Quantum particles and spectral properties of graphs

BEC, confined superfluidity and solitons in inhomogeneous arrays

Raffaella Burioni - Università di Parma

D. Cassi, A. Vezzani, P. Buonsante - Parma

M. Rasetti, V. Penna - Torino

A. Trombettoni - Trieste

P. Sodano - Perugia, Torino, Parma, Trieste, ...

Perugia - QID 2011

- Graphs and complex networks

- Physics and spectral properties of graphs

- Topological Effects: Large Scale and the Spectral Dimension

- Topological Effects: Local Scales

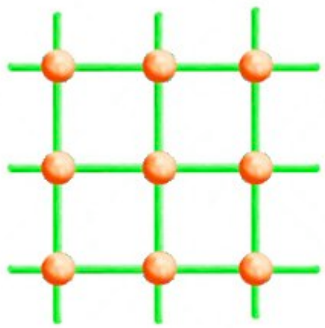
- Quantum particles on inhomogeous networks

- BEC, Topology induced confined superfluidity and topological filters for solitons on inhomogeneous arrays

- Future: Lévy-like graphs

Lattices and Graphs

- Crystals
- Discretized Euclidean spaces $\longrightarrow$ Lattices



$\downarrow$

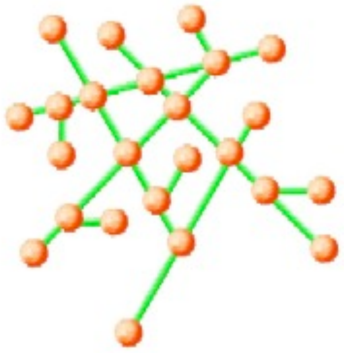
Effects of Geometry and Topology: Translation invariance

- Reciprocal Space, k, Fourier transform
- Bloch states
- Homogeneity
- Euclidean Dimension d of the lattice, Thermodynamic Limit...

$\longrightarrow$

Topologically disordered structures and graphs

- Polymers, glasses, amorphous solids
- Self-similar structures
- Biological matter → Graphs and Networks
- Discretized curved spaces
- Networks, engineered devices



i Points, fields, sites, masses, spins...

(i,j) Links, interactions, couplings, hopping parameters,

Chemical bonds, ...

The graph represents the topology of interactions

Topologically disordered structures and graphs

In general: No translation invariance

↓

- No reciprocal lattice
- No Fourier transform, no k
- No homogeneity
- Site dependent quantities

- Dimension of the graph?
- Thermodynamic limit?
- General geometrical properties of the graph?
- Effects of Dimensionality?
- Effects of Inhomogenenity?

A direct and inverse problem:

Physical structures → Experiments

Topology

Devices with topological effects ← Engineering

- Identify relevant topological features of a graph

- Build a specific structure with given topology (and physical properties)

A Useful tool: Algebraic Graph Theory and Spectral Properties of (Infinite) Graphs (B.Mohar 85)

Spectral properties:

"Global" scale and geometrical parameters for graphs:
Dimension

Local scale: the whole spectrum + eigenvectors

Spectra of what?

GRAPHS: Some Definitions G(V,E) set of vertices V and links E

- Adjacency Matrix

$$A_{ij} = \begin{cases} 1 & \text{if i and j are connected by a link} \\ 0 & \text{otherwise} \end{cases}$$

- Degree (coordination number) of site i

$$z_i = \sum_j A_{ij}$$

- Chemical Distance = # links of the shortest path connecting i and j

On Lattices:

$$A_{ij} \equiv A_{|i-j|}$$

GRAPHS: Some Definitions

- Laplacian Operator on G

$$L_{ij} = z_i - A_{ij}$$

- L is the generalization to networks and graphs of the usual Laplacian on continuous spaces and lattices (rigorous definition on $l_2(G)$)

$$L_{ij} \equiv -\nabla^2$$

Ex: 1d lattice

$$-L_{ij}\phi_j \equiv -L_{|i-j|}\phi_j = -(\phi_{i+1} + \phi_{i-1} - 2\phi_i)$$

- Hamiltonians and differential equations can be reformulated on a topologically disordered networks in terms of the matrices A and L

- The spectral properties of A and L, i.e. the set of their eigenvalues and eigenvectors, enters in many physical problems defined of the network

Some examples that we have been studying in the last few years:

Schroedinger equation on discrete structure with an on site potential

$$\sum_{j=1}^{n} \left(\frac{\hbar}{2m} L_{i,j} + U_i \delta_{ij} \right) \phi_j = i\hbar \frac{\partial \phi_i}{\partial t}$$

Eigenvalues equation:

$$\sum_{j=1}^{n} \left(\frac{\hbar}{2m} L_{i,j} + U_i \delta_{ij} \right) \phi_j^E = E \phi_i^E$$

Tight binding Hamiltonian on a network:

$$H^{TB} = -T \sum_{i,j=1}^{N} A_{i\,j} c_i^{+} c_j - a \sum_{i=1}^{N} z_i c_i^{+} c_i$$

c_i^{+}, c_j creation and annihilation operators for fermions on site i

Classical Spin Models on a network:

$$H = -J \sum_{i,j=1}^{N} A_{i\,j} \vec{S}_i \vec{S}_j$$

$\vec{S}_i$ unitary spin variable on site i

Bose Hubbard Model on a network

$$H = \sum_{j=1}^{M} \left[\frac{U}{2} n_j (n_j - 1) - \mu n_j \right] - T \sum_{i,j=1}^{M} A_{i\,j} a_i a_j^{+}$$

a_i^{+}, a_j	creation and annihilation operators for bosons on site i
$a_i^{+} a_j = n_i$	number of bosons on site i

U	on site repulsion among bosons
T	hopping amplitude between adjacent sites
μ	chemical potential

Discrete non- linear Schroedinger equation on a discrete structure:

$$\sum_{j=1}^{n} \left(\tfrac{\hbar}{2m} L_{i,j} + U_i \delta_{ij} \right) \phi_j + \Lambda |\phi_i|^2 \phi = i\hbar \frac{\partial \phi_i}{\partial t}$$

Stochastic Langevin equation for a phi 4 field:

$$\sum_{j=1}^{n} L_{i,j} \phi_j(t) + \Lambda (\phi_i)^2 \phi + \eta_i = i \frac{\partial \phi_i}{\partial t}$$

$\eta_i(t)$ stochastic gaussian noise

Spectral properties of A and L play a role analogous to k space and plane waves, which are the eigenvalue and eigenvectors of L on the continuum and on the lattice

- They allow for a definition of a "dimension" of a network with properties analogous to the Euclidean dimension

- Their properties can be used to determine the effects of inhomogeneous and disordered topologies on physical quantities (analytical and numerical tools)

