YU. V. ARKHIPOV[1], A.B. ASHIKBAYEVA[1], A. ASKARULY[1],

L. CONDE[2], A.E. DAVLETOV[1], I.M. TKACHENKO[3]

[1]Scientific-Research Institute of Experimental and Theoretical Physics,

al-Farabi Kazakh National University, Almaty, Kazakhstan;

[2]Departamento de Fsica Aplicada, ETSIA, Universidad Politécnica de Madrid, Madrid, Spain;

[3]Instituto de Matemática Pura y Aplicada, Universidad Politécnica de Valencia, Valencia, Spain

ON THE COLLISIONAL ONE-COMPONENT PLASMA DIELECTRIC FUNCTION

Summary

Asymptotic properties of the collisional one-component plasma dielectric function in the random-phase (RPA) and Mermin approximation, with a constant collision frequency, are analyzed from the point of view of the verification of sum rules. The latter are the power frequency moments of the loss function, a positive even function of frequency directly related to the imaginary part of the inverse dielectric function. The zero moment is shown to coincide with that of the RPA, the f-sum rule is satisfied, and the fourth moment sum rule is verified only partly, without taking the correlations into account. These drawbacks of the Mermin model expression for the dielectric function define the realm of applicability of this approximation.

Keywords: static structure factors, sum rules, method of moments.

Кілт сөздер: статикалық құрылымдық факторлар, қосындылар ережелері, моменттер әдісі.

Ключевые слова: статические структурные факторы, правила сумм, метод моментов.

Introduction. Modelling of the dielectric function $\varepsilon(k,\omega)$ (DF) or the inverse dielectric function, $\varepsilon^{-1}(k,\omega)$ (IDF) of Coulomb systems is actively discussed in the literature, in particular, because the corresponding loss function,

$$\mathcal{L}(k,\omega) = -\mathrm{Im}\varepsilon^{-1}(k,\omega)/\omega \geq 0, \qquad (1)$$

which is even for $\forall \omega \in \mathbb{R}$, determines the polarizational stopping power of such systems [1].

The Lindhard dielectric function [1] of a collisionless one-component plasma, $\varepsilon_{RPA}(k,\omega)$, was generalized by Mermin [2] and later, by Das [3] who used the distribution function variation method, to take the collisions into account in the relaxation-time approximation. Mathematical properties and different versions of the Lindhard DF were further considered in a number of elaborate publications, see e.g., [4, 5].

In the present work we study the asymptotic properties of the RPA and Mermin dielectric functions. Precisely, we wish to determine here whether the sum rules (other than the *f*-sum rule) are satisfied by these models.

Though the derivation of the Mermin dielectric function,

$$\varepsilon_M(k,\omega)=1+\frac{(\omega+i\nu)\left(\varepsilon_{RPA}(k,\omega+i\nu)-1\right)}{\omega+i\nu\dfrac{\varepsilon_{RPA}(k,\omega+i\nu)-1}{\varepsilon_{RPA}(k,0)-1}}, \tag{2}$$

guarantees the conservation of the local number of charged particles, this model is valid only in the first order in the total electrostatic potential energy and presumably cannot be applied to describe the properties of the plasma liquid phase at any corresponding value of the coupling parameter $\Gamma=\beta e^2/a$, where $\beta^{-1}=k_BT$ is the system temperature in energy units and $a=\sqrt[3]{3/4\pi n}$ is the Wigner-Seitz radius, *n* being the number density of charged particles, and at any degeneracy. Nevertheless, it is actively employed lately under extreme physical conditions, see, e.g., [6, 7].

The collision frequency ν is determined, e.g., by the Spitzer formula [6] or in the general Green-Kubo context [8]. We will be proceeded with the discussion of the influence of the dynamic collision frequency (see [7] and references therein) elsewhere.

