# Conditions for Bose-Einstein condensation in periodic background

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1. Entropy in Casimir-like structures
2. Basic thermodynamic formulas for BEC
3. Periodic chain of $\delta$-functions and some generalisations
4. On the possibility of BEC in one-dimensional combs
5. BEC in three dimensional lattice of delta functions
6. Conclusions

As known, Bose-Einstein condensation (BEC) is not possible in one and two dimensional systems unless there is some confining potential or interaction. In the present talk we investigate the influence of a periodic background on BEC. Possible applications could include, for instance, optical lattices.

We consider primarily an background composed of potentials with point support (like delta functions). This allows for explicit formulas; generalizations are easier possible.

There is a relation to Casimir physics, see below.

# Free particles and BEC

Given some $2^{nd}$-order elliptic operator $P$ and the related eigenvalue problem $P\phi_{(n)}(x) = \lambda_{(n)}\phi_{(n)}(x)$ ($(n)$ is some multiindex).

We know the spectral functions:

$$\zeta_P(s) = \sum_{(n)} \lambda_{(n)}^{-s}$$ –zeta function

$$K(t) = \sum_{(n)} e^{-t\lambda_{(n)}}$$ –heat kernel

From these one may construct

$$E_0(s) = \frac{\mu^{2s}}{2} \sum_{(n)} \lambda_{(n)}^{\frac{1}{2}-s} = \frac{\mu^{2s}}{2} \zeta_P(s - 1/2)$$ –vacuum ener

$$F = E_0(s) + \Delta F$$ –free energy

with $$\Delta F = T \sum_{(n)} \ln\left(1 - e^{-\beta(\lambda_{(n)}+\mu)}\right) \qquad (\beta = 1/T)$$

$$S = -\frac{d}{dT} F$$ –entropy

note: $E_0$ has uv divergences, $\Delta F$ and $S$ do not have

Dropping empty space contribution, for problem in open space one has a representation

$$\Delta F = T \int_0^\infty \frac{d\omega}{\pi} \ \ln\left(1 - e^{-\beta(\lambda_{(n)}+\mu)}\right) \frac{\partial}{\partial\omega}\delta(\omega)$$

where $\delta(\omega)$ is the scattering phase shift

Remind the role of heat kernel coefficients in uv-renormalization get representation in terms of the heat kernel

$$E_0(s) = \frac{\mu^{2s}}{2} \int_0^\infty \frac{dt}{t} \frac{t^{s-\frac{1}{2}}}{\Gamma(s-\frac{1}{2})} K(t)$$

and the heat kernel expansion: $K(t) = \frac{1}{(4\pi t)^{d/2}} \left(a_0 + a_{\frac{1}{2}}\sqrt{t} + \dots\right)$ in $d = 3$, uv comes from $a_0, \dots, a_2$

# further role of the coefficients

high-T expansion can be expressed in terms of the coefficients

$$F = -\frac{\pi^2}{90} a_0 T^4 - \frac{\zeta(3)}{4\pi^{3/2}} a_{\frac{1}{2}} T^3 - \frac{1}{24} a_1 T^2 + \ldots$$

Now, in Casimir force setups one considers typically separation dependent contributions (having in mind the force), in addition it was advised to separate all contributions which grow for $T \to \infty$ faster than the first power (the 'classical' contribution, this is the $\ell = 0$-contribution in Matsubara representation) as having powers of $\hbar$ in the denominator.

This way it was observed (first in [1]) that negative entropy appears. Later, this effect was intensively studied, see [2] and references therein

[1] B. Geyer, G. L. Klimchitskaya, and V. M. Mostepanenko. Thermal corrections in the Casimir interaction between a metal and dielectric.
*Phys. Rev. A*, 72:022111, 2005

[2] Kimball A. Milton, Yang Li, Pushpa Kalauni, Prachi Parashar, Romain Guerout, Gert-Ludwig Ingold, Astrid Lambrecht, and Serge Reynaud. Negative entropies in Casimir and Casimir-Polder interactions.
*Fortsch. Phys.*, 65(6-8):1600047, 2017

In [1] and [2], in the above aim, the entropy of single standing objects, free standing $\delta$-function plane and sphere was considered, by different approaches; negative entropy was found, whenever there remain discrepancies between the results (see [1] and discussion therein). Also an interesting behavior of the entropy was found in a periodic chain of (generalized) $\delta$-function potentials, see upcoming paper with J.M. Munoz-Castaneda.

