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2010 J. Phys. A: Math. Theor. 43 015402

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On the definition of dielectric permittivity for media with temporal dispersion in the presence of free charge carriers

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Received 1 September 2009, in final form 13 November 2009

Published 7 December 2009

Online at stacks.iop.org/JPhysA/43/015402

Abstract

We show that in the presence of free charge carriers the definition of the frequency-dependent dielectric permittivity requires additional regularization. As an example, the dielectric permittivity of the Drude model is considered and its time-dependent counterpart is derived and analyzed. The respective electric displacement cannot be represented in terms of the standard Fourier integral. The regularization procedure allowing the circumvention of these difficulties is suggested. For the purpose of comparison it is shown that the frequency-dependent dielectric permittivity of insulators satisfies all rigorous mathematical criteria. This permits us to conclude that in the presence of free charge carriers the concept of dielectric permittivity is not as well defined as for insulators and we make a link to widely discussed puzzles in the theory of thermal Casimir force which might be caused by the use of this kind of permittivities.

PACS numbers: 77.22.Ch, 02.30.Nw

1. Introduction

The concept of dielectric permittivity in media with temporal dispersion is commonly used in electrodynamics and condensed matter physics (see e.g. [1, 2]). For not too strong fields the dielectric permittivity $\varepsilon(\tau)$ depending on the time-like variable τ is introduced from the linear integral relation between the electric field $\mathbf{E}(\mathbf{r}, t)$ and the electric displacement $\mathbf{D}(\mathbf{r}, t)$. Then the frequency-dependent permittivity $\varepsilon(\omega)$ is defined using the Fourier transformations of the fields $\mathbf{E}(\mathbf{r}, t)$ and $\mathbf{D}(\mathbf{r}, t)$. Below we argue that this procedure, which is wholly satisfactory for dielectric materials, faces additional regularization problems in an infinite medium containing free charge carriers. This leads us to the conclusion that some applications

of the frequency-dependent dielectric permittivities allowing for free charge carriers might not be rigorously justified. As one such example we discuss the dielectric permittivity of the Drude model which leads to widely discussed difficulties when substituted into the Lifshitz formula for the van der Waals and Casimir forces at nonzero temperature [3].

2. Dielectric permittivity in the presence of temporal dispersion

For simplicity we consider an isotropic nonmagnetic medium of infinite extent. If its properties do not depend on time, the linear dependence between $\mathbf{D}(t)$ and $\mathbf{E}(t)$ satisfying causality (here and below we omit the argument \mathbf{r}) is given by

$$\mathbf{D}(t) = \int_{-\infty}^t dt' \varepsilon(t-t') \mathbf{E}(t'). \quad (1)$$

The kernel $\varepsilon(t-t')$ of the integral operator on the right-hand side of (1) is called the dielectric permittivity for media with temporal dispersion. We represent it in the form

$$\varepsilon(t-t') = 2\delta(t-t') + f(t-t'), \quad (2)$$

where $f(t-t')$ is a continuous real-valued function and the delta function $\delta(t-t')$ is defined on the interval $-\infty < t' \leq t$ in the following manner [4]:

$$\int_{-\infty}^t g(t') \delta(T-t') dt' = \begin{cases} 0, & T > t, \\ \frac{1}{2}g(T-0), & T = t, \\ \frac{1}{2}[g(T-0) + g(T+0)], & -\infty < T < t. \end{cases} \quad (3)$$

Here $g(t)$ is an arbitrary function which has bounded variation in the vicinity of the point $t' = T$. Note that from the physical point of view the function $f(t-t')$ is defined only for $t' \leq t$; for $t' > t$ it can be ascribed any values (including to vanish in that region).

Substituting (2) into (1) with account of (3) and introducing the new variable $\tau = t-t' \geq 0$, we rearrange (1) to [1]

$$\mathbf{D}(t) = \mathbf{E}(t) + \int_{-\infty}^t dt' f(t-t') \mathbf{E}(t') = \mathbf{E}(t) + \int_0^{\infty} d\tau f(\tau) \mathbf{E}(t-\tau). \quad (4)$$

