Towards Bose-Einstein condensation on branched structures: a variational approach

Riccardo Adami
Dipartimento di Scienze Matematiche G.L. Lagrange
Politecnico di Torino

With Simone Dovetta, Enrico Serra and Paolo Tilli

SIMAI 2018, July 2–6, 2018, Roma

Two main topics:

- A theoretical one:
Functional analysis on metric graphs

- An applied one:
Bose-Einstein condensates

Main message: Seeking the ground state of a Bose-Einstein condensate may lead to some mathematical ideas and to applications.
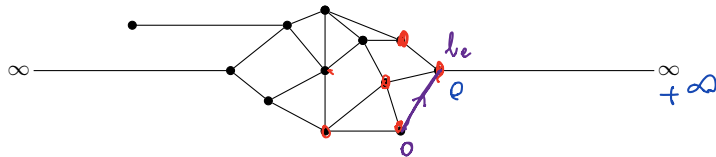
Emerging concept: Criticality.

Outline of the talk

1. Introduction to metric graphs

2. Introduction to Bose-Einstein condensation

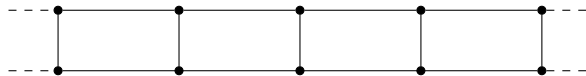3. Critical nonlinearity and critical mass

4. The grid: dimensional crossover

Metric Graphs

Networks: branched structures with edges and vertices
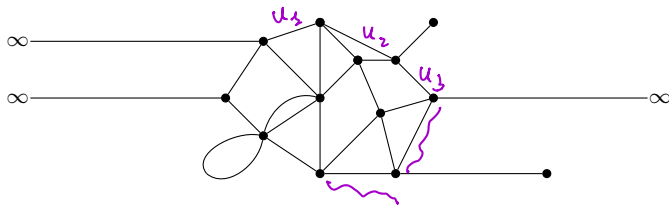
1. Finite non-compact graphs

2. Periodic graphs

- Metric structure: arclength, functions, functional spaces
- Some differential operators

A function u on $\mathcal{G}$ is a collection of functions u_e (e is an edge). Limits, continuity, derivatives are defined naturally

$$I_e \quad [0, \ell_e)$$

- $L^p(\mathcal{G}) := \oplus_e L^p(I_e)$
- $H^1(\mathcal{G}) := \oplus_e H^1(I_e)$ plus continuity at vertices
- $H^1_\mu(\mathcal{G}) = \{u \in H^1(\mathcal{G}) : \|u\|^2_{L^2(\mathcal{G})} = \mu\}$

MASS CONSTRAINT

The problem

Given a non–compact quantum graph $\mathcal{G}$ we investigate the existence of

global minimizers, or ground states of mass μ

for the energy functional

Kinetic   *Focusing*

$$E(u, \mathcal{G}) = \frac{1}{2}\|u'\|^2_{L^2(\mathcal{G})} - \frac{1}{p}\|u\|^p_{L^p(\mathcal{G})} = \frac{1}{2}\int_{\mathcal{G}}|u'|^2\,dx - \frac{1}{p}\int_{\mathcal{G}}|u|^p\,dx$$

NLS

Notation:

$$\mathcal{E}_{\mathcal{G}}(\mu) := \inf_{v \in H^1_\mu(\mathcal{G})} E(v, \mathcal{G}).$$

Euler-Lagrange equations

Any ground state u of $E(\cdot, \mathcal{G})$ satisfies, for some $\lambda \in \mathbb{R}$,

- $$u'' + |u|^{p-2}u = \lambda u \qquad \text{on every edge (NLS)}$$

- $$\sum_{e \succ \mathrm{v}} \frac{du_e}{dx_e}(\mathrm{v}) = 0 \qquad \text{at every vertex } \mathrm{v} \text{ (Kirchhoff)}$$

The sum involves the derivatives of u at v, in the outgoing direction, along every edge e emanating from v

The Kirchhoff condition is the natural condition for u' at the vertices of $\mathcal{G}$: if $\deg(\mathrm{v}) = 1$, it is the usual Neumann condition.

