Quantum integrable systems. Quantitative methods in biology
Systèmes intégrables quantiques. Méthodes quantitatives en biologie

Giovanni Feverati

Soutenance d'habilitation à diriger les recherches

Auditorium, LAPTH, 13 Décembre 2010, 14H00

Membres du jury:

Jean Avan (LPTM, CNRS/Université de Cergy-Pontoise)
Michele Caselle (Dip. fisica teorica, Università di Torino)
Luc Frappat (LAPTH, Université de Savoie)
Francesco Ravanini (Dip. fisica, Università di Bologna)
Jean-Marc Victor (LPTMC, CNRS/Université de Paris VI)
Laurent Vuillon (LAMA, Université de Savoie)

Giovanni Feverati

Thesis (2000): Finite volume spectrum of sine-Gordon model and its restrictions.

Dipartimento di Fisica, Università di Bologna

Supervisor: Francesco Ravanini

Post-docs

1999-2000 Venezia, CNR, Physical oceanography, Luigi Cavaleri

2000-2003 Melbourne, Dept. Mathematics, Paul Pearce

2003-2005 Trieste, SISSA, math. physics, Giuseppe Mussardo

2005- Annecy, LAPTH, math. physics, Luc Frappat, Eric Ragoucy

-2010 Annecy, LAPTH, biophysics, Claire Lesieur, Laurent Vuillon, Paul Sorba

Research subjects

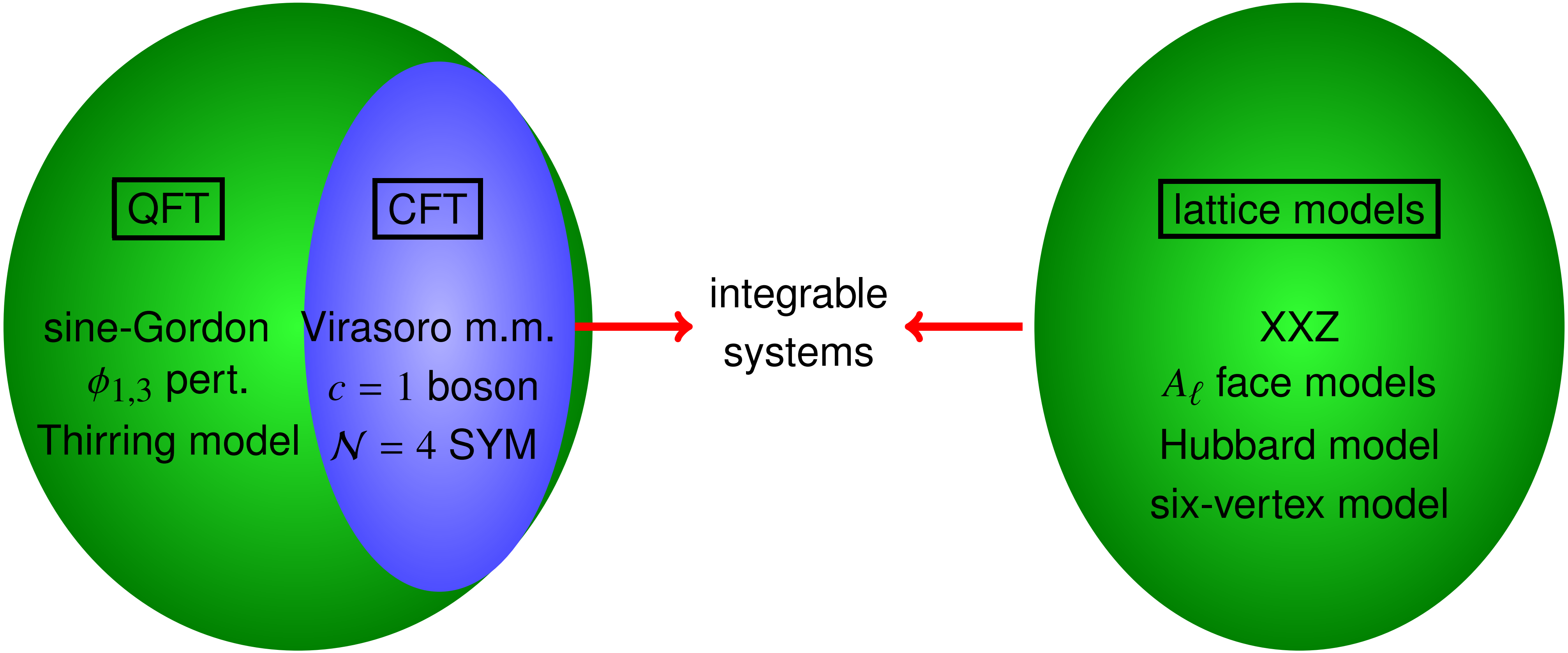
Quantum integrable systems

- sine-Gordon on a cylinder (1997-2000)
- Klümper-Batchelor-Pearce-Destri-de Vega equation NLIE (1997-1999, 2005-2007)
- thermodynamics Bethe ansatz (1995, 2000-2005, 2008)
- integrable models with boundaries (2000-2005)
- truncated conformal space approach (1997-2000, 2005)
- lattice-conformal dictionary (2005)
- physical combinatorics (2002, 2008)
- lattice models and continuum limits
- Hubbard model and AdS/CFT (2005-2008)

Theoretical biophysics

- Darwinian evolution with Turing machines (2006-)
- protein assembly: Gemini graphs (2007-), diffusional association (2010)

Geographical map



QFT: factorized scattering
CFT: Virasoro algebra
Lattice: transfer matrix

continuum limit
lattice-conformal dictionary

XXZ model

$$H_{\mathsf{XXZ}} = -\sum_{i=1}^{N-1}\left[\sigma_i^1\sigma_{i+1}^1 + \sigma_i^2\sigma_{i+1}^2 + \Delta(\sigma_i^3\sigma_{i+1}^3 - 1)\right], \qquad \Delta = \cos\gamma$$

ground state: ferromagnetic (= all spins parallels) if $\Delta \geq 1$, antiferromagnetic if $\Delta < 1$, gapless in the TD limit if $-1 \leq \Delta \leq 1$