Other interesting definitions

•Chemical distance: r_{ij} n. of links of the shortest path connecting i and j

$$\min\left\{n : (A)^n_{ij} \neq 0\right\}$$

•Generalized Van Hove Spheres:

$S_{o,r} \subset G$ Sphere of center o and radius r

Subgraph of G containing $N_{o,r}$ points

Thermodynamic limit $\longrightarrow$ Infinite graphs

Graphs considered here: Physical graphs

- Connected
- Bounded coordination number $\exists z_{\max}, z_i \leq z_{\max} \quad \forall i \in V$
- Polynomial growth $N_i(r) \sim r^c$ for $r \to \infty \quad \forall i \in V$

  n. of points at chemical distance $\leq$ r from i

- Boundary conditions

$$\lim_{r\to\infty} \frac{|\partial S_{o,r}|}{N_o(r)} = 0$$

$$\downarrow$$

Thermodynamic averages

The Laplacian on G and The Spectral Dimension

The gaussian model on a graph

- $\varphi_i \in \mathbb{R}$ $\qquad \ell^\infty(V)$
- m_i $\qquad 0 < m \le m_i \le M < \infty$ uniformly bounded masses

$$H_{o,r} = \frac{1}{2} \sum_{i,j \in S_{o,r}} \varphi_i \varphi_j (L_{ij} + m_i \delta_{ij})$$

Gaussian model

$$\downarrow$$

$$\mu[d\varphi] = Z^{-1}{}_{o,r} e^{-H_{o,r}} \prod_{i \in S_{o,r}} d\phi_i$$

Ferromagnetic Gaussian measure

$r \to \infty$

$$< F(\varphi) >= \int \mu[d\varphi] F(\varphi)$$

•Correlation functions

$$M_{ij} = m_i \delta_{ij} \qquad\qquad <\varphi_i \varphi_j> = (L+M)^{-1}{}_{ij}$$

•Average correlation functions

$$\overline{<\varphi\,\varphi\,>} = \lim_{r\to\infty} \frac{\sum_{i\in S_{o,r}} <\varphi_i \varphi_i>}{N_{o,r}}$$

independent of o on a physical graph

$$\Downarrow$$

The leading massless singularity of $\overline{<\varphi\,\varphi\,>}$

DEF.

Let $m_i = t\mu_i$ with $t > 0$

Define $$\overline{<\varphi\varphi>}^{(n)} = \left(-\frac{d}{dt}\right)^{(n)} \overline{<\varphi\varphi>}$$

If $\exists$ N so that

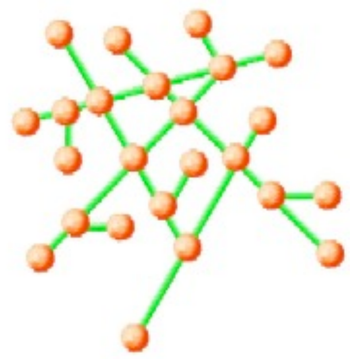
$$\lim_{t\to 0^+} \frac{\ln \overline{<\varphi\varphi>}^{(n)}}{\ln t} = 0 \qquad n = 0,1,\ldots,N-1$$

$$\lim_{t\to 0^+} \frac{\ln \overline{<\varphi\varphi>}^{(N)}}{\ln t} = D \neq 0$$ then

$$\boxed{\bar{d}_{\{m\}} = 2(D+N+1)}$$ Spectral dimension

leading massless singularity $$Sing\overline{<\varphi\varphi>}_{t\to 0} \sim t^{\frac{\bar{d}}{2}-1}$$

L $\longrightarrow$ Eigenvalues of L l



Large N $\longrightarrow$ density of eigenvalues

On a very large graph (in the thermodynamic limit) for $l \to 0$ (large scales)

$$\rho(l) \sim l^{\gamma}$$

$$\gamma = \frac{\bar{d}}{2} - 1$$

density of eigenvalues with power law behavior

$\boxed{\bar{d}}$ Spectral dimension of the graph

The Spectral Dimension is a real dimension:

- it describes the large scale geometry of the graph

  It does not depend on local geometrical details and it is invariant under isospectral transformations, which coincide for example with RG transformations on lattices (review JPA2005)

  it is an intrinsic topological dimension,
  it is different from the fractal dimension, which depends on immersion

  ISOSPECTRAL CLASSES

- it is the extension to general networks of the Euclidean dimension defined on regular lattices, (where $d \equiv \bar{d}$)
  in physical quantities related to bulk properties and large scale

N.B. - It can be experimentally measured (neutron scattering) vibrational modes
- Most of our world is between 1 and 2!

Some examples:

Statistical models on graphs

- Classical ferromagnetic Heisenberg O(n) spin models on graphs

On a Regular Lattice: existence of phase transition at finite temperature for d>2
On a Graph: existence of phase transition at finite temperature for $\bar{d} > 2$

A generalization of the Froelich-Simon-Spencer Bound on lattices

(+ generalized Mermin Wagner Theorem: no continuos symmetry breaking
for $\bar{d} \leq 2$)

- Dynamical critical exponents for phase ordering on graphs depend on $\bar{d}$:
asymptotically out of equilibrium dynamic in quenches at $T < T_c$

$$\sum_{j=1}^{n} L_{i,j}\phi_j(t) + \Lambda(\phi_i)^2\phi + \eta_i = i\frac{\partial \phi_i}{\partial t}$$

- Peierls-Landau vibrational instability in graphs for $\bar{d} \leq 2$, with applications to biological matter and proteins.

Peierls-Landau instability in complex topologies:

Harmonic oscillation of a discrete structure in a thermal bath T>0, mean square displacement of each unit

- On crystalline structures
  - d=1, linear chain with N points
    - Instability of crystalline order
  - d=2, Slowly increasing fluctuations
  - d=3 Bounded fluctuations, Stability

- On non crystalline structures

Effects of vibrations on solid structures ?
Which geometries are thermodynamically stables?

Stable if $\bar{d}$ > 2
Unstable if $\bar{d}$ < 2 , Maximal stability size at a given T when the oscillation exceeds the the typical spacing

-Many spectral dimensions measured in nature are < 2!
-Limited scaling range of fractals observed in nature (Avnir, Science 2002)
-Maximum stability size in globular proteins: experimentally verified!

