On the Casimir entropy for a ball in front of a plane

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outline

- Overview
- Third law, vacuum and free energies
- Parallel planes at low T
- Ball in front of a plane at low T
- Conclusions

The violation of the third law of thermodynamics by the Casimir effect for certain properties of the interacting bodies is still one of the most interesting problems in the field.

The entropy

$$\mathcal{S} = -\frac{\partial \mathcal{F}}{\partial T}$$

It should vanish for $T \to 0$
But sometimes it does not.

first observed in

Bezerra, V.B. and Klimchitskaya, G.L. and Mostepanenko, V.M., PRA, 2002
for metals described by the Drude model

Geyer, B. and Klimchitskaya, G. L. and Mostepanenko, V. M., PRD 2005
for dielectrics with dc conductivity.

At present this is one of the most discussed questions in the theory of the Casimir effect resp of the theory of dispersion forces
Formally, it appears when applying the permittivities of Drude model or *dc* conductivity to the Lifshitz formula

The Drude model, for metals, is characterized by a permittivity

$$\varepsilon^{\mathrm{D}}(i\xi) = 1 + \frac{\omega_p^2}{\xi(\gamma + \xi)}$$

$\omega = i\xi$ is the imaginary frequency
ω_p is the plasma frequency
γ is the relaxation parameter

for $\gamma = 0$ we get the plasma model which does not cause problems with thermodynamics

A dielectric with dc conductivity is characterized by a permittivity

$$\varepsilon^{\mathrm{dc}}(i\xi) = \varepsilon_0(i\xi) + \frac{4\pi\sigma_0}{\xi}$$

σ_0 is the dc conductivity
$\varepsilon_0(i\xi)$ is the permittivity of a dielectric without dc conductivity
(which does not cause problems with TD either)

the violation of TD occurs if the parameters σ_0 or γ are non zero, depend on the temperature and decrease for $T \to 0$:
$\gamma(T) \to 0$
$\sigma(t) \to 0$ for $T \to 0$
This happens for some reasonable idealizations of real materials where σ_0 decreases exponentially fast or γ as a power of T (for metals with perfect crystal lattice).

During the past decade there was quite a number of attempts to avoid a violation of the third law.
Most of them point to a modification by including additional physical effects.
An example is the addition of impurities to a perfect crystal lattice
Another consist in using impedance boundary conditions in place of the Drude model in the Lifshitz formula
It must be admitted that no satisfactory understanding was reached so far.

In this talk I discuss the question whether a finite size of one of the interacting bodies is able to prevent the violation.
For this I consider a ball with the permittivities $\varepsilon^{\mathrm{D}}(i\xi)$ and $\varepsilon^{\mathrm{dc}}(i\xi)$ in front of a conducting plane.

It must be mentioned that the configuration of a ball in front of a plane at finite temperature is under active discussion, see for example papers by Gies&Weber and Canaguier-Durand, Neto, Lambrecht, Reynaud in PRL 2010.

The free energy for parallel planes

Reconsidering parallel planes:
reconfirming the old results
develope a simpler and more direct derivation which is better suited for the spherical case

$$\mathcal{F} = \frac{T}{2} \sum_{l=-\infty}^{\infty} \int \frac{d^2 k}{(2\pi)^2} \sum_{i=\mathrm{TE},\mathrm{TM}} \ln\left(1 - r_i^2\, e^{-2aq}\right)$$

with $q = \sqrt{\xi_l^2 + k^2}$, and the Matsubara frequencies $\xi_l = 2\pi l T$,

The reflection coefficients are

$$r_{\mathrm{TE}} = \frac{q - \sqrt{(\varepsilon - 1)\xi_l^2 + q^2}}{q + \sqrt{(\varepsilon - 1)\xi_l^2 + q^2}} \quad \text{for the TE mode and}$$

$$r_{\mathrm{TM}} = \frac{\varepsilon q - \sqrt{(\varepsilon - 1)\xi_l^2 + q^2}}{\varepsilon q + \sqrt{(\varepsilon - 1)\xi_l^2 + q^2}} \quad \text{for the TM mode}$$

Using the Abel-Plana formula we rewrite the free energy:

$$\mathcal{F} = E_0 + \Delta_{\mathrm{T}}\mathcal{F},$$

vacuum energy (depending on T only through γ or σ):

$$E_0 = \frac{1}{2}\int_0^\infty \frac{d\xi}{\pi}\int \frac{d^2k}{(2\pi)^2}\sum_{i=\mathrm{TE},\mathrm{TM}} \ln\left(1 - r_i^2\, e^{-2aq}\right),$$

temperature dependent part of the free energy:

$$\Delta_{\mathrm{T}}\mathcal{F} = \frac{1}{4\pi^2}\int_0^\infty dx\, n_T(x)\; i\left(\varphi(ix) - \varphi(-ix)\right),$$

with the Boltzmann factor

$$n_T(x) = \frac{1}{e^{x/T} - 1}$$

and

$$\varphi(\xi) = \int_0^\infty dk\, k \sum_{i=\mathrm{TE},\mathrm{TM}} \ln\left(1 - r_i^2\, e^{-2aq}\right),$$