Representing the real functions $\mathbf{D}(t)$ and $\mathbf{E}(t)$ as Fourier integrals,

$$\mathbf{D}(t) = \int_{-\infty}^{\infty} \mathbf{D}(\omega) e^{-i\omega t} d\omega, \quad \mathbf{E}(t) = \int_{-\infty}^{\infty} \mathbf{E}(\omega) e^{-i\omega t} d\omega, \quad (5)$$

one can rewrite (4) in terms of Fourier transforms of the fields [1]

$$\mathbf{D}(\omega) = \varepsilon(\omega) \mathbf{E}(\omega), \quad \varepsilon(\omega) \equiv 1 + \int_0^{\infty} d\tau f(\tau) e^{i\omega\tau} = \int_0^{\infty} d\tau \varepsilon(\tau) e^{i\omega\tau}, \quad (6)$$

here $\mathbf{D}(\omega)$, $\mathbf{E}(\omega)$ and $\varepsilon(\omega)$ are complex-valued functions. From (6) it follows that $\varepsilon(\omega)$ is an analytic function in the upper half-plane of complex ω including the real axis with the possible exception of the point $\omega = 0$. As a result, the real and imaginary parts of $\varepsilon(\omega)$ are connected by means of the Kramers–Kronig relations [1]. Note that in contrast, for instance, to [5] we always consider fields defined in (\mathbf{r}, t) -space as real and only their Fourier transforms might be complex.

The equivalence between (4) and (6) requires the existence of integrals (5) (and respective inverse Fourier transformations) and the possibility of changing the order of integrations with respect to dt' and $d\omega$. In mathematics there are many different conditions on how to assign a rigorous meaning to (5) and respective inverse formulas. The most widely used demand is that the function $\mathbf{D}(t)$ should have a bounded variation and be integrable together with its modulus,

i.e. should belong to $L^1(-\infty, \infty)$. In this case the function $D(\omega)$ is also bounded, uniformly continuous on the axis $(-\infty, \infty)$, and $D(\omega) \rightarrow 0$ when $|\omega| \rightarrow \infty$ [6]. The function $E(t)$ should possess the same properties. The change of order of integrations is possible if both integrals under consideration are uniformly convergent.

3. Media with free charge carriers

It can be easily seen that the above conditions permitting to introduce the frequency-dependent dielectric permittivity $\varepsilon(\omega)$ in accordance with (6) are not directly applicable for media with free charge carriers. As an example we consider the widely used dielectric permittivity of the Drude model, describing such media [7],

$$\varepsilon_D(\omega) = 1 - \frac{\omega_p^2}{\omega(\omega + i\gamma)}, \tag{7}$$

where ω_p is the plasma frequency and $\gamma > 0$ is the relaxation parameter. It is obvious that $\omega = 0$ may lead to mathematical problems in Fourier transformation. To make a link between $\varepsilon_D(\omega)$ and real-valued physical fields $E(t)$ and $D(t)$, it would be of interest to determine the respective function $f_D(\tau)$. The substitution of (7) into (6) leads to the following equations:

$$\begin{aligned} -\frac{\omega_p^2}{\omega^2 + \gamma^2} &= \int_0^\infty f_D(\tau) \cos(\omega\tau) \, d\tau, \\ \frac{\omega_p^2 \gamma}{\omega(\omega^2 + \gamma^2)} &= \int_0^\infty f_D(\tau) \sin(\omega\tau) \, d\tau. \end{aligned} \tag{8}$$

From the first equation, by means of the inverse cosine Fourier transformation performed with the help of the integral 3.723(2) in [8], one finds

$$f_D^{\cos}(\tau) = -\frac{\omega_p^2}{\gamma} e^{-\gamma\tau}. \tag{9}$$

It is easily seen that the substitution of (9) into the first equation of (8) with account of 3.893(2) in [8] leads to a correct identity; however, substitution into the second equation of (8) fails. On the other hand, using the inverse sine Fourier transformation and the integral 3.725(1) in [8], the second equation of (8) leads to a different result:

$$f_D^{\sin}(\tau) = \frac{\omega_p^2}{\gamma} (1 - e^{-\gamma\tau}). \tag{10}$$

Now, the substitution of (10) into the right-hand sides of equations (8) reproduces their left-hand sides up to additional undefined terms and thus also violates the equalities.

The pathological properties under consideration are explained by the fact that $\varepsilon_D(\omega)$ results in $D(\omega)$ which is unbounded in any vicinity of $\omega = 0$. This means that $D(t)$ cannot be represented as a Fourier integral (5) and both the definition of $\varepsilon(\omega)$ in (6) and equivalent equations (8) become unjustified.

