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СРАВНИТЕЛЬНЫЕ РАСЧЕТЫ ДИНАМИЧЕСКИХ ХАРАКТЕРИСТИК ПЛАЗМЫ С ИСПОЛЬЗОВАНИЕМ РАЗЛИЧНЫХ МОДЕЛЕЙ ДИЭЛЕКТРИЧЕСКОЙ ФУНКЦИИ

А.Б. Ашикбаева, А. Аскарулы, Д.Ю. Дубовцев

Проведен сравнительный анализ электродинамических характеристик модельной двухкомпонентной водородной плазмы, как в рамках моментного непертурбативного подхода, так и с использованием формализма диэлектрической функции (ДФ) Мермина. Исследованы динамические структурные факторы (ДСФ), дисперсия и диссипация плазменных волн, распространяющихся в плазме. Полученные в моментном приближении результаты показывают хорошее количественное и качественное согласие с данными моделирования молекулярной динамики, в отличие от модели Мермина.

Ключевые слова: двухкомпонентная плазма; метод моментов; динамическая частота столкновения; диэлектрическая проницаемость; динамический структурный фактор.

ДИЭЛЕКТРДИК ФУНКЦИЯНЫН АР ТҮРДҮҮ МОДЕЛДЕРИН КОЛДОНУУ МЕНЕН ПЛАЗМАНЫН ДИНАМИКАЛЫК МҮНӨЗДӨМӨЛӨРҮНҮН САЛЫШТЫРМА ЭСЕБИ

А.Б. Ашикбаева, А. Аскарулы, Д.Ю. Дубовцев

Бул макалада моделдүү эки компоненттүү суутек плазмасынын электродинамикалык мүнөздөмөсүнө пертурбативдүү эмес учур ыкмасынын алкагында, ошондой эле Мерминдин диэлектрдик функциясынын формалдуулугун пайдалануу менен салыштырма талдоо жүргүзүлдү. Динамикалык түзүмдүк факторлор, плазмада таркалуучу плазма толкундарынын дисперсиясы жана диссипациясы изилдөөгө алынды. Бир учур жакындоодон алынган натыйжалар Мерминдин моделине караганда молекулярдык динамиканын моделдөө маалыматтары менен сапаттык жана сандык жакшы шайкештигин көрсөттү.

Түйүндүү сөздөр: эки компоненттүү плазма; учур ыкмасы; кагылышуулардын динамикалык жыштыгы; диэлектр дик өткөргүчтүк; динамикалык түзүмдүк фактор.

COMPARATIVE CALCULATION OF DYNAMIC CHARA CTERISTICS OF MODERATELY COUPLED PLASMAS USING DIFFERENT DIELECTRIC FUNCTION MODELS

A.B. Ashikbayeva, A. Askaruly, D.Yu. Dubovtsev

A comparative analysis of the electrodynamic characteristics of a model twocomponent hydrogen plasma is carried out, both within the moment non-perturbative approach and using the Mermin dielectric function (DF) formalism. Dynamic structural factors (DSFs), dispersion and dissipation of plasma waves propagating in a plasma have been studied. The results obtained in the moment approximation show good quantitative agreement with the molecular-dynamics simulation data.

Keywords: two-component plasmas; method of moments; dynamic collision frequency; dielectric permeability; dynamic structure factor.

Introduction. Dense plasmas are found in various astrophysical objects (white dwarfs, neutron stars) [1], and in several experimental facilities (electrolytes, colloidal systems, dusty plasma, etc.) [2, 3]. In this case, the potential energy of the interparticle interaction is usually greater than or equal to the thermal energy of motion of the plasma particles. The dielectric properties of plasmas are usually investigated using both numerical simulations and theoretical approaches using various interparticle interaction potentials. Numerical methods using the *ab initio* approach provide direct access to

the investigation of collective processes described by the dynamic structural factors [4, 5].

Advanced theoretical research methods include the quasi-localized charge approximation method (QLCA), which allows calculating the dispersion of plasma waves, while the question of the dissipation of the latter remains open [6]. In a dense plasma medium, when correlations between charged particles become significant compared with the kinetic characteristics of the particles, that is, when there are no small parameters in the system, the question arises about the quality of the applied dielectric function (DF) models. In this paper, we compare dielectric functions calculated using the moment method [7] and the Mermin model [8].