In order to get some idea about the physical relevance, one needs to consider different physical processes. This was the motivation to consider Bose-Einstein condensation (BEC) in similar systems, specifically in periodic lattices of $\delta$-functions.

So in this talk I will consider BEC in one-dimensional systems, subsequently discuss another approach (using heat kernel expan.)

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[1] Kimball A. Milton, Pushpa Kalauni, Prachi Parashar, and Yang Li. Remarks on the Casimir self-entropy of a spherical electromagnetic $\delta$-function shell. *Phys. Rev.*, D99(4):045013, 2019

[2] M Bordag and K Kirsten. On the entropy of a spherical plasma shell. *J. Phys. A: Math. Gen.*, 51:455001, 2018

# Basic thermodynamic formulas for BEC

basic object is average total particle number in great canonical ensemble, given by

$$N = \frac{z}{1-z} + V \int \frac{d^d k}{(2\pi)^d} \frac{1}{z^{-1} e^{\beta\varepsilon(k)} - 1}.$$

the first term is the ground state contribution, $z$ is the fugacity
for relativistic dynamics, the one particle energy is $\varepsilon(k) = \hbar ck$
the temperature dependence can be scaled out,

$$N = \frac{z}{1-z} + V\Omega_d \Gamma(d) T^d g_d(z)$$

with the frequently used notation

$$g_d(z) = \frac{1}{\Gamma(d)} \int_0^\infty dk \, \frac{k^{d-1}}{z^{-1} e^k - 1}$$

For BEC, the contribution from the second terms must be bounded in order that additional particles may go to the ground state. This is the case if its contribution at $z = 1$ is finite.

# Basic thermodynamic formulas for BEC

The transition temperature is then

$$T_c = \left( \frac{N}{V} \frac{1}{\Omega_d \Gamma(d) g_d(1)} \right)^{1/d} .$$

For a free Bose gas we have

$$g_d(1) = \frac{1}{\Gamma(d)} \int_0^\infty dk \, \frac{k^{d-1}}{e^k - 1} = \zeta(d)$$

which is finite for $d > 1$.
(For non relativistic dynamics, i.e., $2^{nd}$ order operator, $d > 2$.)
[these are the formulas one can find in any textbook]

# One dimensional chain of $\delta$-functions

The wave equation within this model

$$\left(-\omega^2 - \frac{\partial^2}{\partial x^2} + \alpha \sum_n \delta(x - an)\right)\phi(x) = 0$$

The spectrum is determined by the zeros of the function ($k$ is the quasi momentum)

$$\tilde{\Phi}(\omega, k) = \frac{1}{\alpha} + \frac{\sin(\omega)}{\cos(k) - \cos(\omega)} = \frac{1}{\alpha} + \sum_N \frac{1}{-\omega^2 + (k + 2\pi N)^2}$$

it can be rewritten in the more popular form

$$\cos(k) = \cos(\omega) + \frac{\alpha}{\omega}\sin(\omega) = \frac{\cos(\omega + \delta(\omega))}{|t(\omega)|}$$

which is the well known frequency condition of the Dirac comb. Solutions show the well known band structure.

# Specific models

we consider some specific models

1. The generalized comb
   has in addition a delta'-contribution, $V(x) = \alpha\delta(x) + 2\beta\delta'(x)$

$$t(\omega) = \frac{2\omega(1-\beta^2)}{2\omega(\beta^2+1) + i\alpha}.$$

2. Double delta function
   In this model there are two delta function in each cell, representing for example two species of scattering centers, with $V(x) = \alpha_1\delta(x) + \alpha_2\delta(x-L)$.

$$t(\omega) = \left(\left(1 - \frac{\alpha_1}{i\omega}\right)\left(1 - \frac{\alpha_2}{i\omega}\right) + \frac{\alpha_1\alpha_2}{\omega^2}\, e^{2i\omega L}\right)^{-1}.$$

   The case of a single delta function can be obtained from here by $L = 0$ and $\alpha_1 = \alpha_2 = \alpha$.

