Phase transitions in finite size systems

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Abstract. We follow recent developments of a finite size thermal field theoretic formalism, which is mainly relevant to the investigation of small size corrections to the thermodynamical properties of the quark-gluon plasma. In doing so, we rely on statistical mechanics and large deviation theory arguments, and investigate geometrically confined systems of infinite volume $V$ with a finite spatial extent $L$. More specifically, we focus on systems in contact with a heat bath as well as on isolated ones. We find and present in detail the characteristic behaviors of a first and a second order phase transition, respectively. In the former case, we establish a connection between the phase transition and the mechanical support of the system. In the latter one, we identify a critical length $L_c \sim (V/EL)^{1/3}$, where $E$ is the total energy of the system which is fixed. We also briefly comment on the relevance of our findings, for respectively both the Casimir experiments and the future quark-gluon plasma phenomenology.

1. Introduction

1.1. Context and outline

In this proceedings, we briefly report on recent advances in identifying and fully characterizing a new type of geometrically driven phase transition [1, 2]. We use the recent developments made in investigating the finite size thermodynamics of relativistic quantum fields, with especially [3, 1, 4]. These developments are mostly relevant to the need for understanding and incorporating small size corrections to the thermodynamical properties of the quark-gluon plasma, and ultimately to all its medium properties [5]. However, the procedure can and will [2] be applied following section 2 to Casimir systems such as those featuring the so called force [6, 7].

It should be noticed that we work in the thermodynamic limit ($V \to \infty$), and thus chose to implicitly rescale all thermodynamic functions by the fixed asymptotically large area parameter $V_2 \equiv V/L$, in order to be able to properly manipulate the functions. We use two simplified models of a massless single neutral scalar field, with Dirichlet spatial boundary conditions, in a geometry defined by the space in between two asymptotically large and perfectly conducting parallel plates separated by a distance $L$, as inspired from [1].

In section 1.2, we first present our main argument regarding the relevance and equivalence of ensembles. Our argument is based on the theory of large ensemble deviation, and fully supported by the references [8, 9]. We then describe, in section 2, a very simple model of Casimir systems in thermal equilibrium with their environments. Such a crude model is nonetheless qualitatively relevant to isothermal realistic Casimir systems in such a geometry. Furthermore, in section 3 we describe a very simple model of a non interacting gluon plasma, in the same geometry, following in a simplified manner what has been recently studied in [1, 4]. Such a simplified model is nonetheless qualitatively relevant to small size isolated systems which are created in
heavy ion collisions. Finally, we conclude in section I with a special emphasis on the relevance of
our findings for the interpretation of Casimir experimental data, as well as for the development
of an improved quark-gluon plasma phenomenology.

1.2. Equivalence of ensembles

From an experimental point of view, the \{T, L\} set of variables is not relevant in any of the
experimental setups which are at the center of this work (see both sections 2 and 3), even if
it is extremely convenient from a theoretical point of view when computing any quantity. In
particular, the L variable only makes sense – experimentally speaking – for truly macroscopic
systems, where one can actually use a ruler in order to measure distances and the lengths can
be considered to be exactly fixed. For non-macroscopic systems\footnote{With sizes ranging from the micro/nano-meter to the femto-meter, and involving energy scales which make them comparatively small such as the ones we consider here.}, lengths cannot be measured
exactly: They fluctuate. Therefore, in such a system, and apart from possibly the temperature
T, the force or the pressure p which is applied to the system is actually what can be triggered, and
thus is the pressure of the system itself. One can see that, for example, the direct measurements
in Casimir systems concern forces instead of lengths \cite{10, 7, 11, 2}.

This being said, the presently investigated Phase Transitions (PT) require the promotion of
\{T, p\} and \{e, p\} (e \equiv E/V_2, the scaled total energy of the system) – for the isothermal Casimir
systems and those isolated which are relevant to small relativistic collisions, respectively – to the
rank of experimentally relevant set of variables. Regarding the former type of system, we will,
however, only consider here the \{e, L\} set of variables, and refer to \cite{1} for a complete treatment
further using a refined model. Thus, we will consider the \{T, p\}- and \{e, L\}-ensembles to be the
physically relevant ones for each of the system type, and analyze their respective equivalence, if
any, to the \{T, L\}-ensemble which is used in order to perform the calculations.