In [7, 9], a theoretical approach was proposed based on the nonperturbative method of moments [10], the basic relations of which satisfy the sum rules and other exact relations. Knowledge of the moments of the sought functions and static characteristics allows us to find and investigate the dynamic properties of a dense plasma. In accordance with the results of [11], the method of moments used in the present work does not require preliminary knowledge of the experimental or simulation data under study and allows us to find a parametric function that is used for calculations within the method of moments from certain physical considerations.

By calculating the dynamic structure factor (DSF) of a two-component nonideal plasma, using, inter alia, the ideas developed in [11], it is possible to compare them with available simulation data. In the present work, we use both dynamic and static models for the so-called Nevanlinna parameter function, obtained in the framework of [12], which turned out to be quite productive for calculating the DSF in the two-component model. From the analysis of the obtained relations, it is easy to see that the values obtained for the DPF are quite close to the experimental results [4].

On the other hand, the analysis of dynamic relations found within the framework of the formalism of the Mermin dielectric function shows their significant difference from both experimental results and in the values of the moments calculated in the framework of the method, which was noted earlier in [9].

Plasma parameters. In this paper, we study a two-component fully ionized hydrogen plasma, which is described by the dimensionless parameters of nonideality, density, and degeneracy:

$$\Gamma = \frac{\beta e^2}{a}, \quad \beta = \frac{1}{k_B T}, \; r_s = \frac{a}{a_0}$$

$$\theta = \frac{1}{\beta E_F} = 2\left(\frac{4}{9\pi}\right)^{2/3} \frac{r_s}{\Gamma}$$

The Wigner-Seitz radius $a = \sqrt[3]{3/4\pi n}$, is introduced here along the elementary charge e, the Boltzmann constant k_B, temperature T, number density of particles n (we presume that the densities of electrons and ions coincide, $n_e = n_i$), the Bohr radius a_0, and the system Fermi energy E_F.

In this work we use the Deutsch interaction potential is used, which takes into account the quantum-mechanical effect of diffraction,

$$\Phi_{ab}(r) = \frac{e_a e_b}{r}\left[1 - \exp\left(-\frac{r}{\lambda_{ab}}\right)\right]. \qquad (1)$$

Here e_a, e_b are the charges of particles of the species a and b, respectively, $\lambda_{ab} = \hbar/\sqrt{\pi\mu_{ab}k_B T}$ being the distance between them, $\lambda_{ab} = \hbar/\sqrt{\pi\mu_{ab}k_B T}$ is the de Broglie wavelength, $\hbar$ is the Planck constant, and $\mu_{ab} = \frac{m_a m_b}{m_a + m_b}$ is the reduced mass.

Method of moments. The method of moments allows one to determine the dielectric properties of the Coulomb system using the first few power frequency moments of the loss function $L(k,\omega)$,

$$C_\nu(k) = \frac{1}{\pi}\int_{-\infty}^{\infty} \omega^\nu L(k,\omega) d\omega, \qquad (2)$$

which are the so-called sum rules [9]. They can be calculated independently, knowing the interparticle interaction potential and the partial static structural factors. The latter in turn can be found, for example from the solution of the Ornstein-Zernike equation in the hyper-netted chain approximation [13]. By definition, the loss function is related to the dielectric function as follows:

$$L(k,\omega) = -\frac{\mathrm{Im}\,\varepsilon^{-1}(k,\omega)}{\omega}. \qquad (3)$$

The inverse (longitudinal) dielectric function obtained in the framework of the method of moments, see [7], can be written as

$$\varepsilon^{-1}(k,\omega)=1+\frac{\omega_p^2(Q(k)+\omega)}{\omega(\omega^2-\omega_2^2(k))+Q(k)(\omega^2-\omega_1^2(k))}, \quad (4)$$

where $\omega_1^2(k)=C_2(k)/C_0(k)$, $\omega_2^2(k)=C_4(k)/C_2(k)$ and the Nevanlinna parameter function (NPF) can be defined, in the static approximation, as in [11]:

$$Q(k)=\frac{i}{\sqrt{2}}\frac{\omega_2^2(k)}{\omega_1(k)}. \quad (5)$$

The moments $C_v(k)$ are defined explicitly as

$$C_0(k)=\frac{k_{De}^2}{k^2}(Z_e^2S_{ee}(k)+Z_i^2S_{ii}(k)-2Z_iS_{ei}(k)),$$

$$k_{De}^2=4\pi n_e e^2\beta, \quad (6)$$

$$C_2=\omega_p^2, \quad (7)$$

$$C_4=\omega_p^4(\zeta_{ee}(q)+K(k)+U(k)+H), \quad (8)$$

where

$$K(k)=\frac{\langle\upsilon_e\rangle^2k^2}{\omega_p^2}+\left(\frac{\hbar}{2m}\right)^2\frac{k^2}{\omega_p^2},$$

