Comment on “Analytical and numerical verification of the Nernst heat theorem for metals”

G. L. Klimchitskaya\textsuperscript{1} and V. M. Mostepanenko,\textsuperscript{2}

\textsuperscript{1}North-West Technical University, Millionnaya Street 5, St.Petersburg, 191065, Russia
\textsuperscript{2}Noncommercial Partnership “Scientific Instruments”, Tverskaya Street 11, Moscow, 103905, Russia

Abstract

Recently, Høye, Brevik, Ellingsen and Aarseth (\texttt{quant-ph/0703174}) claimed that the use of the Drude dielectric function leads to zero Casimir entropy at zero temperature in accordance with Nernst’s theorem. We demonstrate that their proof is not applicable to metals with perfect crystal lattices having no impurities. Thus there is no any contradiction with previous results in the literature proving that the Drude dielectric function violates the Nernst theorem for the Casimir entropy in the case of perfect crystal lattices. We also indicate mistakes in the coefficients of their asymptotic expressions for metals with impurities.

PACS numbers: 05.30.-d, 12.20.Ds, 42.50.Nn, 65.40.Gr
As correctly mentioned in the Introduction of Ref. \[1\], the relaxation frequency of a metal \(\nu(T)\) goes to zero when temperature \(T\) goes to zero. In accordance with the Bloch-Grüneisen law at low temperatures \(\nu(T) \sim T^5\). It should be particularly emphasized that the Bloch-Grüneisen law is established for metals with perfect crystal lattices having no impurities. This law is also valid for metals with impurities at temperatures larger than 3–4 K. Although real metals have some small fraction of impurities, the model of perfect crystal lattice is basic in all theoretical condensed matter physics. Many important results in this field, including the theory of electron-phonon interactions, are obtained for perfect crystal lattices. The Casimir entropy in the case of a perfect crystal lattice, if calculated correctly, must satisfy the Nernst theorem and all other requirements of thermodynamics. The reason is that the perfect crystal lattice is a truly equilibrium system with a nondegenerate dynamical state of lowest energy. Consequently, in accordance with quantum statistical physics, the entropy at zero temperature must be equal to zero [2].

The analytical derivation of the thermal correction to the Casimir energy between two Au plates in Ref. \[1\] is based on the Drude model and uses the condition

\[
\zeta_m(T) \ll \nu(T).
\]

This condition should be satisfied by sufficient number of Matsubara frequencies \(\zeta_m\) with \(m = 1, 2, 3, \ldots\) [see Eqs.(5) and (9) in Ref. \[1\]; note that Ref. \[1\] omits the lower index \(m\) and the argument \(T\)]. Here \(\zeta_m(T) = \frac{2\pi kmT}{\hbar}\), \(k\) is the Boltzmann constant and \(m = 0, 1, 2, \ldots\)

It is easily seen that in the case of perfect crystal lattice the condition \(1\) does not hold for any nonzero Matsubara frequency. In fact, according to Ref. \[1\], for Au \(\nu(T = 300\, \text{K}) = 34.5\, \text{meV}\) whereas \(\zeta_1(T = 300\, \text{K}) = 161.9\, \text{meV}\). Thus \(\nu(T = 300\, \text{K}) < \zeta_1(T = 300\, \text{K})\) in contradiction with assumption \(1\). Taking into account that \(\zeta_m = m\zeta_1\), the same inequality is valid for all nonzero Matsubara frequencies. When \(T\) decreases from room temperature up to approximately \(T_D/4\), where \(T_D\) is the Debye temperature (\(T_D = 165\, \text{K}\) for Au \[3\]), \(\nu(T) \sim T\), i.e., decreases with decreasing temperature following the same law as \(\zeta_m\). This preserves the inequality

\[
\nu(T) < \zeta_m(T), \quad m = 1, 2, 3, \ldots
\]