The quantum Case:

Other effects of complex geometry? Local Scales and Local Topological defects?
Bose-Einstein Condensates

- Inhomogeneous topology can give rise to anomalous spectral properties of A and L: Hidden States

- Hidden States can induce Bose-Einstein Condensation on inhomogeneous networks even at low dimensionality ($\bar{d}$ matters but is not enough) and without a confining external potential

- “Topological” potentials: Condensation induced by inhomogeneous geometry

- Topological defects can act as Filters for solitons

- An example: The Comb Lattice, a simple low dimensional inhomogeneous graph, where non interacting bosons can condense

- General condition for the occurrence of BEC on inhomogeneous structures for non interacting bosons

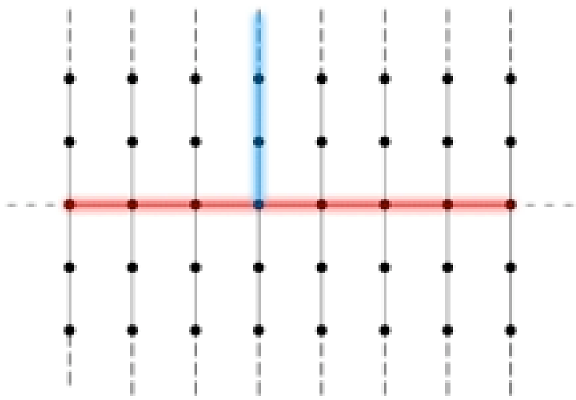
- Interactions: Bose Hubbard Model on a Comb Lattice
  Topology Induced confined superfluidity

- DNSE and Topological filters for solitons on graphs

Topology induced confined superfluidity on a comb network

Bose-Hubbard model on a comb

$$H = \sum_{j=1}^{N} \left[\frac{U}{2} n_j (n_j - 1) - \mu n_j \right] - T \sum_{i,j=1}^{N} A_{i\,j} a_i a_j^{+}$$



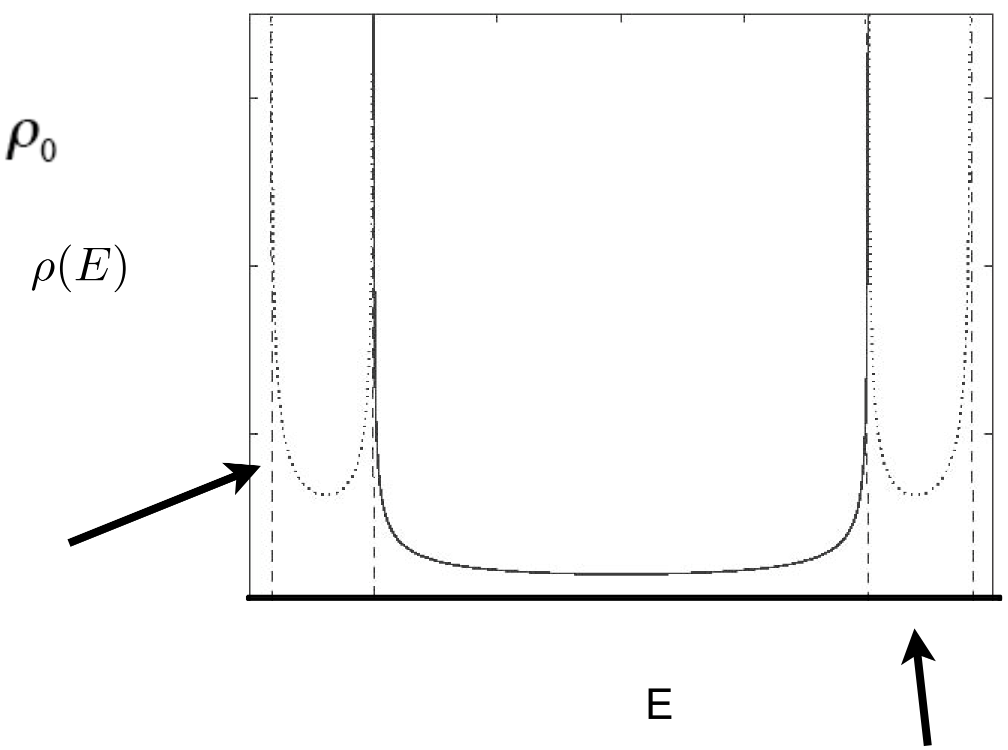
Already in the non interacting case there are interesting phenomena

Non interacting case

Exact solution: spectral region with “Hidden states” at low energy in single particle energy spectrum

N sites

$$\rho^r(E) = \frac{1}{N^r}\sum_k \delta(E - E_k^r) \qquad \rho^r(E) = \rho_+ + \rho_- + \rho_0$$



$\sqrt{N}$ states in the low energy region

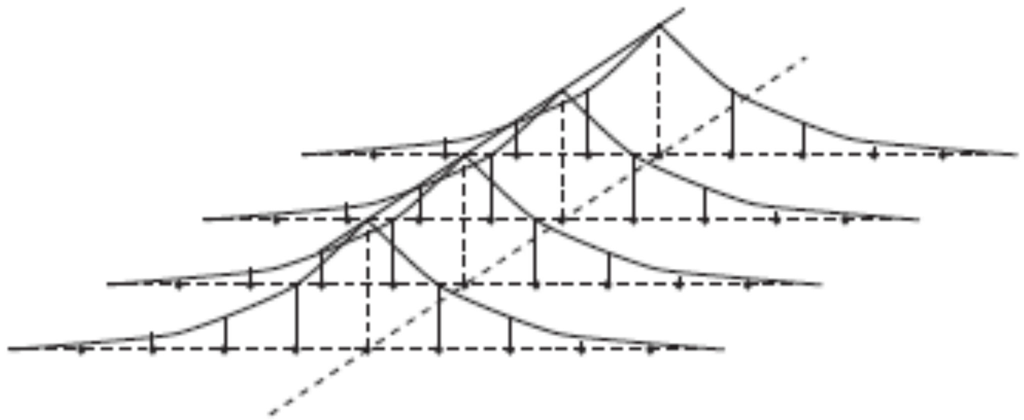
This is a zero measure set of states,which do no influence the thermodynamic density of states, but where bosons can condense.

Hidden States: An energy interval [E_1,E_2] such that

$$[E_1, E_2] \cap Supp(\rho(E)) = 0$$

$$\lim_{r\to\infty} N_r > 0$$

N_r is the number of eigenvalues in that region



- The ground state, i.e. the eigenvector with lowest energy: exponentially decreasing on the fingers and delocalized along the backbone

- Inhomogeneous localization properties

- Finite size: Bose Einstein condensation at finite temperature with anomalous mesoscopic properties. A whole bunch of states is filled in the hidden region.