$$H=-\frac{1}{6\pi^2n_e}\int_0^\infty q^2S_{ei}(k)\zeta_{ei}(k)dk,$$

$$U(k)=\frac{1}{16\pi^2n_e}\int_0^\infty q^2(S_{ee}(q)-1)\left(Z_{ee}(k,q)-\frac{8\zeta_{ee}(q)}{3}\right)d,$$

$$Z_{ee}(k,q)=\int_{q-k}^{q+k}\zeta_{ee}(p)\left(q^2-k^2-p^2\right)^2\frac{dp}{qk^3p}.$$

Here $\zeta_{ab}(q)$ is the formfactor of the interaction potential Fourier transform, $\Phi_{ab}(q)=\frac{4\pi e^2}{q^2}\zeta_{ab}(q)$, $\zeta_{ab}(q)=\zeta_{ba}(q)$, $\langle\upsilon_e^2\rangle=3\frac{\theta}{m\beta}F_{3/2}(\eta)$ is the averaged electron thermal velocity squared, m is the electron mass, ω_p is the system plasma frequency, and F_v is the Fermi integral, which is defined as

$$F_v(\eta)=\int_0^\infty\frac{x^v}{\exp(x-\eta)+1}dx;$$

$\eta=\beta\mu$ being the dimensionless chemical potential defined by the normalization condition:

$$F_{1/2}(\eta)=\frac{2}{3}\theta^{-3/2}.$$

Alternative dynamic NPF model. In addition to (5), we can use the dynamic NPF corresponding to the DF asymptotic form of Perel' and Eliashberg [14],

$$Q_2(k,\omega)=\frac{\sqrt{2}}{3^{5/4}}\frac{r_s^{3/4}\sqrt{\omega}(1+i)}{\omega_2^2(k)-\omega_1^2(k)}, \quad (9)$$

it was employed in the article [12] to reproduce the simulation data of [4].

Mermin's dielectric model. On the other hand, in ideal plasmas the random-phase approximation (RPA), can de used with the electronic dielectric function determined as in [15]:

$$\varepsilon_{RPA}(k,\omega)=\varepsilon_r(k,\omega)+i\varepsilon_i(k,\omega),$$

where the real part is written as

$$\varepsilon_r(k,\omega)=1+\frac{1}{4z^3\pi k_F}\left[g(u+z)-g(u-z)\right],$$

and the function $g(x)=\int_0^\infty\frac{ydy}{\exp(Dy^2-\eta)+1}\ln\left|\frac{x+y}{x-y}\right|$

and $D=\theta^{-1}$.

The imaginary part of the RPA DF is defined explicitly as

$$\varepsilon_i(k,\omega)=\frac{1}{8z^3k_F}\theta\ln\left[\frac{1+\exp\left(D\left[1-(u-z)^2\right]\right)}{1+\exp\left(D\left[1-(u+z)^2\right]\right)}\right].$$

The following traditional notations are introduced here: $u=\omega/k\upsilon_F$ and $z=k/2k_F$, υ_F, k_F stand for the Fermi velocity and wavenumber, $\upsilon_F=k_F$, $k_F=(3\pi^2n)^{(1/3)}$.

The collisionless one-component (usually electronic) dielectric permeability of Lindhard [16] was summarized by Mermin [8] and then by Das [17], who used an alternative method of variation of the distribution function to take into account collisions of charged particles:

$$\varepsilon_M(k,\omega)=1+\frac{(\omega+i\nu)\left[\varepsilon_{RPA}(k,\omega+i\nu)-1\right]}{\omega+i\nu\left[\varepsilon_{RPA}(k,\omega+i\nu)-1\right]/\left[\varepsilon_{RPA}(k,0)-1\right]}. \quad (10)$$

Here

$$\nu=\frac{2}{3}\sqrt{\frac{2\pi}{m}}\frac{e^4n}{(k_BT)^{3/2}}\Lambda \quad (11)$$

is the static collision frequency. To find it, it is necessary to know the generalized Coulomb logarithm, which can be determined in terms of the partial static structural factors $S_{ab}(k)$ (a, b define the species of the charged particles) using the Green – Kubo formula [13]:

$$\Lambda=\int_0^\infty\frac{dk}{k}\frac{S_{ee}(k)S_{ii}(k)-S_{ei}^2(k)}{(1+k^2\lambda_{ei}^2)^2}.$$