The subdivision

$$\mathcal{F} = E_0 + \Delta_{\mathrm{T}}\mathcal{F},$$

introduced using the Abel-Plana formula is according to the photonic dof

for temperature dependent excitations of the interacting bodies also the vacuum energy dependes on temperature

the entropy thus consists of two parts, $\mathcal{S} = \mathcal{S}_0 + \mathcal{S}_1$

The more conventional approach to derive the violation terms, used in the literature, rests on the observation that the interesting terms result from the $(l = 0)$-contribution to the Matsubara sum
For metallic bodies described by the Drude model:

$$\mathcal{F}^{\mathrm{Drude}} = -\mathcal{F}_{l=0}^{\mathrm{plasma,TE}} + \ldots = -\frac{T}{16\pi a^2}\,\zeta(3) + \ldots$$

For a dielectric body with dc conductivity,

$$\mathcal{F}^{\mathrm{dc}} = \mathcal{F}_{l=0}^{\mathrm{dc,TM}} - \mathcal{F}_{l=0}^{\mathrm{no\ dc,TM}} + \ldots \ = -\frac{T}{16\pi a^2}\left(\zeta(3) - \mathrm{Li}_3(r_0^2)\right) + \ldots$$

The vacuum energy in the Drude model

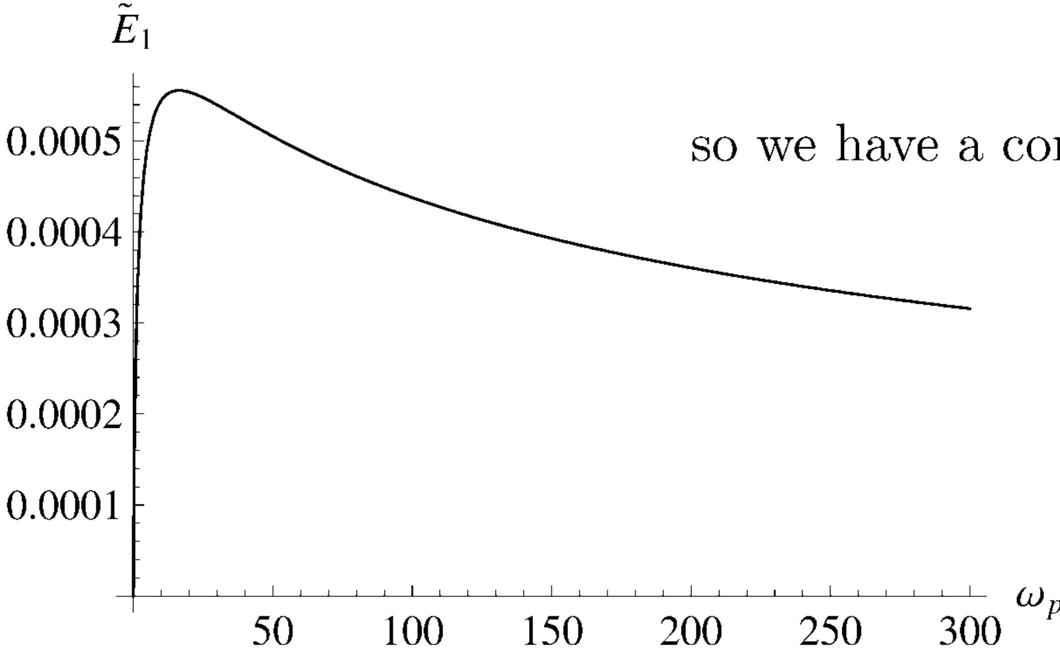
we assume $\gamma(T) = \gamma_1 T^\alpha + \dots$

$$S_0 = -\frac{\partial E_0(\gamma)}{\partial \gamma}\,\frac{\partial \gamma}{\partial T} \qquad \text{and} \qquad \frac{\partial \gamma}{\partial T} = \alpha\gamma_1 T^{\alpha-1}$$

the expansion reads

$$E_0(\gamma) = E_0(0) + \gamma\left(-\ln(2a\gamma)\,\tilde{E}_1 + E_1\right) + \dots.$$