The question arises of whether there is a possibility to consistently define the function $f_D(\tau)$ related to the frequency-dependent permittivity (7). Keeping in mind that in the case of the Drude model the second equality in (6) cannot be considered as a classical Fourier transformation, we make an attempt to assign a definite meaning to the function $f_D(\tau)$ by considering the generalized inverse transformation of the quantity $\varepsilon_D(\omega) - 1$ defined as

$$\begin{aligned} f_D^{(0)}(\tau) &\equiv -\frac{\omega_p^2}{2\pi} \int_{-\infty}^\infty d\omega \frac{1}{(\omega + i0)(\omega + i\gamma)} e^{-i\omega\tau} \\ &= -\frac{\omega_p^2}{2\pi} \int_{-\infty}^\infty d\omega \frac{\omega - i\gamma}{(\omega + i0)(\omega^2 + \gamma^2)} e^{-i\omega\tau} \equiv I_1 + I_2. \end{aligned} \tag{11}$$

Here, the addition of an infinitesimally small quantity $+i0$ establishes the rule on how to bypass the pole of $\text{Im}\varepsilon_D(\omega)$ at $\omega = 0$ and the following notations are used:

$$\begin{aligned} I_1 &= -\frac{\omega_p^2}{2\pi} \int_{-\infty}^{\infty} d\omega \frac{1}{\omega^2 + \gamma^2} e^{-i\omega\tau}, \\ I_2 &= \frac{i\omega_p^2\gamma}{2\pi} \int_{-\infty}^{\infty} d\omega \frac{1}{(\omega + i0)(\omega^2 + \gamma^2)} e^{-i\omega\tau}. \end{aligned} \tag{12}$$

In I_1 the integrated function is regular at $\omega = 0$. This integral can be found in 3.354(5) [8],

$$I_1 = -\frac{\omega_p^2}{2\gamma} \begin{cases} e^{-\gamma\tau}, & \tau > 0, \\ e^{\gamma\tau}, & \tau < 0. \end{cases} \tag{13}$$

The second integral in (12) can be calculated using the contours consisting of the real axis in the complex ω -plane and semicircles of infinitely large radii centered at the origin in the lower half-plane (for $\tau > 0$) and in the upper half-plane (for $\tau < 0$). The result is

$$I_2 = \frac{\omega_p^2}{2\gamma} \begin{cases} 2 - e^{-\gamma\tau}, & \tau > 0, \\ e^{\gamma\tau}, & \tau < 0, \end{cases} \tag{14}$$

where for $\tau > 0$ the contributions from the two poles at $\omega_1 = -i0$ and $\omega_2 = -i\gamma$ were taken into account, whereas for $\tau < 0$ only one pole at $\omega_3 = i\gamma$ determines the value of I_2 . Substituting (13) and (14) into the right-hand side of (11) we arrive at

$$f_D^{(0)}(\tau) = \begin{cases} \frac{\omega_p^2}{\gamma} (1 - e^{-\gamma\tau}), & \tau > 0, \\ 0, & \tau < 0. \end{cases} \tag{15}$$

It is seen that the suggested rule leads to the same result (10), as was obtained by the inverse sine Fourier transformation from the imaginary part of $\varepsilon_D(\omega)$ in (8).

A similar situation occurs for other dielectric permittivities taking into account free charge carriers, e.g. for the dielectric permittivities of the plasma model and of the normal skin effect,

$$\varepsilon_p(\omega) = 1 - \frac{\omega_p^2}{\omega^2}, \quad \varepsilon_n(\omega) = 1 + i\frac{4\pi\sigma_0}{\omega}, \tag{16}$$

where σ_0 is the dc conductivity. In both cases the mathematical conditions permitting to perform the Fourier transformation in the classical understanding are violated. However, by using the same considerations as presented above in the case of the Drude model, one may assign a meaning analogous to (10) to the second formula in (6) and obtain the following dielectric permittivities as functions of τ :

$$f_p^{(0)}(\tau) = \begin{cases} \omega_p^2\tau, & \tau > 0, \\ 0, & \tau < 0. \end{cases} \quad f_n^{(0)}(\tau) = \begin{cases} 4\pi\sigma_0, & \tau > 0, \\ 0, & \tau < 0. \end{cases} \tag{17}$$

It should be remarked that $f_p^{(0)}(\tau)$ is obtainable also from (15) in the limiting case $\gamma \rightarrow 0$.