Indeed, in order to make a point potentially relevant to the experiments, one must make
sure that the theoretically chosen set of parameters \{T, L\} gives the same answer as the
aforementioned physically relevant one: One must pay attention that the two statistical
ensembles are (at least locally; where applicable) equivalent, which is to say here that for example
\{T, L\} \iff \{T, p\} over part or all of the domains of variables. For the present purpose, we consider
the thermodynamic equivalence of our ensembles and not the macrostate equivalence. Then,
one can establish the local equivalence over some sub-domains of two ensembles – one being fully
convex or concave (i.e. fully canonical or microcanonical), and the other convex in one variable
and concave in the other (i.e. mixed canonical and microcanonical), which is the case here with
the \{T, p\}- or \{e, L\}-ensembles and the \{T, L\}-ensemble, respectively – by means of the
following \footnote{Defining supporting hulls in mixed canonical and microcanonical ensembles, or simply defining them in the usual manner given that the curvature (in the sense of the second order derivative test) has the wrong sign on a whole half of the domain, are examples of such difficulties.}: The difference between the thermodynamic potential of, say, the \{T, L\}-ensemble, i.e., the Helmholtz free energy \(F(T, L)\), and its single Legendre-Fenchel transform \footnote{In \cite{12} the single Legendre-Fenchel transform is in fact equivalent to the full Legendre-Fenchel transform of manipulating supporting hulls within our setups.} back and forth \(F(T, L)^{**}\) must be vanishing over the said sub-domain of local equivalence \footnote{In \cite{8, 9} the single Legendre-Fenchel transform is in fact equivalent to the full Legendre-Fenchel transform of manipulating supporting hulls within our setups.}. In other
words, \(F(T, L) - F(T, L)^{**} = 0\) when \(F(T, L)^{**} \equiv S(e, L)\) proves the equivalence between the
\{T, L\}-ensemble and the \{e, L\} one over the related domain.

Regarding the Legendre-Fenchel transform, which is necessary in order to assess the
thermodynamic equivalence of two ensembles, we use here the following procedure given that
we expect our ensembles not to be globally equivalent anyway: We perform only the Legendre
transform of the thermodynamic potentials over one of their variables, but restrict the domains of
definition of these potentials to the sub-domains where their Hessians are not singular. On such
sub-domains indeed, the Legendre-Fenchel and the Legendre Transforms are in fact equivalent,
which allow us to circumvent the difficulty of manipulating supporting hulls within our setups.
Using this procedure, the sub-domain of ensemble equivalence is defined by the overlap of both the region in which we have $F(T, L) - F(T, L)^{**} = 0$, and the region in which the Legendre and the Legendre-Fenchel transforms are equivalent, i.e., in which the Hessian is non singular. If such a non empty region exists, then we can claim to have local equivalence of the two ensembles wherever on this domain [2].

2. Isothermal Casimir systems

We now present our isothermal Casimir system model, defined by the \( \{ T, L \} \)-ensemble free energy

\[
F_{cs}(T, L) = -\frac{1}{L^3} - LT^4 + \frac{\kappa}{2}(L - L_0)^2.
\]  

(1)

A few comments are in order regarding the above definition: (a) Regarding the thermal Casimir contribution to our model, we only kept both the high temperatures and short distances leading (respectively second and first above) terms, compared to the corresponding full free energy [1]. (b) For the sake of simplicity, we set the constants of these terms to one, following an unphysical but very convenient unit system \([\mathcal{U}]\). This is done, with no loss of generality, by defining specific units of temperature and length. (c) Regarding the mechanical support contribution to our model, we incorporated a spring-like term (the last above one; relevant to cantilevers in actual experimental setups [10, 7, 11, 2]). (d) This last term features a stiffness parameter \( \kappa \), and a rest length parameter \( L_0 \). (e) The setting of such a new dimensionfull parameter \( \kappa \) to some arbitrary numerical value is done by defining a convenient unit of energy. (f) At last, we have checked that changing the unit system, hence the numerical values of the constants and \( \kappa \) does not qualitatively affect the findings which we report in the following.

In figure [1][left], we present the phase diagram of the \( \{ T, L \} \)-ensemble.

![Figure 1](image)

**Figure 1.** (Left) The \( \{ T, L \} \)-ensemble phase diagram. The blue region marks a non singular Hessian. The pink meshed and blue sub-region marks ensemble equivalence. The red line is the line of phase transition. The Mechanical equilibrium paths, for which the total pressure vanishes, are the green and dashed black lines, each set at different values of \( L_0 \). (Right) The pressure obtained from the \( \{ T, L \} \)-ensemble versus the length of the system, with critical point.