these functions can be calculated quite easily, the most interesting is



so we have a contribution for $0 < \alpha \leq 1$

The vacuum energy for a dielectric with dc conductivity

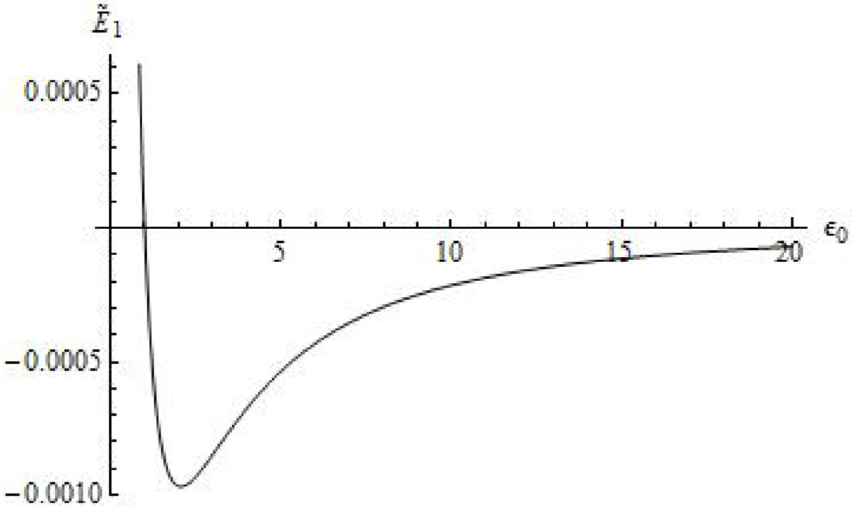
similar to the Drude model

$$S_0 = -\frac{\partial E_0(\sigma)}{\partial \sigma} \frac{\partial \sigma}{\partial T}, \qquad \sigma(T) = \sigma_1 T^\alpha + \ldots$$

Again we will observe a logarithmic contribution for $T \to 0$. This time it comes from the TM mode

$$E_0(\sigma) = E_0(0) + \sigma \left(-\ln(2a\sigma)\, \tilde{E}_1 + E_1 \right) + \ldots ,$$

in this case the function $\tilde{E}_1$ can be calculated explicitely



$$\tilde{E}_1 = \frac{1}{4\pi^2} \frac{\mathrm{Li}_2(r_0^2)}{(1-\varepsilon_0^2)a^2},$$

again, contribution for $0 < \alpha \leq 1$

The temperature dependent part of the free energy in the Drude model

So we have to consider

$$\varphi(ix) = \int_0^\infty dk\, k \sum_{i=\mathrm{TE,TM}} \ln\left(1 - r_i^2\, e^{-2aq}\right),$$

with $q = \sqrt{k^2 - x^2}$. We divide the integration into a first region, $k \in [0, x]$, and a second region, $k \in [x, \infty)$. We need the function $\varphi(ix)$ for small $x \sim T$. Therefore, in the first part of the integration region we have $k \le T$ and a factor $\sim T^2$ from $dk\, k$. As a consequence, the contribution from this region is by two additional powers of T suppressed as compared with the second region where the integration region is infinite. Hence a contribution to the linear in T term can come from the second region only. In that region we change the variable of integration from k for $q = \sqrt{k^2 - x^2}$ (which is real) and arrive at a representation of the temperature dependent part of the free energy, up to higher orders in T, given by the above formulas but now with

$$\varphi(ix) = \int_0^\infty dq\, q \sum_{i=\mathrm{TE,TM}} \ln\left(1 - r_i^2\, e^{-2aq}\right).$$

Drude model:

the leading contribution results from the TE mode.

$$\Delta_T \mathcal{F}^{\text{Drude,TE}} = \frac{1}{4\pi^2} \int_0^\infty \frac{dx}{e^{x/T}-1} \int_0^\infty dq\, q\, i \left(h_q\left(\frac{\gamma}{ix}\right) - h_q\left(\frac{\gamma}{-ix}\right)\right) + \dots$$

with

$$h_q(z) = \ln \left[1 - \left(\frac{q - \sqrt{\frac{\omega_p^2}{1+z} + q^2}}{q + \sqrt{\frac{\omega_p^2}{1+z} + q^2}} \right)^2 e^{-2aq} \right] .$$