1931: (coordinate) Bethe ansatz

Bethe equations $$\left(\frac{\sinh\frac{\gamma}{\pi}(\theta_j + i\frac{\pi}{2})}{\sinh\frac{\gamma}{\pi}(\theta_j - i\frac{\pi}{2})}\right)^N = -\prod_{k=1}^{M}\frac{\sinh\frac{\gamma}{\pi}(\theta_j - \theta_k + i\pi)}{\sinh\frac{\gamma}{\pi}(\theta_j - \theta_k - i\pi)}$$

spectrum $$E = -2\sum_{j=1}^{M}\frac{\sin^2\gamma}{\sinh\frac{\gamma}{\pi}(\theta_j + i\pi)\sinh\frac{\gamma}{\pi}(\theta_j - i\pi)} = \sum_{j=1}^{M} f_E(\theta_j) \qquad 0 \leq M \leq \frac{N}{2}$$

θ_j (Bethe roots): *quasiparticles* — completeness of spectrum, $\theta_j \neq \theta_k$

Six-vertex model

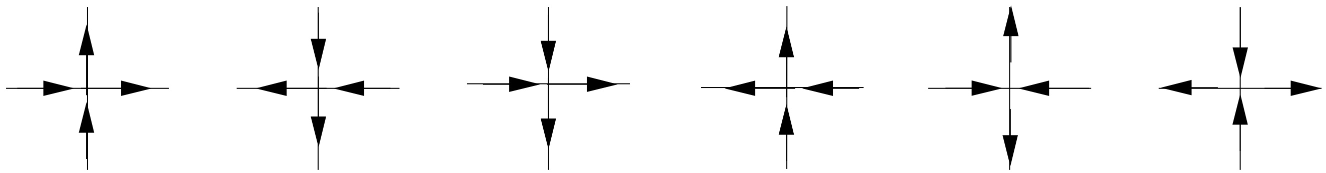
The XXZ Hamiltonian comes from a transfer matrix

$$H_{\mathrm{XXZ}} \propto \frac{d \log \mathbf{T}(\theta)}{d\theta}\Big|_{\frac{i\pi}{2}} \qquad \text{where} \qquad \mathbf{T} = \operatorname*{Tr}_A \, R_{A\,1} R_{A\,2} \ldots R_{A\,N}$$

and

$$R_{A\,i}(\theta) = \begin{pmatrix} \sinh \frac{\gamma}{\pi}(\theta + i\pi) & & & \\ & \sinh \frac{\gamma}{\pi}\theta & i \sin\gamma & \\ & i\sin\gamma & \sinh\frac{\gamma}{\pi}\theta & \\ & & & \sinh\frac{\gamma}{\pi}(\theta + i\pi) \end{pmatrix}$$

$\mathbf{T}$ describes the partition function of a classical two dimensional six vertex model



1 2 3 4 5 6

$\sinh \frac{\gamma}{\pi}(\theta + i\pi)$ $\sinh \frac{\gamma}{\pi}\theta$ $i \sin\gamma$

Yang-Baxter equation $\quad R_{12}(\lambda - \mu) R_{13}(\lambda) R_{23}(\mu) = R_{23}(\mu) R_{13}(\lambda) R_{12}(\lambda - \mu)$

XXZ as a reference model

XXZ → sine-Gordon: Destri-de Vega NLIE

XXZ → $c = 1$ (free massless boson), thermodynamic Bethe ansatz

XXZ → ("reduction") A_ℓ face models, thermodynamic Bethe ansatz → lattice conformal dictionary

XXZ ↔ Hubbard model (XXX)

NLIE: nonlinear integral equations

The Klümper-Batchelor-Pearce-Destri-de Vega NLIE equation *re-writes* the Bethe equations by changing the fundamental set of *quasiparticles*: roots/holes duality

Klümper, Batchelor, Pearce 1991
Destri-de Vega 1992
Feverati, Ravanini, Takács 1997-2000
G. Feverati, D. Fioravanti, P. Grinza, M. Rossi, 2006, 2007

take the log of Bethe equations: $\boxed{Z(\theta_j) = 2\pi I_j}$ $\quad (\star)$

I_j : quantum numbers

$$I_j = \begin{cases} \text{half-integer} & \text{if } N - M \text{ even} \\ \text{integer} & \text{if } N - M \text{ odd} \end{cases}$$

counting function (XXX): $$Z(x) = iN \ln \frac{\frac{i}{2} + x}{\frac{i}{2} - x} - \sum_{k=1}^{M} i \ln \frac{i + x - \theta_k}{i - x + \theta_k} \qquad (\star\star)$$

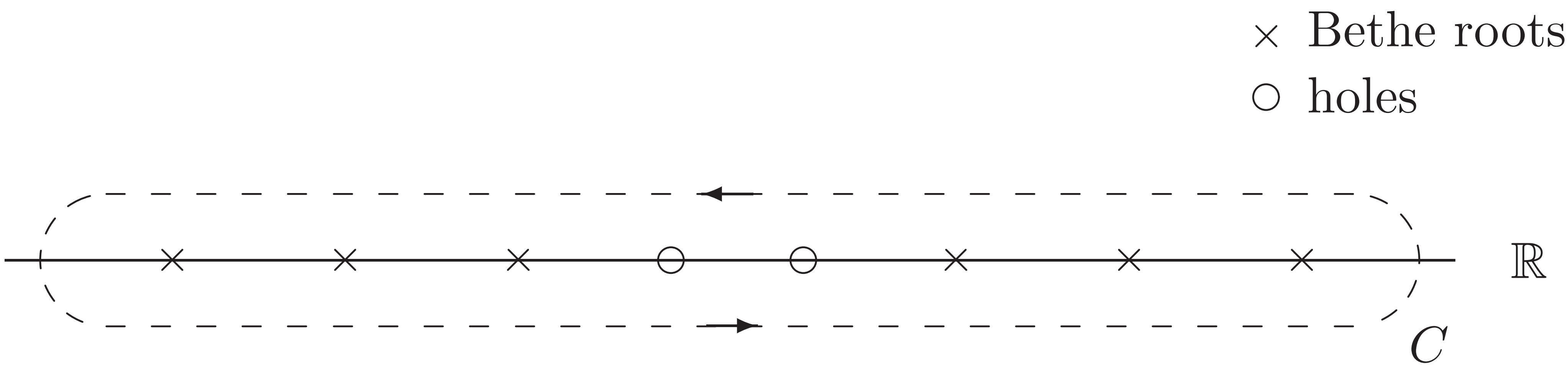
volume　　　scattering

$$\theta_k \in \begin{cases} \mathbb{R} \\ \mathbb{C} - \mathbb{R} \end{cases}$$

"hole" = real solution of ($\star$) not in ($\star\star$)

Is there a state with many real roots (order of N)?

