A proposal for the thermodynamics of certain open systems

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abstract

Motivated by the fact that the (inverse) temperature might be a function of the energy levels in the Planck distribution $n_\varepsilon = \frac{1}{z^{-1}e^{\beta(\varepsilon)\varepsilon}-1}$ for the occupation number n_ε of the level ε for free bosons, we show that it can be naturally achieved by imposing the constraint concerning the conservation of a weighted sum $\sum_\varepsilon f(\varepsilon)\varepsilon n_\varepsilon$, with a fixed positive weight function f, of the contributions of the single energy levels occupation in the Microcanonical Ensemble scheme, obtaining $\beta(\varepsilon) \propto f(\varepsilon)$. This immediately addresses the possibility that also a weighted sum $\sum_\varepsilon g(\varepsilon)n_\varepsilon$ of the particles occupation number is conserved, having as a consequence that the chemical potential might be a function of the energy levels of the system as well. This scheme leads to a thermodynamics of open systems in the following way:

the equilibrium is reached when the entropy function is maximised under the constraints that some weighed sums of occupation of the energy levels and the occupation numbers are conserved.

The standard case of isolated systems corresponds to the weight functions being trivial (i.e. f, g are identically 1).

Concerning the theoretical investigation of such open systems, new and unexpected phenomena can appear. Among them, we mention the appearance of the Bose Einstein Condensation both in dimension less than 3 in configuration space, and even in excited levels of the energy spectrum. In addition, this suggests a new approach to the condensation which allows an unified analysis involving also the condensation of q-particles, $-1 \leq q \leq 1$, where $q = \pm 1$ corresponds to the Bose/Fermi alternative. For such q-particles, it is shown that the condensation can occur only if $0 < q \leq 1$, the case 1 corresponding to the standard Bose-Einstein condensation. In this more general approach, completely new and unexpected states exhibiting condensation phenomena naturally occur even in the usual situation of equilibrium thermodynamics involving bosons.

The new approach proposed for the situation of 2^{nd} quantisation of free particles, is based on the theory of the distributions, which might hopefully be extended to more general cases involving nontrivial interaction.

The talk is based on the following papers:

Accardi L., Fidaleo F. *Condensation of Bose and q-particles in equilibrium and non equilibrium thermodynamics*, Rep. Math. Phys. **77** (2016), 153-182.

Fidaleo F., Viaggiu S. *A proposal for the thermodynamics of certain open systems*, Physica A **468** (2017), 677-690.

introduction

The present project on which is based the talk was suggested/based on the phenomenon of the Bose–Einstein Condensation (BEC for short). Such a phenomenon is a well–known one concerning the fact that at high density/low temperature regime, a macroscopic portion of Bose particles (i.e. quantum particles of integer spin) can occupy the ground level in the infinite volume limit of finite volume states constructed by using the Gibbs grand canonical ensemble prescription. All such states satisfy the Kubo–Martin–Schwinger (KMS for short) boundary condition. The KMS boundary condition can be then considered essentially the unique surviving condition after the infinite volume limit, in order to select states which are meaningful in the thermodynamics of the equilibrium. Due to Pauli exclusion principle, it is well know that the condensation cannot occur for half–integer spin quantum particle (i.e. Fermi particles). This can be seen by considering the (parallel) analysis involving the ideal Bose and Fermi gas, see e.g. the seminal book(s) by O. Bratteli and D. Robinson and the huge literature cited therein. Even if the ideal Bose gas (as well as the Fermi one) is only a theoretical model, it explain in a very clear way the motivation of the occurrence of the BEC. On the other hand, several phenomena are more or less directly connected with the BEC. Among them we mention the superfluidity of He_4, and the superconductivity of the Bardeen–Cooper–Schrieffer (BCS for short) pairs of electrons in superconductors.* Recently, it seems that some BEC condensation of photons has been also observed.†

All these states describing these very important condensation phenomena are then equilibrium states w.r.t. a fixed dynamics, hence automatically stationary. The aim of the present talk is to discuss such condensation phenomena in the light of the so–called *Local Equilibrium Principle* recently pointed out by Accardi, Fagnola and Quezada (cf. Weighted detailed balance and local KMS condition for non–equilibrium stationary states, Bussei Kenkyu **97** (2011),

*Also the other isotope He_3 presents the λ-point transition at around $\approx 0.2K$ which is a combined effect of the formation of the BCS pairs of He_3.

†The photon gas (together with the massive Z_0 Boson entering in the electroweak interaction), is the unique gas of Bosons which does not interact at any high density/low temperature regime. Recently (cf. Klaers et. al. doi:10.1038/nature09567) the BEC of photons in optical micro cavity was experimentally proved.

318–356), which roughly asserts that *the (inverse) temperature is a function of the energy of the levels*, and can be considered for all the cases under consideration as a generalization of the KMS boundary condition.[‡] Such a local principle, which is perfectly meaningful for systems with compact resolvent Hamiltonian, cannot be easily generalised to more complicated systems. Indeed, such a description is possible for the pivotal model describing a gas of infinitely many non interacting (boson) particles.[§]

The results we are going to describe are summarised as follows:

[‡]Probably, the idea to consider the temperature as a function of the energy levels is an old idea already present in literature. In addition, a similar but not equivalent approach was carried out by De Cannière from a mathematical point of view by using the modular theory, see below.

[§]Such a generalisation is still possible for systems described by quadratic Hamiltonians.

(i) The Local Equilibrium Principle can be easily generalised for quasi free states of the CCR algebra when the dynamics arises by a one parameter group of Bogoliubov automorphisms of the one–particle space, without any additional condition.

(ii) We exhibit states satisfying Local Equilibrium Principle and exhibiting BEC, not only on the ground state, but also (or only) on exited level, depending on the function $\beta(h)$, entering in the definition of the Local Equilibrium Principle.