Now we consider $\alpha \geq 1$, i.e., γ decreases not slower than the first power of the temperature. We make the substitution $x = \gamma\zeta$,

$$\Delta_T \mathcal{F}^{\text{Drude,TE}} = \frac{1}{4\pi^2} \int_0^\infty d\zeta \frac{\gamma}{e^{\gamma\zeta/T}-1} \int_0^\infty dq\, q\, i \left(h_q\left(\frac{1}{i\zeta}\right) - h_q\left(\frac{1}{-i\zeta}\right)\right)$$

and observe

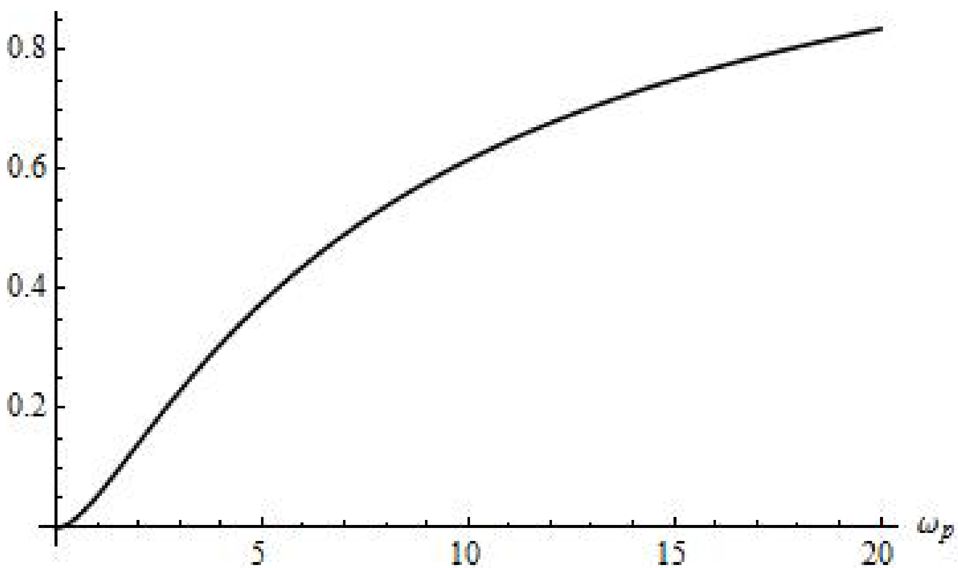
$$\frac{\gamma}{e^{\gamma\zeta/T}-1} = \frac{T}{\zeta} + \dots$$

the remaining integration is finite and results in

$$\Delta_T \mathcal{F}^{\mathrm{Drude,TE}} = \frac{T}{16\pi a^2}\, f^{\mathrm{D}}$$

with

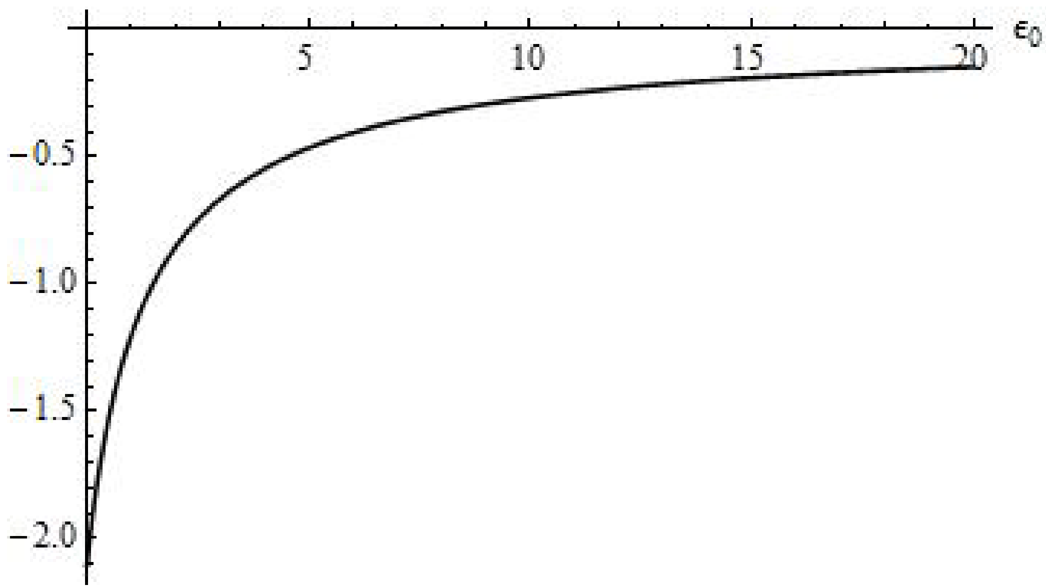
$$f^{\mathrm{D}} = (2a)^2 \int_0^\infty d\zeta \frac{1}{\zeta} \int_0^\infty dq\, q\, i \left(h_q\left(\frac{1}{i\zeta}\right) - h_q\left(\frac{1}{-i\zeta}\right)\right) .$$