Antiferromagnetic state = Dirac sea of real roots; excitations above it: “holes”, complex roots



Bethe roots $\{\theta_j\}$ are simple poles of $\dfrac{1}{1+e^{iZ(z)}}$ so use Cauchy formula to replace the sum on real roots:

$$\sum_{\text{real roots}} f(\theta_k) = \frac{1}{2\pi i}\int_C \frac{f(z)}{1+e^{iZ(z)}} e^{iZ(z)} iZ'(z)\, dz - \sum_{\text{holes}} f(x_h)$$

Exchange the degrees of freedom “real root” and “hole”

XXX: unknown function $Z(x)$

$$Z(\theta_j) = 2\pi I_j$$

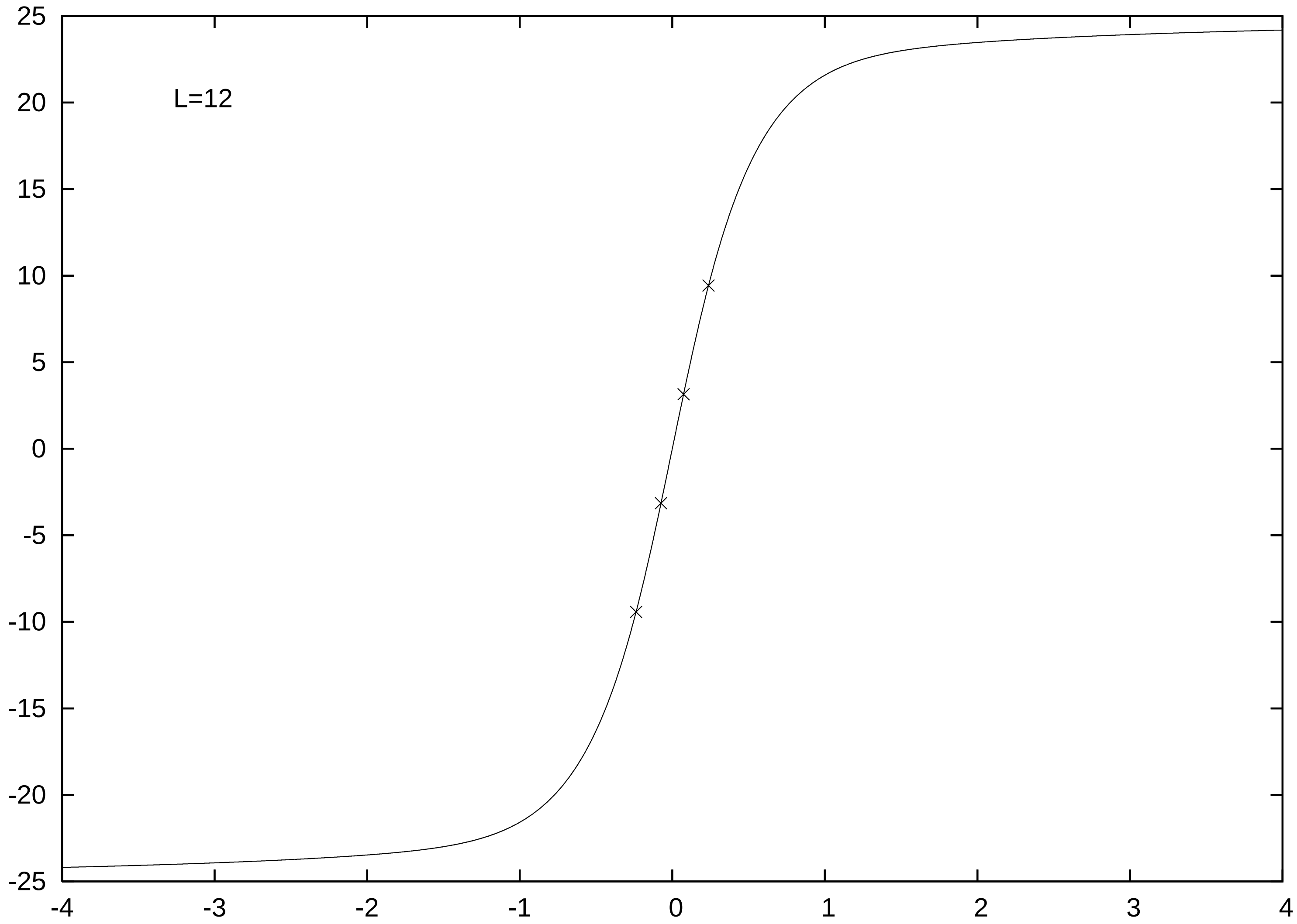
$$Z(x) = F(x) + \textit{sources} + 2\int_{-\infty}^{\infty} dy\, G(x-y)\, \mathrm{Im}\ln\left[1 + e^{iZ(y+i0)}\right]$$

forcing term: $F(x) = N \arctan\sinh \pi x$; $\quad G(x) = \int_{-\infty}^{\infty} \frac{dp}{2\pi} \frac{e^{ipx}}{1+e^{|p|}}$