Now let us check for consistency the respective results for $D(t)$. For example, we choose the electric field in the form

$$\mathbf{E}(t) = \mathbf{E}_0 e^{-\beta t^2} = \int_{-\infty}^{\infty} \mathbf{E}(\omega) e^{-i\omega t} d\omega, \tag{18}$$

where $\beta > 0$ and $\mathbf{E}_0 \equiv \mathbf{E}_0(\mathbf{r})$ describes the spatial dependence of the field. As already stated (18), the function $\mathbf{E}(t)$ satisfies all required conditions and can be presented as a Fourier integral. Its Fourier transform is calculated using the formula 3.896(4) in [8],

$$\mathbf{E}(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathbf{E}(t) e^{i\omega t} dt = \frac{1}{2\sqrt{\pi\beta}} \mathbf{E}_0 e^{-\frac{\omega^2}{4\beta}}. \tag{19}$$

Substituting (15) and (18) into (4) and using the formula 3.322(2) in [8] we arrive at

$$D(t) = E(t) + E_0 \frac{\omega_p^2}{2\gamma} \sqrt{\frac{\pi}{\beta}} \left[1 + \operatorname{erf}(\sqrt{\beta}t) - e^{\frac{\gamma^2}{4\beta} - \gamma t} \operatorname{erfc}\left(\frac{\gamma}{2\sqrt{\beta}} - \sqrt{\beta}t\right) \right], \quad (20)$$

where $\operatorname{erf}(x)$ is the error function and $\operatorname{erfc}(x) = 1 - \operatorname{erf}(x)$. Keeping in mind that [8]

$$\operatorname{erf}(-x) = -\operatorname{erf}(x), \quad \operatorname{erf}(x) = 1 - \frac{1}{\sqrt{\pi}} \frac{e^{-x^2}}{x} + \dots, \quad (21)$$

we obtain for $t \rightarrow \pm\infty$

$$D(\infty) = E_0 \frac{\omega_p^2}{\gamma} \sqrt{\frac{\pi}{\beta}}, \quad D(-\infty) = 0. \quad (22)$$

This is what one expects on physical grounds because for an infinite medium containing free charge carriers the action of switching on and then switching off the electric field should result in a nonzero residual displacement (for a finite medium, the presence of external electric field leads to the accumulation of positive and negative charges on the opposite boundary surfaces and to the vanishing of the total electric field inside such a medium [9]; after the external electric field switches off, the accumulated charges are distributed uniformly over the volume of the medium leading to zero electric displacement at $t \rightarrow +\infty$). However, the first equality in (22) means that $D(t)$ is not an integrable function over the interval $(-\infty, \infty)$. This makes impossible the use of the standard Fourier transformation (5) and resulting equality (6), and makes the whole formalism not self-consistent.

This can be seen even more clearly if one defines $D(\omega)$ in accordance with the first equality in (6), where $\varepsilon_D(\omega) = \varepsilon_D(\omega)$ and $E(\omega)$ is given in (19), and then calculates the electric displacement using the first equality in (5). The obtained quantity which we denote $\tilde{D}(t)$ is calculated using the formulas 3.954(2) in [8] and 2.5.36(6, 11) in [10]. The result is

$$\tilde{D}(t) = D(t) - E_0 \frac{\omega_p^2}{2\gamma} \sqrt{\frac{\pi}{\beta}}, \quad (23)$$

where $D(t)$ is defined in (20). It has nonzero values at both $t \rightarrow \infty$ and $t \rightarrow -\infty$:

$$\tilde{D}(\infty) = E_0 \frac{\omega_p^2}{2\gamma} \sqrt{\frac{\pi}{\beta}}, \quad \tilde{D}(-\infty) = -E_0 \frac{\omega_p^2}{2\gamma} \sqrt{\frac{\pi}{\beta}}. \quad (24)$$

Derivation of a different electric displacement than in (20), which does not vanish at $t \rightarrow -\infty$, i.e. before the switching on of the electric field, can be understood as an artifact resulting from the use of the Fourier integral of a nonintegrable function $D(\omega)$ (the definition of the Fourier integral as a generalized function used in mathematics in this case seems to be not appropriate in our physical situation because it is natural to understand the electric displacement as a usual function). This suggests that in the presence of free charge carriers, the standard definition of the frequency-dependent dielectric permittivity based on the formal representations of $E(t)$ and $D(t)$ in terms of Fourier integrals is not satisfactory and requires some additional regularization procedure.