reproducing the result of the $l = 0$-mode similar calculation for the dc conductivity

$$\Delta_T \mathcal{F}^{\mathrm{dc,TM}} = -\frac{T}{16\pi a^2}\left(\mathrm{Li}_3(r_0^2) - \zeta(3)\right)$$

also confirming the old result



The free energy for a sphere in front of a plane

basic formula,

$$\Delta_T \mathcal{F} = \frac{1}{2\pi} \int_0^\infty dx\, n_T(x)\; i\mathrm{Tr}\left[\ln\left(1 - \mathbb{M}(ix)\right) - \ln\left(1 - \mathbb{M}(-ix)\right)\right] ,$$

The matrix $\mathbb{M}(\xi)$ has the entries

$$M_{l,l'} = \sqrt{\frac{\pi}{4\xi L}} \sum_{l''=|l-l'|}^{l+l'} K_{\nu''}(2\xi L) H_{ll'}^{l''} \begin{pmatrix} \Lambda_{l,l'}^{l''} & \tilde{\Lambda}_{l,l'} \\ \tilde{\Lambda}_{l,l'} & \Lambda_{l,l'}^{l''} \end{pmatrix} \begin{pmatrix} d_l^{\mathrm{TE}}(\xi R) & 0 \\ 0 & -d_l^{\mathrm{TM}}(\xi R) \end{pmatrix}$$

$$d_l^{\mathrm{TE}}(\xi) = \frac{2}{\pi} \frac{\sqrt{\varepsilon} s_l(\xi) s_l'(n\xi) - \sqrt{\mu} s_l'(\xi) s_l(n\xi)}{\sqrt{\varepsilon} e_l(\xi) s_l'(n\xi) - \sqrt{\mu} e_l'(\xi) s_l(n\xi)} ,$$

$s_l(z) = \sqrt{\pi z/2} I_{l+1/2}(z)$, $e_l(z) = \sqrt{2z/\pi} K_{l+1/2}(z)$

the lowest orders for $\xi \to 0$,

$$\mathbb{M} = \mathbb{M}_0 + \mathbb{M}_1 \xi + \dots .$$

From the powers of ξ it follows that only $l'' = l + l'$ contributes and that $\mathbb{M}_0$ is diagonal in the polarizations. The latter follows form the additional factor of ξ in $\tilde{\Lambda}_{l,l'}^{l''}$. For this reason, and because of the trace, the temperature dependent part of the free energy becomes a sum of the two polarizations,

$$\Delta\mathcal{F} = \Delta\mathcal{F}^{\mathrm{TE}} + \Delta\mathcal{F}^{\mathrm{TM}} + \dots ,$$

which holds in the orders of T we are interested in.

Ball described by the Drude model

Because of the Boltzmann factor $n_T(x) = \frac{1}{e^{x/T}-1}$, we make the substitution $x = \gamma\zeta$

$$\frac{1}{\varepsilon^{\mathrm{D}}(\gamma\zeta)} = \frac{\gamma\sqrt{\zeta(1+\zeta)}}{\omega_p} + \ldots \qquad \text{and} \qquad \sqrt{\varepsilon^{\mathrm{D}}(\gamma\zeta)}\,\gamma\zeta = \omega_p\sqrt{\frac{\zeta}{1+\zeta}} + \ldots$$

now we expand d^{TX} for small ζ:
for the TE mode

$$t^{\mathrm{TE}}(\gamma\zeta) = t_0^{\mathrm{TE}}(\zeta, \omega_p) + \ldots$$

with

$$t_0^{\mathrm{TE}}(\zeta, \omega_p) = \frac{i_l(0)\,\tilde{i}_l\left(\omega_p\sqrt{\frac{\zeta}{1+\zeta}}\right) - \tilde{i}_l(0)\,i_l\left(\omega_p\sqrt{\frac{\zeta}{1+\zeta}}\right)}{k_l(0)\,\tilde{i}_l\left(\omega_p\sqrt{\frac{\zeta}{1+\zeta}}\right) - \tilde{k}_l(0)\,i_l\left(\omega_p\sqrt{\frac{\zeta}{1+\zeta}}\right)},$$