At \(T < T_D/4\) the relaxation frequency decreases even more rapidly than \(\zeta_m\) with decreasing \(T\) (i.e., as \(\sim T^5\) according to the Bloch-Grüneisen law due to electron-phonon collisions and as \(\sim T^2\) at liquid helium temperatures due to electron-electron scattering). As a result, with
the decrease of temperature for perfect crystal lattices it holds

$$\nu(T) \ll \zeta_m(T), \quad m = 1, 2, 3, \ldots \tag{3}$$

This inequality is just the opposite of the inequality (1) used in the derivation of Ref. [1]. Thus, all the results, obtained in Ref. [1], are inapplicable to perfect crystal lattices. According to Ref. [1] “the Nernst theorem is not violated when using the realistic Drude dispersion model” and this conclusion “is clearly in contrast to that presented in various works [4, 5, 6, 7, 8]”. These formulations are, however, misleading. References [4, 5, 6, 7, 8] deal with perfect crystal lattices and prove that for such lattices the use of the Drude model leads to the violation of the Nernst heat theorem. As explained above, the derivation in Ref. [1] is not applicable to perfect crystal lattices because it uses the inequality (1) which is just the opposite to the inequality (3) satisfied for perfect lattices. Thus, there is no contradiction between the results of Ref. [1] and Refs. [4, 5, 6, 7, 8]. Note that all above explanations concerning the inequalities (1)–(3) are contained in Ref. [4]. However, they were simply ignored in Ref. [1].

What is in fact found in Ref. [1] [see Eq.(31)] is the analytic behavior of the low-temperature thermal correction to the Casimir energy using the Drude model for crystal lattices with impurities:

$$\Delta F = C_1 T^2 (1 - C_2 T^{1/2} + \ldots), \tag{4}$$

where $C_1$ and $C_2$ are constants. According to this correction, at very low temperatures the Casimir entropy abruptly jumps to zero starting from negative values. Thus formally the Nernst heat theorem is satisfied when impurities are present. This result is not new. It was first found by B.E. Sernelius in Ref. [9] and has been acknowledged in Refs. [4, 5, 6, 7, 8]. Previously this result was proven only numerically. Reference [1] provides an analytical proof.

However, the values of numerical coefficients $C_1$ and $C_2$ for Au in Eq. (4) are determined in Ref. [1] incorrectly. To calculate these coefficients, Ref. [1] uses the Au relaxation frequency $\nu(T = 300\text{ K}) = 34.5\text{ meV}$ and the inequality (1). However, as explained above, at room temperature and also at much lower temperatures in the application range of the Bloch-Grüneisen law, the inequality (1) is violated and exactly the opposite inequality (3) is valid. The inequality (1) used in Ref. [1] becomes valid only for imperfect lattices at very low $T$ when, due to the presence of impurities, the relaxation frequency deviates from the Bloch-
Grüneisen law and takes a nonzero $T$-independent residual value $\nu_0$. For typical Au samples the residual relaxation frequency is approximately equal to $\nu_0 \approx 34.5 \times 10^{-3}$ meV, and for the best samples which are most close to the perfect crystal it is even 3 orders of magnitude lower: $\nu_0 \approx 34.5 \times 10^{-6}$ meV [3]. In order that at least the first 10 Matsubara frequencies satisfy the inequality

$$\zeta_m(T) \ll \nu_0,$$

the temperature must be $T < 10^{-3}$ K for typical Au samples and $T < 10^{-6}$ K for the best Au samples. For the applicability of asymptotic expression (4) [Eq.(31) in Ref. [1]] the temperatures must be additionally at least one order of magnitude less.

As was mentioned above, to calculate the values of the coefficients $C_1$ and $C_2$ Ref. [1] uses the value $\nu(T = 300 \text{ K}) = 34.5$ meV. The correct values to be used instead are $\nu_0 = 34.5 \times 10^{-3}$ meV for typical Au samples and $\nu_0 = 34.5 \times 10^{-6}$ meV for the best Au samples. As a result, Eqs.(13), (18) and (30) in Ref. [1] lead to the following values of coefficients in Eq. (4):

$$C_1 = 5.81 \times 10^{-10} \text{ J/}(\text{m}^2 \text{ K}^2), \quad C_2 = 95.75 \text{ K}^{-1/2} \quad \text{(typical Au samples)},$$

$$C_1 = 5.81 \times 10^{-7} \text{ J/}(\text{m}^2 \text{ K}^2), \quad C_2 = 3028.0 \text{ K}^{-1/2} \quad \text{(best Au samples)}. \quad (6)$$

This should be compared with the values presented in Ref. [1]:

$$C_1 = 5.81 \times 10^{-13} \text{ J/}(\text{m}^2 \text{ K}^2), \quad C_2 = 3.03 \text{ K}^{-1/2}. \quad (7)$$

The results of numerical computations in Ref. [1] were found to be in agreement with the asymptotic expression [1] containing the wrong coefficients [7]. The reason is that in numerical computations the room temperature relaxation frequency $\nu(T = 300 \text{ K}) = 34.5$ meV was also used incorrectly within the wide temperature region from 0.01 K to 800 K. To obtain the correct computation results, from 4–5 K to 800 K the actual temperature dependence of the relaxation frequency on $T$ should be employed (given by the Bloch-Grüneisen law and the linear dependence). For temperatures around zero the residual relaxation frequency for Au, $\nu_0$, depending on the concentration of impurities, must be applied.