The functional aimed at minimizing is the conserved energy of the focusing NLS

$$i\partial_t u(t) = -\Delta u(t) - |u(t)|^{p-2}u(t)$$

on a metric graph $\mathcal{G}$
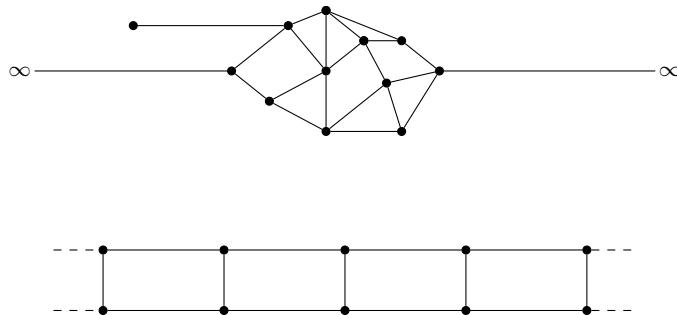
where Δ is the Kirchoff's or "free" Laplacian

Well-posedness is well-known (Ali Mehmeti 94)

Conservation laws of mass

$$\mu = \int_{\mathcal{G}} |u|^2$$

and energy

$$E(u, \mathcal{G}) = \frac{1}{2} \int_{\mathcal{G}} |u'|^2 - \frac{1}{p} \int_{\mathcal{G}} |u|^p$$

If $p < 6$, then all solutions are global in time, otherwise there exist blow up solutions that explode in a finite amount of time.

In the line, the only stationary states are the solitons. If $p < 6$, then they are also ground states.

Bound and Ground states

A bound state is a solution $\psi(x, t)$ to NLS s.t.

$$\psi(x, t) = e^{i\omega t} u(x)$$

A ground state u_{GS} is a standing wave that *minimizes the energy among the functions with the same mass μ*

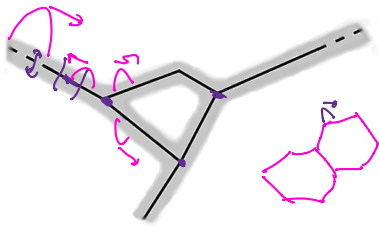$$E(u_{GS}, \mathcal{G}) := \min_{u \in H^1_\mu(\mathcal{G})} E(u, G)$$

$H^1_\mu(\mathcal{G}) :=$

$\{u \in H^1 \text{ inside edges}, \int_{\mathcal{G}} |u|^2 = \mu, u \text{ is continuous at nodes}\}$

u_{GS} is a ground state at mass $\mu \Longleftrightarrow$
1. $\mathcal{E}_{\mathcal{G}}(\mu) := \inf_{u \in H^1_\mu} E(u, \mathcal{G}) > -\infty$
2. $E(u_{GS}) = \mathcal{E}_{\mathcal{G}}(\mu)$

Some physical motivations

- Graphs provide approximations for dynamics in which transverse dimensions are negligible compared to longitudinal ones.

- Spectrum of valence electrons in organic molecules (Ruedenberg-Scherr 53)
- Nanotechnologies (circuits of quantum wires)
- Spectra of electromagnetic waves in thin dielectrics
- Quantum chaos
- Nonlinear effects in branched structures (Von Below '90s, Cacciapuoti-Finco-Noja 14, Noja-Pelinovsky-Shaikhova 15, Marzuola-Pelinovsky 15, Gnutzmann-Waltner 15, Tentarelli 16, Serra-Tentarelli 15, Dovetta 18)
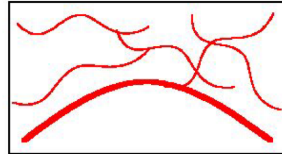
What is Bose-Einstein condensation (BEC)?
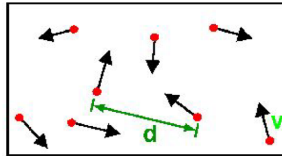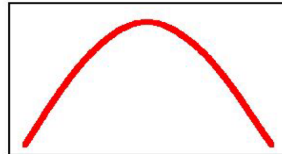

High Temperature T:
thermal velocity v
density d^{-3}
"Billiard balls"