- β_c $$1=\frac{1}{\pi f}\int_{\rho_o}\frac{dE}{e^{\beta_c(E+t\sqrt{8})}}\frac{1}{\sqrt{4t^2-E^2}}$$ $T_c \propto -(\ln f)^{-1}$ $\quad f \ll 1.$

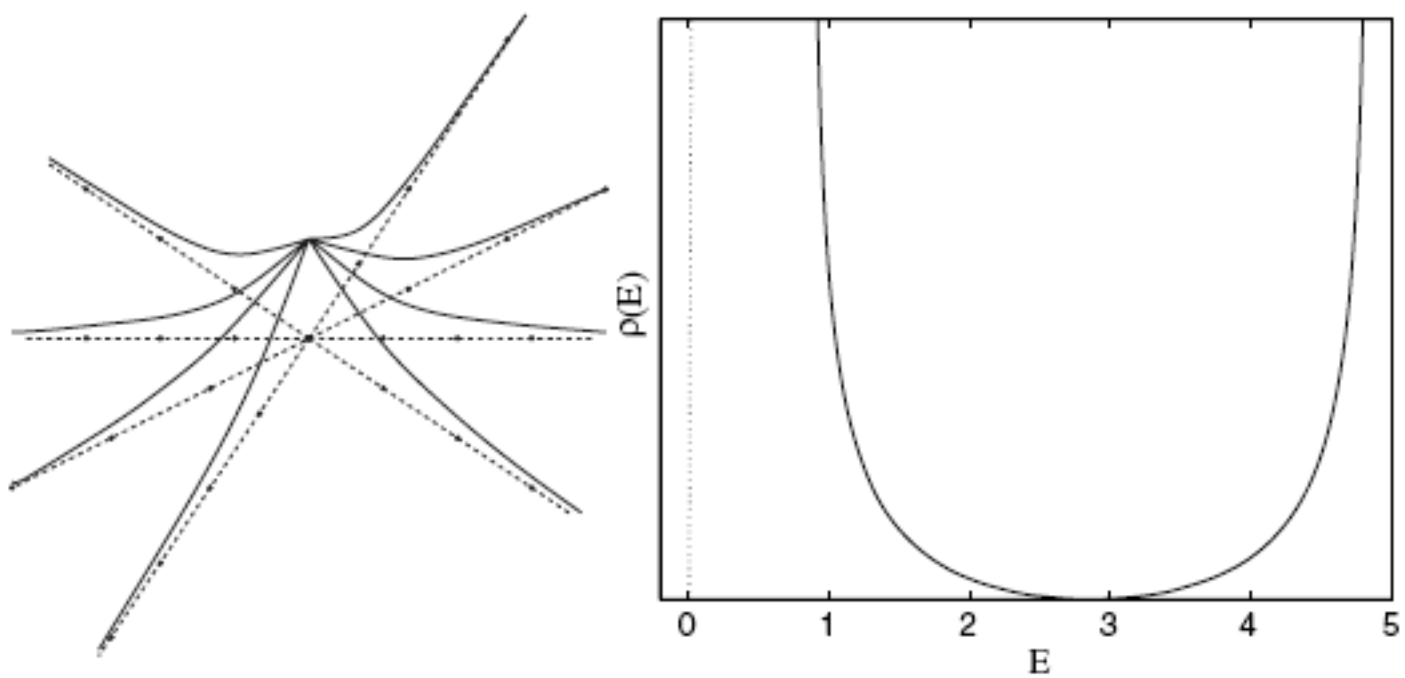
- n_0 $$n_0=1-\frac{1}{\pi f}\int_{\rho_0}\frac{dE}{e^{\beta(E+t\sqrt{8})}-1}\frac{1}{\sqrt{4t^2-E^2}}$$ $n_0 \propto (T-T_c)$

- Rigorous Result on the occurrence of BEC on a general network from the spectral properties of the adjacency matrix A:

  $\bar{d} > 2$ or existence of low energy hidden states region

- The non interacting case can be solved exactly on many graphs star network, fractals, trees, bundled structures. Analogous results.