# Sturm-Liouville problem framed by generalized delta functions

Consider a potential $V(x)$ with support $x \in [-\frac{L}{2}, \frac{L}{2}]$ with $L < 1$ and the related Sturm-Liouville equation,

$$\left(-\frac{\partial}{\partial x^2} + V(x)\right) u(x) = \omega^2 u(x).$$

Besides $u(x)$, this equation has a second independent solution, $v(x)$, with non-vanishing Wronskian $w = uv' - u'v$.
scattering setup:

$$\Phi(x) = \left(e^{i\omega x} + re^{-i\omega x}\right)\Theta\left(\frac{a}{2} - x\right) + \left(\mu\, u(x) + \nu\, v(x)\right)\Theta\left(\left(\frac{a}{2}\right)^2 - x^2\right) + te^{i\omega x}\Theta\left(x - \frac{a}{2}\right).$$

we impose the boundary conditions corresponding to the generalized delta function at $x = \pm\frac{L}{2}$. Transmission coefficient

$$t(\omega) = \frac{2i\omega w}{\Delta} e^{-2i\omega a}$$

# Sturm-Liouville problem framed by generalized delta functions

with

$$\Delta = \left[\frac{1+\beta'}{1-\beta'}v'_+ + \left(-i\omega\frac{1-\beta'}{1+\beta'} + \frac{\alpha'}{1-\beta'^2}\right)v_+\right]$$
$$\times\left[\frac{1-\beta}{1+\beta}u'_- + \left(i\omega\frac{1+\beta}{1-\beta} - \frac{\alpha}{1-\beta^2}\right)u_-\right]$$
$$+\left[-\frac{1+\beta'}{1-\beta'}u'_+ + \left(i\omega\frac{1-\beta'}{1+\beta'} - \frac{\alpha'}{1-\beta'^2}\right)u_+\right]$$
$$\times\left[\frac{1-\beta}{1+\beta}v'_- + \left(i\omega\frac{1+\beta}{1-\beta} - \frac{\alpha}{1-\beta^2}\right)v_-\right].$$

Specific examples were
Pöschl-Teller potential

$$V(x) = \frac{-2}{\cosh^2(x)}$$

and rectangular potential $V(x) = V_0\Theta\left(\left(\frac{a}{2}\right)^2 - x^2\right)$

# On the possibility of BEC in one-dimensional combs

let $\omega_n(k)$ be the solution of the dispersion relation
the particle number turns into

$$N = \frac{z}{1-z} + V \sum_n \int_0^\pi dk \frac{1}{z^{-1} e^{\beta \omega_n(k)} - 1}.$$

Since now the temperature dependence cannot be scaled out as before, we define a function

$$g(z) = \sum_n \int_0^\pi dk \frac{1}{z^{-1} e^{\beta \omega_n(k)} - 1}$$

the above equation after division by the volume turns into

$$n = \frac{1}{V}\frac{z}{1-z} + g(z)$$

Advancing, the discussion about a possible condensation in the thermodynamic limit goes the same way as before and reduces to the question whether $g(1)$ is finite.
To answer this question we change the integration over the quasimomentum $k$ for $\omega$ and come with $J(\omega) = \frac{\partial k}{\partial \omega}$ to the representation

$$g(z) = \sum_n \int_{\omega_n^{(u)}}^{\omega_n^{(o)}} d\omega \; \frac{J(\omega)}{z^{-1}\exp\left(\beta(\omega - \omega_1^{(u)})\right) - 1}$$

Now, for $z = 1$ we have a simple zero in the denominator and have to look for the behavior of the Jacobian at the lowest energy. It should be mentioned that this Jacobian, which is equivalent to the density of states, is formally the only difference to the case of a free field,