(iii) We can exhibit states satisfying Local Equilibrium Principle, for which the condensation can occur also for models living in spatial dimensions d different from the usual ones $d \geq 3$.

(iv) For such states describing the condensation on excited levels, the rotation symmetry can be spontaneously broken, so we can obtain in a natural way states exhibiting BEC which are rotationally invariant or not.

(v) By using a quite natural principle involving the theory of the distributions in order to derive the BEC for the Local Equilibrium Principle (where the standard KMS condition is a particular case corresponding to thermodynamic equilibrium), we can consider the general case of the q–Deformed Commutation Relations with $q \in [-1,1]$, the cases $q = \pm 1$ corresponding to the Bose and Fermi cases, respectively. We prove that the BEC can occur also for the q–relations provided that $q \in (0,1]$. In addition, the distribution describing all such states must solve an equation in the space of the distribution, where the appearance of the BEC corresponds to additional (distributional) terms concentrated on a hyper–surface of codimension one in the space of momenta (typically a disjoint union of spheres).

(vi) By using the last result, even in the usual case of equilibrium thermodynamics we exhibit new states describing BEC, which are mathematically (and possibly also physically) meaningful, but are unknown at the knowledge of the author.¶

After such an analysis, some natural questions can be naturally addressed. Among them, we

¶This is due to the fact that the spatial distribution of the condensate has an infinite mean density, which excludes the appearance of such states after a standard thermodynamic limit process obtained by fixing a (finite) mean density.

mention the main one concerning the appearance of the Local Equilibrium Principle from the prescriptions of the basic concepts of the thermodynamics which is never explained in the previous analysis.

(vii) We can show that it will naturally emerge by enlarging the natural prescription in dealing with the Microcanonical Ensemble:

- on one hand, the computable function is still the Entropy, and the equilibrium is reached always when the Entropy Functional reaches the maximum;

- on the other hand, such a maximum is reached relaxing the constrains relative to the conserved energy and particle number of the system as explained before.

Local Equilibrium Principle

We start with a physical system whose observables are described by the C^*–algebra of all the bounded operators $\mathcal{B}(\mathcal{H})$ acting on a separable Hilbert space $\mathcal{H}$, and the time evolution is given in Heisenberg picture as

$$a \in \mathcal{B}(\mathcal{H}) \mapsto \alpha_t(a) = e^{\imath Ht} a e^{-\imath Ht} \in \mathcal{B}(\mathcal{H})\,, \quad t \in \mathbb{R}\,,$$

being H, acting on $\mathcal{H}$, the Hamiltonian of the system. To simplify the matter, we suppose that $H = \sum_{n=0}^{\infty} \varepsilon_n |\psi_n\rangle\langle\psi_n|$ is a the densely defined closed positive operator with compact resolvent, with eigenvalues and eigenvectors (repeated according the multiplicity) rearranged in increasing order. Fix any positive function (i.e. the *local inverse temperature*) $\beta : \mathbb{R}_+ \to \mathbb{R}_+$ such that $e^{-\beta(H)H}$ is a trace–class operator. According to the *Local Equilibrium Principle*, define the state

$$\omega_\beta(a) := \mathrm{Tr}\Big(e^{-\beta(H)H} a\Big)\,, \quad a \in \mathcal{B}(\mathcal{H})\,.$$

Denoting $\mathcal{F}(\mathcal{H})$ the sub algebra consisting of all the finite–rank operators acting on $\mathcal{H}$, it is immediate to show that

$$z \in \mathbb{C} \mapsto \omega_\beta(a\alpha_z(b))\,, \quad a \in \mathcal{B}(\mathcal{H})\,, b \in \mathcal{F}(\mathcal{H})\,,$$

is well defined and entire. The Local Equilibrium Principle simply means

$$\begin{aligned} &\omega_\beta(a\alpha_{t+i\beta(\varepsilon_i)}(|\psi_i\rangle\langle\psi_j|)) \\ =&e^{[\beta(\varepsilon_i)-\beta(\varepsilon_j)]\varepsilon_j}\omega_\beta(\alpha_t(|\psi_i\rangle\langle\psi_j|a)\,, \quad a \in \mathcal{B}(\mathcal{H})\,. \end{aligned}$$

The Local Equilibrium Principle, which reduces to the usual Kubo–Martin–Schwinger boundary condition when β is the constant function, is not immediately generalizable to arbitrary dynamical systems $(\mathfrak{A}, \alpha_t)$ consisting of a C^*–algebra, and an action α_t by possibly outer $*$–automorphisms. A way to get such a possible generalisation is to look at the modified evolution

$$\alpha_t^{(\beta)}(a) = e^{\imath\beta(H)Ht}ae^{-\imath\beta(H)Ht} \in \mathcal{B}(\mathcal{H})\,.$$

There is no way to define this modified evolution in the general case, but it is perfectly meaningful in the previous setting. Even in this modified evolution,

$$z \in \mathbb{C} \mapsto \omega_\beta(a\alpha_z^{(\beta)}(b))\,, \quad a \in \mathcal{B}(\mathcal{H})\,, b \in \mathcal{F}(\mathcal{H})\,,$$

is well defined and entire. The state ω_β satisfies for $a \in \mathcal{B}(\mathcal{H})\,, b \in \mathcal{F}(\mathcal{H})\,, t \in \mathbb{R}$,

$$\omega_\beta(a\alpha_{t+\imath}^{(\beta)}(b)) = \omega_\beta(\alpha_t^{(\beta)}(b)a)\,. \tag{1}$$

which can be extended to the whole $\mathcal{B}(\mathcal{H})$ as α is inner. Roughly speaking, for inner dynamics on $\mathcal{B}(\mathcal{H})$:
a state ω satisfies the Local Equilibrium Principle for the function β and the dynamics α, if it satisfies the KMS boundary condition at inverse temperature $\beta = 1$ for the modified dynamics $\alpha^{(\beta)}$.