- All of them feature anomalous localization properties of the eigenvectors

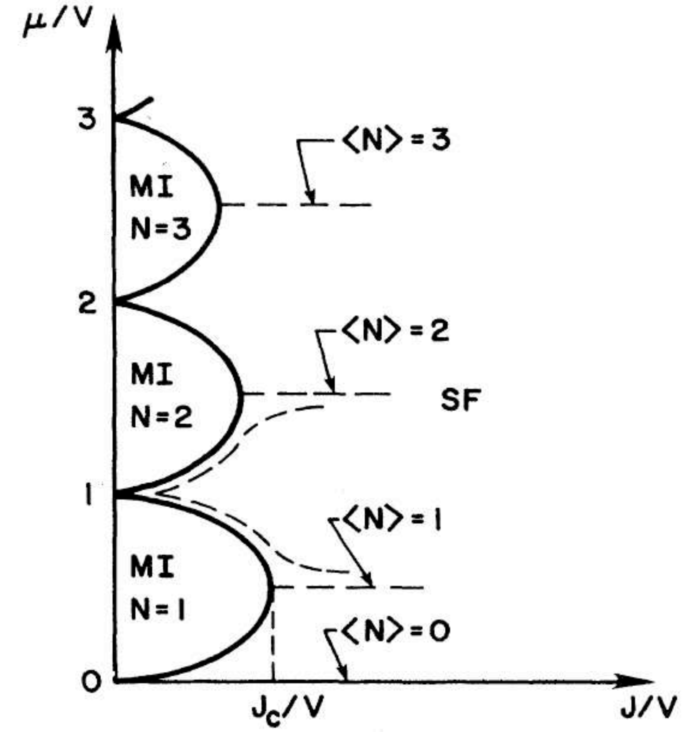


The star graph: spatial localization

Interacting case: Mott-Superfluid transition on the comb

$\rho_i = < n_i >$ Local density of bosons on site i in the ground state

$$k_i = \frac{\partial \rho_i}{\partial \mu}$$ Local compressibility



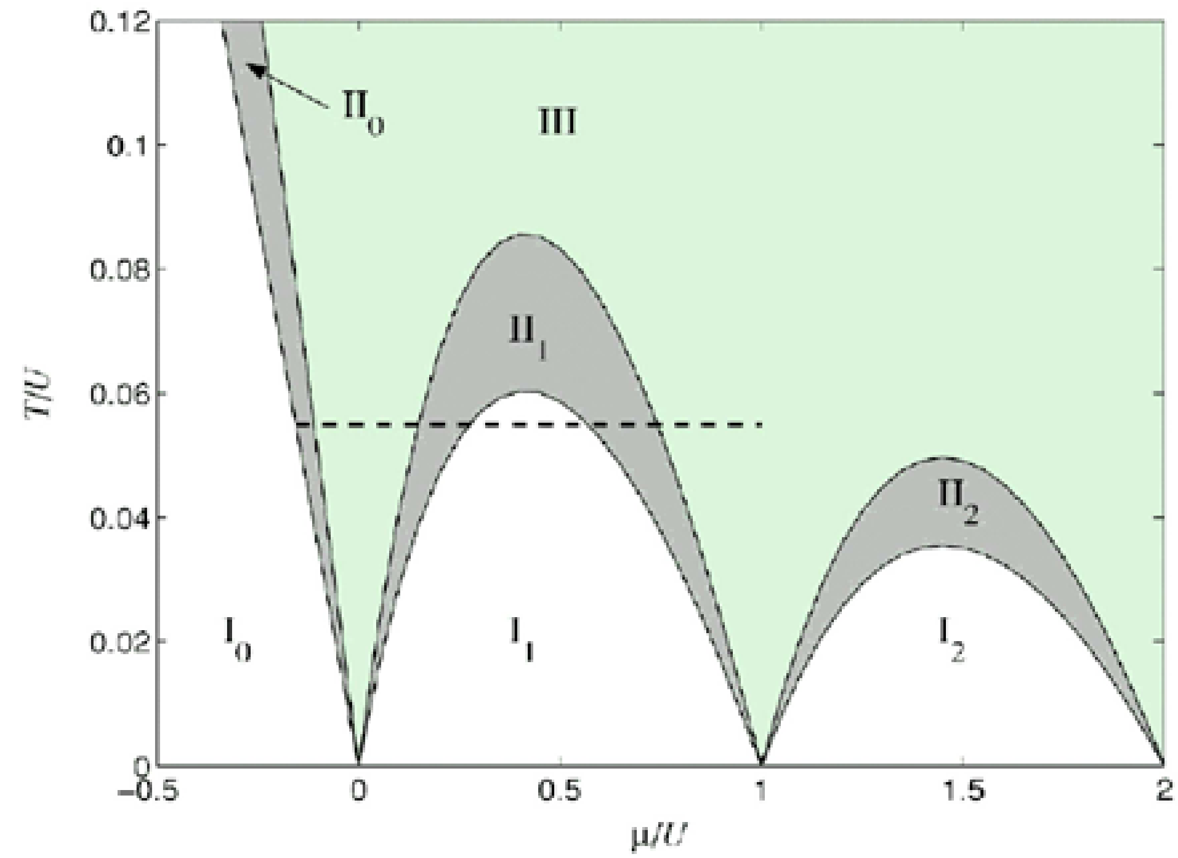
Homogeneous topology: phase diagram at T=0

- Superfluid Phase: k finite

- Incompressible Mott Insulator Phase: k vanishing

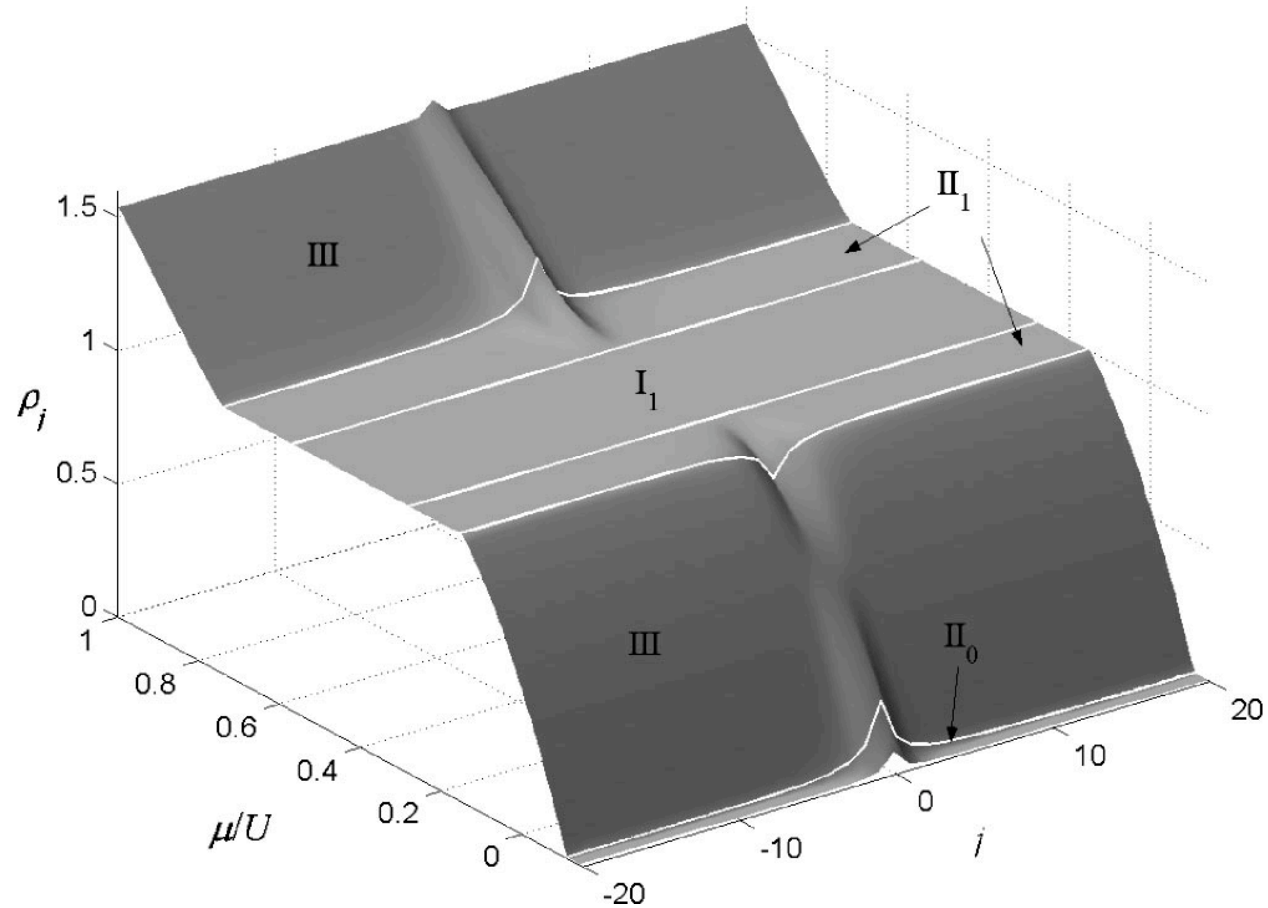
filling pinned to an integer value $f = \frac{M}{N}$

mean field
(Fisher et al 89)



I_f	$k_i = 0$	for all sites and M=fN Mott
III	$k_i \neq 0$	extended superfluidity
II_f	k_i	finite but vanishes exponentially along the fingers - confined superfluidity