If in (10) instead of the constant collision frequency we use the so-called dynamic collision frequency (DCF), then the range of applicability of this expression expands and it can be used in dense non-ideal plasma, as it was done in the generalized

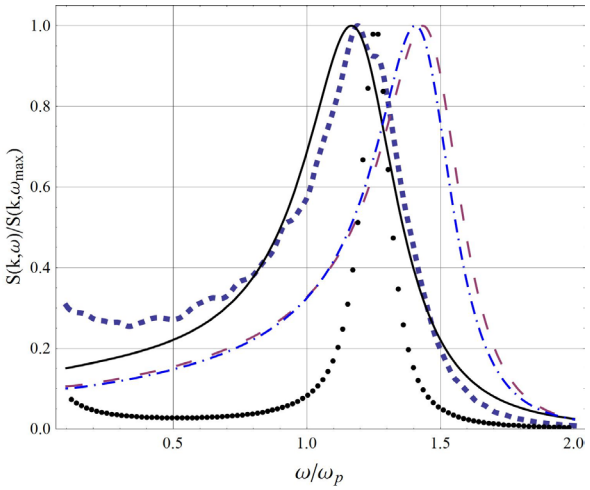

Fig. 1. The normalized dynamic structure factor "charge-charge" for $\Gamma = 1,\ r_s = 1,\ ka = 0.7795$

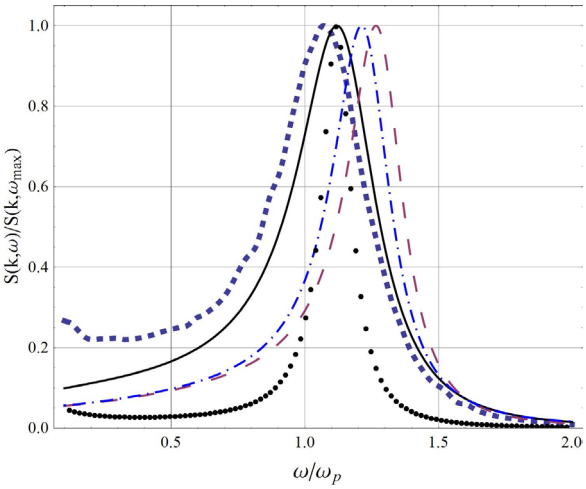

Fig. 2. As in Fig. 1 but for $\Gamma = 2,\ r_s = 2,\ ka = 0.7795$

Drude-Lorentz model for the two-component plasma (TCP) inverse dielectric function of [18].

In this paper, the DCF is calculated in the first Born approximation in terms of the ion-ion static structural factor [19]:

$$\nu(\omega) = \frac{n_i}{6\pi^2 m_e^2}\int_0^\infty q^6 V_{ei}^2(q) S_{ii}(q) \frac{\varepsilon_{RPA,e}(q,\omega) - \varepsilon_{RPA,e}(q,0)}{i\omega\omega_p^2} dq. \quad (12)$$

Here, n_i is the number density of ions and is the electron mass,

$$V_{ei}(q) = -\frac{4\pi e^2}{q^2 \varepsilon_{RPA}(q,0)}$$

is the Fourier transform of the electron-ion interaction potential statically screened by the electrons.

Dynamic structure factor. According to the fluctuation-dissipation theorem, we can write the following expression for the "charge-charge" dynamic structure factor:

$$S(k,\omega) = \frac{L(k,\omega)}{\pi\beta\phi(k)B(\beta\hbar\omega)}, \quad (13)$$

where $\phi(k) = 4\pi e^2 / k^2$, and the Bose factor $B(x) = (1 - \exp(-x))/x$ is always positive.

Substituting into (13) the expressions for the dielectric function obtained by the method of moments (4) or the Mermin dielectric function (10), we obtain the DSF *S (k, ω)*. The results are presented in Figures 1–3 in comparison with the simulation results of [4]. Precisely, the continuous lines were obtained by the method of moments with the static NPF (5), the black circles correspond to the method of moments but with the dynamic NPF (9), the blue squares stand for the simulation results of [4], the dash-dotted line was obtained with the Mermin DF with the dynamic collision frequency (12), while the dashed line displays the results found within the Mermin model but with the static collision frequency (11).