Consider any continuous compactly supported function f on $\mathbb{R}$, together with its Fourier anti transform $\check{f}$. It is almost immediate to see that for each $a \in \mathcal{B}(\mathcal{H})$

$$\mu(f) := \int_{-\infty}^{+\infty} \check{f}(t)\omega_\beta(a^*\alpha_t^{(\beta)}(a))\,,$$
$$\nu(f) := \int_{-\infty}^{+\infty} \check{f}(t)\omega_\beta(\alpha_t^{(\beta)}(a)a^*)$$

define Radon measures on $\mathbb{R}$. It can be straightforwardly seen that μ and ν are linear combination of Dirac measures supported in a subset of $\{\beta(\varepsilon_n)\varepsilon_n - \beta(\varepsilon_m)\varepsilon_m \mid n, m \in \mathbb{N}\}$, depending on a. In addition, these are equivalent measures with Radon–Nikodym derivative given by

$$\frac{\mathrm{d}\mu}{\mathrm{d}\nu}(k) = e^{-k}$$

where

$$k \in \{\beta(\varepsilon_n)\varepsilon_n - \beta(\varepsilon_m)\varepsilon_m \mid n, m \in \mathbb{N}\}\,.$$

The last observation provides the bridge between the Local Equilibrium Principle and the related related condition involving directly the spectrum of the extension of the action α_t

on the sector $\pi_\omega(\mathfrak{A})''$. To conclude, we also mention some connections with the *strongly 2–spectrally passive states* investigated by De Cannière (cf. Commun. Math. Phys., **84** (1982),187–205; Publ. Res. Inst. Math. Sci. **20** (1984), 79–96).[‖]

[‖]The spectrum of an action describing the time evolution as in the present situation is given by $\{\varepsilon_n - \varepsilon_m \mid n, m \in \mathbb{N}\}$ and is known as the set of the *Bohr Frequencies*. The general case consisting of the spectrum of an action of an Abelian group on a C^*–algebra is denoted in mathematics as the *Arveson Spectrum*.

Local Equilibrium Principle for Quasi–Free Bosons

The C^*–algebra describing Bosons is that generated by the so–called Canonical Commutation Relations (CCR for short) and

$$a(f)a^\dagger(g) - a^\dagger(g)a(f) = \langle f|g\rangle \quad f, g \in \mathfrak{h}\,. \quad (2)$$

Here, $\mathfrak{h}$ is the *one–particle Hilbert space* equipped with the *one–particle Hamiltonian* $h > 0$, and the CCR C^*–algebra is meant in the Weyl form. The time evolution is generated by a one–parameter group of Bogoliubov automorphisms which, on the on the Weyl generators $\{W(u) \mid u \in \mathfrak{h}\}$, assumes the form

$$\alpha_t(W(f)) := e^{\imath t\,\mathsf{d}\Gamma(h)}W(u)e^{-\imath t\,\mathsf{d}\Gamma(h)} = W(e^{\imath th}f)\,. \quad (3)$$

Here, $\mathsf{d}\Gamma(h)$ is the second quantised Hamiltonian $H = \mathsf{d}\Gamma(h)$. For systems with finite degrees of freedom (i.e. when $\mathfrak{h}$ is finite–dimensional), the second quantised Hamiltonian $H := \mathsf{d}\Gamma(h)$ has compact resolvent and, in our framework

$e^{-\beta(H)H}$ is automatically trace–class. In this situation, it is almost immediate to show that the unique state ω_β satisfying the Local Equilibrium Principle w.r.t. the time evolution (3) is the quasi–free state uniquely determined by the two–point function

$$\omega_\beta(a^\dagger(g)a(f)) = \left\langle f \middle| \left(e^{\beta(h)h} - 1\right)^{-1} \middle| g \right\rangle , \quad f, g \in \mathfrak{h} .$$

In addition, we have

$$\omega_\beta(a(g)a^\dagger(e^{-\beta(h)h}f)) = \omega_\beta(a^\dagger(f)a(g)) , \quad (4)$$

or equivalently

$$\omega_\beta(a^\dagger(g)a(e^{\beta(h)h}f)) = \omega_\beta(a(f)a^\dagger(g)) . \quad (5)$$

The boundary conditions (4), (5) can be easily proved by using the commutation relations (2), and they are nothing else than the boundary condition (1) for the (unbounded) annihilator and creator operators a, $a^\dagger$. Even if the Local Equilibrium Principle is not immediately generalizable to arbitrary C^*–dynamical systems, it is now possible to provide its definition for CCR.

Fix on $\mathfrak{h}$ a quadratic form $Q : \mathfrak{h} \to [0, +\infty]$ with domain D_Q. Consider the sesquilinear form $F : \mathcal{D}_F \times \mathcal{D}_F \to \mathbb{C}$ uniquely determined by polarisation, $\mathcal{D}_F = \operatorname{span} D_Q$ being the linear span of D_Q. In order to achieve the chemical potential, we fix a Borel function $\gamma : (0, +\infty) \to (1, +\infty)$, which satisfies $\gamma > 1$ almost everywhere w.r.t. the Lebesgue measure.** Let $\mathfrak{h}_0 \subset \mathfrak{h}$ be a dense subspace such that, $\mathfrak{h}_0 \subset \mathcal{D}_F$, $\gamma(h)^{-1}\mathfrak{h}_0 \subset \mathcal{D}_F$, and consider the CCR algebra (always in the Weyl form) CCR($\mathfrak{h}_0$) generated by the annihilators in $\mathfrak{h}_0$. In order to have a reasonable dynamical behaviour of the physical system under consideration, we also suppose that $e^{\imath th}\mathfrak{h}_0 = \mathfrak{h}_0$, even if the last condition plays no role in the foregoing analysis.