Region II: confined superfluidity

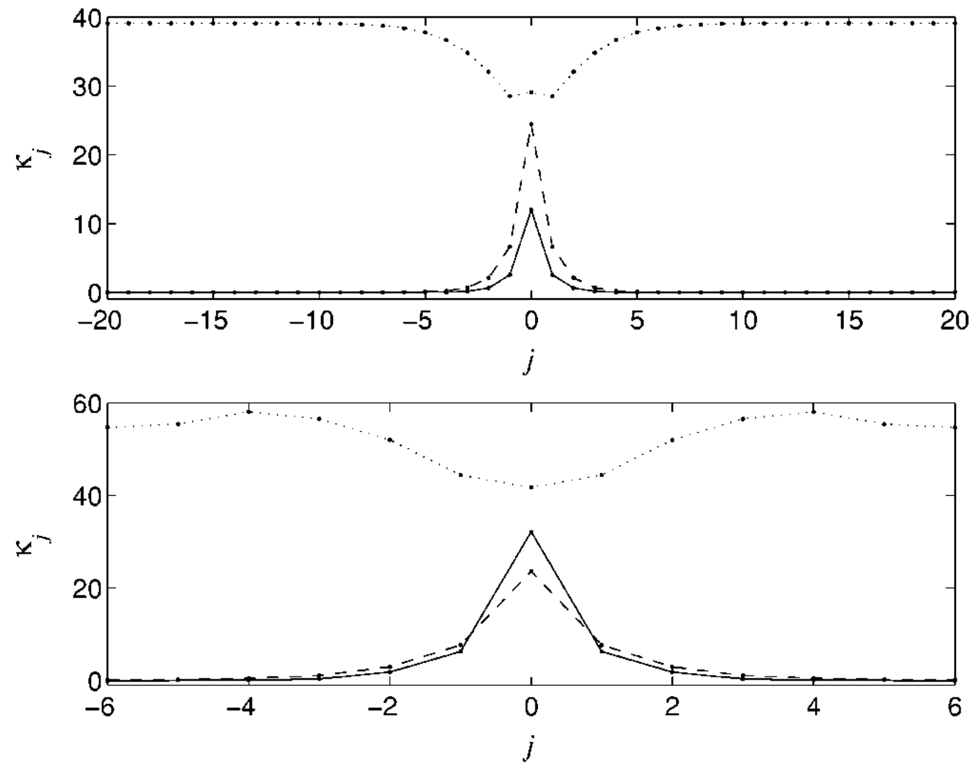


in region II_f $\rho_i \to f$ exponentially along the fingers

local compressibility

mf

qmc



II_0

II_1

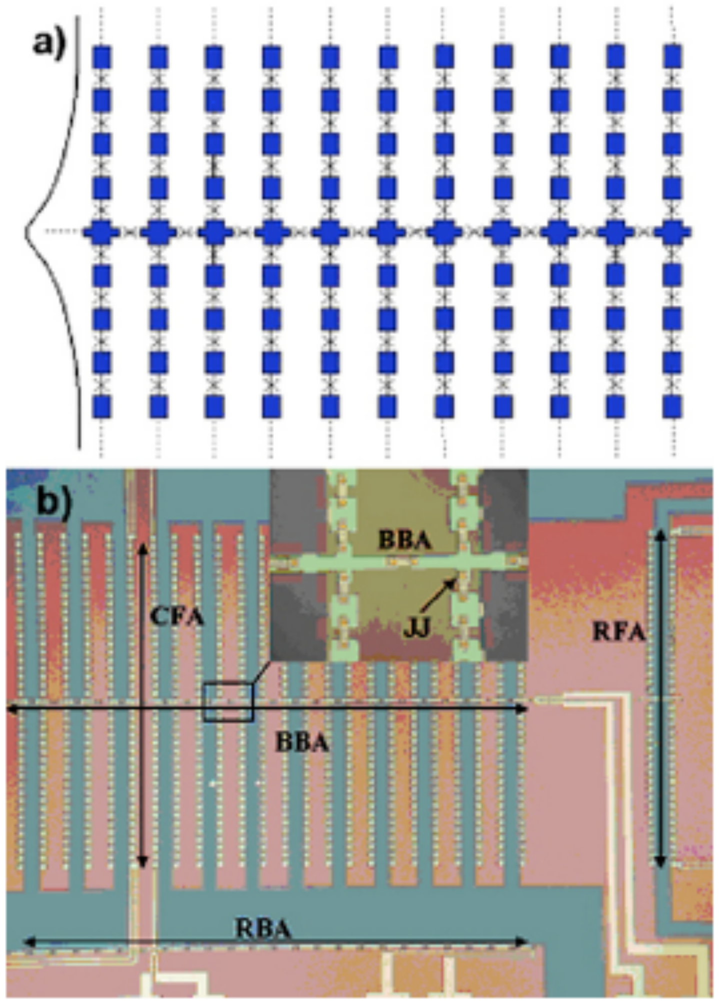
III

+ strong coupling expansion based on spectral properties of A

The Superfluid Phase is confined along the backbone

- a possible experimental setup in cold atoms for the BH case: change from a 2d to a 1d interference pattern once the lattice is released when crossing from region III to region II, as in the experiment of Greiner et al.

- a real experimental set up for the non interacting case: a comb array of Josephson junctions (critical current)



P. Sodano, M. Cirillo et al 2006, 2007, Enhancement of the critical current along the backbone - explained through Bogoliubov-De Gennes eq.
(P. Sodano et al. 2006)

- work in progress

Topological filters for solitons in inhomogeneous chains:

