Breathers in Quantum Lattices

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HPC-EUROPA project at the EPCC in collaboration with the group of Professor J.C. Eilbeck. Department of Mathematics, Heriot-Watt University. Edinburgh (U.K.)

Summary

- Introduction.
- Quantum breathers. Hubbard models. Overview.
- Computational problems.
  - Algebraic routines.
  - Spectrum calculations.
- Some results.
  - Rotational invariant systems.
  - Non-rotational invariant systems.
- HPC-Europa project. Breathers in quantum lattices.
- Work in progress and perspectives.

Introduction

Discrete breathers in classical lattices

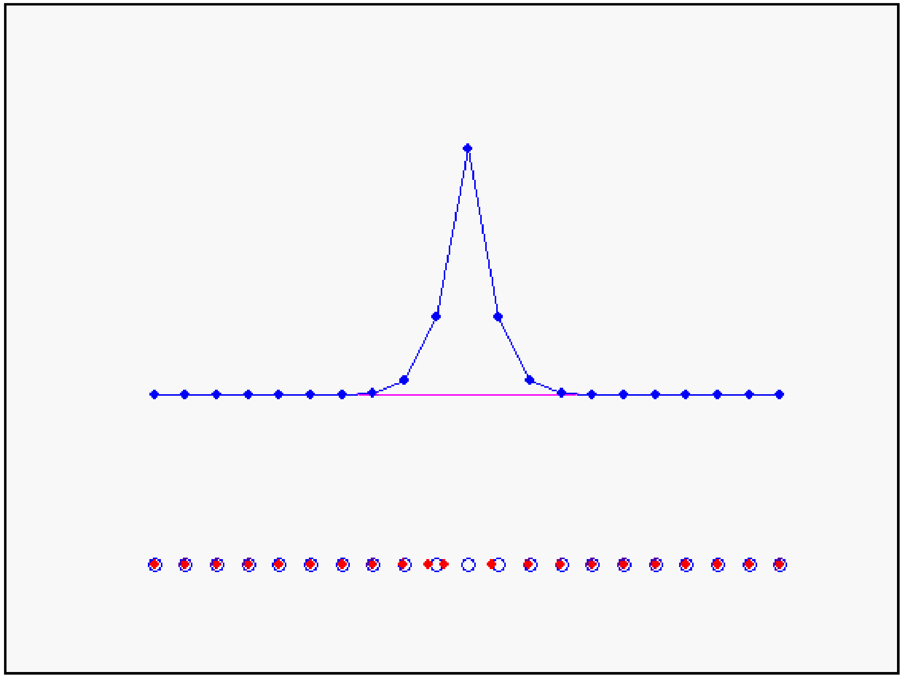
- Nonlinear lattices:

$$H = \sum_{\vec{n}} \left(\frac{1}{2} m_n \dot{\vec{u}}_{\vec{n}}^2 + V_{\vec{n}}(\vec{u}_{\vec{n}}) + C \sum_{\vec{m}} W_{\vec{n},\vec{m}}(\vec{u}_{\vec{n}}, \vec{u}_{\vec{n}+\vec{m}}) \right)$$

- Spatial localization by nonlinearity. General conditions for its existence and stability.
- Some analytical results. Standard numerical methods.
- Static and moving breathers.
- Experimental evidences.

Example: Klein–Gordon lattices

$$H = \sum_n \left(\frac{1}{2}\dot{u}_n^2 + \frac{1}{2}(e^{-u_n} - 1)^2 + C(u_n - u_{n-1})^2 \right)$$



Quantum breathers

Quantum equivalence of discrete breathers: open question.

- Hubbard models (fermions or bosons). QDNLS systems.

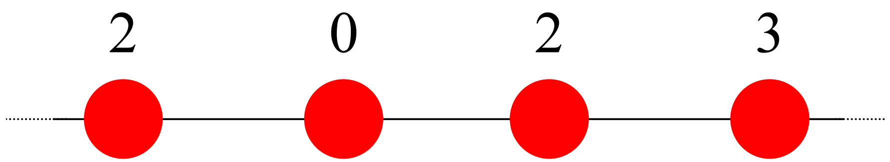
$$\hat{H} = -\sum_{j=1}^{f^D} \frac{\gamma_j}{2} b_j^\dagger b_j^\dagger b_j b_j - \sum_{j=1}^{f^D} \sum_p \epsilon_{jp} b_j^\dagger b_{j+p}.$$

  Index j and p a D-dimensional index, ranges over the D-dimensional lattice).