Low Temperature T:
De Broglie wavelength
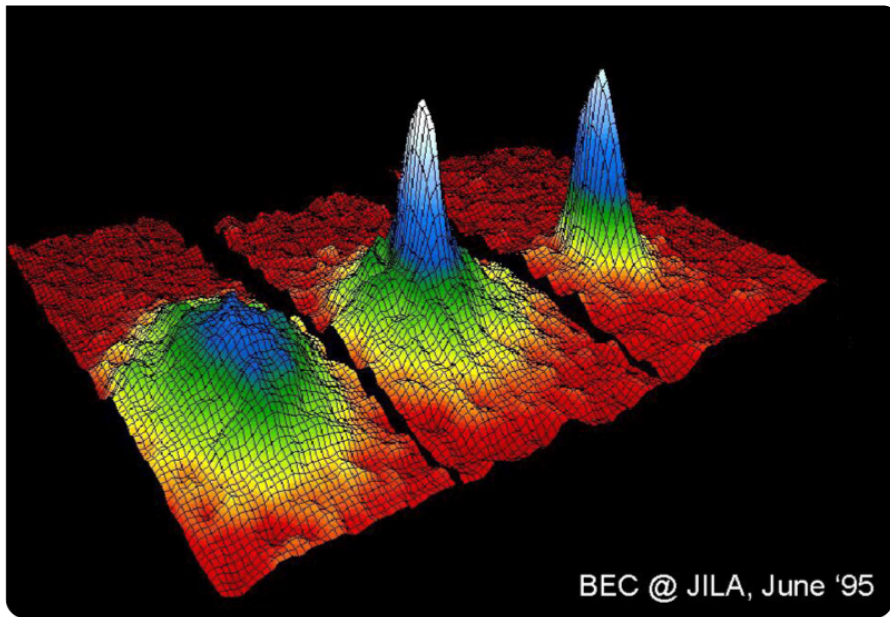$\lambda_{dB} = h/mv \propto T^{-1/2}$
"Wave packets"

$T = T_{crit}$:
Bose-Einstein Condensation
$\lambda_{dB} \approx d$
"Matter wave overlap"

T=0:
Pure Bose condensate
"Giant matter wave"

Ketterle
NP '01

25

BEC @ JILA, June '95

September

Ultracold boson gases undergo a phase transition in which all particles collapse to the same quantum state.

Such a quantum state is represented by the minimizer of the energy

$$E(u, \Omega) = \frac{1}{2}\|\nabla u\|^2_{L^2(\Omega)} + g\|u\|^4_{L^4(\Omega)} + \gamma\|u\|^6_{L^6(\Omega)}$$

where Ω is the region occupied by the magneto-optical trap that confines the condensate.

- The quartic term summarizes the two-body interaction between the particles of the gas

- The sixth power term summarizes the three-body interaction between the particles in the gas.

From the two-body interaction to the quartic term

1. Denoting V the two-body interaction potential, a particle feels any other in the state ψ by the effective potential

$$V_e(t, x) = \int_\Omega V(x - y)|\psi(t, y)|^2 \, dy$$

2. After the transition, the wave function spreads all over the (physically) admissible domain, so that V can be considered as a Dirac's delta and

$$V_e(t, x) = \left(\int V \right) |\psi(t, x)|^2$$

3. The Schrödinger equation for the first particle (in the same state ψ) then becomes

$$i\partial_t \psi(t, x) = -\Delta\psi(t, x) + \left(\int V \right) |\psi(t, x)|^2\psi(t, x)$$

4. The associated conserved energy reads

$$E(\psi(t)) = \frac{1}{2}\|\nabla\psi(t)\|_2^2 + \left(\int V\right)\|\psi(t)\|_4^4 \qquad \textit{Lieb}$$

5. The actual deduction of the energy is extremely more involved: Bogoliubov '50s, Gross 61, Pitaevskii 63, Lieb-Seiringer-Solovej-Yngvason '00s, A.-Golse-Teta 07, Erdős-Schlein-Yau 07-10, Benedikter-De Oliveira-Porta-Schlein 14.

In particular, the right coupling constant is not $\int V$.

6. A highly non-trivial physical mechanism, called Feshbach resonance allows tuning the coupling constant.

In most cases, only the quartic term is considered.

However, several nonlinearity powers have physical meaning.

The nonlinearity can be either focusing (positive sign) or defocusing (negative sign). We restrict to the focusing case.

Furthermore, we allow nonlinearity with an arbitrary power.

There exist quasi one-dimensional (cigar-shaped) condensates and ramified condensates (Vidal-Lima-Lyra 11, Lorenzo et al. 14), for which the minimization problem is related to ours.