1. **The asymptotic expansion and the sum rules.** Since the definition of the dielectric function of homoge-neous non-magnetized (multi-species) plasmas is just $\mathbf{D}(k,\omega)=\varepsilon(k,\omega)\mathbf{E}(k,\omega)$, and the «cause» is the external field/displacement $\mathbf{D}(k,\omega)$, the IDF is a genuine response function, i.e., the Kramers-Kronig relations are definitely valid for this function:

$$\varepsilon^{-1}(k,w)=1+\int_{-\infty}^{\infty}\frac{\operatorname{Im}\varepsilon^{-1}(k,\omega)}{\omega-w}\frac{d\omega}{\pi},\quad \operatorname{Im}w>0. \tag{3}$$

or, particularly,

$$\varepsilon^{-1}(k,0)=1+P\int_{-\infty}^{\infty}\operatorname{Im}\varepsilon^{-1}(k,\omega)\frac{d\omega}{\pi\omega}, \tag{4}$$

P standing for the principal value of the integral.

Consider the *convergent* sum rules for the IDF $\varepsilon^{-1}(k,w)$, which are effectively the first three finite non-zero power moments of the loss function [9]:

$$\begin{aligned} C_l(k) &= \frac{1}{\pi}\int_{-\infty}^{\infty}\omega^l \mathcal{L}(k,\omega)\,d\omega,\quad l=0,2,4,\\ C_0(k) &= 1-\varepsilon^{-1}(k,0),\quad C_2=\omega_p^2,\quad C_4(k)>0. \end{aligned} \tag{5}$$

Consider also the characteristic frequencies,

$$\omega_1(k) = \sqrt{C_2 / C_0(k)} = \omega_p / \sqrt{1-\varepsilon^{-1}(k,0)}, \quad \omega_2(k) = \sqrt{C_4(k)} / \omega_p . \tag{6}$$

It is important that the explicit forms of these characteristics can be derived independently of a particular DF or IDF model of an equilibrium plasma.

The expression for the zero moment follows immediately from (3) and (4):

$$C_0(k) = -\frac{1}{\pi}\int_{-\infty}^{\infty} \frac{\mathrm{Im}\,\varepsilon^{-1}(k,\omega)}{\omega} d\omega = 1-\varepsilon^{-1}(k,0) > 0. \tag{7}$$

Then, it is easy to see that

$$\varepsilon^{-1}(k,w) = \varepsilon^{-1}(k,0) + \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{\Lambda(k,\omega)\,d\omega}{1-\omega/w}, \tag{8}$$

and thus construct the IDF asymptotic expansion along any ray in the upper half-plane,

$$\varepsilon^{-1}(k, w\to\infty) \underset{w\to\infty}{\simeq} \varepsilon^{-1}(k,0) + \frac{1}{\pi}\int_{-\infty}^{\infty}\left(1+\frac{\omega}{w}+\left(\frac{\omega}{w}\right)^2+\cdots\right)\Lambda(k,\omega)\,d\omega = \tag{9}$$

$$= 1 + \frac{\omega_p^2}{w^2} + \frac{\omega_p^2\omega_2^2(k)}{w^4} + \cdots. \tag{10}$$

Within the RPA the static dielectric function is defined as

$$\varepsilon_{RPA}(k,0) = 1 + \frac{4}{\pi a_B k^3}\int_0^{\infty} p f_{FD}(p) \ln\left|\frac{k/2+p}{k/2-p}\right| dp.$$

Here a_B is the Bohr radius and $f_{FD}(p) = \left[\exp\left(\beta E(p) - \eta\right)+1\right]^{-1}$ is the Fermi-Dirac distribution density with $E(p) = \hbar^2 p^2/(2m)$. The dimensionless chemical potential $\eta = \beta\mu$ is defined by the normalization condition, $F_{1/2}(\eta) = \frac{2}{3}D^{3/2}$ with

$$F_\nu = \int_0^{\infty} \frac{x^\nu dx}{\exp(x-\eta)+1},$$

$$D = \beta E_F = \beta m \upsilon_F^2/2 = \beta\hbar^2 k_F^2/2m = \beta\hbar^2\left(3\pi^2 n\right)^{2/3}/2m, \tag{11}$$

where $F_\nu(\eta)$, E_F, υ_F, and k_F are the ν-th order Fermi integral, Fermi energy, velocity, and wavenumber, respectively.