**In our situation, γ is nothing else $e^{\beta(h)h}$.

Definition The quasi–free state $\omega \in \mathcal{S}(\mathrm{CCR}(\mathfrak{h}_0))$ uniquely defined by the two–point function

$$\omega(a^\dagger(f)a(g)) := F(g,f)$$

satisfies the Local Equilibrium Principle w.r.t. γ if it fulfils the boundary condition

$$\omega(a(g)a^\dagger(\gamma(h)^{-1}f)) = \omega(a^\dagger(f)a(g)) \,. \qquad (6)$$

It is possible to prove for many interesting situations, and by direct inspection for the cases of interests exhibiting BEC, that states satisfying the Local Equilibrium Principle are automatically invariant under the dynamics generated by the one–parameter Bogoliubov automorphisms given on the one particle space by $f \mapsto e^{\imath t h} f$.

Now we exhibit in details concrete quasi–free states satisfying the Local Equilibrium Principle and exhibiting BEC possibly in excited levels. We specialise the matter to the simplest models describing free Bosons living on $\mathbb{R}^d$. To simplify, we put $m = 1/2$ for their mass. Analogous considerations can be done for Bosons on lattices $\mathbb{Z}^d$. Indeed, fix the functions in the Schwartz class $\mathcal{S}(\mathbb{R}^d) \subset L^2(\mathbb{R}^d, \mathrm{d}^d\mathbf{x})$ equipped with the Hamiltonian

$$h = -\sum_{j=1}^{d} \frac{\partial^2}{\partial x_j^2} \equiv -\Delta$$

given by the opposite of the Laplace operator on $\mathbb{R}^d$, and consider the CCR algebra $\mathfrak{A} := \mathrm{CCR}(\mathcal{S}(\mathbb{R}^d))$. By passing to the momentum space, the Hamiltonian will be the multiplication function $h(\mathbf{k}) = k^2$. Another situation of interest will be the photon/phonon hamiltonian (in suitable unity) $h(\mathbf{k}) = k$. Let $\beta : (0, +\infty) \to (0, +\infty)$ be a Borel function with $\beta > 0$ almost everywhere w.r.t. the Lebesgue measure, such that

$$\rho_c(\beta) = \int_{\mathbb{R}^d} \frac{\mathrm{d}^d\mathbf{p}}{e^{\beta(p^2)p^2} - 1} < +\infty\,, \qquad (7)$$

Consider the set $S \subset [0, +\infty)$ made of points x_0 such that

$$\lim_{x \to x_0} \beta(x) x = 0 \,. \tag{8}$$

and, to simplify, choose a finite set of vectors $F \subset \mathbb{R}^d$ such that $\mathbf{p} \in F \Rightarrow p^2 \in S$. For a vector with non negative entries $\mathbf{D} := (D_{\mathbf{k}})_{k^2 \in F}$ define

$$\omega_{\beta,\mathbf{D}}(a^\dagger(f)a(g)) := \int_{\mathbb{R}^d} \frac{\widehat{f}(\mathbf{p})\overline{\widehat{g}(\mathbf{p})}}{e^{\beta(p^2)p^2} - 1} \mathrm{d}^d\mathbf{p} \tag{9}$$
$$+ \sum_{\mathbf{k} \in F} D_{\mathbf{k}} \widehat{f}(\mathbf{k}) \overline{\widehat{g}(\mathbf{k})} \,, \qquad f, g \in \mathcal{S}(\mathbb{R}^d) \,.$$

If some coefficient $D_{\mathbf{k_0}} > o$ in (9), then the state $\omega_{\beta,\mathbf{D}}$ exhibits the BEC on the energy level k_0^2.

Proposition The states $\omega_{\beta,\mathbf{D}}$ with two–point function given in (9) satisfy the Local Equilibrium Principle w.r.t. the function $\gamma(x) = e^{\beta(x)x}$.

proof (scketch) As noticed that the sesquilinear form defining $\omega_{\beta,\mathbf{D}}$ is well defined on $\mathcal{S}(\mathbb{R}^d) \times$

$\mathcal{S}(\mathbb{R}^d)$. In addition, thanks to (8), $e^{-\beta(h)h}f$ determines an equivalence class of functions which admits a representative such that its Fourier transform $\widehat{e^{-\beta(h)h}f}(\mathbf{p})$ is continuous in 0, with $\widehat{e^{-\beta(h)h}f}(\mathbf{0}) = \widehat{f}(\mathbf{0})$. Finally,

$$\int_{\mathbb{R}^d} \left|\widehat{f}(\mathbf{p})\overline{\widehat{g}(\mathbf{p})}\right| \frac{e^{-\beta(p^2)p^2}}{e^{\beta(p^2)p^2}-1}\,\mathrm{d}^d\mathbf{p} \leq \int_{\mathbb{R}^d} \frac{\mathrm{d}^d\mathbf{p}}{e^{\beta(p^2)p^2}-1} < +\infty\,.$$