whereas for the TM mode

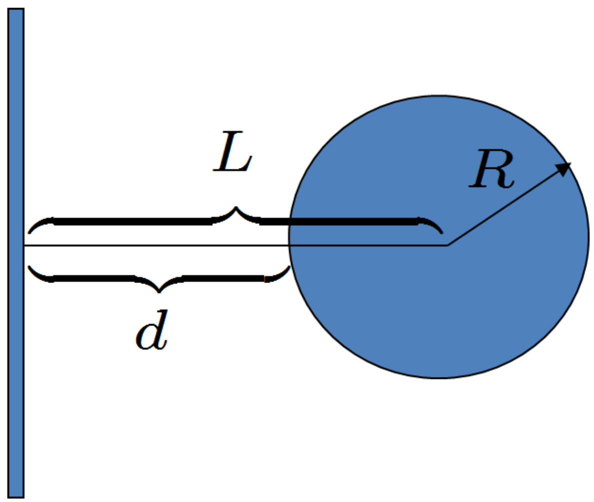
$$t^{\mathrm{TM}}(\gamma\zeta) = O(\gamma^2)$$

hence we get

$$
\begin{aligned}
M_{l,l'}^{\mathrm{Drude}}(\zeta) &\equiv M_{l,l'}(\gamma\zeta)_{|_{\gamma=0}}\,, \\
&= \frac{\sqrt{\pi}}{2}\left(\frac{\rho}{2}\right)^{2l+1} k_{l+l'}(0) H_{l,l'}^{l+l'} \Lambda_{l,l'}^{l+l'} t_0^{\mathrm{TE}}(\zeta, \omega_p R)\,,
\end{aligned}
$$

where we defined

$$\rho = \frac{R}{L}$$



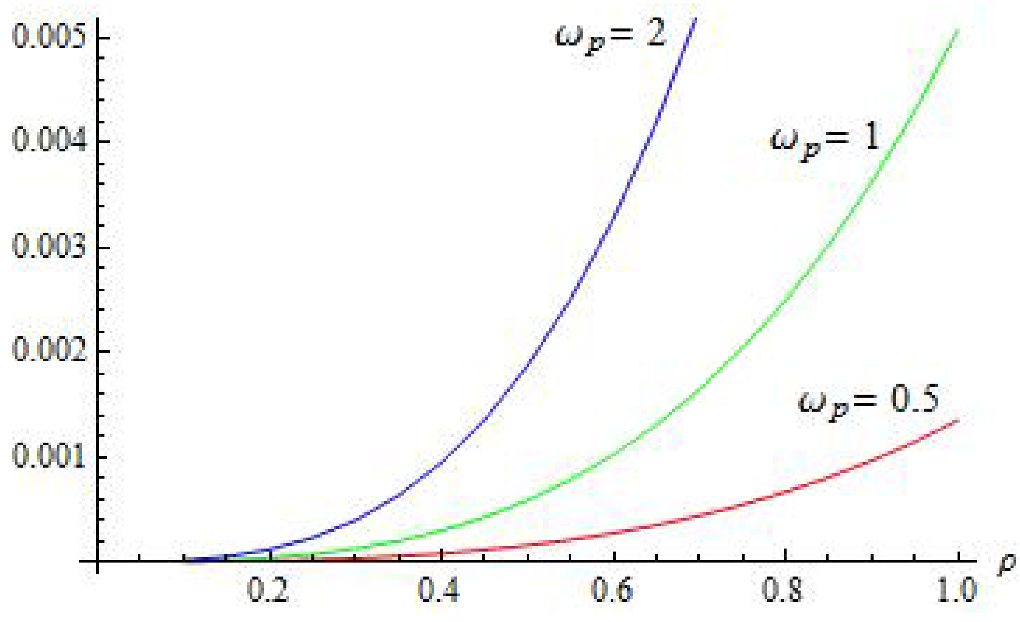
we come to a formula

$$\Delta_T \mathcal{F} = \frac{T}{2\pi} \int_0^\infty d\zeta \, \frac{1}{\zeta} \, i\mathrm{Tr} \left[\left(1 - \mathbb{M}^{\mathrm{Drude}}(i\zeta)\right) - \left(1 - \mathbb{M}^{\mathrm{Drude}}(-i\zeta)\right) \right] .$$

where it 'remains' to take the trace, i.e., to sum over the orbital momenta.

$$\Delta_T \mathcal{F} = \frac{T}{2\pi} \, f^{\mathrm{D}}_{\mathrm{ball}}(\rho, \omega_p R) + O(T^2)$$