In the Mermin approximation $\varepsilon_M(k,\omega=0)=\varepsilon_{RPA}(k,0)$, i.e., the zero sum rule is not satisfied since the static IDF $\varepsilon^{-1}(k,0)$ (related via the fluctuation-dissipation theorem to the system dynamic structure factor) takes the correlations into account while $\varepsilon_{RPA}(k,0)$ does not.

Notice also that the second moment is exactly the *f*-sum rule ($C_2=\omega_p^2$). We provide also an explicit expression for the 4$^{\text{th}}$ moment. In a coupled OCP (see [9] and references therein):

$$C_4(k)=\omega_p^4\left[1+W_0(k)\right], \tag{12}$$

and the correction of the fourth moment contains only two contributions:

$$W_0(k)=V(k)+U(k). \tag{13}$$

The first contribution is produced by the kinetic term of the system Hamiltonian, in the classical case $V(k)$ coincides with the known Vlasov contribution to the dispersion relation, $V_{cl}(k)=3k^2/\left(4\pi ne^2\beta\right)$. The second contribution to the fourth moment stems from the interaction contribution to the system Hamiltonian:

$$U(k)=\frac{1}{2\pi^2 n}\int_0^\infty p^2\left(S(p)-1\right)f(p,k)\,dp, \tag{14}$$

where we have introduced the angular factor $f(p,k)=\frac{5}{12}-\frac{p^2}{4k^2}+\frac{\left(k^2-p^2\right)^2}{8pk^3}\ln\left|\frac{p+k}{p-k}\right|$ and the static structure factor $S(k)$.

Let us now study the power moments of the OCP model dielectric functions.

The RPA dielectric function asymptotic form for $\mathrm{Im}\,w \geq 0$ was determined in [5]:

$$\varepsilon_{RPA}(k,w\to\infty)\simeq$$

$$\simeq 1-\frac{\omega_p^2}{w^2}\left(1+A_2(k)\left(\frac{k\upsilon_F}{w}\right)^2+A_4(k)\left(\frac{k\upsilon_F}{w}\right)^4+O\left(\left(\frac{k\upsilon_F}{w}\right)^6\right)\right), \tag{15}$$

where $A_2(k)=\omega_p^2 V(k)/k^2\upsilon_F^2$ and

$$A_4(k)=\frac{3}{2}\frac{F_{5/2}(\eta)}{D^{7/2}}+\frac{\hbar^2k^2}{4m_e^2\upsilon_F^2}\frac{5F_{3/2}(\eta)}{D^{5/2}}+\frac{15}{4}\frac{\hbar^4k^4}{m_e^4\upsilon_F^4}.$$

We conclude that, as expected, within the RPA the sum rule (12) is satisfied only partially, without taking the correlation contribution $U(k)$ into account.

The Mermin loss function satisfies the *f*-sum rule by construction. The situation with the fourth sum rule is quite different. It is not very difficult to calculate the high-frequency limit of the fourth power moment integrand to see that if the collision frequency is kept constant,

$$\lim_{\omega\to\infty}\left(-\frac{\omega^3 \operatorname{Im}\varepsilon_M^{-1}(k,\omega)}{\omega_p^3}\right)=\frac{\nu}{\omega_p},$$

which means that in the «classical» Mermin approximation the fourth power moment of the loss function diverges and the corresponding sum rule (12) is not satisfied at all. In other words, the asymptotic expansion of the Mermin model DF with a constant collision frequency is just

$$\varepsilon_M(k, w\to\infty) \simeq 1-\frac{\omega_p^2}{w^2}. \tag{16}$$

This behavior takes place because at high frequencies the imaginary part of the Mermin DF is determined by the imaginary part of the product $(1+i\nu/\omega)(\varepsilon_{RPA}(k,\omega+i\nu)-1)$ and is reduced to the rational form $(-\nu\omega_p^2/\omega^3)$, which significantly differs from the corresponding exponential factor characteristic for the RPA. This latter factor with the zero asymptotic expansion guarantees the convergence of all power moments of the RPA loss function, while in the Mermin approximation only the second power moment «survives».

Numerical results. In this Section we wish to check the numerical importance of the above drawbacks of the Mermin approximation of the OCP dielectric function. It is clear that in a TCP the inconsistencies of the Mermin model will reveal themselves even stronger, we hope to demonstrate it in our further publications.