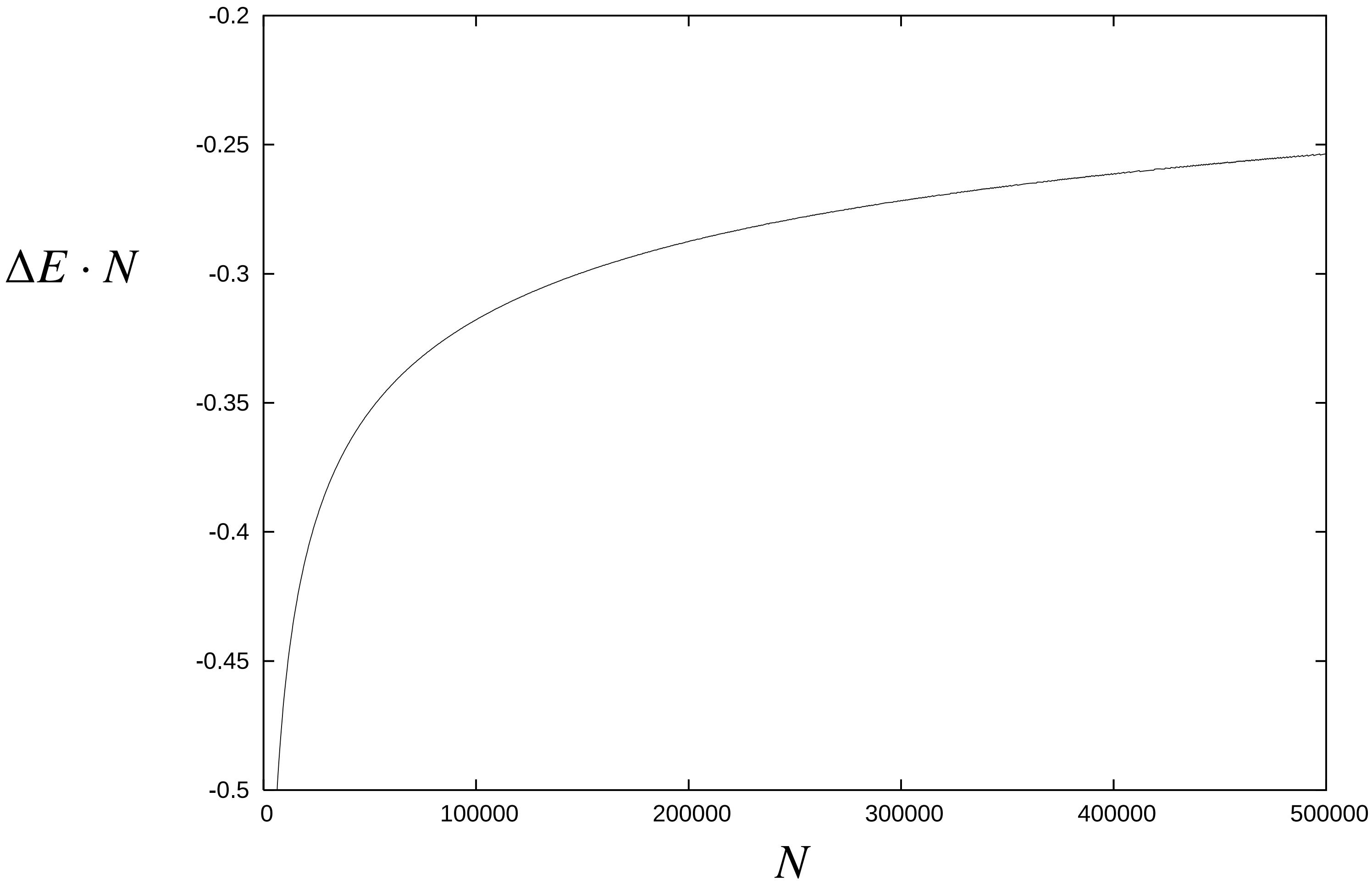
$$E = 2N\ln 2 + \textit{sources} + \int_{-\infty}^{\infty} dy \left(-\pi \frac{\sinh \pi y}{\cosh^2 \pi y}\right) \mathrm{Im}\ln\left[1 + e^{iZ(y+i0)}\right]$$

roots/holes duality	before	after
	Bethe equations	equation for Z
sources (quasiparticles)	real roots + complex roots	holes + complex roots

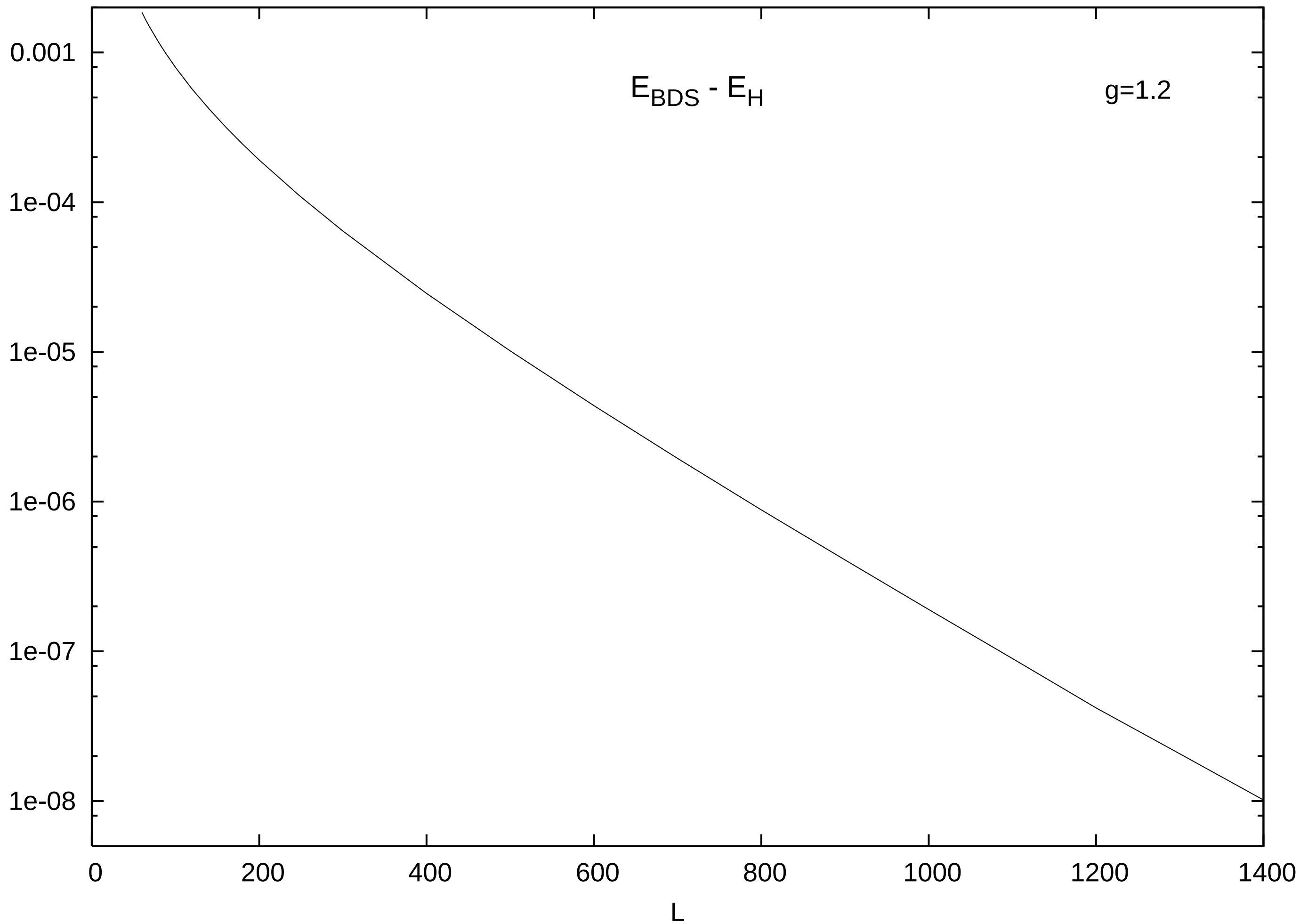
- useful to describe excitations of the *antiferromagnetic state*
- large N (chain length) development (XXX, SO(6) spin chain)
- strong and weak coupling limits (Hubbard)
- IR limit (scattering theory) and UV limit (conformal limit), sine-Gordon
- numerical analysis



Plot of the counting function $Z(x)$ for the four holes state $I = (-\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2})$ of the XXX chain.