Discrete non linear Scroedinger equation on a network

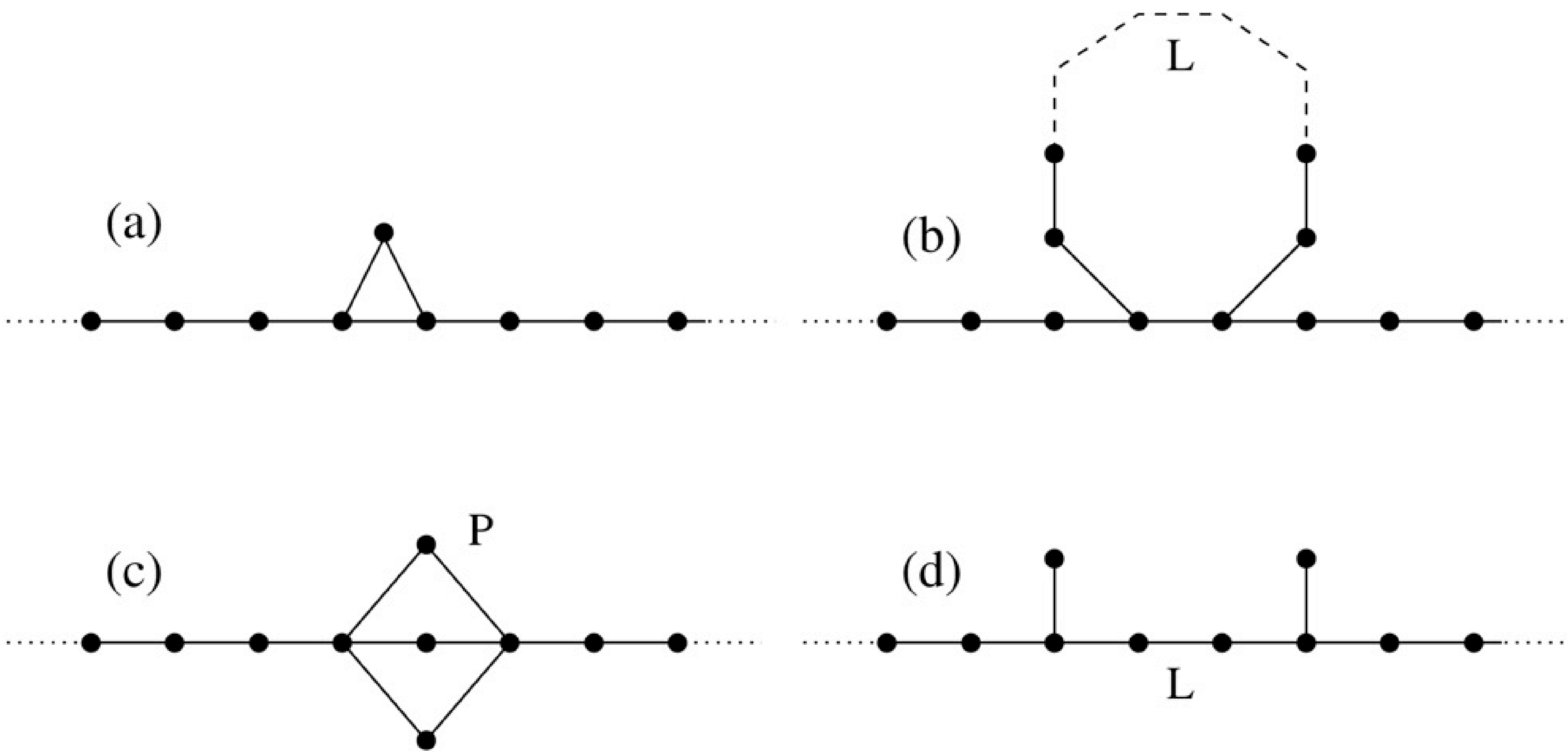
$$-\frac{1}{2}\sum_{j=1}^{N} A_{ij}\varphi_j(t) + \Lambda |\varphi_i|^2 \varphi_i = i\frac{\partial \varphi_i(t)}{\partial t}$$

Λ non linear coefficient

A_{ij} adjacency matrix of the network

$$-\frac{1}{2}(\varphi_{j+1}(t) - \varphi_{j-1}(t)) + \Lambda |\varphi_i|^2 \varphi_i = i\frac{\partial \varphi_i(t)}{\partial t}$$ on a chain

Inserting a simple topological defect on the chain

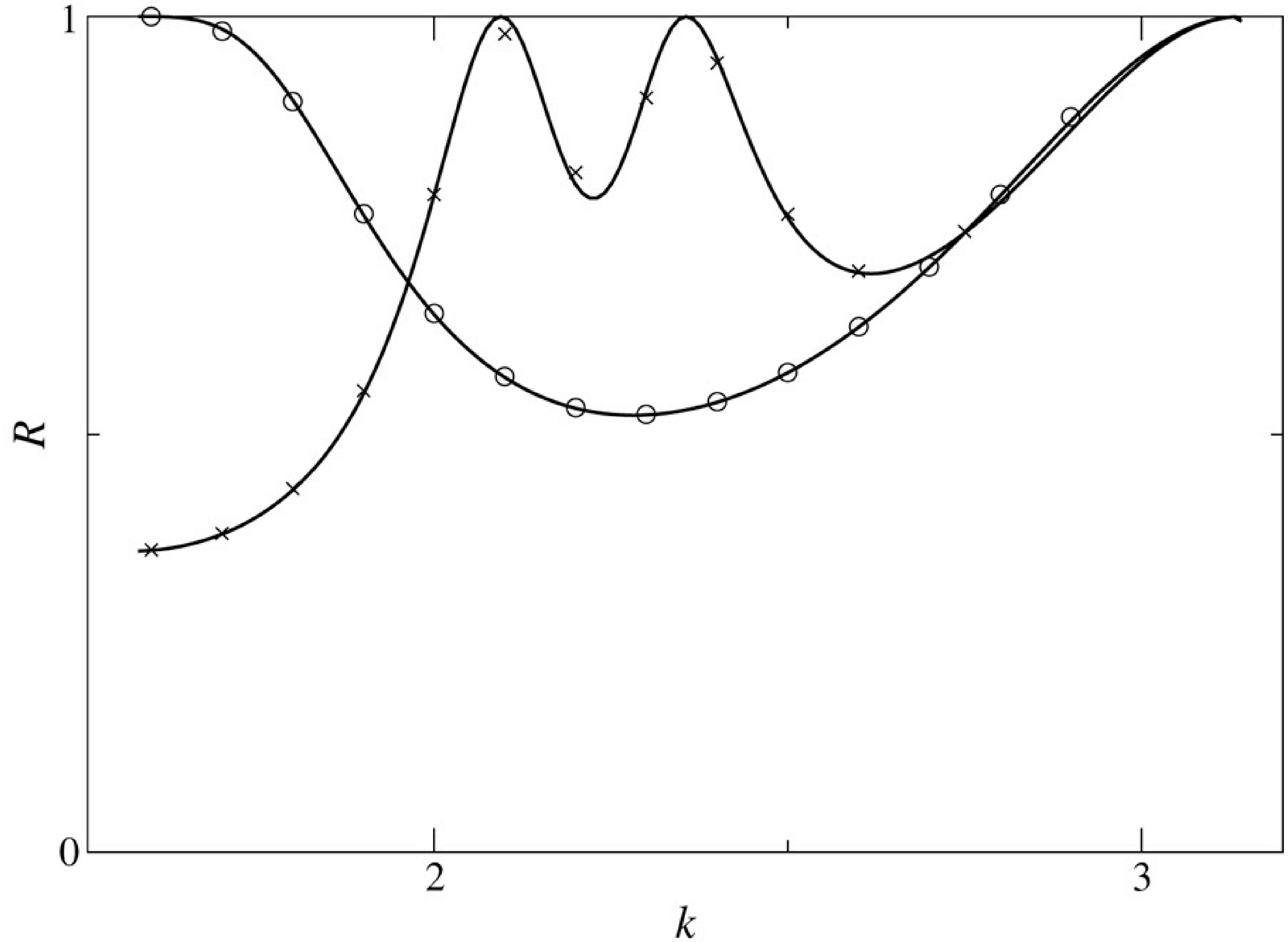


•Soliton-like solutions can propagate for a long time (variational approach: $\Lambda \approx \cos(k)$)