This implies that $\omega_{\beta,D}(a(g)a^\dagger(e^{-\beta(p^2)p^2}f))$ is well defined, obtaining

$$\begin{aligned}
&\omega_{\beta,D}(a(g)a^\dagger(e^{-\beta(h)h}f)) \\
=&\omega_{\beta,D}(a^\dagger(e^{-\beta(h)h}f)a(g)) + \left\langle g\middle|e^{-\beta(h)h}\middle|f\right\rangle \\
=&\int_{\mathbb{R}^d} \left|\widehat{f}(\mathbf{p})\overline{\widehat{g}(\mathbf{p})}\right| \left(\frac{e^{-\beta(p^2)p^2}}{e^{\beta(p^2)p^2}-1} + e^{-\beta(p^2)p^2}\right)\mathrm{d}^d\mathbf{p} \\
&+D\widehat{e^{-\beta(h)h}f}(\mathbf{0})\overline{\widehat{g}(\mathbf{0})} = \int_{\mathbb{R}^d} \frac{\widehat{f}(\mathbf{p})\overline{\widehat{g}(\mathbf{p})}}{e^{\beta(p^2)p^2}-1}\,\mathrm{d}^d\mathbf{p} \\
&+D\widehat{f}(\mathbf{0})\overline{\widehat{g}(\mathbf{0})} = \omega_{\beta,D}(a^\dagger(f)a(g))
\end{aligned}$$

Notice that, the density of $\omega_{\beta,\mathbf{D}}$ is heuristically described as

$$\rho(\omega_{\beta,\mathbf{D}}) = \lim_{\Lambda\uparrow\mathbb{R}^d}\left(\frac{1}{\mathrm{vol}(\Lambda)}\int_\Lambda \omega_{\beta,\mathbf{D}}(a^\dagger(\delta_{\mathbf{x}})a(\delta_{\mathbf{x}}))\,\mathrm{d}^d\mathbf{x}\right)$$
$$= \int_{\mathbb{R}^d}\frac{\mathrm{d}^d\mathbf{p}}{e^{\beta(p^2)p^2}-1} + \rho_{cond}(\omega_{\beta,\mathbf{D}})\,,$$

where $\delta_{\mathbf{x}}$ is Dirac point mass concentred in the point $\mathbf{x}\in\mathbb{R}^d$, and $\rho_{cond}(\omega_{\beta,\mathbf{D}})$ is the portion of the condensed given by

$$\rho_{cond}(\omega_{\beta,\mathbf{D}}) = \lim_{\Lambda\uparrow\mathbb{R}^d}\frac{\sum_{k\in F} D_k}{\mathrm{vol}(\Lambda)}\int_\Lambda \left|\widehat{\delta_{\mathbf{x}}}(\mathbf{0})\right|^2 \mathrm{d}^d\mathbf{x}$$
$$= \sum_{k\in F} D_k\,.$$

By averaging on the spheres, we provide states $\omega_{\beta,\mathbf{D}}$ satisfying the Local Equilibrium principle, and exhibiting BEC whose condensed is equidistributed on the shell $k^2 = x$, provided $x \in S$. Let $\mathbb{S}_k \subset \mathbb{R}^d$ be the sphere in $\mathbb{R}^d$ of radius k, together with the rotationally invariant measure $\mathrm{d}\Omega_k$ on it. As before, for $F\subset S$,

$\mathbf{D} := (D_k)_{k^2 \in F}$ is a vector with non negative entries. Their two–point function is given by

$$\omega_{\beta,\mathbf{D}}(a^\dagger(f)a(g)) := \int_{\mathbb{R}^d} \frac{\widehat{f}(\mathbf{p})\overline{\widehat{g}(\mathbf{p})}}{e^{\beta(p^2)p^2}-1}\,\mathrm{d}^d\mathbf{p} \quad (10)$$
$$+\sum_{k\in F} D_k \int_{\mathbb{S}_k} \widehat{f}(\mathbf{p})\overline{\widehat{g}(\mathbf{p})}\,\mathrm{d}\Omega_k(\mathbf{p})\,,\ f,g\in\mathcal{S}(\mathbb{R}^d)\,.$$

We end by showing that the Local Equilibrium Principle allows condensation phenomena also for spatial dimensions different than the usual ones $d \geq 3$. Suppose that β is continuous with $\beta(x) > 0$, and

$$\beta(x) \approx x^{\alpha_0} \text{ for } x \to 0^+\,; \quad \beta(x) \approx \alpha_\infty \frac{\ln x}{x} \text{ for } x \to +\infty\,.$$

Conditions (8) and (7) implies $\alpha_0 + 1 > 0$ and $\alpha_\infty > 0$. We then compute

$$\int_0^{+\infty} \frac{\mathrm{d}^d\mathbf{p}}{e^{\beta(p^2)p^2}-1}$$
$$\approx \int_0^1 p^{d-1-2(\alpha_0+1)}\,\mathrm{d}p + \int_1^{+\infty} p^{d-1-2\alpha_\infty}\,\mathrm{d}p\,,$$

which converges if and only if

$$2(\alpha_0+1) < d < 2\alpha_\infty\,.$$

A new approach to the condensation

The difficulty to obtain the above mentioned stationary states as infinite volume limit of finite volume Gibbs states subjected to suitable boundary conditions suggests to approach to the problem of the BEC, directly by considering conditions on the infinite volume states. The idea is that to work directly by using distributions. The simplest model will be that describing free Bosons, that is to work directly in momentum space. The technique we are going to outline might be generalised to other situations involving Hamiltonians with a potential.[††]

For our purposes we treat the case for which the one–particle Hamiltonian $h(\mathbf{k}) = k^{\nu}$, $\nu > 0$

[††]Here, the possible generalisations can involve one–particle Hamiltonians of the form $h = p^2/2m + V(q)$, or multi–particle quadratic Hamiltonians.

(denoted with an abuse of notation directly as $h(k)$). It includes the massive (non relativistic) Hamiltonian $h(k) = k^2$ and the massless (relativistic) one $h(k) = k$.[‡‡] In order to avoid technicalities which do not add anything more to the understanding of the analysis, we make some reasonable restrictions to the function $\beta : \mathbb{R}_+ \to \mathbb{R}_+$. In fact we assume that

(i) $\lim_{x\downarrow 0} \beta(x)x = l \in [0, +\infty) \cup \{+\infty\}$ exists.

