5–8. Figure 5 shows that as the coupling parameter increases, the weight of the negative correlation contribution in (10) increases and the dispersion of plasma waves becomes negative. It is also worth noting that the static characteristics taken from [19] provide reliable results for the calculation of DSF for $\Gamma < 100$ as well. Considering the opportunities for further studies, interpolation formulas are constructed for both the dispersion and the decrement of the plasma waves, see appendix.

Conclusion. – We present the self-consistent interpolational method of moments and show that to describe collective processes in a quasi-classical one-component plasma in a wide range of variation of the coupling parameter Γ, it is sufficient to use the data of the interpolation [19] of the static structure factor numerical modelling results. Thus, the robustness of the results of the moment approach with respect to the accuracy of the static input data is demonstrated.

* * *

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Data availability statement: The data generated and/or analysed during the current study are not publicly available for legal/ethical reasons but are available from the corresponding author on reasonable request.

Appendix

These are the interpolation formulae for the dispersion and the decrement of the quasi-classical UEG plasmon mode valid for $\Gamma \in [1, 150]$ and $q \in [0, 3.1]$:

$$\begin{aligned}\omega(\Gamma, q) = {} & \left(-0.01553q^3\right) + \left(-0.00288q^3 \ln\left(\Gamma^2\right)\right) \\ & + \left(0.01338q^3 \ln(\Gamma)\right) + \left(0.13707q^2\right) \\ & + \left(0.02093q^2 \ln\left(\Gamma^2\right)\right) \\ & + \left(-0.11324q^2 \ln(\Gamma)\right) \\ & + \left(-0.00049q^2 \ln\left(\Gamma^3\right)\right) \\ & + \left(-0.00001\Gamma^2 q\right) + (0.15192q) \\ & + (-0.14533q \ln(\Gamma)) \\ & + \left(0.05201q \ln\left(\Gamma^2\right)\right) \\ & + \left(-0.00890q \ln\left(\Gamma^3\right)\right) \\ & + (0.00279q\Gamma) + (0.00492 \ln(\Gamma)) \\ & + (0.98468); \end{aligned} \qquad (A.1)$$

$$\begin{aligned}\delta(\Gamma, q) = {} & \left(0.00051 \ln\left(\Gamma^3\right)\right) + \left(-0.03716q^3\right) \\ & + \left(-0.00201q^3 \ln\left(\Gamma^2\right)\right) + \left(0.01840q^3 \ln(\Gamma)\right) \\ & + \left(-0.07158q^2 \ln(\Gamma)\right) + \left(0.00132q^2 \ln\left(\Gamma^3\right)\right) \\ & + \left(-0.00434 \ln\left(\Gamma^2\right)\right) + \left(0.21369q^2\right) \\ & + (0.00901 \ln(\Gamma)) \\ & + \left(-0.00443q \ln\left(\Gamma^3\right)\right) \\ & + \left(0.036989q \ln\left(\Gamma^2\right)\right) \\ & + (-0.07431q \ln(\Gamma)). \end{aligned} \qquad (A.2)$$

These interpolations obtained from the solutions of eq. (15) using the static structure factor of [19] predict the onset of the negative dispersion at $\Gamma = 8.6$, which is in a reasonable agreement with the known results. Since these interpolations are valid in a wide range of variation of the parameters Γ and q, they do not permit to localize the onset value of the coupling parameter with a higher level of precision. It is also clear that this value depends on the precision of calculation of the static structure factor.

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