To conclude, Ref. [1] finds (up to incorrectly determined coefficients) the low-temperature behavior of the thermal correction to the Casimir energy in the configuration of two Au plates with impurities, using the permittivity of the Drude model. Although the results of Ref. [1] are in formal agreement with the Nernst theorem, there is no contradiction with the results...
of Refs. [4, 5, 6, 7, 8] demonstrating the violation of the Nernst theorem in the Drude model approach for perfect crystal lattices. The reason is that the condition used by the authors of Ref. [1] in their derivation is violated for perfect lattices and can be applied to only lattices with impurities.

It must be emphasized that the results of Ref. [1] do not solve the problem of inconsistency of the Drude model with basic thermodynamic principles in the application to the Casimir entropy, as the authors claim. Reference [1] recognizes that “a simple physical model of course cannot be permitted to run into conflict with thermodynamics”. However, as is clearly seen in the above and from Refs. [4, 5, 6, 7, 8], the Drude model violates the Nernst heat theorem for the Casimir entropy in the case of metals with perfect crystal lattices. This alone makes the Drude model approach to the Casimir force unacceptable as being in contradiction with quantum statistical physics. According to the authors of Ref. [1], the approaches with nonzero contributions of the transverse electric term at zero frequency (recall that in the Drude model approach this term does not contribute at \( \zeta = 0 \)) would violate the Nernst theorem. This is misinformation. As is rigorously proved in Refs. [4, 10], both the plasma model approach and the impedance approach are in agreement with the Nernst theorem, and both of them include a nonzero contribution from the transverse electric term at zero frequency. Thus, although for metals with impurities the Drude model approach leads to zero Casimir entropy at zero temperature, this approach is theoretically invalid and fails to provide a consistent description of the thermal Casimir force in the framework of the Lifshitz theory.

**Acknowledgments**

The authors are grateful for helpful discussions with all co-authors of our publications on this subject, i.e., V. B. Bezerra, M. Bordag, R. S. Decca, E. Fischbach, B. Geyer, D. E. Krause, D. López, U. Mohideen and C. Romero.

[1] J. S. Høye, I. Brevik, S. A. Ellingsen, and J. B. Aarseth, quant-ph/0703174(v.1).

[2] L. D. Landau and E. M. Lifshitz, *Statistical Physics*, Part 1 (Pergamon, Oxford, 1980).

[3] C. Kittel, *Introduction to Solid State Physics* (Wiley, New York, 1996).
[4] V. B. Bezerra, G. L. Klimchitskaya, V. M. Mostepanenko, and C. Romero, Phys. Rev. A 69, 022119 (2004).
[5] R. S. Decca, D. López, E. Fischbach, G. L. Klimchitskaya, D. E. Krause, and V. M. Mostepanenko, Ann. Phys. (N.Y.) 318, 37 (2005).
[6] V. B. Bezerra, R. S. Decca, E. Fischbach, G. L. Klimchitskaya, D. E. Krause, D. López, V. M. Mostepanenko, and C. Romero, Phys. Rev. E 73, 028101 (2006).
[7] V. M. Mostepanenko, V. B. Bezerra, R. S. Decca, E. Fischbach, B. Geyer, G. L. Klimchitskaya, D. E. Krause, D. López, and C. Romero, J. Phys. A: Math. Gen. 39, 6589 (2006).
[8] V. M. Mostepanenko, quant-ph/0702061; G. L. Klimchitskaya, U. Mohideen, and V. M. Mostepanenko, quant-ph/0703139, to appear in J. Phys. A: Math. Theor.
[9] M. Boström and B. E. Sernelius, Physica A 339, 53 (2004).
[10] B. Geyer, G. L. Klimchitskaya, and V. M. Mostepanenko, Phys. Rev. A 67, 062102 (2003).