We have estimated the static collision frequency as it was suggested in [8]:

$$\frac{\nu}{\omega_p}=0.2387\Gamma^{3/2}\int_0^\infty \frac{dk}{k}\frac{\left[S_{ee}(k)S_{ii}(k)-S_{ei}^2(k)\right]}{\left(1+k^2\lambda_{ei}^2\right)}, \tag{17}$$

where the partial static structure factors were obtained within the HNC approximation [10] for the Deutsch pseudopotential,

$$\varphi_{ab}(r)=Z_aZ_b\left(e^2/r\right)\left[1-\exp\left(-r/\lambda_{ab}\right)\right], \tag{18}$$

without the exchange corrections,

$$\lambda_{ab}^2=\frac{\beta\hbar^2}{2\pi\mu_{ab}},\quad \mu_{ab}=\frac{m_am_b}{m_a+m_b}.$$

The values of the moments $C_0(k_F)$, C_2, and $C_4(k_F)$ presented in Table 1 were calculated for $n=10^{23}cm^{-1}$ ($r_s=2.5256$). The values marked «HNC» were obtained within the HNC approximation for the pseudopotential (18) and those marked «Mermin» were evaluated by direct integration of the power moments of the Mermin loss function. As it was expected, the *f*-sum rule is satisfied by the Mermin model with a high precision. The deviations of the Mermin power moments $C_0(k_F)$ and $C_4(k_F)$ from the sum rule values are quite significant.

Table 1 – The values of the moments

	$\beta^{-1} = 5\ \ eV$		$\beta^{-1} = 10\ \ eV$		$\beta^{-1} = 100\ \ eV$	
Moments	HNC	Mermin	HNC	Mermin	HNC	Mermin
C_0	0.8163	0.4835	0.5396	0.2944	0.0813	0.0071
C_2 / ω_p^2	1.0000	1.0004	1.0000	1.0004	1.000	1.004
C_4 / ω_p^4	3.4101	4.9582	5.0299	6.8365	35.690	40.068

We believe that these deviations once more stress that the Mermin IDF is not exactly a response function. This question deserves further investigation.

Conclusions. It is shown that even the «collision-corrected» Mermin approximation does not satisfy the exact sum rules and other exact relations valid for one-component plasmas.

In other words, the realm of applicability of some widely used approximations is established.

The problem to be studied soon is to which extent the above defects of the Mermin approximation might influence the utility of the Mermin model for the calculation of the stopping power of strongly coupled plasmas at finite temperature [11].

Acknowledgement. *This work was partially supported by the Spanish Ministerio de Ciencia e Innovación under Grant No. ENE2010-21116-C02-02. The authors acknowledge the financial support of KazNU and I.M. T. is grateful to the KazNU for its hospitality.*

REFERENCES

1 Lindhard J., Dan K., On the properties of a gas of charged particles, *Vidensk Selsk. Mat. Fys. Medd.,* **1954**, Vol. 28, Issue 8, P. 1-57.

2 Mermin N.D., Lindhard Dielect ric Function in the Relaxation-Time Approximation, *Phys. Rev. B.,* **1970**, Vol. 1, P. 2362-2363.

3 Das A.K., The relaxation-time approximation in the RPA dielectric formulation, *J. Phys. F.*, **1975**, Vol. 5, Issue 11, P. 2035-2040.

4 Gouedard C., Deutsch C., Dense electron-gas response at any degeneracy, *J. Math. Phys.*, **1978**, Vol. 19, No1, P. 32-39.

5 Arista N.R., Brandt W., Dielectric response of quantum plasmas in thermal equilibrium, *Phys. Rev. A.*, **1984**, Vol. 29, P. 1471-1780.

6 Barriga-Carrasco M.D., Dynamical local field corrections on energy loss in plasmas of all degeneracies, *Phys. Rev. E.,* **2009**, Vol. 79, Article 027401 (4pages).

7 Thiele R. et al., Thomson scattering on inhomogeneous targets, *Phys. Rev. E.*, **2010**, Vol. 82, Article 056404 (7 pages).

8 Baus M., Hansen J.-P., Sjögren L., Electrical conductivity of a strongly coupled hydrogen plasma, *Phys. Lett. A.*, **1981**, Vol. 82, P. 180-182.