Plot of the subleading corrections for the four holes state $I = (-\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2})$ of the XXX spin chain: $E = 2\ln 2N - 4\pi + \frac{\pi^2}{6N} + \Delta E;\quad \Delta E = \frac{\pi^2}{6N}\Big(\frac{c1}{\ln^2 N} + \dots\Big)$

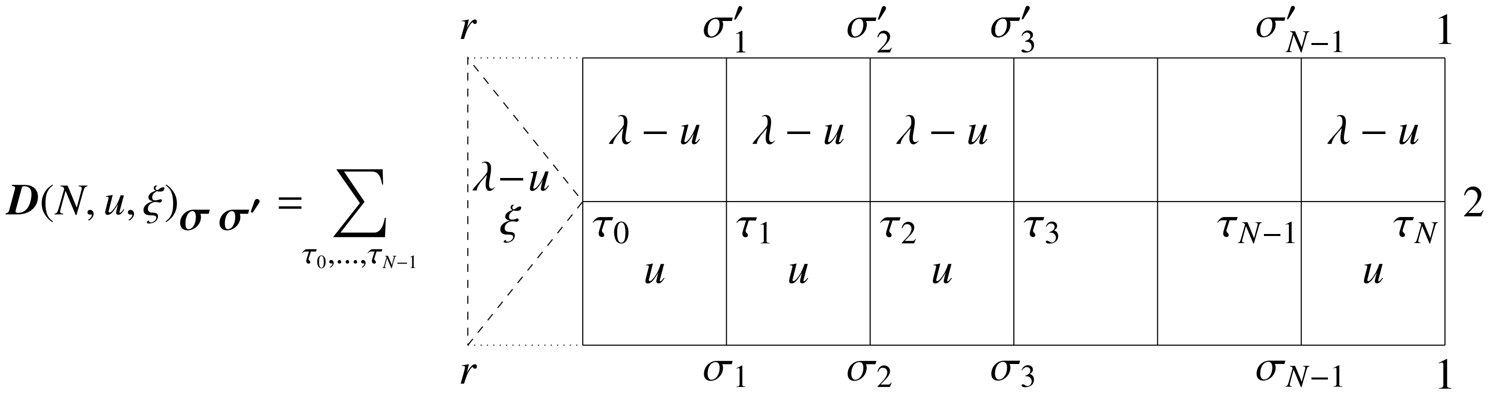


Difference of BDS and Hubbard energies (anomalous dimensions) at different sizes of the system and fixed $g = 1.2$ in a logarithmic scale.

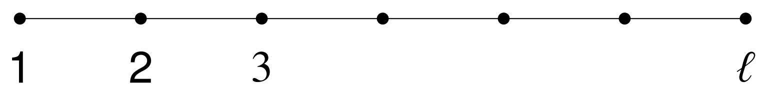
Exponential damping: $|E_{\mathrm{BDS}} - E_{\mathrm{H}}| \propto e^{-a(g)N}$

Thermodynamic Bethe ansatz

Face models A_ℓ: classical 2 dim. models with interaction defined on a square



heights: $\sigma_j = 1, \dots \ell$; A_ℓ adjacency rule:



Fusion hierarchy: $\boldsymbol{D}^0 \propto \boldsymbol{I}$; $\boldsymbol{D}^1 = \boldsymbol{D}$; recursively $\boldsymbol{D}^1 \to \boldsymbol{D}^2 \to \dots \boldsymbol{D}^{\ell-1}$; $\boldsymbol{D}^\ell = 0$

Functional equations: $\tilde{\boldsymbol{d}}^q(u+\lambda/2)\, \tilde{\boldsymbol{d}}^q(u-\lambda/2) = \prod_r (1+\tilde{\boldsymbol{d}}^r(u))^{A_{qr}}$

Al. Zamolodchikov Y-system for RSOS scattering theories (1991), $\tilde{\boldsymbol{d}} = \exp(-\varepsilon) = Y$

Zeros of the transfer matrix eigenvalues

Thermodynamic Bethe ansatz equations

$$\log \hat{d}^q(x) = -4\,\delta_{1,q}\,e^{-x} + \log \prod_{j=1}^{L-2} \prod_{k=1}^{m_j} \Big[\tanh \frac{x-\hat{y}_k^{(j)}}{2}\Big]^{A_{q,j}}$$
$$+ \sum_{j=1}^{L-2} A_{q,j} \int_{-\infty}^{\infty} dy\, \frac{\log(1+\hat{d}^j(x))}{2\pi\cosh(x-y)}, \qquad q=1,\ldots,\ell-2$$

Quantization conditions

$$\hat{\Psi}^q(x) = 4\delta_{1,q}\,e^{-x} + i\sum_{r=1}^{L-2} A_{q,r} \sum_{k=1}^{m_r} \log\tanh\Big(\frac{x-\hat{y}_k^{(r)}}{2} - i\frac{\pi}{4}\Big)$$
$$- \sum_{r=1}^{L-2} A_{q,r} \fint_{-\infty}^{\infty} dy\, \frac{\log(1+\hat{d}^r(y))}{2\pi\sinh(x-y)}$$
$$\hat{\Psi}^q(\hat{y}_k^{(q)}) = \pi\, n_k^{(q)} = \pi[1+2(I_k^{(q)}+m_q-k)]$$

Continuum limit of the lattice model A_ℓ: integrable perturbation of a CFT $\mathcal{M}_{\ell,\ell+1}$ (unitary minimal model)

All excited states. If no sources (=zeros): ground state

Physical combinatorics: classification of the zeros of the transfer matrix eigenvalues

Continuum limit

$$-\tfrac{1}{2}\log D(N,0) = N\log\kappa_{\text{bulk}} + \tfrac{1}{2}\log\kappa_{\text{bound}} + \tfrac{\pi}{N}E + \text{higher order corrections in } \tfrac{1}{N}$$

At the critical (conformal) point

$$E = -\frac{c_\ell}{24} + \frac{1}{4}\boldsymbol{m}^T C \boldsymbol{m} + \sum_{q=1}^{\ell-2}\sum_{k=1}^{m_q} I_k^{(q)}; \qquad \text{central charge } c_\ell = 1 - \tfrac{6}{\ell(\ell+1)}$$