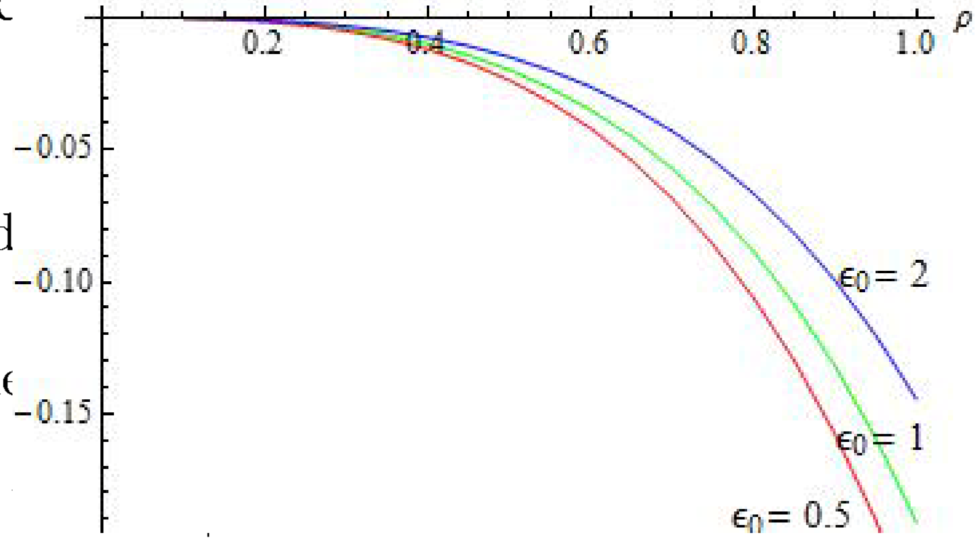
For the calculation of the trace one needs to make a truncation of the orbital momenta, $l \le l_m$. In this case it turned out that for all values of the parameters ρ and ω_p a few lowest $l \lesssim 4$ are sufficient.



Dielectric ball with DC c

now we have the combinations

$$\frac{1}{\varepsilon^{dc}(\sigma\zeta)} = \frac{\zeta}{\varepsilon_0 + \zeta} + \dots, \quad \text{and}$$



the dominating contribution come

$$t_0^{\rm TM}(\zeta,\sigma) \equiv$$

$$= \frac{\left(\frac{\zeta}{\varepsilon_0+\zeta} - 1\right) i_l(0)\tilde{i}_l(0)}{\frac{\zeta}{\varepsilon_0+\zeta} k_l(0)\tilde{i}_l(0) - \tilde{k}_l(0) i_l(0)},$$

we get

$$\Delta_T \mathcal{F} = \frac{T}{2\pi}\, f^{dc}_{\rm ball}(\rho,\varepsilon_0) + O(T^2)$$

In this way we have seen that the violation of thermodynamics 3rd law appears for a ball in front of a plane in much the same way as for infinite parallel planes

For completeness, we also calculated the case of fixed parameters, γ and σ, where no violation occures
for $\xi \to 0$ we note

$$\frac{1}{\varepsilon^{\mathrm{D}}} = \frac{\gamma}{\omega_p^2}\,\xi + \ldots, \qquad \sqrt{\varepsilon^{\mathrm{D}}}\xi R = \frac{\omega_p R}{\sqrt{\gamma}}\,\sqrt{\xi} + \ldots\,,$$

$$\frac{1}{\varepsilon^{\mathrm{dc}}} = \frac{1}{\sigma}\xi + \ldots, \qquad \sqrt{\varepsilon^{\mathrm{dc}}}\xi R = \sqrt{\sigma} R\,\sqrt{\xi} + \ldots\,,$$