9 Arkhipov Yu.V. et al., Dynamic properties of one-component strongly coupled plasmas: The sum-rule approach, *Phys. Rev. E.*, **2010**, Vol. 81, Article 026402 (9 pages) and references therein.

10 Fisher I.Z., Statistical Theory of Liquids. University of Chicago Press, 1964, 335 p.

11 Tkachenko I.M., Muñoz-Cobo J.L., Muñoz A., Comment on "Stopping power of nonmonochromatic heavy-ion clusters with two-ion correlation effects", *Phys. Rev. E.*, **1997**, Vol. 56, Issue 5, P. 6208-6210.

Резюме

Ю. В. Архипов[1], Ә. Б. Ашықбаева[1], Ә. Асқарұлы[1], Л. Конде[2], А. Е. Дәулетов[1], И. М. Ткаченко[3]

[1]ЭТФҒЗИ, әл-Фараби атындағы Қазақ ұлттық университеті, Алматы, Қазақстан;

[2]Мадрид политехникалық университеті, аэронавтика факультеті,

қолданбалы физика кафедрасы, Мадрид қ., Испания;

[3]Таза және қолданбалы математика институты,

Валенсия политехникалық университеті, Валенсия қ., Испания

СОҚТЫҒЫСТЫ БІР КОМПОНЕНТТІ ПЛАЗМАНЫҢ ДИЭЛЕКТР ФУНКЦИЯЛАРЫ ТУРАЛЫ

Тұрақты соқтығысу жиілігімен хаосты фазалардың (ХФЖ) және Мермин жуықтауларында қосындылар заңдарың тексеру көмегімен соқтығысты, бір компанентті плазманың диэлектр функцияларының асимпто-тикалық қасиеттері зерттелінді. Бұл реттегі қосындылар жойылу функцияның жиілік моменттері болып табылады, яғни кері диэлектр функцияларының жорамал бөлігімен тікелей байланысатын оң жұп жиілік бойынша функциялар. Нөлдік момент ХФЖ мәнімен дәл келетіні, f-қосындылар заңы орындалатыны және жүйедегі өзара байланыстар ескерілмеген төртінші моменттік қосындылар заңы жартылай қанағаттан-дырылатыны көрсетілген. Бұл диэлектр функциясы үшін модельдік Мермин шамасының кемшіліктері осы жуықтаудың қолданылатын аймағын анықтайды.

Кілт сөздер: статикалық құрылымдық факторлар, қосындылар ережелері, моменттер әдісі.

Резюме

Ю. В. Архипов[1], А. Б. Ашикбаева[1], А. Аскарулы[1], Л. Конде[2], А. Е. Давлетов[1], И. М. Ткаченко[3]

[1]НИИ Экспериментальной и теоретической физики,

Казахский национальный университет им. аль-Фараби, г. Алматы, Казахстан;

[2]Кафедра прикладной физики факультета аэронавтики

Мадридского политехнического университета, г. Мадрид, Испания;

[3]Институт чистой и прикладной математики

Валенсийского политехнического университета, г. Валенсия, Испания

О ДИЭЛЕКТРИЧЕСКОЙ ФУНКЦИИ

СТОЛКНОВИТЕЛЬНОЙ ОДНОКОМПОНЕНТНОЙ ПЛАЗМЫ

Изучены асимптотические свойства и проведена проверка выполнения правил сумм для диэлектрической функции столкновительной однокомпонентной плазмы в приближениях хаотических фаз (ПХФ) и Мермина с постоянной частотой столкновения. При этом правилами сумм являются частотные моменты функции потерь, являющейся положительной четной функцией частоты, непосредственно связанной с мнимой частью обратной диэлектрической функции. Показано, что нулевой момент совпадает с таковым в ПХФ, f-правило сумм выполняется, а четвертое моментное правило сумм удовлетворяется лишь частично, в нем не учитываются корреляции в системе. Эти недостатки модельного выражения Мермина для диэлектрической функции определяют область применимости данного приближения.

Ключевые слова: статические структурные факторы, правила сумм, метод моментов.

Поступила 27.03.2013г