$A_\ell \longrightarrow \mathcal{M}_{\ell,\ell+1}$ = Virasoro minimal model

A_3 Ising model
A_4 tricritical Ising
A_5 (related to) three states Potts

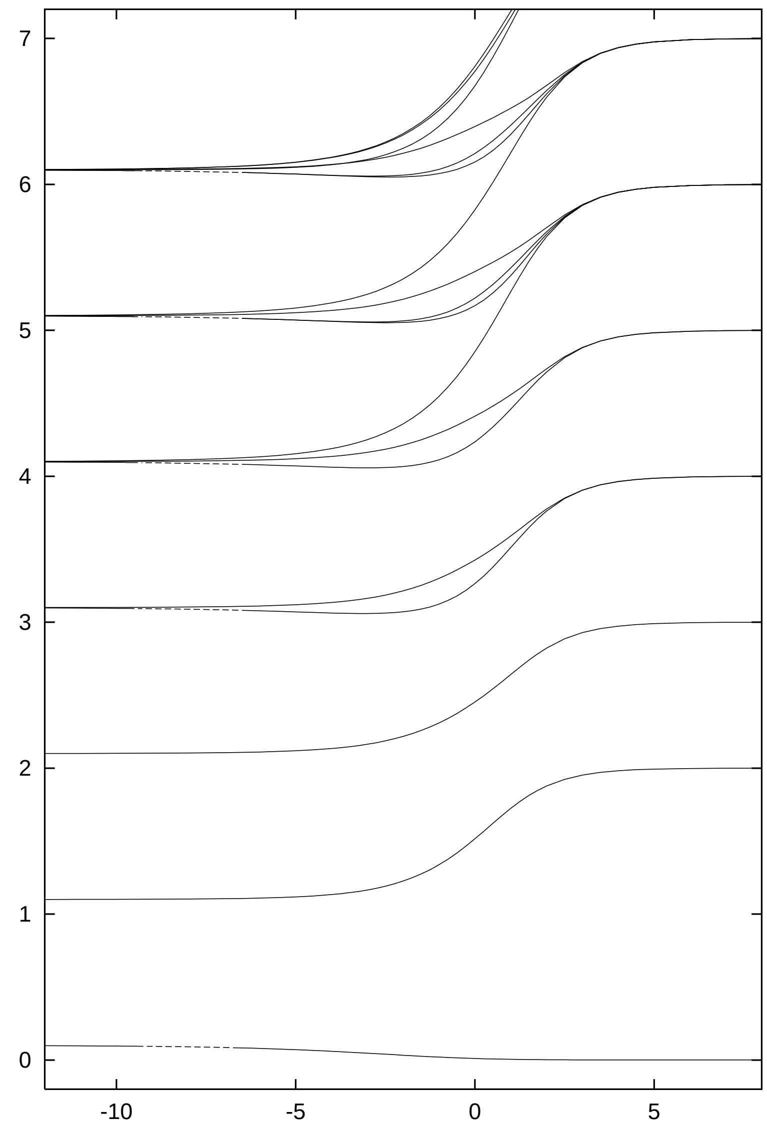
Feverati, Grinza, Pearce, Ravanini, Witte ...
2000-2005, 2009

Numerical solutions

Scaling energies for the boundary flow $\chi_{1,2} \to \chi_{1,1}$ of the tricritical Ising model.

Geometry: infinitely long strip.

At the two extremes: exact solutions (as above). Possible description as quasi-particles gaz (physical combinatorics)



$(1,2)$ $(1,1)$

Lattice-conformal dictionary

Where are the eigenstates?

Comparison of the eigenvalues of $\boldsymbol{I}_3$ and $\boldsymbol{I}_5$ from conformal field theory and from TBA in the vacuum sector of the tricritical Ising model. The left column contains the level degeneracy (l.d.) as indicated in the conformal character (conformal partition function): dq^l

Numerical evaluation but exact results

l.d.	lattice-conformal dictionary	I_3 (CFT)	I_3 (TBA)	I_5 (CFT)	I_5 (TBA)
1	$(\,) \longleftrightarrow \lvert 0\rangle$	0.0061979	0.0061979	−0.0028301	−0.0028301
$1q^2$	$(00) \longleftrightarrow L_{-2}\lvert 0\rangle$	4.2561979	4.2561979	8.1731074	8.1731074
$1q^3$	$(10) \longleftrightarrow L_{-3}\lvert 0\rangle$	19.131198	19.131197	104.14545	104.14545
$2q^4$	$(20) \longleftrightarrow 3(\frac{4+\sqrt{151}}{5}L_{-4} + 2\,L_{-2}^2)\lvert 0\rangle$	52.052045	52.052042	556.20159	556.20155
	$(11) \longleftrightarrow 3(\frac{4-\sqrt{151}}{5}L_{-4} + 2\,L_{-2}^2)\lvert 0\rangle$	22.560351	22.560348	108.29650	108.29648
$2q^5$	$(30) \longleftrightarrow (\frac{7+\sqrt{1345}}{2}L_{-5} + 20\,L_{-3}L_{-2})\lvert 0\rangle$	110.13688	110.13687	1943.8246	1943.8244
	$(21) \longleftrightarrow (\frac{7-\sqrt{1345}}{2}L_{-5} + 20\,L_{-3}L_{-2})\lvert 0\rangle$	55.125517	55.125511	551.34946	551.34937
$4q^6$	$(40) \longleftrightarrow (11.124748\,L_{-6} + 9.6451291\,L_{-4}L_{-2} + 4.4320186\,L_{-3}^2 + L_{-2}^3)\lvert 0\rangle$	200.49775	200.49773	5280.2710	5280.2705
	$(31) \longleftrightarrow (-4.9655743\,L_{-6} + 2.3354391\,L_{-4}L_{-2} + 0.71473858\,L_{-3}^2 + L_{-2})\lvert 0\rangle$	112.78147	112.78146	1919.0972	1919.0969
	$(22) \longleftrightarrow (0.66457527\,L_{-6} - 1.2909210\,L_{-4}L_{-2} - 1.2605013\,L_{-3}^2 + L_{-2}^3)\lvert 0\rangle$	69.265146	69.265138	636.39114	636.39101
	$(0000\lvert 00) \longleftrightarrow (-1.6612491\,L_{-6} - 4.0646472\,L_{-4}L_{-2} + 1.4118691\,L_{-3}^2 + L_{-2}^3)\lvert 0\rangle$	35.980431	35.980428	209.28433	209.28430