- $b_j^\dagger$ and b_j are standard bosonic (fermionic) creation and destruction operators.
- $\hat{H}$ conserves the number of quanta $\hat{N} = \sum_{j=1}^{f} b_j^\dagger b_j$.

Number of states method

- Main problem: Determination of matrix representation of the Hamiltonian operator and its total/partial spectrum. Block-diagonalize the Hamiltonian for a fixed number of quanta N.
- The operators b_j and $b_j^\dagger$ acts on *number states* basis $|\psi_n\rangle = [n_1, n_2, ..., n_f]$,$N = \sum n_i$.
- General wave function:$|\Psi_n\rangle = \sum_n a_n |\psi_n\rangle$.
  Example: 1D lattice, 4 sites and 7 quanta (bosons): [2,0,2,3].



Algebraic routines

Quantum Mechanics in Maple

- For a given value of the number of quanta, determination of the *number of states* basis.
- Definition operators $b_j^\dagger$ and b_j over a vector of the basis. Determination of matrix representation of the Hamiltonian operator.
- Main problem: Number of basis vectors p grows rapidly with n and f. For a one dimensional lattice of f sites and n bosons $p=(n+f-1)!/(f-1)!n!$.
- Project: Parallel Maple: J.C Eilbeck. Department of Mathematics, Heriot-Watt University, Edinburgh, U.K.

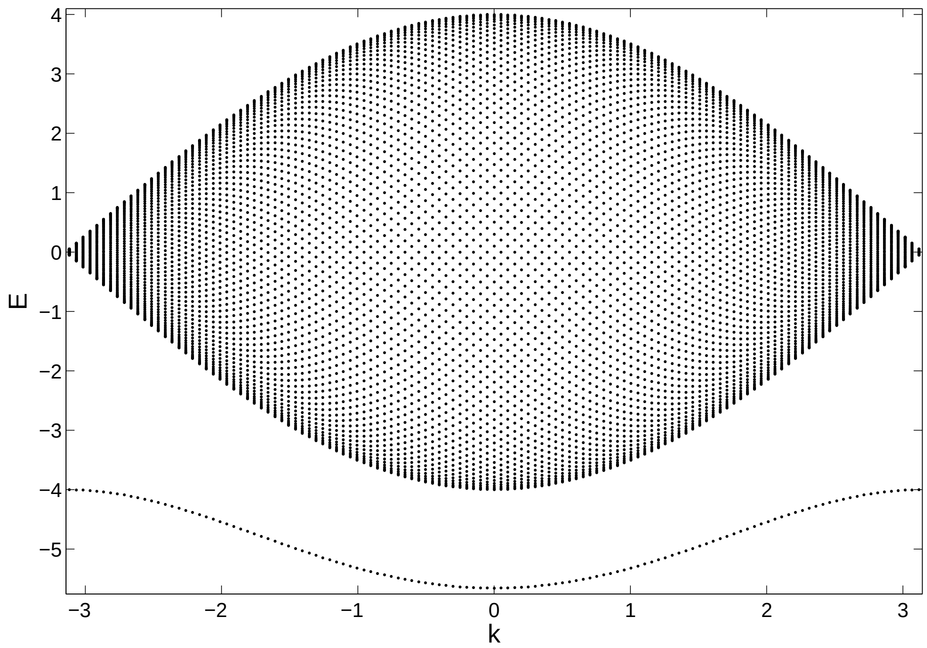
Rotational symmetry

In homogeneous quantum lattices with periodic boundary conditions, it is possible to block–diagonalize the Hamiltonian using eigenfunctions of the rotation operator $\hat{R}$, given states with fixed momentum $\vec{k}$. That implies a reduction of the size of the matrix.

- Some analytical results in some cases ($n = 2$, infinite lattices, n large in infinite lattices ...). Numerics: standard numerical spectrum calculations.
- In general, if anharmonic parameter is high enough, the spectrum shows a characteristic band structure where the ground state is a localized in the sense that there exist a high probability to find the two quanta on the same site, but with equal probability at any site of the chain.

Spectrum

Example: Eigenvalues of the energy $E(k)$ as function of the momentum k for a QDNLS one–dimensional bosons system. $f = 125$ and $n = 2$.



On a lattice of length f, the unnormalized coefficients of the first f terms are equal to unity and the rest are $O(\gamma^{-1})$. At $k = 0$ for simplicity, the ground state is $|\Psi\rangle = [20\ldots0] + [020\ldots0] + \cdots + [0\ldots02] + O(\gamma^{-1})$..

