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Fundamental limitations of the mode temperature concept in strongly coupled systems

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Abstract: We theoretically analyze heat exchange between two quantum systems in interaction with external thermostats. We show that in the strong coupling limit the widely used concept of mode temperatures loses its thermodynamic foundation and therefore cannot be employed to make a valid statement on cooling and heating in such systems; instead, the incorrectly applied concept may result in a severe misinterpretation of the underlying physics. We illustrate these general conclusions by discussing recent experimental results reported on the nanoscale heat transfer through quantum fluctuations between two nanomechanical membranes separated by a vacuum gap.

Keywords: Casimir force; coupled harmonic oscillators; mode temperature concept; near-field thermal radiation.

1 Introduction

Recently, experimental results [1] on coupled nanomechanical oscillators have been interpreted as an important heat transfer mechanism driven by quantum fluctuations. As claimed by the authors and subsequent comments [2], this startling phenomenon could have major practical implications in the field of thermal management in nanometer-scale technologies. On a fundamental level, it has even been suggested that the traditional three channels for heat transport — namely, conduction, convection, and radiation — should actually become four. This "new" heat flux channel could potentially revolutionize our understanding of heat exchanged between systems out of thermal equilibrium, and it could also pave the way to a new cooling technology which could have a huge societal impact [1, 2]. Therefore, these findings have met with high interest within the scientific community, and consequently, have triggered a large number of feature articles in the popular press.

In this work, we point out that the commonly accepted concept of a mode temperature should not be applied to the analysis of the experimental data in the manner suggested in a study by Fong et al. [1] because these mode temperatures lose their thermodynamical meaning under the conditions of that experiment. As we will demonstrate, an uncritical use of such mode temperatures may lead to a profoundly incorrect interpretation of the actual physical processes. In conclusion, we argue that Fong et al. [1] actually have measured an increase of the coupling strength between their coupled nanomechanical oscillators at short distances which is due to the Casimir force but definitely no real temperature change of the physical heat bath and no heat flux. Hence, this experiment provides no direct experimental evidence of a Casimir force driven heat flux (CFDHF). We show further that the CFDHF as derived from theory will certainly have no technological impact for cooling because it is simply negligibly small compared to many other ubiquitous heat transfer mechanisms.

2 Theoretical model

To start with let us consider a simple system described by two harmonic oscillators A and B as depicted in Figure 1 which corresponds to the experimental situation in a study by Fong et al. [1], where two heat baths were coupled by means of two micromechanical oscillators. These oscillators, fabricated as thin membranes, possess a high quality factor which leads to a weak coupling with the corresponding heat bath. In the course of the experiment, the coupling between the two harmonic oscillators is tuned by varying the separation distance between them. The oscillation frequencies of both oscillators are chosen to be equal as in the experiment, i.e., we set $\Omega_A = \Omega_B \equiv \Omega$. The phenomenological damping rates $\gamma_A = \Omega/2Q_A$ and $\gamma_B = \Omega/2Q_B$ are inversely proportional to the quality factors of the membranes which are large in the experiment,

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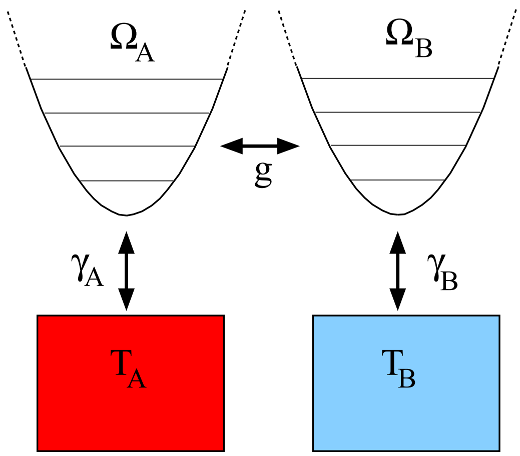

Figure 1: Sketch of the two harmonic oscillators of frequencies Ω_A and Ω_B in interaction which are coupled to two thermostats at temperature T_A and T_B with coupling strengths γ_A and γ_B. Here g denotes the coupling strength between the two systems A and B.

$Q_A = 4.5 \times 10^4$ and $Q_B = 2 \times 10^4$. They describe the coupling strength of the vibrational oscillator modes to the heat baths provided by the atoms in the membrane and membrane frame which are held at different temperatures T_A and T_B. Hence, T_A and T_B are temperatures in the thermodynamic sense of the electron and phonon system of the membrane. We further assume that the two membranes are coupled via a force whose strength is described by a coupling constant g.