Hubbard models with arbitrary symmetries

Hopping electrons

$$H = \sum_{i=1}^{L} \Big[\sum_{\sigma=\uparrow,\downarrow} \big(c^\dagger_{i,\sigma} c_{i+1,\sigma} + c^\dagger_{i+1,\sigma} c_{i,\sigma} \big) + U\, n_{i,\uparrow} n_{i,\downarrow} \Big] \qquad n_{i,\sigma} = c^\dagger_{i,\sigma} c_{i,\sigma}$$

$su(2)$ symmmetry ($gl(1|1)$ algebra); superconductivity, Mott transition

$\mathcal{N} = 4$ super Yang-Mills: $\frac{1}{U} = g$, where $g^2 = \frac{\lambda}{8\pi^2}$ = t'Hooft coupling

arbitrary simmetries: find integrable generalizations

$P^\sigma_{j,j+1}$ =permutation, π^σ_j =projector; $\Sigma^\sigma_{j,j+1} = \pi^\sigma_j (1 - \pi^\sigma_{j+1}) + (1 - \pi^\sigma_j) \pi^\sigma_{j+1}$; $C^\sigma_j = 2\pi^\sigma_j - 1$

$$H = \sum_{j=1}^{L} \left[\Sigma^\uparrow_{j,j+1} P^\uparrow_{j,j+1} + \Sigma^\downarrow_{j,j+1} P^\downarrow_{j,j+1} + U\, C^\uparrow_j C^\downarrow_j \right]$$

Interacting fermions: several particle types; screening effects; Bethe equations

J. Drummond, G. Feverati, L. Frappat, E. Ragoucy, 2007
G. Feverati, L. Frappat, E. Ragoucy, 2009

AdS/CFT and integrability

$AdS_5 \times S^5$ string energy

AdS/CFT duality

$\mathcal{N} = 4$ SYM dilatation operator anomalous dimensions

sigma models, integrable quantum spin chain

dilatation operator, sector SU(2): 1 dim. Hubbard model 2005-2007

So:

1) generalizations to other sectors (arbitrary simmetry)

2) NLIE for the Hubbard model

Example: $gl(2|2) \oplus gl(2|2)$ Hubbard Hamiltonian

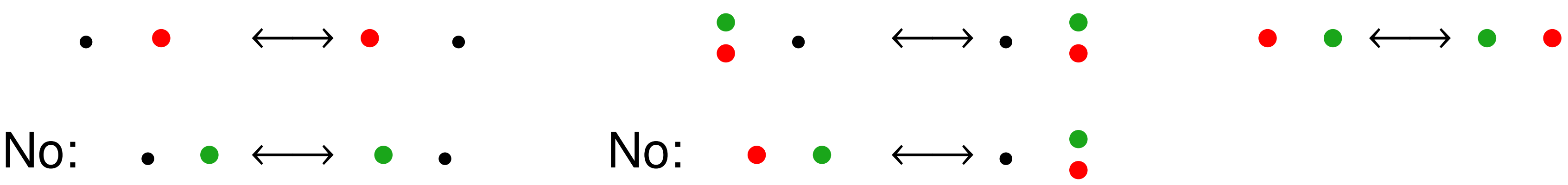
$$H_{\text{Hub}} = \sum_{i=1}^{L} \Big\{ \sum_{\sigma=\uparrow,\downarrow} (c^\dagger_{\sigma,i} c_{\sigma,i+1} + c^\dagger_{\sigma,i+1} c_{\sigma,i}) \overbrace{(c'^\dagger_{\sigma,i} c'_{\sigma,i+1} + c'^\dagger_{\sigma,i+1} c'_{\sigma,i} + 1 - n'_{\sigma,i} - n'_{\sigma,i+1})}^{\mathcal{N}'_{\sigma,i,i+1}} + U(1-2n_{\uparrow,i})(1-2n_{\downarrow,i}) \Big\}$$

symmetry: $gl(1|1) \oplus gl(1|1) \oplus gl(1|1) \oplus gl(1|1)$

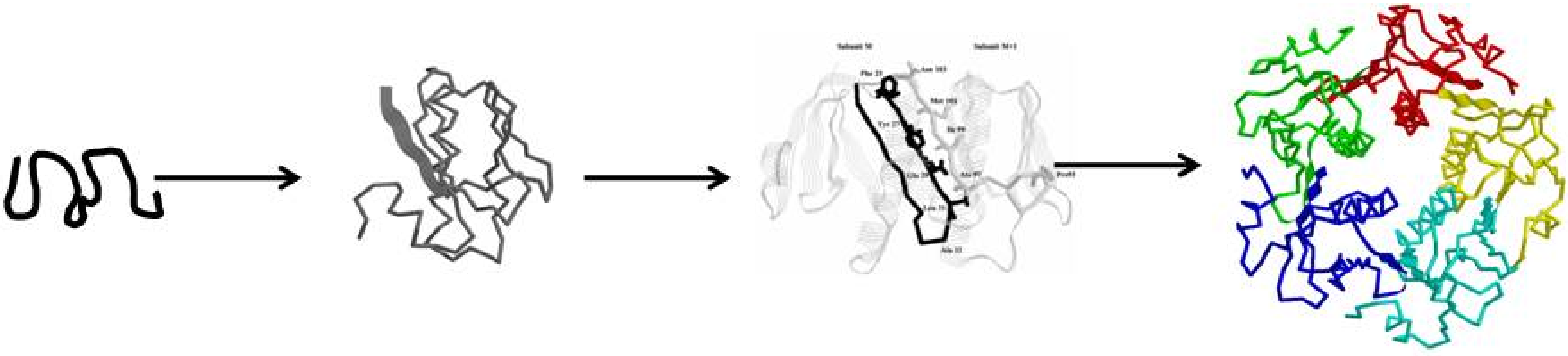
Perturbative calculation in $\frac{1}{U}$; second order:

$$H^{(2)}_{\text{eff}} = -\frac{1}{U} \sum_{i=1}^{L} \Big[(\frac{1}{2} - 2S^z_i S^z_{i+1}) - (S^+_i S^-_{i+1} + S^-_i S^+_{i+1})\, \mathcal{N}'_{\uparrow,i,i+1}\, \mathcal{N}'_{\downarrow,i,i+1} \Big]$$

unprimed particles: charged (=repel each other) ● ; primed particles: neutral ●



Assembly of oligomeric proteins



Estimations in E.C. indicate that 18% only of proteins is strictly monomeric (D. Goodsell, 2000) the remaining ones are oligomeric, from dimeric on. Formation of interfaces

Public health: Alzheimer, Anthrax, Cholera ...