Non-rotational inv. systems (NRI)

Computational effort increases. Expectation value of momentum k

- Finite lattices.
- Localized impurities in anharmonic term:

$$\hat{H} = -\sum_{j=1}^{f^D} \frac{\widetilde{\gamma}_j}{2} b_j^\dagger b_j^\dagger b_j b_j - \sum_{j=1}^{f^D} b_j^\dagger b_{j+1},$$

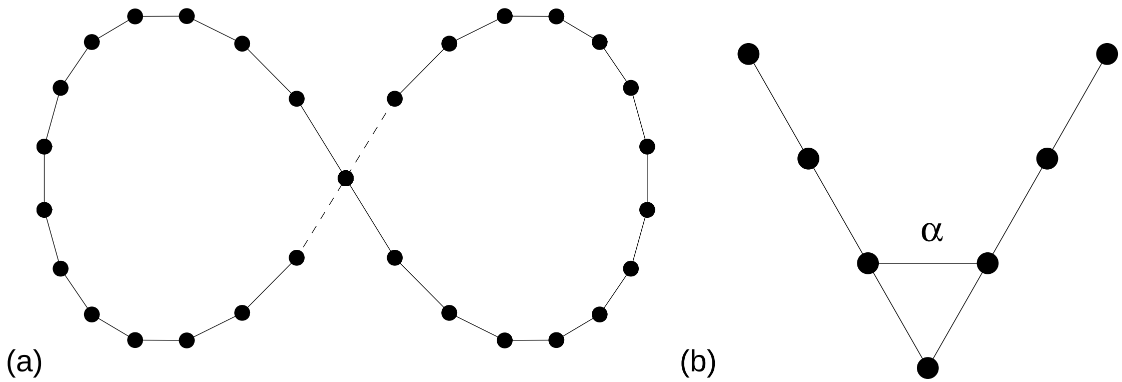
  where $\widetilde{\gamma}_j = \gamma$, $j \neq m$ and $\widetilde{\gamma}_j = \gamma_1$ for some fixed choice of impurity site(s) m.

- Long range interactions. Long range hopping terms:

$$\hat{H} = -\sum_{j=1}^{f^D} \frac{\widetilde{\gamma}_j}{2} b_j^\dagger b_j^\dagger b_j b_j - \sum_{j=1}^{f^D} b_j^\dagger b_{j+1} - \alpha_{\ell,m}(b_\ell^\dagger b_m + b_m^\dagger b_\ell).$$

Non-rotational invariant systems II

- Example: Two non-uniform chain geometries



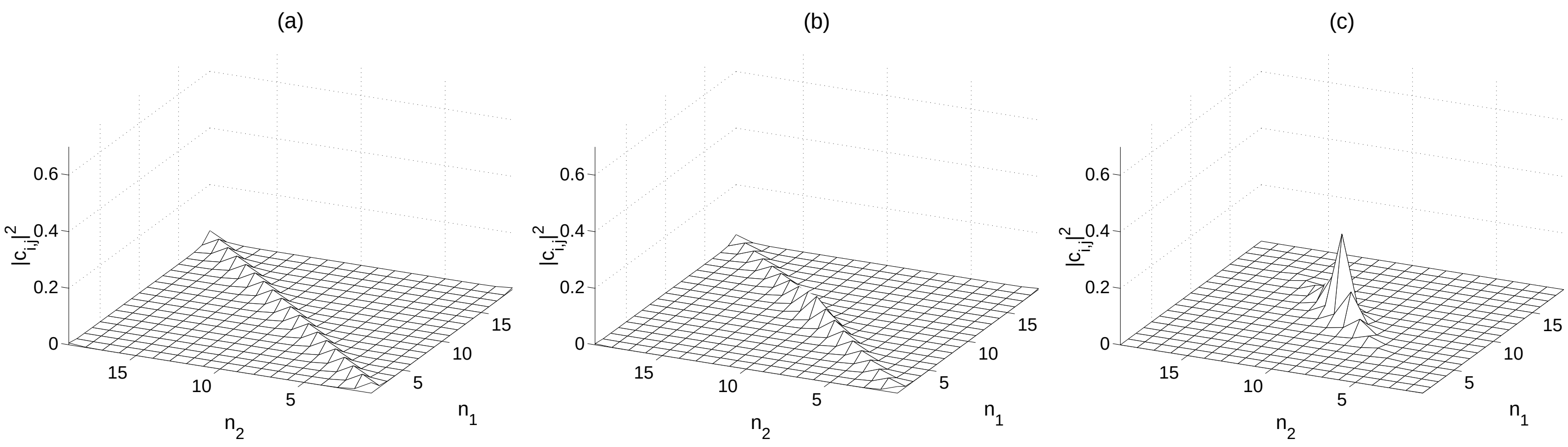
- Random noise (Anderson localization)

$$\hat{H}_{ran} = -\sum_{j=1}^{f^D} W_j b_j^\dagger b_j,$$

where W_j is a random parameter and $W_j \in [-W, W]$.