As it can be seen from the displayed results, our calculations of the dynamic structure factor using the method of moments with both static and dynamic models for the Nevanlinna parameter function, (5) or (9), respectively, have led to a good agreement with available simulation data of [4].

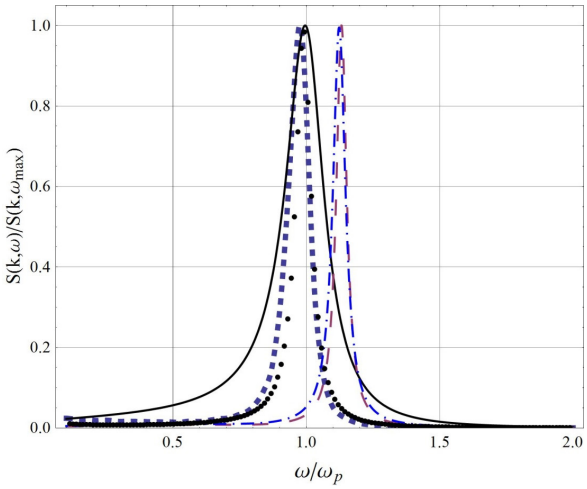

Fig. 3. As in Fig. 1 but for $\Gamma = 2,\ r_s = 0.5,\ ka = 0.3898$.

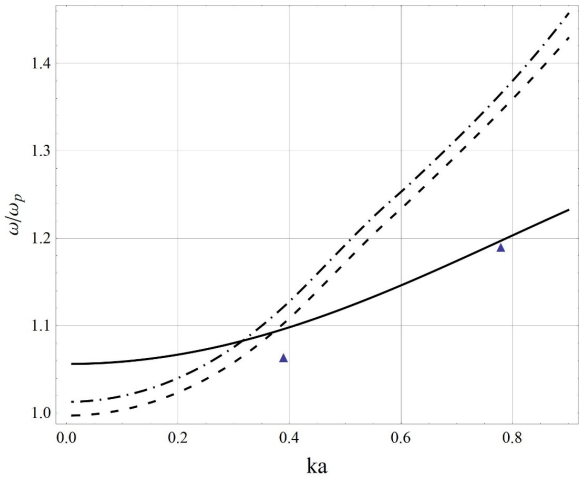

Fig. 4. The plasma waves dispersion.
The types of the lines are as in Fig. 1.
Triangles were obtained from the DSF data of [4]

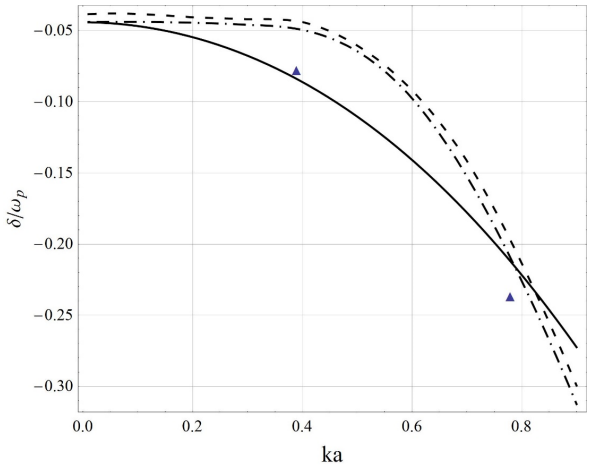

Fig. 5. The decrement of the plasma waves,
notations are as in Fig. 4, $\Gamma = 1,\ r_s = 1$.

On the other hand, the DSF calculations in the framework of the Mermin model either with the static or dynamic collision frequencies produced disagreement with the simulation data, specifically, with respect to the positions of the DSF maxima. We conclude that the method of moments, at least, for the above conditions, reproduces the data of numerical experiments better than the Mermin model.

Dispersion and decay of the plasma waves. The dispersion equation for the (longitudinal) plasma waves in a plasma medium can be written as:

$$\varepsilon(k,\omega) = 0\,. \qquad (14)$$

The roots of this equation (14) are complex, say, equal to $z = \omega + i\delta$, the real part of which represents the dispersion of the plasma waves, and the imaginary part indicates their dissipation.

When the decrement of the waves is relatively small, the dynamic structure factor allows determining the dispersion and dissipation of the plasma waves: from the positions of the DSF peaks on the frequency axis with fixed wavenumbers it is easy to determine the dispersion of the waves, and the half-width of the dynamic structure factor at half-height is proportional to the decrement of these waves.