# Comb with single delta functions

From the above explicit expression we get

$$J(\omega) = \frac{\left(1 + \frac{\alpha}{\omega^2}\right)\sin(\omega) - \frac{\alpha}{\omega}\cos(\omega)}{\sqrt{1 - \left(\cos(\omega) + \frac{\alpha}{\omega}\sin(\omega)\right)^2}},$$

Expanding in $\omega - \omega_1^{(u)}$ we get

$$J(\omega) = \frac{1}{\sqrt{(\omega - \omega_1^{(u)})}} \sqrt{\frac{1}{2}\left(1 + \frac{\alpha}{(\omega_1^{(u)})^2}\right)\sin(\omega - \omega_1^{(u)}) + \frac{\alpha}{\omega_1^{(u)}}\cos(\omega_1^{(u)})}$$
$$+ O\left((\omega - \omega_1^{(u)})^0\right).$$

So, the Jacobian is singular which makes the condensation even more suppressed as compared to the free case.

# Thermodynamic properties of more general combs

for convenience we introduce the notation $h(\omega)$ for the frequency equation

$$h(\omega) = \frac{\cos(\omega + \delta(\omega))}{|t(\omega)|}.$$

and its expansion $h(\omega) = h(\omega_1^{(u)}) + (\omega - \omega_1^{(u)})h'(\omega_1^{(u)}) + \dots,$ now the expansion of the Jacobian reads

$$J(\omega) = -\frac{h'(\omega)}{\sqrt{1 - h(\omega)^2}} = \frac{\sqrt{-h'(\omega_1^{(u)})}}{\sqrt{2(\omega - \omega_1^{(u)})}} + \dots .$$

From here we conclude that for BEC in the one dimensional case to be possible, the function $h(\omega)$ must have vanishing first and second order derivatives in $\omega = \omega_1^{(u)}$ (together with the condition $h(\omega_1^{(u)}) = 1$).

*At the moment we do not know whether such condition is in conflict with all other necessary conditions or not*. We restrict ourselves to the consideration of the mentioned specific examples (which do not fulfill this condition).

# Examples: generalized delta

$$h(\omega) = \frac{\cos(\omega + \delta(\omega))}{|t(\omega)|}, \quad J(\omega) = -\frac{h'(\omega)}{\sqrt{1 - h(\omega)^2}} = \frac{\sqrt{-h'(\omega_1^{(u)})}}{\sqrt{2(\omega - \omega_1^{(u)})}} + \dots$$

need to have $h(\omega_1^{(u)}) = 1$ and $h'(\omega_1^{(u)}) = 0$
generalized comb:

$$h(\omega) = \frac{1 + \beta^2}{1 - \beta^2} \cos(\omega) + \frac{\alpha}{2\omega(1 - \beta^2)} \sin(\omega).$$

no solution for real parameters

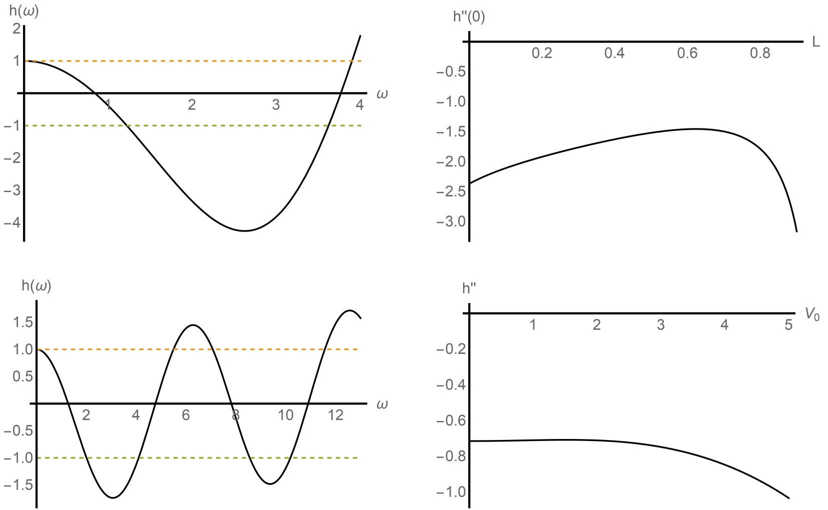
$$h(\omega) = \left(1 - \alpha_1\alpha_2 \frac{1-\cos(2\omega L)}{\omega^2}\right)\cos(\omega) + \left(\alpha_1 + \alpha_2 + \alpha_1\alpha_2 \frac{\sin(2\omega L)}{\omega}\right)$$