In a full quantum description [3], the mean occupation number $\langle \hat{a}^\dagger \hat{a} \rangle$ (resp. $\langle \hat{b}^\dagger \hat{b} \rangle$) of two coupled harmonic oscillators in thermal equilibrium with two thermal baths at temperatures T_A and T_B reads under the standard Born–Markov assumption

$$\langle \hat{a}^\dagger \hat{a} \rangle = \frac{g^2 \frac{\gamma_A n_A + \gamma_B n_B}{\gamma_A + \gamma_B} + \gamma_A \gamma_B n_A}{g^2 + \gamma_A \gamma_B}, \tag{1}$$

$$\langle \hat{b}^\dagger \hat{b} \rangle = \frac{g^2 \frac{\gamma_A n_A + \gamma_B n_B}{\gamma_A + \gamma_B} + \gamma_A \gamma_B n_B}{g^2 + \gamma_A \gamma_B} \tag{2}$$

where $\hat{a}$ (resp. $\hat{b}$) denotes the ladder operator of oscillator A (resp. B) which fulfill the standard commutation relations $[\hat{a}, \hat{a}^\dagger] = 1$ (resp. $[\hat{b}, \hat{b}^\dagger] = 1$) and $n_{A/B} = 1/(\exp(\hbar\Omega/k_B T_{A/B}) - 1)$ is the Bose distribution function. Note, that in the experiment the frequencies of both oscillations of the membranes are $\Omega/2\pi = 191.6$ kHz so that $\hbar\Omega \ll k_B T_{A/B}$ and, therefore, the classical limit $n_{A/B} \approx \frac{k_B T_{A/B}}{\hbar\Omega}$ is applicable and will be used further.

Before we discuss the heat flow between the coupled harmonic oscillators, let us consider two very important limiting cases. In the weak coupling limit ($g \ll \gamma_A, \gamma_B$) we find

$$\langle \hat{a}^\dagger \hat{a} \rangle = n_A \approx \frac{k_B T_A}{\hbar\Omega} \quad \text{and} \quad \langle \hat{b}^\dagger \hat{b} \rangle = n_B \approx \frac{k_B T_B}{\hbar\Omega}. \tag{3}$$

Hence, in this limit the oscillators are thermalized by their heat baths at the corresponding bath temperature. Now, in the strong coupling limit ($g \gg \gamma_A, \gamma_B$) we have

$$\langle \hat{a}^\dagger \hat{a} \rangle \approx \langle \hat{b}^\dagger \hat{b} \rangle \approx \frac{k_B}{\hbar\Omega} \frac{\gamma_A T_A + \gamma_B T_B}{\gamma_A + \gamma_B}. \tag{4}$$

Thus, in the strong coupling limit, the mean occupation numbers are the same for both oscillators. It must be noted that the two oscillators are not in equilibrium at the same temperature, but their mean occupation number is in some sense the weighted mean value of the occupation numbers of the decoupled oscillators.

The heat flowing between the two reservoirs which are coupled via the oscillators by the coupling constant g in steady state reads in the classical limit [3]

$$P_{A\to B} \approx 2g^2 \frac{\gamma_A \gamma_B}{(\gamma_A + \gamma_B)(g^2 + \gamma_A \gamma_B)} k_B (T_A - T_B). \tag{5}$$

From this expression, it can be seen that any coupling g leads to a heat transfer between the reservoirs as predicted by several authors in recent theoretical studies [4–6] considering different models for phonon tunneling including the CFDHF. In the strong coupling limit, the power simplifies to the following form,

$$P_{A\to B} \approx 2 \frac{\gamma_A \gamma_B}{\gamma_A + \gamma_B} k_B (T_A - T_B) \tag{6}$$

which gives the maximal value of the heat transfer achievable in this model.