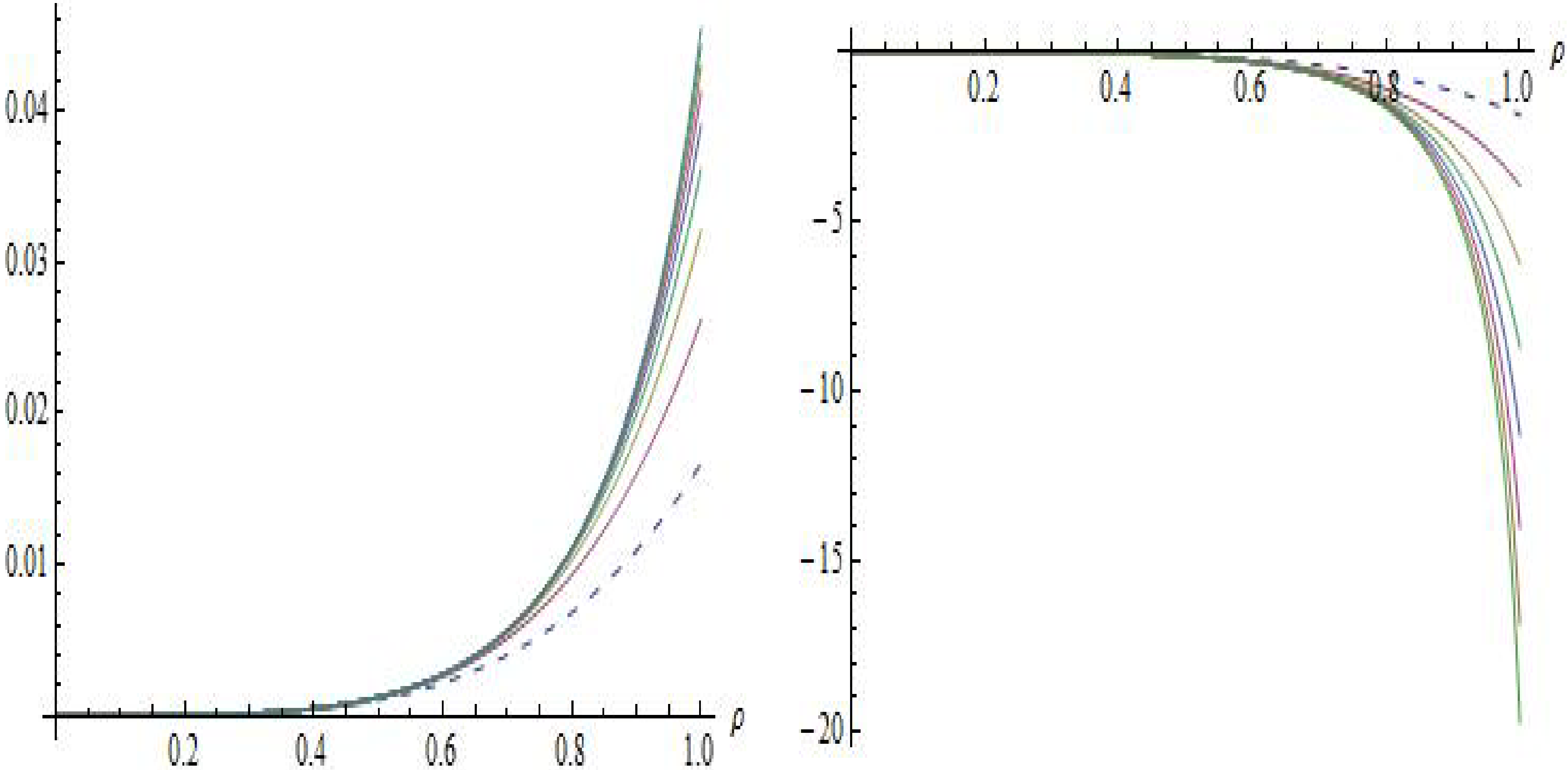
in this approximation both models are related by the substitution $\sigma \to \omega_p^2/\gamma$

the general structure of the expansion is

$$\mathrm{Tr}\ln\left(1-\mathbb{M}^{\mathrm{TM}}(\xi)\right) = \mathrm{Tr}\ln\left(1-\mathbb{M}_0^{\mathrm{TM}}\right) - \mathrm{Tr}\left(1-\mathbb{M}_0^{\mathrm{TM}}\right)^{-1}\mathbb{M}_1^{\mathrm{TM}}\,\xi + \ldots\,.$$

only the odd term survives the ξ-integration

$$\Delta_T \mathcal{F}^{\mathrm{TX}} = g^{\mathrm{TX}}(\rho)\,\frac{\gamma\,T^2}{\omega_p^2} + \ldots$$



$\rho = 1$ corresponds to contact

Conclusions

We have now the following cases withand without violation of 3rd law of TD

	Drude model	dc conductivity
parallel planes		
$\gamma \to 0$ resp. $\sigma \to 0$		
vacuum Energy	TE, $\mathcal{S} < 0$	TM, $\mathcal{S} > 0$
$\Delta_T \mathcal{F}$	TE, $\mathcal{S} < 0$	TM, $\mathcal{S} > 0$
γ resp σ fixed		
$\Delta_T \mathcal{F}$	TE, $\mathcal{S} < 0$	TM, $\mathcal{S} > 0$
	and TM, $\mathcal{S} > 0$	
ball-plane		
$\gamma \to 0$ resp. $\sigma \to 0$		
$\Delta_T \mathcal{F}$	TE, $\mathcal{S} < 0$	TM, $\mathcal{S} > 0$
γ resp σ fixed		
$\Delta_T \mathcal{F}$	TE, $\mathcal{S} < 0$	same as Drude
	and TM, $\mathcal{S} > 0$	with $\frac{\omega_p^2}{\gamma} \leftrightarrow \sigma$

TD violation occurs for $\gamma \sim T^\alpha$ and σT^α with $0 < \alpha$

at the moment it is not clear whether this is really a defect or, whether such a behavior does not happen for real materials (in a sense of a meaningful idealization)

Thank you for attention!