can have $\omega_1^{(u)} = 0$ for $\alpha_1 = -\alpha_2/(1 + 2\alpha_2 L(1-L))$
This implies that one of the delta functions in each cell of the lattice is attractive. However, inspection shows that nevertheless the spectrum starts at $\omega = 0$.
Further expansion

$$h(\omega) = 1 - \frac{3 + 6\alpha L(1-L) + 4\alpha^2 L^2(1-L)^2}{6(1 + 2\alpha L(1-L))}\omega^2 + \ldots .$$

As can be seen, the numerator has no real zeros. This way, the Jacobian is not singular in the ground state, but it does not vanish since the second derivative is nonzero. This is better than in the case with the generalized comb or with the single comb, but still not sufficient to have BEC.

# 'framed' Pöschl-Teller potential




'framed' Pöschl-Teller and rectangular potentials; the function $h(\omega)$ in the left panel, $h''(0)$ as function of the width $L$ in the right panel. ( $h'(0) =$) from symmetry), no solution!

# Three dimensional lattice of delta functions

$$\left(-\omega^2 - \Delta + \alpha \sum_{\mathbf{n}\in\mathbb{Z}^3} \delta^3(\mathbf{x} - a\mathbf{n})\right) \phi(x) = 0,$$

where **n** is a vector of integers and the delta function is in 3d
As well know, a delta function as potential in the wave equation is ill defined in three dimensions. There are several possibilities to give them a precise meaning. These possibilities, which are all equivalent, were recently discussed and compared in [1].
Frequency condition is $\tilde{\Phi}(\omega, \mathbf{k}) = 0$

$$\tilde{\Phi}(\omega, \mathbf{k}) = \frac{1}{\alpha} + \frac{i\omega}{4\pi} + \frac{J_1(\omega\mathbf{k})}{4\pi}, \qquad J_s(\omega, \mathbf{k}) = {\sum_{\mathbf{n}}}' \frac{1}{(a|\mathbf{n}|)^s}\, e^{ia\omega|\mathbf{n}| + ia\mathbf{k}\mathbf{n}},$$

[1] M. Bordag and J.M. Muñoz Castañeda. Dirac Lattices, Zero-Range Potentials and Self Adjoint Extension.
*Phys. Rev. D*, 91:065027, 2015

# Three dimensional lattice of delta functions

the critical temperature follows from the equation $n = g(1)$. For small $\alpha$, expansion of energy follws from above equations

$$\varepsilon(\omega) = \sqrt{(\mathbf{k} + 2\pi\mathbf{N}_0)^2 + \alpha\mu_1 + \dots}$$
$$= \sqrt{(\mathbf{k} + 2\pi\mathbf{N}_0)^2} + \frac{\alpha}{2\sqrt{(\mathbf{k} + 2\pi\mathbf{N}_0)^2}} + \dots .$$

expand further,

$$g(z) = \int_{\mathbb{R}^3} \frac{dk}{(2\pi)^3} \frac{1}{z^{-1}\exp(\beta\sqrt{k^2+\alpha}) - 1}.$$

we get

$$g(1) = \frac{T^3}{2\pi^2}\left(2\zeta(3) + \left(\frac{1}{2}\ln\left(\frac{\sqrt{\alpha}}{T}\right) - \frac{1 + 2\ln 2}{4}\right)\frac{\alpha}{T^2} + \dots\right).$$

# Three dimensional lattice of delta functions

solving this equation by iteration,

$$T_c = T_c^{(0)} \left( 1 + \frac{1}{4\zeta(3)} \left( \ln \left( \frac{\sqrt{\alpha}}{T_c^{(0)}} \right) - \frac{1 + 2\ln 2}{2} \right) \frac{\alpha}{\left(T_c^{(0)}\right)^2} + \dots \right) ,$$

of the critical temperature for small $\alpha$, where $T_c^{(0)} = \left(\frac{n\pi^2}{\zeta(3)}\right)^{1/3}$ is the critical temperature in the free case.