Some results in NRI

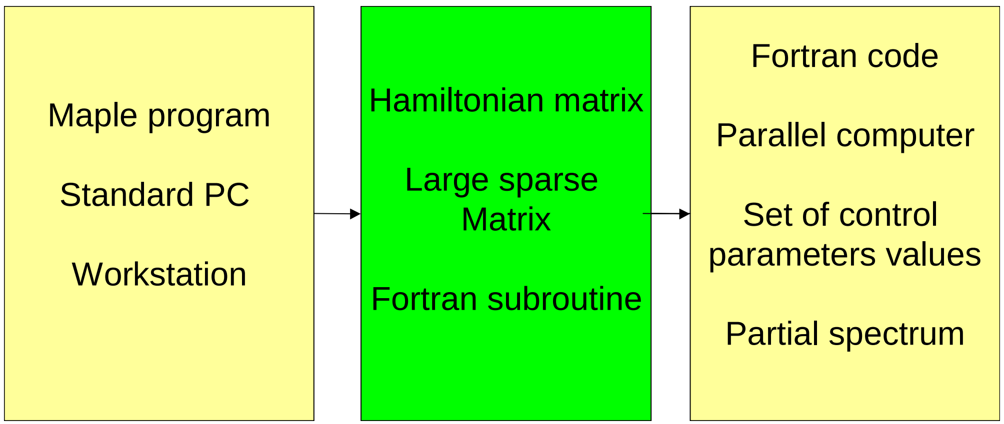
- Local inhomogeneities, due to geometrical factors and to long–range interactions or impurities in the anharmonicity parameter, break the translational invariance of the system and localize the ground state around a particular site of the chain.



QDNLS. Square wave function amplitudes corresponding to the ground state as a function of the positions n_1, n_2 of the two bosons on the chain. We have $f = 19$ and $\gamma = 4$ and a point impurity at $\ell = 10$. (a) Homogeneous chain, (b) $\gamma_{\rm im} = 4.1$, (c) $\gamma_{\rm im} = 4.4$.

HPC-Europa project

- **Objective:** Study of quantum breathers in QDNLS systems with non–rotational symmetry.
- **Strategy:**
  - Optimize Maple programs to generate Hamiltonian matrix representation for a different non-rotational invariant systems.
  - Parallel fortran code to calculate the partial spectrum of the system.