3 Definition of mode temperatures

Before analyzing the measurement of the CFDHF, it is now important to recall some standard features of harmonic oscillators. Here we focus, for clarity reasons, only on oscillator A but of course corresponding relations also hold for the oscillator B. Quantum mechanics predicts that its mean kinetic and mean potential energy reads [3]

$$\langle E_A^{\rm kin} \rangle = \frac{1}{2} m_A \langle \dot{\hat{x}}_A^2 \rangle = \langle \hat{a}^\dagger \hat{a} \rangle \frac{\hbar\Omega}{2}, \tag{7}$$

$$\langle E_A^{\rm pot} \rangle = \frac{1}{2} m_A \Omega^2 \langle \hat{x}_A^2 \rangle = \langle \hat{a}^\dagger \hat{a} \rangle \frac{\hbar\Omega}{2}. \tag{8}$$

In the weak coupling limit, Eq. (3) allows us to obtain the simplified expressions

$$\langle E_A^{\rm kin} \rangle = \langle E_A^{\rm pot} \rangle \approx n_A \frac{\hbar\Omega}{2} \approx \frac{k_B T_A}{2} \tag{9}$$

showing the classical result that each degree of freedom contributes $k_B T_A/2$ to the mean energy in equilibrium. Of course, in this limit, the oscillator is in equilibrium with its heat bath completely and decoupled from its surrounding. On the other hand, in the strong coupling limit, we have with Eq. (4)

$$\langle E_A^{\mathrm{kin}}\rangle = \langle E_A^{\mathrm{pot}}\rangle \approx \frac{\gamma_A}{\gamma_A+\gamma_B}\frac{k_B T_A}{2} + \frac{\gamma_B}{\gamma_A+\gamma_B}\frac{k_B T_B}{2}. \quad (10)$$

As already noted before, in this coupling regime, the oscillators are not in equilibrium with their baths anymore and each bath contributes a value of $k_B T_A/2$ and $k_B T_B/2$ weighted by the relative coupling of the oscillators to the baths.

Despite the fact that due to the coupling the oscillators are in general not in thermal equilibrium, in a study by Fong et al. [1], the mode temperature T_A' is defined by the authors as to be

$$\langle E_A^{\mathrm{kin}}\rangle = \langle E_A^{\mathrm{pot}}\rangle \approx n_A \frac{\hbar\Omega}{2} \approx \frac{k_B T_A'}{2}, \quad (11)$$

for all values of g. Setting this definition equal to Eq. (7) we have

$$T_A' = \frac{\hbar\Omega}{k_B}\langle \hat{a}^\dagger \hat{a}\rangle \quad (12)$$

which provides in the classical limit of Eq. (1) a relation to the bath temperatures which can be expressed as

$$T_A' = T_A + \frac{g^2\gamma_B (T_B - T_A)}{(\gamma_A+\gamma_B)(g^2+\gamma_A\gamma_B)}. \quad (13)$$

Hence, in the weak coupling limit, ($g \ll \gamma_A, \gamma_B$) one has $T_A' = T_A$ and in the strong coupling limit ($g \gg \gamma_A, \gamma_B$), one has obviously

$$T_A' \approx T_B' \approx \frac{\gamma_A}{\gamma_A+\gamma_B} T_A + \frac{\gamma_B}{\gamma_A+\gamma_B} T_B. \quad (14)$$

Therefore, the mode temperatures associated with the mean square displacement only coincide with the bath temperatures in the weak coupling limit. In that case, the mode temperatures are resembling real temperatures which could also be measured with any other thermometer. In contrast, in the strong coupling limit, the values of the mean square displacements of both oscillators become equal. This just reflects the fact that in the strong coupling regime the mean occupation numbers of the two oscillators become equal due to the coupling. Note that from the theoretical point of view, it is right from the start excluding that the bath temperature changes.

4 Discussion

After we have laid the theoretical foundation, we turn now to the analysis of the experiment in a study by Fong et al. [1]. If we use the values of the experiment, where $T_A = 312.5$ K and $T_B = 287$ K we obtain $T_A' \approx T_B' \approx 304.7$ K in the strong coupling regime which agrees very well with the value measured at 350 nm separation distance. Apparently, the membranes cool down (heat up) by about 8 K (18 K). But what's the meaning of these temperatures and the cooling or heating effect? The concept of a temperature is solely well defined for systems with an infinite large number of degrees of freedom. If all the contained modes in this system are thermalized it is possible to look at a single mode of the system and measure its energy content to deduce the temperature of the entire system. One can therefore introduce an additional oscillator like a membrane and couple it strongly to the system, determine its energy content, and deduce the temperature from it, i.e., the oscillator functions as a thermometer. This method is widely used in science and is absolutely correct if and only if the oscillator is strongly coupled to the system under investigation and thermally insulated from the surrounding. The latter mentioned necessary condition is imperative for all temperature measurements with any kind of thermometer. If this is not fulfilled one measures anything but the temperature of the system of interest. Exactly this is the case in a study by Fong et al. [1] in the strong coupling regime. Hence, T_A' and T_B' have no thermodynamical meaning in the strong coupling regime which also means that they allow for no statement on cooling or heating of the membranes.