Mathematical and physical breakthrough: Criticality - 0

Consider $\mathcal{G} = \mathbb{R}$ and the mass-preserving transformation

$$u_\lambda(x) \;=\; \sqrt{\lambda}u(\lambda x).$$

Then,

$$E(u_\lambda, \mathcal{G}) \;=\; \frac{\lambda^2}{2}\int |u'|^2 - \frac{\lambda^{\frac{p}{2}-1}}{p}\int |u|^p$$

so that

- If $p < 6$ then the kinetic energy overwhelms the potential term.
- If $p = 6$ then the two terms scale in the same way.
- If $p > 6$ then the potential prevails

More generally, in all graphs with a half-line the one-dimensional Gagliardo-Nirenberg inequalities hold.

Criticality - I

Gagliardo-Nirenberg inequalities:

$$\int |u|^p \leq C_p \, \mu^{\frac{p}{4}+\frac{1}{2}} \left(\int |u'|^2 \right)^{\frac{p}{4}-\frac{1}{2}}$$

$$\implies E(u, \mathcal{G}) \geq \frac{1}{2} \int |u'|^2 - \frac{C_p}{p} \mu^{\frac{p}{4}+\frac{1}{2}} \left(\int |u'|^2 \right)^{\frac{p}{4}-\frac{1}{2}}$$

- If $p < 6$, then E is lower bounded
- If $p = 6$, (critical power) then

$$E(u, \mathcal{G}) \geq \left(\frac{1}{2} - \frac{C_6}{6} \mu^2 \right) \int |u'|^2$$

so that there exists a critical mass under which all states have positive energy.
- If $p > 6$ no relevant information is provided, however the functional is not lower bounded

Subcritical, critical and supercritical nonlinearity

According to the different phenomenology, nonlinearity powers are classified as:
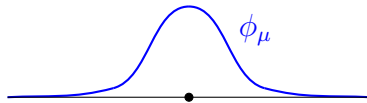
1. Subcritical: $2 < p < 6$.

2. Critical: $p = 6$.

3. Supercritical: $p > 6$.

Results are expected to vary sensitively as p crosses 6.

Subcritical case on the line

(Zakharov-Shabat 72, Cazenave-Lions 82)
For $p \in (2, 6)$ and every $\mu > 0$ ground states exist and are the translates of the soliton

$$\phi_\mu(x) = C\mu^{\frac{2}{6-p}} \operatorname{sech}^{\frac{2}{p-2}}(c\mu^{\frac{p-2}{6-p}} x).$$

ϕ_μ

Solitons have negative energy
When $p = 4$ (cubic NLS)

$$\phi_\mu(x) = \frac{\mu}{2\sqrt{2}} \operatorname{sech}\left(\frac{\mu}{4}x\right), \qquad \mathcal{E}_\mathbb{R}(\mu) = -\frac{\mu^3}{96}$$

Solitons are orbitally stable

Critical case in the line

Let $p = 6$.

- Denoted $\mu_{\mathbb{R}} = \pi\sqrt{3}/2$,

$$\mathcal{E}_{\mathbb{R}}(\mu) = \begin{cases} -\infty & \text{if } \mu > \mu_{\mathbb{R}} \\ 0 & \text{if } \mu \leq \mu_{\mathbb{R}} \end{cases}$$

- Ground states only for $\mu = \mu_{\mathbb{R}}$ and $\mathcal{E}_{\mathbb{R}}(\mu_{\mathbb{R}}) = 0$
  They are

$$\phi_\lambda(x) = \sqrt{\lambda}\phi(\lambda x), \qquad \lambda > 0,$$

  where $\phi(x) = \text{sech}^{1/2}(\frac{2}{\sqrt{3}}x)$.
- The dynamical problem is globally well-posed for all initial data with $\mu < \mu_{\mathbb{R}}$, while for $\mu \geq \mu_{\mathbb{R}}$ blow up arises
- Stationary solutions are orbitally unstable

The appearance of the critical mass

In the critical case $p = 6$, the value $\mu_{\mathbb{R}} = \pi\sqrt{3}/2$ marks two sudden transitions:

- Reached from below, $\mu_{\mathbb{R}}$ marks the transition from nonexistence to existence of ground states.
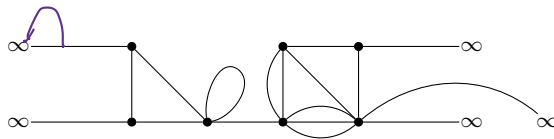- Reached from above, $\mu_{\mathbb{R}}$ marks the transition from lower boundedness to non-lower boundedness.

One gives to this value the name of critical mass.