As an example of such a procedure, we consider the modified dielectric permittivity of the Drude model

$$\varepsilon_D^{(\theta)}(\omega) = 1 - \frac{\omega_p^2}{(\omega + i\theta)(\omega + i\gamma)}, \quad (25)$$

where, in contrast with (11), the quantity $\theta > 0$ is not infinitesimally small. In accordance with (25) $\varepsilon_D^{(\theta)}$ is regular at $\omega = 0$. The substitution of (25) into (6) leads to

$$\begin{aligned} -\omega_p^2 \frac{\omega^2 - \theta\gamma}{(\omega^2 + \theta^2)(\omega^2 + \gamma^2)} &= \int_0^\infty f_D^{(\theta)}(\tau) \cos(\omega\tau) \, d\tau, \\ \omega_p^2(\theta + \gamma) \frac{\omega}{(\omega^2 + \theta^2)(\omega^2 + \gamma^2)} &= \int_0^\infty f_D^{(\theta)}(\tau) \sin(\omega\tau) \, d\tau. \end{aligned} \tag{26}$$

It can be easily seen that both the inverse cosine and sine Fourier transformations performed in (26) lead to the common result

$$f_D^{(\theta)}(\tau) = \frac{\omega_p^2}{\gamma - \theta} (e^{-\theta\tau} - e^{-\gamma\tau}). \tag{27}$$

Substituting this into (4) and performing calculations with the electric field (18), we arrive at the modified electric displacement

$$\begin{aligned} \mathbf{D}^{(\theta)}(t) = \mathbf{E}(t) + \mathbf{E}_0 \frac{\omega_p^2}{2(\gamma - \theta)} \sqrt{\frac{\pi}{\beta}} \left[e^{\frac{\theta^2}{4\beta} - \theta t} \operatorname{erfc}\left(\frac{\theta}{2\sqrt{\beta}} - \sqrt{\beta}t\right) \right. \\ \left. - e^{\frac{\gamma^2}{4\beta} - \gamma t} \operatorname{erfc}\left(\frac{\gamma}{2\sqrt{\beta}} - \sqrt{\beta}t\right) \right]. \end{aligned} \tag{28}$$

In the limiting case $\theta \rightarrow 0$ (28) coincides with (20).

Precisely the same result, as in (28), is obtained if one considers $\mathbf{D}^{(\theta)}(\omega) = \varepsilon_D^{(\theta)}(\omega)\mathbf{E}(\omega)$ and then finds $\mathbf{D}^{(\theta)}(t)$ from the first equality in (5). Thus, when we assume $\theta > 0$, both methods of the calculation of the electric displacement are in agreement. The reason is that for $\theta > 0$ the functions $\mathbf{D}(t)$ and $\mathbf{D}(\omega)$ belong to $L^1(-\infty, \infty)$ and all Fourier transformations are well defined. However, to obtain the correct physical results for an infinite medium, one must put $\theta = 0$ in (28) and return to (20). The point is that (28) with $\theta > 0$ leads to $\mathbf{D}^{(\theta)}(t) \rightarrow 0$ when $t \rightarrow \pm\infty$ (as it must be for functions belonging to $L^1(-\infty, \infty)$). At the same time, in the presence of free charge carriers, the electric displacement in an infinite medium remains nonzero in accordance with (22) after the electric field is switched off. Thus, the limiting transitions $t \rightarrow \pm\infty$ and $\theta \rightarrow 0$ are not interchangeable.

4. Insulating media

The situation is quite different for dielectric materials at zero temperature which do not contain free charge carriers (i.e. for true insulators). In this case the dielectric permittivity can be represented in the form [11]

$$\varepsilon_I(\omega) = 1 + \sum_{j=1}^K \frac{g_j}{\omega_j^2 - \omega^2 - i\gamma_j\omega}, \tag{29}$$

where $\omega_j \neq 0$ are the oscillator frequencies, γ_j are the relaxation parameters and g_j are the oscillator strengths of K oscillators. In this case the second equality of (6) results in

$$\begin{aligned} \sum_{j=1}^K \frac{g_j(\omega_j^2 - \omega^2)}{(\omega_j^2 - \omega^2)^2 + \gamma_j^2\omega^2} &= \int_0^\infty f_I(\tau) \cos(\omega\tau) \, d\tau, \\ \sum_{j=1}^K \frac{g_j\gamma_j\omega}{(\omega_j^2 - \omega^2)^2 + \gamma_j^2\omega^2} &= \int_0^\infty f_I(\tau) \sin(\omega\tau) \, d\tau. \end{aligned} \tag{30}$$