Actually, the temperatures of the membranes are fixed at $T_A = 312.5$ K and $T_B = 287$ K during the experiment, which is also the underlying assumption of the theory. This is due to the fact that the CFDHF is extremely small. From Eq. (6), we can determine the maximal possible value of the CFDHF and obtain $P_{A\to B} = P_{\mathrm{Casimir}} \approx 6.5 \times 10^{-21}$ W. How big is this CFDHF compared to other heat flux mechanisms? In Figure 2, we show the distance dependence of the CFDHF in comparison to the radiative heat flux between the membranes used in Ref. [1]. The radiative heat flux has been determined in an exact calculation based on the framework of fluctuational electrodynamics so that it also includes the near-field enhancement effect [7]. Obviously, the radiative heat flux is 14–16 (in average about 15) orders of magnitude larger than the CFDHF. As estimated in [1] a heat flux of about 3.5 μW would lead to a temperature change of the membranes of only 0.02 K. Hence, the CFDHF will lead to a

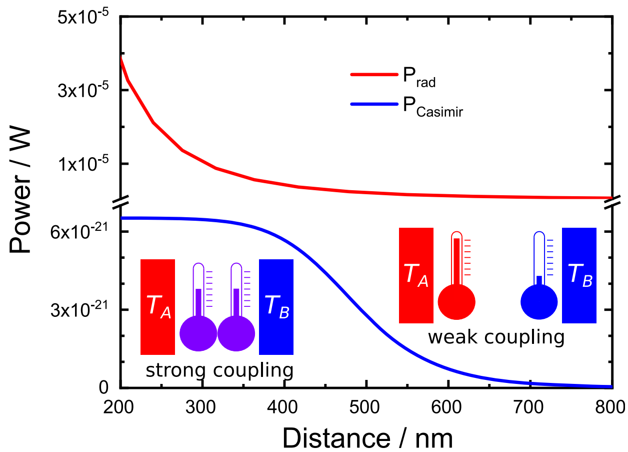

Figure 2: Comparison of heat flux $P_{A\to B} = P_{\text{Casimir}}$ mediated by the Casimir force using Eq. (5) with the values from the experiment for $T_{A/B}$, $\gamma_{A/B}$ and the measured coupling constant g from [1] with the radiative heat flux P_{rad} between the membranes using fluctuational electrodynamics [9]. It can be seen that for small distances the strong coupling regime for $P_{A\to B}$ is reached and the flux converges to 6.5×10^{-21}. Note, that the radiative heat flux is by 14–16 orders of magnitude larger than the CFDHF. Inset: Illustration of the different mode temperatures in weak and strong coupling regime.

temperature change of 0.02×10^{-15} K. This seems to be in strong contradiction to the experimental results allegedly suggesting that the CFDHF leads to a temperature change of several Kelvin. But as discussed before, the mode temperatures have no thermodynamical meaning and indeed the temperatures of the membranes do not change at all by the CFDHF. A comparison to heat conduction leads to a similar result. For example, the heat conductance of single molecules is on the order of 18×10^{-12} W/K [8]. This means, for a temperature difference of 25 K applied at both ends of a single molecule one would have a heat flowing through the molecule at a rate of about 4.5×10^{-10} W, i.e., a value which is 11 orders of magnitude larger than the CFDHF given by P_{Casimir}. Hence, even a single molecule is by many orders of magnitude more efficient in heating or cooling than the CFCHF.

How could then a "heat flux" be measured? To answer this question, let us compare Eqs. (14) and (5). By doing so, we find

$$P_{A\to B} = 2\gamma_A k_B\left(T_A - T_A'\right) = -2\gamma_B k_B\left(T_B - T_B'\right) \qquad (15)$$