Its appearance can be easily explained by using Gagliardo-Nirenberg inequality and the behaviour of E under mass-preserving transformation:

$$E(u_\lambda, \mathbb{R}) = \lambda^2 E(u, \mathbb{R})$$

(A.-Serra-Tilli 15-17)


- Let $p < 6$. Fix a mass $\mu > 0$

- Halflines host quasi-solitons approximating solitons

- The compact core of the graph possibly hosts bound states.

- If a bound state based on the compact core does better than the soliton, then a ground state at mass μ exists.

- The existence or nonexistence of a ground state results from a competition between halfilnes and compact core

Critical case for graphs with a halfline

(A.-Serra-Tilli 17) Let $\mathcal{G}$ be a graph with exactly one halfline. Then there exist
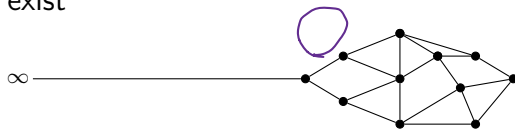
- A lower critical mass $\mu_{\mathcal{G}}^- = \mu_{\mathbb{R}}/2$ s.t. if $\mu < \mu_{\mathcal{G}}^-$, then $\mathcal{E}_{\mathcal{G}}(\mu) = 0$ and a ground state does not exist.

- A upper critical mass $\mu_{\mathcal{G}}^+ = \mu_{\mathbb{R}}$ s.t. if $\mu > \mu_{\mathcal{G}}^+$, then $\mathcal{E}_{\mathcal{G}}(\mu) = -\infty$.

- For $\mu_{\mathcal{G}}^- < \mu \leq \mu_{\mathcal{G}}^+$, a ground state with negative energy exists.

Some class of graphs with more than one halfline behaves similarly

Graphs distinguish the two roles of the critical mass

Criticality - II

1. In prevuois cases, the critical power $p_c \, (= 6)$ yields:
   1. If $p < p_c$, then $-\infty < \mathcal{E}_\mathcal{G}(\mu) < 0$
   2. If $p > p_c$, then $\mathcal{E}_\mathcal{G}(\mu) = -\infty$ for every μ

2. For $\mathcal{G} = \mathbb{R}$, a critical mass $\mu_\mathbb{R}$ s.t. at critical power:
   1. If $\mu < \mu_\mathbb{R}$, then $\mathcal{E}_\mathbb{R}(\mu) = 0$ is not attained
   2. If $\mu > \mu_\mathbb{R}$, then $\mathcal{E}_\mathbb{R}(\mu) = -\infty$

3. For a class of graphs made of a compact core and some haflines, two critical masses $\mu_\mathcal{G}^-, \mu_\mathcal{G}^+$ s.t.
   1. If $\mu < \mu_\mathcal{G}^-$, then $E(u, \mathcal{G}) > 0$ and $\mathcal{E}_\mathcal{G}(\mu) = 0$
   2. If $\mu > \mu_\mathcal{G}^+$, then the constrained energy is not lower bounded.

The grid splits the two roles of the critical power

The two-dimensional grid
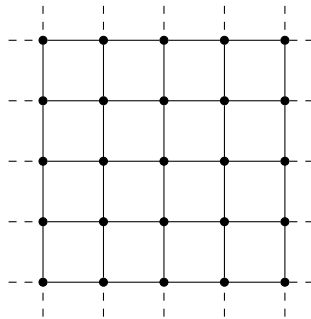
- Macroscale: $\mathcal{G} \to \mathbb{R}^2$. Critical exponent: $p = 4$

- Microscale: $\mathcal{G} \to \mathbb{R}$. Critical exponent: $p = 6$

In the middle?

Grid: preliminaries

1. *Quasi-solitons* are not available since there are no halflines

2. The only competitor to ground state is "spreading along the grid", reaching zero energy.

3. Therefore, if there is a function with negative energy, then there exists a ground state.

For instance, let $\mu > 0$.