Performing the inverse cosine Fourier transformation in the first equation of (30) with the help of the integrals 3.733(1, 3) in [8] we obtain

$$f_I(\tau) = \sum_{j=1}^K \frac{g_j e^{-\frac{1}{2}\gamma_j \tau}}{\sqrt{\omega_j^2 - \frac{1}{4}\gamma_j^2}} \sin\left(\sqrt{\omega_j^2 - \frac{1}{4}\gamma_j^2} \tau\right). \quad (31)$$

Precisely the same result is obtained by means of the inverse sine Fourier transformation from the second equation in (30) when one uses the integral 3.733(2) in [8]. In this case all involved Fourier integrals exist in the classical sense with no use of regularization and $\varepsilon_I(\omega)$ is well defined.

Substituting the electric field (18) into (4) and using the integral 3.897(1) in [8], we obtain the electric displacement in an insulating media,

$$\mathbf{D}(t) = \mathbf{E}(t) \left\{ 1 + \sqrt{\frac{\pi}{\beta}} \sum_{j=1}^K \frac{g_j}{\sqrt{4\omega_j^2 - \gamma_j^2}} \text{Im}[e^{B^2} \text{erfc}(B)] \right\}, \quad (32)$$

where

$$B \equiv B(t) = \frac{\gamma_j - 4\beta t - i\sqrt{4\omega_j^2 - \gamma_j^2}}{4\sqrt{\beta}}. \quad (33)$$

The same result is obtained by means of the inverse Fourier transformation from $\mathbf{D}(\omega)$ found using the first equality in (6), as it should be. From (32) and (21) it can be easily seen that $\mathbf{D}(t) \rightarrow 0$ when $t \rightarrow \pm\infty$, as it should be for insulating materials, and that both $\mathbf{D}(t)$ and $\mathbf{D}(\omega)$ belong to $L^1(-\infty, \infty)$.

5. Conclusions and discussion

To conclude, we have shown that the definition of the frequency-dependent dielectric permittivity for materials containing free charge carriers by means of Fourier transformation of the fields is not as straightforward as in the case of insulators. The essence of the problem is in the use of the idealization of an infinite medium. For insulators this idealization is applicable if the sizes of the bodies are much greater than some characteristic parameter (e.g. the width of a gap between the bodies). However, for media with movable free charge carriers this kind of conditions fails. The physical situation for an infinite medium turns out to be totally different from the case of finite bodies of any conceivable size. In fact for conductors $\varepsilon(\omega)$ is a quantity obtained through formal application of Fourier transformation in the region where it needs additional regularization. In spite of a great number of successful applications (see e.g. [1, 2, 5]) there are delicate cases where such a procedure leads to problems. As an example one could mention the use of $\varepsilon_D(\omega) - 1$ as a response function in the fluctuation-dissipation theorem and related puzzles in the theory of thermal Casimir force [3, 12, 13]. During the last 10 years the thermal Casimir force has been the subject of considerable discussion. It was suggested [14, 15] to describe it using the Lifshitz theory combined with the Drude model (7). In the limit of large separations between the test bodies the predictions of the Drude model approach were found to be in agreement with classical statistical physics [16, 17]. On the other hand, at short separations the predictions of this approach were excluded experimentally, whereas the predictions based on the use of the plasma model in (16) were found to be consistent with the data [18]. The question of how to correctly calculate the thermal Casimir force still remains to be answered. Keeping in mind that the Lifshitz theory is based on the fluctuation-dissipation theorem, we would like to emphasize that the application of this theorem with poorly defined

response functions cannot be considered as either exact or rigorous and might cause currently discussed problems.

Acknowledgments

The authors are grateful to VN Marachevsky for helpful discussions. GLK and VMM are grateful to the Institute for Theoretical Physics, Leipzig University for their kind hospitality. This work was supported by Deutsche Forschungsgemeinschaft, grant no GE 696/9–1.

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