Thus, based on the simulation data of [4], the above characteristics were determined and compared to the dispersion and decrement of the plasma waves found from the dispersion equation (14) using dielectric functions found by the method of moments (4) and the model proposed by Mermin (10).

The graphs presented in Figures 4 and 5 confirm that the results of the method of moments are in better agreement with the simulation data, than those found using the Mermin model.

The sum rules. This can also be verified by calculating the sum rules studied in detail in [9] for different models of the dielectric function. Notice that the second frequency moment of the loss function (the f – sum rule) normalized to the plasma frequency squared should be equal to unity, (7), and the fourth frequency moment satisfies the exact relation (8). The advantage of the moment method is that the inverse dielectric function (4) satisfies all convergent sum rules (6) – (8) automatically. The results of calculation of the sum rules are provided in Table 1, wherefrom it becomes clear that, as expected, the second sum rule (the second moment), both in the Mermin model and the method of moments are satisfied, while the values of the zero and the fourth moments obtained by the moment method and the Mermin model (8) do not coincide.

One of the important conditions for the loss function (3) stemming from different models of the dielectric function is compliance with the Cauchy-Schwarz inequality [7], which can be represented in terms of frequency moments as follows [20],

$$b(k) = \omega_2(k) - \omega_1(k) > 0\,. \qquad (15)$$

The function (15) is plotted in Figure 6 for the plasma parameters $\Gamma = 1,\ r_s = 1$.

Table 1 – The loss function power moments

Plasma parameters	The moments / DF	C_0	C_2/ω_p^2	C_4/ω_p^4	The fourth moment contributions (8)
$\Gamma = 1,\ r_s = 1,$ $ka = 0.7795$	Mermin's DF	0,8878	1	2,269	$\zeta_{ee} = 0{,}837$ $K = 0{,}835$ $U = -0{,}001$ $H = 0{,}184$
	DF, moments method	0,9997	1	1,855	
$\Gamma = 2,\ r_s = 2,$ $ka = 0.7795$	Mermin's DF	0,9420	1	1,988	$\zeta_{ee} = 0{,}837$ $K = 0{,}418$ $U = -0{,}0005$ $H = 0{,}375$
	DF, moments method	1,0693	1	1,629	
$\Gamma = 2,\ r_s = 0.5,$ $ka = 0.3898$	Mermin's DF	0,9236	1	2,232	$\zeta_{ee} = 0{,}837$ $K = 0{,}245$ $U = -0{,}0001$ $H = 0{,}051$
	DF, moments method	1,2337	1	1,134	

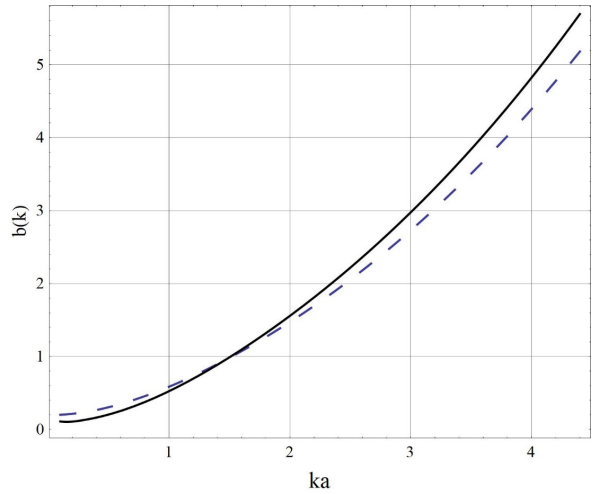

Fig. 6. Graphical analysis of the implementation of the Cauchy-Schwartz condition (15)

The fulfillment of the inequality (15), see Fig. 6, shows that both models analyzed in the present work, satisfy this important condition.

Conclusion. In this paper, using the method of moments and the Mermin model, we have described the dynamic structure factor, the dispersion and decay of the plasma waves in comparison with the results of numerical experiments [4]. From the results, which are reflected graphically (Figures 1–3, 4–5), it follows that the results obtained within the method of moments agree much better with the experimental ones than those obtained in the framework of the Mermin model. Apparently, this is due to the fact that Mermin DF does not satisfy the fourth sum rule, as it was shown in [9] and in the Table above. Nevertheless, it satisfies the Cauchy-Schwartz condition and the f – sum rule, which indicates its possible use in certain specific physical problems.

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