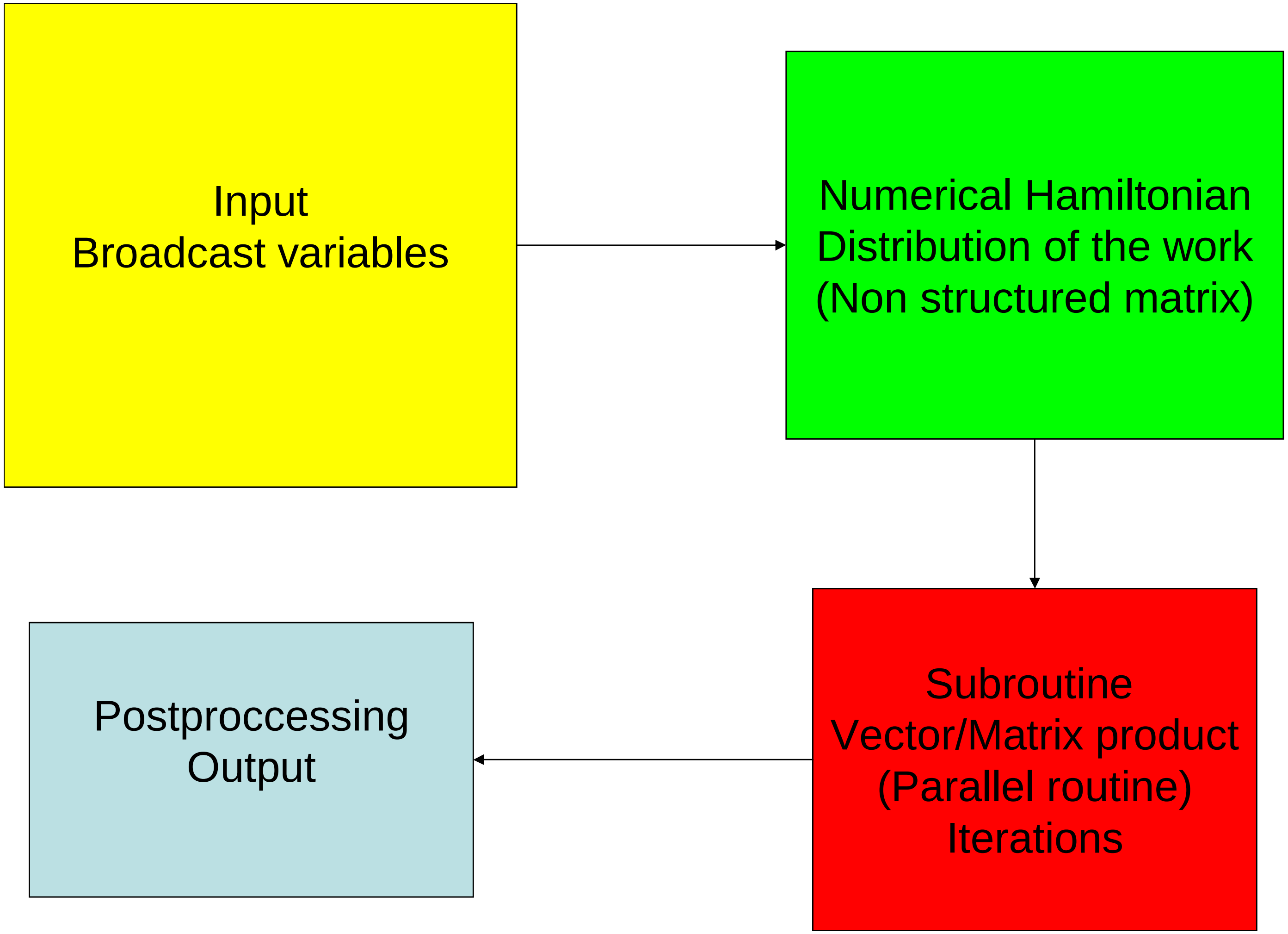
Results

- **Maple routines:** A careful optimization of algorithms has allowed to obtain the symbolic matrix representation of the Hamiltonian operator for translational and non–translational invariant systems, for one or two–dimensional systems, and with a number of sites and quanta high enough to obtain physical relevant results. In general the output is a very large hermitian sparse matrix.
  - **Example:** One–dimensional non–translational invariant system with $f = 7$ and $n = 9$ bosons, with first–neighbor interaction, the metrics of the matrix is 5005×5005 and the number of nonzero elements 47047.
- **Fortran routine:**Parallel Fortran program . We have used MPI and the parallel version of the free numerical library ARPACK (PARPACK).http://www.caam.rice.edu/ kristyn/parpack_home.html.

MPI-PARPACK

- PARPACK: Collection of Fortran 77 subroutines designed to solve large scale eigenvalue problems. Implicitly Restarted Arnoldi Method. In symmetric cases reduces to a variant of the Lanczos process called the Implicitly Restarted Lanczos Method.
- Designed to compute a few ($neig$) eigenvalues with user specified features.
  - User should provide their own matrix–vector multiplication routine. Reverse communication interface.
- Matlab. Command *eigs* based on this package (serial version ARPACK).
- **Objective:** To write up a standard program, based in free software libraries, and highly portable.