$$u_\varepsilon(x) := \begin{cases} \sqrt{\mu}\, n_\varepsilon\, e^{-\varepsilon(|x|+|k|)} & \text{if } x \in V_k \\ \sqrt{\mu}\, n_\varepsilon\, e^{-\varepsilon(|x|+|h|)} & \text{if } x \in H_h \end{cases} \quad , \quad \lambda \in \mathbb{R}^+, \varepsilon > 0$$

where V_k is the k.th vertical line and H_h the h.th horizontal line,

$$n_\varepsilon = \sqrt{\frac{\varepsilon}{2}\frac{e^{2\varepsilon}-1}{e^{2\varepsilon}+1}}, \quad \int_{\mathcal{G}} |u_\varepsilon|^2 = \mu$$

$$\int_{\mathcal{G}} |u'_\varepsilon|^2 = \varepsilon^2 \mu$$

$$\int_{\mathcal{G}} |u_\varepsilon|^p = \frac{4\mu^{\frac{p}{2}} n_\varepsilon^p}{p\varepsilon} \left(\frac{e^{p\varepsilon}+1}{e^{p\varepsilon}-1} \right) \sim \frac{2^{3-\frac{p}{2}}}{p^2} \mu^{\frac{p}{2}} \varepsilon^{p-2}$$

Thus

$$E(u_\varepsilon, \mathcal{G}) = -\frac{2^{3-\frac{p}{2}}}{p^3} \mu^{\frac{p}{2}} \varepsilon^{p-2} + o(\varepsilon^{p-2}), \quad \varepsilon \to 0.$$

Therefore, choosing ε small enough one gets $E(u, \mathcal{G}_1) < 0$ and then there exists a ground state provided that $p < 4$!

(Two-dimensional effect!)

Gagliardo-Nirenberg inequalities

1. One-dimensional Gagliardo-Nirenberg inequality

$$\int |u|^p \; \leq \; C_p \, \mu^{\frac{p}{4}+\frac{1}{2}} \left(\int |u'|^2 \right)^{\frac{p}{4}-\frac{1}{2}}$$

holds for every graph

2. Two-dimensional Gagliardo-Nirenberg inequality

$$\int |u|^p \; \leq \; M_p \, \mu \left(\int |u'|^2 \right)^{\frac{p}{2}-1}$$

Quite astonishingly, both hold in the grid!

Then, by interpolation, for every $4 \leq p \leq 6$

$$\int |u|^p \; \leq \; K_p \, \mu^{\frac{p}{2}-1} \int |u'|^2$$

Thus for every $4 \leq p \leq 6$

$$E(u, \mathcal{G}) \geq \frac{1}{2}\left(1 - \frac{K_p}{p}\mu^{\frac{p}{2}-1}\right)\int |u'|^2$$

That show the occurrence of a critical mass μ_p below which energy is always positive

However, if $p < 6$, then for $\mu > \mu_p$ energy remains lower bounded, since, according to 1D Gagliardo-Nirenberg inequality, for every $u \in H^1_\mu(\mathcal{G})$

$$E(u, \mathcal{G}) \geq \frac{1}{2}\int |u'|^2 - \frac{C_p}{p}\mu^{\frac{p}{4}+\frac{1}{2}}\left(\int |u'|^2\right)^{\frac{p}{4}-\frac{1}{2}}$$

We finally obtain

> **Theorem (Dimensional Crossover)**
>
> *For every $4 \leq p \leq 6$ there exists a critical mass $\mu_p > 0$ s.t.*
>
> (i) *if $p = 4$ then ground states exist if $\mu > \mu_4$ and do not exist if $\mu < \mu_4$.*
>
> (ii) *if $4 < p < 6$ then ground states exist if and only if $\mu \geq \mu_p$*
>
> (iii) *if $p = 6$ then ground states never exist. Furthermore,*
>
> $$\inf_{u \in H^1_\mu(\mathcal{G})} E(u, \mathcal{G}) = \begin{cases} 0 & \text{if } \mu \leq \mu_6 \\ -\infty & \text{if } \mu > \mu_6 \end{cases}$$

Final remarks and open questions

We showed that the grid graph distinguishes two features of the critical power, i.e. the fact of being

1. the maximal power below which $\mathcal{E}_\mathcal{G}(\mu) < 0$ for every μ

2. the minimal power over which $\mathcal{E}_\mathcal{G}(\mu) = -\infty$ for every μ

Many issues are to be investigated, for instance:

- $\mu = \mu_4$?
- excited states and their stability
- Reconstructing $\mathbb{R}^2$ as a more and more dense grid
- N-dimensional grid with $N > 2$
- Other periodic graphs

...and the Physics?

The (few) experiments on Bose-Einstein condensates on branched structures show that the role of the junction can be crucial in a way that is not modelable by Kirchhoff conditions.

In our language, the functional to be minimized could remain the same, but the domain should change!. We are currently working on that.