From Eq. (15), it becomes clear that to measure a heat flux between the reservoirs it suffices to determine either the mode temperature T_A' or T_B' together with the bath temperatures T_A or T_B which are fixed during the experiment. But it is not necessary to use the concept of mode temperatures because what really counts is simply $\langle \hat{a}^\dagger \hat{a}\rangle$ or equivalently $\langle E_A^{\text{pot}}\rangle$ or $\langle \hat{x}_A^2\rangle$. And in the experiment in a Fong et al. [1] exactly the quantities $\langle \hat{x}_A^2\rangle$ and $\langle \hat{x}_B^2\rangle$ have been measured. This is done by measuring the values for the quadrature of the displacements of the membranes which allow for determining the distribution of the displacement. This distribution can be mapped to an energy distribution which, under the assumption that it is excited by a heat bath, can be fitted with a Boltzmann distribution $\propto \exp\left(-E_{A/B}^{\text{total}}/k_B T'_{A/B}\right)$ allowing us to determine the mode temperature. This gives the wrong impression that the membranes are equilibrated at their temperatures T_A' and T_B' so that the displacement measurement corresponds to a temperature measurement. But it must be kept in mind that only in the weak coupling limit ($g \ll \gamma_A, \gamma_B$) the vibrational modes are equilibrated to their bath temperatures and in general the mode temperatures have no thermodynamic meaning. Actually the displacement of the membranes or oscillators has the Gaussian property so that in phase space the quadrature can be fitted by a two dimensional Gaussian distribution. The distribution of the displacement itself is a one dimensional Gaussian $\propto \exp\left(-x_{A/B}^2/2\langle \hat{x}_{A/B}^2\rangle\right)$ which resembles the Boltzmann distribution. A fit with this function yields $\langle \hat{x}_{A/B}^2\rangle$, i.e., the quantity which is really measured in the experiment. With relation (11), we can associate it to mode temperatures T_A' and T_B', but this step is not necessary at all but is even dangerously misleading for the interpretation as we have seen before.

Finally, is the experiment of Fong et al. [1] a heat flux measurement and therefore an experimental proof of the CFDHF? As discussed the distance dependent ratio of the coupling strength between the membranes to the coupling strength of the membranes to their heat baths is measured by determining the energy content of the membrane oscillations $\langle \hat{x}_A^2\rangle$ so that at the end g is measured via Eqs. (1) and (12). There is no measurement of a temperature change of the membranes and definitely no heat flux measurement because there is no experimental calibration relating $\langle \hat{x}_A^2\rangle$ to the heat flux. Actually, the experimentalists simply calculate the associated heat flux from the theoretical expression of $P_{A\to B}$ knowing g, γ_A, and γ_B as we have done to calculate P_{Casimir} in Figure 2 by using the g from Casimir force measurements. Indeed, any measurement of the coupling constant g, i.e., Casimir force measurement with membranes, could have been used to calculate $P_{A\to B}$ from the model. Therefore, the calculation of the heat flux from measured mean square displacement of the membranes completely hinges on the validity of the theoretical model for $P_{A\to B}$ which is a priori assumed to be valid. Or differently stated, without the model giving the expression for

$P_{A\to B}$ the experiment could not give any value for the CFDHF, and it is hence no independent measure of it and is furthermore certainly no proof of the validity of the model for $P_{A\to B}$ nor of the existence of the CFDHF.

5 Conclusion

To summarize, the "new heat transfer mechanism" [2] introduced by Fong et al. [1] relies on a coupling via the Casimir force known since many decades. The experiment does not measure directly any heat flux, but the determination of the heat flux completely hinges on the model used to interpret the results. Furthermore, the interpretation of the energy content of the membranes in terms of a "mode temperature" is misleading. If applied in a naive manner, it seems to suggest the existence of a temperature change caused by the Casimir coupling which is larger than the change caused by any other known heat transfer mechanism. This spurious finding unfortunately has led to some exuberant claims concerning the alleged new channel, to the effect that it "has practical implications to thermal management in nanometer-scale technologies" and "paves the way for the exploitation of quantum vacuum in energy transport at the nanoscale" [1]. The list of untenable promises has been further extended in Ref. [2], claiming that "Phonon heat transfer through vacuum could have implications for managing heat in integrated circuits. The mechanism may provide a new way to intentionally dissipate heat in high-density transistor circuits, and it is an important consideration for keeping close elements thermally isolated in, for example, optical communication devices, which are sensitive to temperature cross talk. On a fundamental level, the conventional three methods of heat transfer — conduction, convection, and radiation — must now become four." Our theoretical analysis has clearly revealed that these ideas cannot be upheld and that the interpretation of the experiment [1] requires a profound revision. As we have shown, CFDHF indeed is 15 orders of magnitude smaller than the radiative heat flux and 11 orders magnitudes smaller than the heat conduction through a single molecule. Therefore, it is clear that the CFDHF can hardly be used in thermal management application. We therefore conclude that although of fundamental interest it is difficult to anticipate practical applications for the CFDHF whose detectability remains today questionable. Hence, for the moment, the "methods of heat transfer" remain three.

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