A. Trombettoni, A. Smerzi PRL 2001

•The spectral properties of the network plus the defect selects, for large fast solitons, the transmission and reflection properties

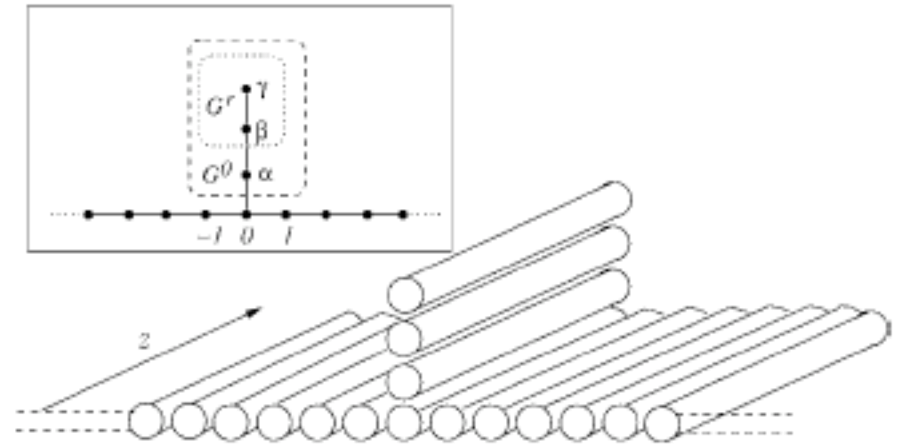
•Topological filters for solitons: total reflection and transmission, low pass, high pass, depeding on the topological defect



Reflection coefficient for loop of size L=2 and L=4
(numerical and analytical results)

Topological Filters for solitons:

$$-\sum_{j=1}^{N} \beta_{n,j} E_j + \Lambda |E_n|^2 E_n = i \frac{\partial E_n}{\partial t}$$



E_n electrical field on the n-th waveguide in the z direction

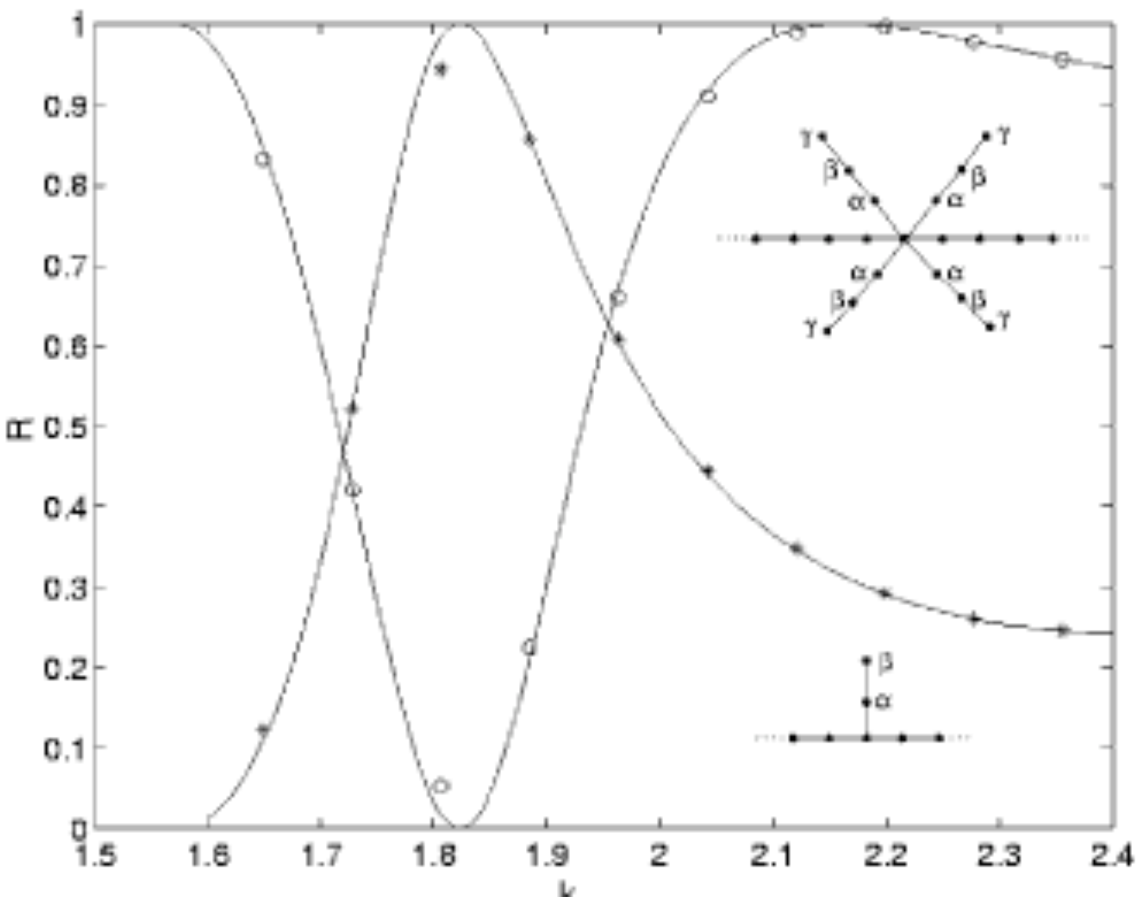
Λ non linear Kerr coefficient (focusing/defocusing for negative/positive values)

$\beta_{n,j}$ coupling between adjacent waveguides, proportional to the mode overlap of the corresponding electrical fields

Soliton-like solution can propagate for a long time: variational approach

total reflection, total trasmission, low pass, high pass

$$\Lambda_{sol} \approx 4\beta_c\sqrt{\pi}\frac{|\cos k|}{\gamma_0}.$$



Present and Future:

- the 2d Lévy Glass at LENS
  (P. Barthelemy, J. Bertolotti and
  D. Wiersma, Nature 2009)
  We studied trasport in the
  classical case, for the moment.

- Lévy-distributed disorder in the
  topology, strong effects on
  transport

- Quantum case? Localization?

- the Spectral Dimension?
- Inhomogeneous Disorder?

a