The blue region corresponds to the region in which the Hessian of the thermodynamic potential from equation [1] is not singular (i.e. in which the second law of thermodynamic

\[^3\text{In the following, } \kappa = 15 \, \mathcal{U} \text{ always.}\]
is not violated), and the meshed pink region corresponds to the region in which we have $F(T, L) - F(T, L)^{**} = 0$. Therefore, the overlap of the two regions is the domain of equivalence between the ensembles $\{T, L\}$ and $\{T, p\}$, as discussed in section 1.2. The red (horizontal, due to the simplicity of the model) line is the line of isothermal compressibility divergence (where the first derivative of the pressure vanishes [1]), i.e., in the $\{T, L\}$-ensemble then, the line of second order phase transition. The lines in green and dotted black represent possible paths of mechanical equilibrium (vanishing pressure), for different values of the spring rest length $L_0$.

One can see that this parameter is compared to a specific value, namely $L_0^c$ which happens to be the $L_0$ value above which no mechanical equilibrium line can meet the second order phase transition. Below that critical value, such a phase transition occurs in this ensemble.

In figure 1 right, we then show the pressure obtained from the $\{T, L\}$-ensemble versus the length of the system. We see a critical $(T, L)$ point at a given rest length $L_0 < L_0^c$, where the pressure changes its first order derivative sign with respect to $L$ [1]. This point lays onto the red line in the left part of the same figure, and features the said second order phase transition.

We then move to the $\{T, p\}$-ensemble, which is physically relevant for this model as we saw in section 1.2 and show in figure 2 left, the phase diagram of the $\{T, p\}$-ensemble with same notation as in figure 1. It is interesting to see that again, a phase transition features in this ensemble, in the very same manner as for the $\{T, L\}$-ensemble. However, in figure 2 right, where we display the length obtained from the $\{T, p\}$-ensemble versus the pressure of the system, that the phase transition featuring for mechanical support with rest length $L_0 < L_0^c$ is a first order one.

**Figure 2.** (Left) The phase diagram of the $\{T, p\}$-ensemble, with same notation as in figure 1. (Right) The length obtained from the $\{T, p\}$-ensemble versus the pressure of the system, with critical point.

Given the relevance of this system, it would appear that isothermal Casimir systems feature a first order phase transition for certain mechanical support setups (here reflected by the constraint $L_0 < L_0^c$).

### 3. Isolated systems from relativistic collisions

We now present our isolated small system model, defined by the $\{T, L\}$-ensemble free energy

$$F_{Is}(T, L) = -\frac{1}{L^3} - LT^4,$$  \hspace{1cm} (2)
where we see the exact same expressions than in equation 1, except for the mechanical support which disappeared here. Thus, the same comments than for equation (a), (b), and (f) hold for the present model.

In figure 3, we show the phase diagrams of the \( \{T, L\} \)- and \( \{e, L\} \)-ensembles, respectively, with the same notation as in figure 1. The red phase transition line in figure 3 left is reported only for guidance purposes, since it is coming from the divergence of the iso-energetic compressibility which is relevant to (and computed in) the ensemble \( \{e, L\} \).

![Phase Diagrams](image)

**Figure 3.** (Left) The phase diagram of the \( \{T, L\} \)-ensemble, with same notation as in figure 1. We notice the ensemble equivalence is no restricted by the necessity to keep the Hessian non singular. A red phase transition line is reported, for guidance purposes, from the divergence of the iso-energetic compressibility (pertaining then to the ensemble \( \{e, L\} \)). (Right) The phase diagram of the \( \{e, L\} \)-ensemble, with same notation as in figure 1. We also notice the ensemble equivalence is no restricted by the necessity to keep the Hessian non singular. The red line is no pertaining to the actual second order phase transition.

Finally, in figure 4, we show the divergence of the iso-energetic compressibility as computed from the (correct) \( \{e, L\} \)-ensemble.

The relevant ensemble for such systems is however not the \( \{e, L\} \)-ensemble, but the \( \{e, p\} \)-one, and we refer to the reference [1] for a complete treatment using a somewhat more realistic model.

### 4. Conclusion

We have reported some evidence about the possible existence of phase transitions in very different finite size systems: First, isothermal Casimir systems with a first order phase transition providing certain mechanical support settings. A further investigation with more realist models is currently underway [2]. Then, a possible second order phase transition into finite size systems relevant to small (quark-)gluon plasma as created in current heavy-ion collisions. A more complete such investigation is reported in reference [1].

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Figure 4. Iso-energetic compressibility obtained from the \( \{e, L\} \)-ensemble, with critical point.

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