(ii) $\beta : \mathbb{R}_+ \to \mathbb{R}_+$ is continuous but a possibly finite number of points, including the empty set, such that if x_0 is one of such points, $\lim_{x\to x_0} \beta(x) = 0$.

(iii) $\inf_{\mathbb{R}_+} x\beta(x) = 0$

‡‡As in relativistic physics there is an upper limit to the velocity, the physical meaningful situations might correspond to $\nu \geq 1$.

(iv) If on $\mathbb{R}^d$, $h(k) = k^\nu$, $\nu > 0$, we assume that

$$\int_1^{+\infty} x^{\frac{d}{\nu}-1} e^{-\beta(x)x}\, \mathrm{d}x < +\infty\,.$$

Denote $F := \{r \in [0,+\infty) \mid \lim_{x\to r} x\beta(x) = 0\}$, and for $r \geq 0$, the shell $\mathbb{S}_r \subset \mathbb{R}\times\mathbb{R}$ defined as

$$\mathbb{S}_r := \{(\mathbf{p},\mathbf{k}) \in \mathbb{R}\times\mathbb{R} \mid h(p) = h(q) = r\}\,.$$

In order to unify the q–commutation relations, we consider the cases with the parameters $q \in [-1,1]$, the Bose and Fermi case being $q = \pm 1$, respectively. By using Fourier Transform, we can consider the density creators and annihilators in momentum space by putting

$$a^\dagger(f) = \int f(\mathbf{k}) a^\dagger(\mathbf{k})\, \mathrm{d}^d\mathbf{k}\,.$$

Then the q–Commutation Relations can be formally rewritten as

$$a(\mathbf{k})a^\dagger(\mathbf{p}) - q a^\dagger(\mathbf{p}) a(\mathbf{k}) = \delta(\mathbf{k}-\mathbf{p})\mathbf{1}\,.$$

Under the usual assumptions, we limit our analysis to two–point function defining the state ω which are described by a distribution on $\mathcal{D}(\mathbb{R}^d \times \mathbb{R}^d)$ as follows

$$\omega(a^\dagger(\check{f})a(\check{g}) = F_\omega(f \otimes \bar{g})\,, \qquad (11)$$

where $^-$ stands for the complex conjugate. Fix the one–particle Hamiltonian as a function of the momenta as before. In addition, we introduce a chemical potential λ by using the principle that the Local Equilibrium Principle for the function β and the Hamiltonian H corresponds to the standard equilibrium at (inverse) temperature 1 for the Hamiltonian $\beta(H)H$. In the equilibrium case for which $\beta(H) = \beta$, then $\lambda = \beta\mu$ where μ is the standard equilibrium chemical potential. Another choice in introducing the chemical potential is to pass to the shifted Hamiltonian $H_\mu := H - \mu$. Although being the last possibility more reasonable from a physical point of view, it seems to introduce many technical difficulties in order to capture the appearance of the BEC. By using the commutation relation (11), the Local Equilibrium Principle (6) for the chemical potential λ that for now we suppose to be any real number,

$$M_{\gamma_\lambda\otimes\mathrm{id}-q}F_\omega=\delta\,, \tag{12}$$

where $M_{\gamma_\lambda\otimes\mathrm{id}-q}$ is the multiplication operator for the function

$$G(\mathbf{k},\mathbf{p})=e^{\beta(h(k))k-\lambda}-q\,,$$

and δ is the Dirac distribution supported on the diagonal. If $q>0$ with $\lambda_q:=-\ln q$, define

$$\rho_c^{(q)}:=\int_{\mathbb{R}^d}\frac{\mathrm{d}^d\mathbf{p}}{e^{\beta(h(p))h(p)-\lambda_q}-q}=\frac{\rho_c}{q}\,.$$

Now we are ready to show how the condensation regime naturally emerge without using the thermodynamic limit of finite volume theories. The results are summarised in the following

Theorem

Suppose that the inverse temperature function β fulfils (i)–(iv) above, and a state ω satisfying the Local Equilibrium Principle uniquely defines a distribution on $\mathcal{D}(\mathbb{R}^d \times \mathbb{R}^d)$ as in (11) (hence it is a quasi–free state). Then the following assertions hold true.

(i) If $\lambda > -\ln(0 \vee q)$ (with the convention that $-\ln 0 = +\infty$), no of such states can exist.

(ii) **non condensation regime**: For each $\lambda < -\ln(0 \vee q)$, the quasi–free state ω with kernel

$$F_\omega(\mathbf{k}, \mathbf{p}) = \frac{\delta(\mathbf{k} - \mathbf{p})}{e^{\beta(h(p))h(p)-\lambda} - q} \tag{13}$$

is the unique quasi–free state in the selected class as above.

(iii) **condensation regime** (corresponding to $q > 0$ and $\lambda = \lambda_q$): The critical case can occur only if $\rho_c < +\infty$. If this is the case, each F_ω assumes the form

$$F_\omega(\mathbf{k},\mathbf{p}) = \frac{\delta(\mathbf{k}-\mathbf{p})}{q(e^{\beta(h(p))h(p)}-1)} + G(\mathbf{k},\mathbf{p})\,, \tag{14}$$

where G is supported in $\bigcup_{r\in F}\mathbb{S}_r$.

proof (sketch) We have already seen that the Local Equilibrium principle leads to (12), which can be uniquely solved provided $\lambda \neq -\ln(0\vee q)$, by giving (13).

(i) and (ii) Being

$$n_{\mathbf{p}} = \frac{1}{e^{\beta(h(p))h(p)-\lambda}-q}$$

the occupation number at momentum $\mathbf{p}$ and chemical potential λ, it must be positive, almost everywhere w.r.t. the Lebesgue measure.