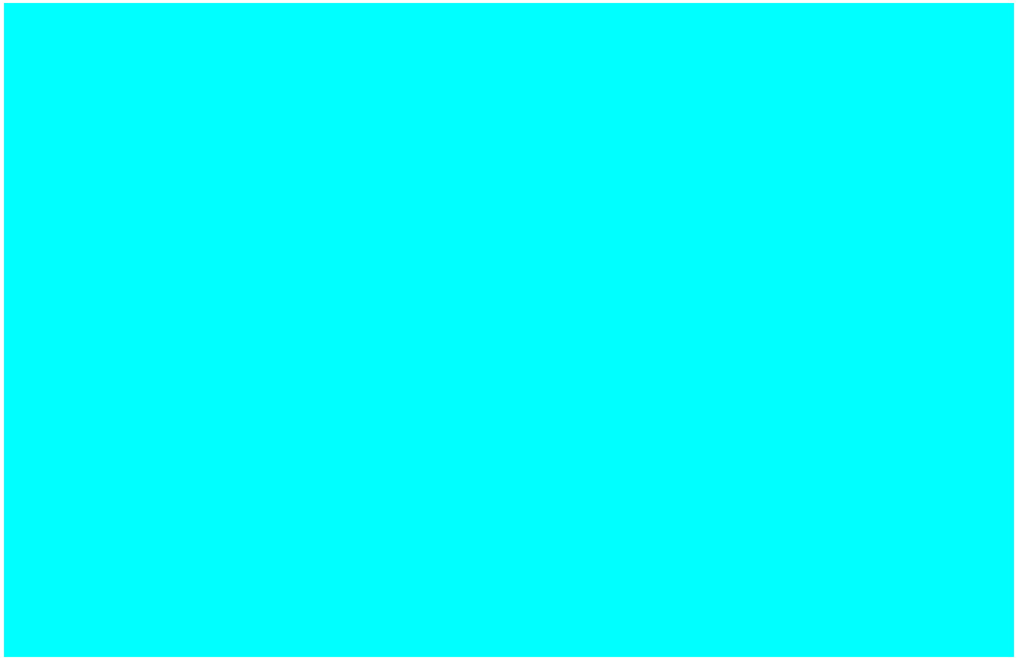
Program structure



Test

- **Test:** One–dimensional non–translational invariant system with $f = 7$ and $n = 9$ bosons, first–neighbor interaction.
  - Matrix 5005×5005. Nonzero elements 47047 and 100 eigenvalues/eigenvectors (largest magnitude). No structure (fractal–like structure!). 52 processor Sun Fire E15k, located at the EPCC in Edinburgh.

N. proc	1	2	3	4	8
Time (s)	19.38	10.35	7.10	6.55	5.42

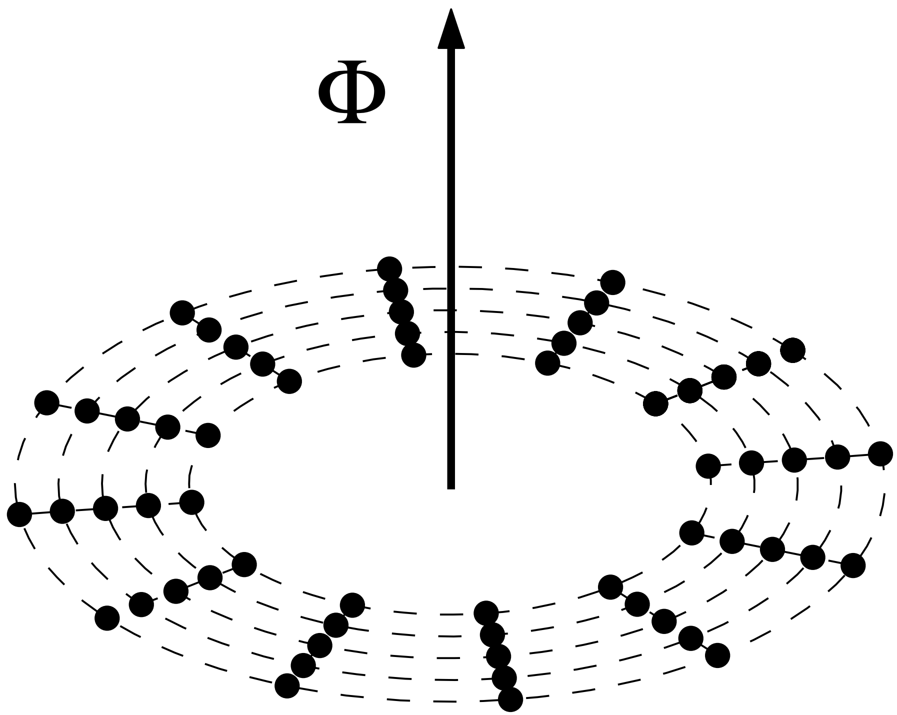


Open problems

- Analytical results?.
- Differences with harmonic localization (Anderson localization). Hubbard models with diagonal disorder Question: Anderson localization/Anharmonic localization. Two faces of the same phenomenon?.
- Classical limit.
- Soliton wave packets.

Nanorings structures

- An electron and a hole. Bound state.
- Magnetic flux. Aharonov-Bohm effect.



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