This is our final result in the three dimensional case. It is valid if $\alpha/(T_c^{(0)})^2$ is a small parameter, which is equivalent to large density, $n \gg \alpha^{2/3}$. The coefficient in front of $\alpha$ is negative and lowers the critical temperature. Due to the presence of $\ln\sqrt{\alpha}$ the correction is not analytic in the coupling $\alpha$.

For decreasing (non-periodic) potential; return to finite particle number (and finite volume)

$$N = \frac{z}{1-z} + \sum_{(n)}{}' \frac{1}{z^{-1}e^{\beta\lambda_{(n)}} - 1}.$$

(primed sum: without ground state)
rewrite using $1/(x-1) = \sum_{k\geq 1} x^{-k}$,

$$N = \frac{z}{1-z} + \sum_{k\geq 1} z^{-k} \sum_{(n)}{}' e^{-k\beta\lambda_{(n)}} = \frac{z}{1-z} + \sum_{k\geq 1} z^{-k} K(\beta k)$$

now use heat kernel expansion

$$N = \frac{z}{1-z} + \sum_{k\geq 1} z^{-k} \left(\frac{T}{4\pi k}\right)^{d/2} a_0 \left(1 + \frac{a_{\frac{1}{2}}}{a_0}\sqrt{\frac{k}{T}} + \dots\right)$$

$$= \frac{z}{1-z} + a_0 \left(\frac{T}{4\pi}\right)^{d/2} \mathrm{Li}_{\frac{d}{2}}(z) \left(1 + \frac{a_{\frac{1}{2}}}{a_0}\frac{1}{\sqrt{T}}\frac{\mathrm{Li}_{\frac{d-1}{2}}(z)}{\mathrm{Li}_{\frac{d}{2}}(z)} + \dots\right)$$

# Critical temperature

put z=1 and divide by $V$, use $\mathrm{Li}_n(1) = \zeta(n)$, get equation for $T_c$,

$$n = \frac{N}{V} = \frac{a_0}{V}\left(\frac{T_c}{4\pi}\right)^{d/2} \zeta(\frac{d}{2}) \left(1 + \frac{a_{\frac{1}{2}}}{a_0} \frac{1}{\sqrt{T_c}} \frac{\zeta(\frac{d-1}{2})}{\zeta(\frac{d}{2})} + \dots \right)$$

and solve by iteration,

$$\frac{T_c}{4\pi} = \left(\frac{V}{a_0}\frac{n}{\zeta(\frac{d}{2})}\right)^{2/d} \left(1 - \frac{2}{d}\frac{a_{\frac{1}{2}}}{a_0}\frac{\zeta(\frac{d-1}{2})}{\zeta(\frac{d}{2})}\left(\frac{a_0}{V}\frac{\zeta(\frac{d}{2})}{n}\right)^{1/d} + \dots \right)$$

for BEC to happen one needs $d > 2$ ($2^{nd}$ order operator)
in open geometry we have $a_0 \sim V$, $a_{1/2} \sim S$,...
thus $\frac{a_0}{V}$ is finite, $\frac{a_{1/2}}{a_0} \sim \frac{S}{V} \to 0$ in the thermodynamic limit
[different picture in confining potential with finite number of atoms in condensate]

# Conclusions

Initial question: what is physical relevance of entropy in Casimir like systems

No direct answer, but physical effect of Bose-Einstein condensation can be considered in such systems and may be of interest in its own

So far no correlation observed between non standard behavior of entropy and BEC, the only hint says that volume contribution is dominating for BEC

As for BEC:

1. in 1d periodic background no BEC in considered examples, condition on spectral function formulated, question whether corresponding systems exist, is still opened
2. in higher dimension (especially $d = 3$), in periodic lattice of delta functions, BEC happens, $T_c$ and first correction can be calculated even without calculating lattice sums [presentation of results in preparation]