This leads to $\lambda < -\ln(0 \vee q)$, for which the unique quasi–free states ω whose two–point function is determined by a distribution F_ω as above are those for which F_ω is given in (13).

(iii) By (ii), the condensation regime can occur only if $q \in (0,1]$ and $\lambda = -\ln q$. So we consider this case. By solving (12), we obtain (14), provided

$$f \mapsto \int_{\mathbb{R}^d} \frac{|f(\mathbf{p})|^2}{q(e^{\beta(h(p))h(p)} - 1)} \mathrm{d}^d\mathbf{p} < +\infty$$

for each $f \in \mathcal{D}(\mathbb{R}^d)$. If $F = \emptyset$, $\rho_c < +\infty$ by (iv) above. Then for $f \in \mathcal{D}(\mathbb{R}^d)$,

$$\int_{\mathbb{R}^d} \frac{|f(\mathbf{p})|^2}{q(e^{\beta(h(p))h(p)} - 1)} \mathrm{d}^d\mathbf{p} \leq \frac{\|f\|_\infty^2}{q}\rho_c < +\infty\,.$$

Thus, for the kernel we obtain (14) with G identically zero because $\bigcup_{r\in F}\mathbb{S}_r = \emptyset$. Thanks to the conditions (i)–(iv) imposed to β, $\rho_c = +\infty$ if and only if, for some $r_0 \in F$

$$\int_{B_\varepsilon(r_0)} \frac{\mathrm{d}^d\mathbf{p}}{e^{\beta(h(p))h(p)} - 1} = +\infty\,.$$

Here, $B_\varepsilon(r_0)$ is a spherical shell of thickness ε around $h(p) = r_0$. Choose any $f \in \mathcal{D}(\mathbb{R}^d)$ which is identically 1 on $B_\varepsilon(r_0)$. We compute

$$F_\omega(f \otimes \bar{f}) \geq \frac{1}{q} \int_{\mathbb{R}^d} \frac{|f(\mathbf{p})|^2}{e^{\beta(h(p))h(p)} - 1} \, \mathrm{d}^d\mathbf{p}$$
$$\geq \frac{1}{q} \int_{B_\varepsilon(r_0)} \frac{|f(\mathbf{p})|^2}{e^{\beta(h(p))h(p)} - 1} \, \mathrm{d}^d\mathbf{p}$$
$$\geq \frac{1}{q} \int_{B_\varepsilon(r_0)} \frac{\mathrm{d}^d\mathbf{p}}{e^{\beta(h(p))h(p)} - 1} = +\infty \,,$$

that is F_ω cannot define any distribution which is the kernel of some two–point function. Conversely, if $\rho_c < +\infty$, $\lambda = -\ln q$ is allowed as we have already proven that the states in (9), (10) have the form as in (14), and provides states exhibiting BEC, the latter being the uniques rotationally invariant because they are equidistributed on the hyper surfaces $h(k) = r$ for $r \in F$.

We end by showing that, also in the standard case of equilibrium, we can find states, mathematically meaningful, satisfying the usual KMS boundary condition, and exhibiting BEC. To simplify matter we reduce the analysis to the simplest case corresponding to the equilibrium situation at inverse temperature $\beta = 1$ corresponding to usual Bosons with one–particle Hamiltonian $h(k) = k^{\nu}$. We start with states which are not rotationally invariant, that is there is a privileged direction which we can suppose to be the first one x_1 in the configuration space, which correspond to k_1 in momentum space. Fix $D > 0$ and supposed that the critical density $\rho_c < +\infty$. It is straightforward to check that the states whose two–point function is given by

$$\omega(a^{\dagger}(\check{f})a(\check{g})) = \int_{\mathbb{R}^d} \frac{f(\mathbf{p})\overline{g(\mathbf{p})}}{e^{p^{\nu}} - 1}\,\mathrm{d}^d\mathbf{p} + D\frac{\partial f}{\partial p_1}(\mathbf{0})\frac{\partial \bar{g}}{\partial p_1}(\mathbf{0})$$

are equilibrium states for the dynamics generated by the one–particle Hamiltonian $h(p) = p^{\nu}$, provided $\nu > 1$ Such states cannot be obtained in the usual way as infinite volume limit of finite volume Gibbs states constructed by fixing the density of the environment, because the local density

$$
\begin{aligned}
\rho_\omega(x) &:= \omega(a^\dagger(\delta_{\mathbf{x}})a(\delta_{\mathbf{x}})) \\
&= \int_{\mathbb{R}^d} \frac{\mathrm{d}^d\mathbf{p}}{e^{p^\nu}-1} + D\left|\frac{\partial\widehat{\delta_{\mathbf{x}}}}{\partial p_1}(\mathbf{0})\right|^2 \\
&= \int_{\mathbb{R}^d} \frac{\mathrm{d}^d\mathbf{p}}{e^{p^\nu}-1} + Dx_1^2
\end{aligned}
$$

leads to an infinite mean density for the presence of the density of the condensate $\propto x_1^2$. The corresponding isotropic state has the two–point function given by

$$
\begin{aligned}
\omega(a^\dagger(\check{f})a(\check{g})) = \int_{\mathbb{R}^d} \frac{f(\mathbf{p})\overline{g(\mathbf{p})}}{e^{p^\nu}-1}\,\mathrm{d}^d\mathbf{p} \\
+D\Big\langle\nabla_{\mathbf{p}}g(\mathbf{0})\Big|\nabla_{\mathbf{p}}f(\mathbf{0})\Big\rangle\,.
\end{aligned}
$$

Remark For free q-particles whose one–particle Hamiltonian is $h(k)=k^\nu$ as before, we point out that we can search quasi–free states satisfying the (Local) Equilibrium Principle, exhibiting or not BEC, for a fixed chemical potential λ, among all positive–defined solutions in the space of the distributions of the equation (12) which assume the form

$$(e^{\beta(h(k))k^{\nu}-\lambda} - 1)F(\mathbf{k},\mathbf{p}) = \delta(\mathbf{k}-\mathbf{p})\,.$$

Already in the equilibrium case (i.e. $\beta(h) = const$), it provides new and unexpected simple nontrivial solutions.

The thermodynamics of certain open systems

The main question arising from the previous analysis is then to derive from the basic principles of statistical mechanics the analogous of the Planck distribution (for excited levels) of the form

$$n_{\varepsilon} = \frac{1}{z^{-1}e^{\beta(\varepsilon)\varepsilon} - 1}\,.$$

We now show that it will be a particular case of the following simple consideration.

We start as usual from the microcanonical ensemble corresponding to the (finite but "huge") system whose hamiltonian H is a selfadjoint strictly positive matrix

$$H=\sum_{\varepsilon_i\in\sigma(H)}\varepsilon_i P_{\varepsilon_i}$$

uniquely characterised up to unitary equivalence, by the set $\{\varepsilon_i\}$ of its eigenvalues and its degeneracy of the levels (i.e. the multiplicity)

$$g_i := \mathrm{dimR}(P_{\varepsilon_i})\,.$$

We can suppose equally well that H is a densely defined positive selfadjoint unbounded operator with compact resolvent acting on an infinite dimensional Hilbert space, obtaining an extreme problem on an infinite dimensional space. As this technicality is not adding anything else to our analysis, we decide not to pursue such a generalisation.

Suppose that N indistinguishable particles are occupying the levels ε_i with occupation numbers n_i under the obvious condition $N=\sum_i n_i$.

According to the three cases Bose/Fermi and Boltzmann respectively, the number $W(\{n_i\})$ of such possible configurations is given by

$$W(\{n_i\}) = \prod_i w_i \,,$$

with

$$w_i = \begin{cases} \binom{n_i+g_i-1}{n_i} & \text{Bose}\,, \\ \binom{g_i}{n_i} & \text{Fermi}\,, \\ \frac{g_i^{n_i}}{n_i!} & \text{Boltzmann}\,, \end{cases}$$

after dividing $W(\{n_i\})$ by $N!$ in the Boltzmann one. As usual, we suppose that all g_i and n_i go to infinity justifying the replacement of the factorials with their asymptotic by Stirling formula $m! \approx m^m e^{-m}$, obtaining for the entropy $S(\{\nu_i\}) := \ln W(\{n_i\})$ (in the units for which $k_B = 1$)

$$S(\{\nu_i\}) = \begin{cases} \sum_i g_i[\nu_i \ln(1/\nu_i + 1) + \ln(1+\nu_i)] & \text{Bose}\,, \\ \sum_i g_i[\nu_i \ln(1/\nu_i - 1) - \ln(1-\nu_i)] & \text{Fermi}\,, \\ \sum_i g_i \nu_i (1 - \ln \nu_i) & \text{Boltz.}\,. \end{cases} \tag{15}$$

Here, we have put $\nu_i := n_i/g_i$.

The entropies given in (15) for the Bose/Fermi and Boltzmann alternative can be considered as particular cases of of the q-*entropy* defined for $q \in [-1, 0) \cup (0, 1]$,

$$S_q(\{\nu_i\}) := \sum_i g_i \left[\frac{(1 + q\nu_i)}{q} \ln(1 + q\nu_i) - \nu_i \ln \nu_i \right]. \tag{16}$$

In fact, the Bose/Fermi cases correspond to the evaluation of S_q for $q = \pm 1$, respectively:

$$S_{+1/-1}(\{\nu_i\}) = S_{\text{Bose/Fermi}}(\{\nu_i\}).$$

Concerning the Boltzmann case, we get

$$\lim_{q \to 0} S_q(\{\nu_i\}) = S_{\text{Boltzmann}}(\{\nu_i\}),$$

pointwise in the variables ν_i, and uniformly on all bounded subsets (in the variables $\{\nu_i\}$).

To avoid unpleasant situations, we fix two strictly positive functions f, g on the spectrum $\{\varepsilon_i\}$ of the hamiltonian H. Concerning the continuum case, we can allow the functions f, g to be zero on a negligible subset w.r.t. the measure determined by the resolution of the identity of the one particle hamiltonian.

The main point of the present paper is to consider the extreme problem for the Entropy Functional (16) with the constraints

$$\sum_i f(\varepsilon_i)\varepsilon_i n_i = e\,, \quad \sum_i g(\varepsilon_i) n_i = n\,. \tag{17}$$

Here, e, n correspond to the weighted sums involving the number of particles and the energy of the system which, in our thermodynamical scheme, are considered as conserved quantities. They depend on the chosen functions f and g, which are not explicitly mentioned to shorten the notation. Notice that we can recover the usual thermodynamics when they are identically 1, obtaining $e = E$ the total energy of the system, and $n = N$ the total number of particles respectively.

Theorem
The values $\{\bar{\nu}_i\}$ which maximise the q-entropy S_q in (16) subjected to the constraints (17) are given by

$$\bar{\nu}_i = \frac{1}{e^{b(f(\varepsilon_i)\varepsilon_i - mg(\varepsilon_i))} - q}\,. \qquad (18)$$

As usual, In order to obtain the entropy as function of the conserved quantities e, n, the Lagrange multipliers will be determined by using the constrains (17).

To end, we note that the case corresponding to the Local Equilibrium Principle corresponds to $g(\varepsilon_i) = 1$, identically.