Interface = geometrical and chemical complementarity

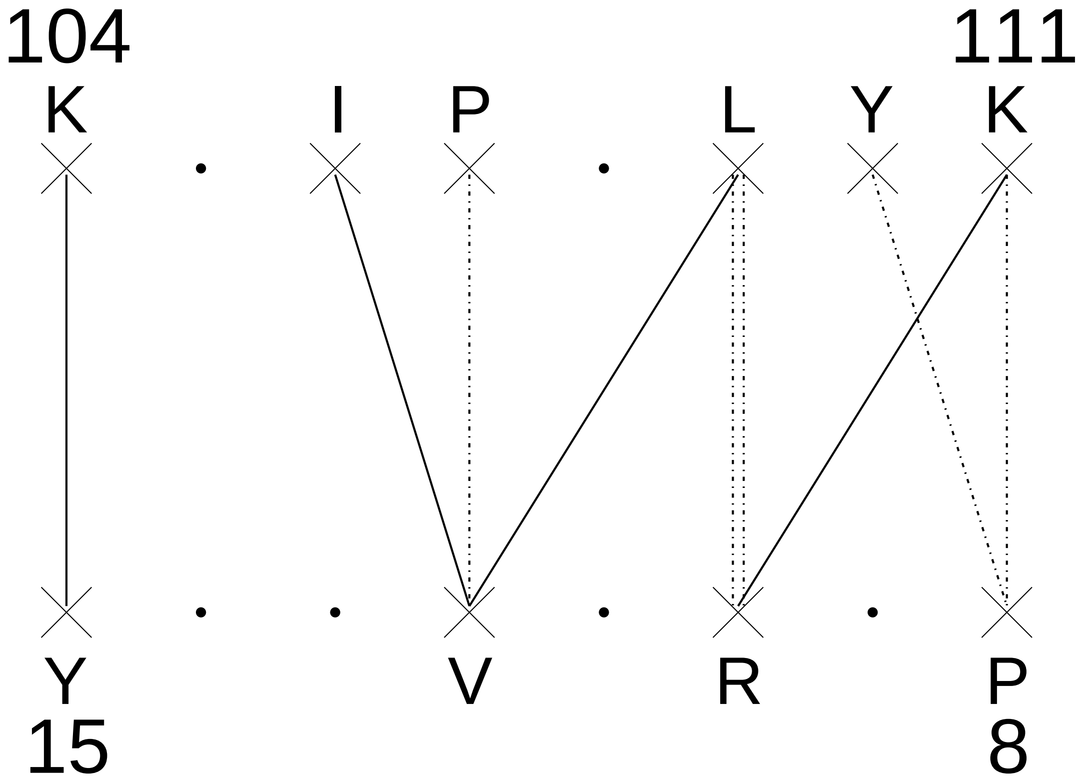
Goal: systematic analysis of 3D structures to find the key of interface formation

Interfaces are specific (no erroneous mixing of protein interfaces), no “chimeric” interfaces, oligomeric proteins are chemically stable; still ...

Gemini: a tool to investigate interfaces

- GeminiDistances: from PDB 3D structure, detect the interface.
- GeminiRegions: interface is broken into non-interacting regions.
- GeminiGraph: representing the network of interactions.
- ...
- GeminiData: database

Code deposited to the “Agence pour la protection des programmes”, 2009



solid: side chain-side chain or side chain-backbone

dashed: backbone-backbone

7-1G31-3-9

ladder: 2β structures

Feverati, Lesieur (2010), Vuillon

GeminiDistances: from PDB structure, detect the interface

- distance between atoms of adjacent subunits <0.5 nm
- symmetrization (the closest, for the two subunits)

The symmetrization makes the interface weakly cut-off dependent

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Protein: 1G31     Program Version: 2      Number of monomers:   7        Simmetry:circula
Amino acids for each monomer: 107  107  107  107  107  107  107
Distance cutoffs:  20.0   5.0 Angstrom        Algorithm: simmetrized interface
Bonded atoms (PDB atom serial numbers)
A:     181    197    268    300    473    486    500    753    767    775    776    785    788    790    7
       OE2    CG2    NE     OE2    CD2    OG     CG     O      O      O      CB     N      O      CG     C
G:    5545   5546   5148   5429   5491   5451   5426   4979   4954   4948   5610   4935   4932   4953   49
       CE     NZ     CD     NH1    O      CG     CD     OH     CG2    N      OG1    O      N      CG1    C
      3.48   4.25   3.92   3.18   3.82   3.28   3.72   2.66   3.15   2.91   3.69   2.94   2.90   3.61   3.
Bonded amino acids (PDB serial numbers)
A:      28     30     40     44     68     70     72    104    106    107    107    109    109    109    1
         E      V      R      E      L      S      P      K      I      P      P      L      L      L
         1      0      1      1      0      1      0      1      0      0      0      0      0      0
         -      -      a      a      b      b      b      a      -      -      -      -      -      -
G:      92     92     39     77     85     80     77     15     12     12    100     10     10     12
         K      K      K      R      A      P      R      Y      V      V      T      R      R      V
         1      1      1      1      0      0      1      1      0      0      1      1      1      0
         a      a      a      b      a      -      b      b      -      -      b      -      -      -
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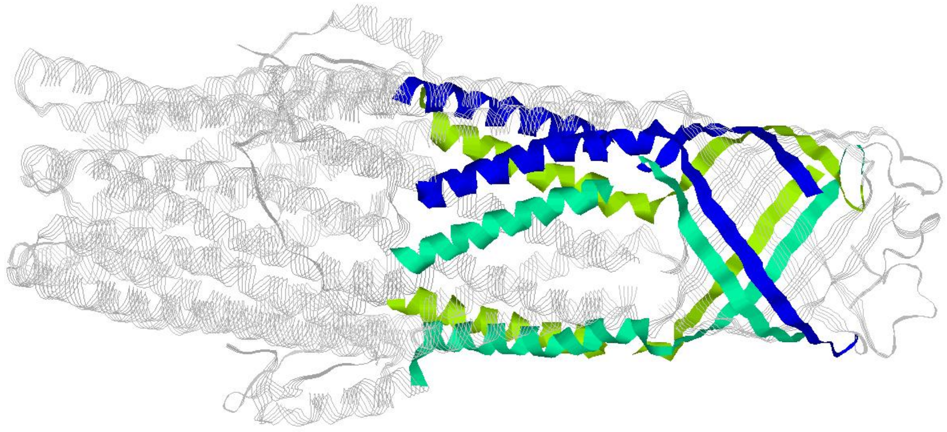
Geometrical and chemical validation

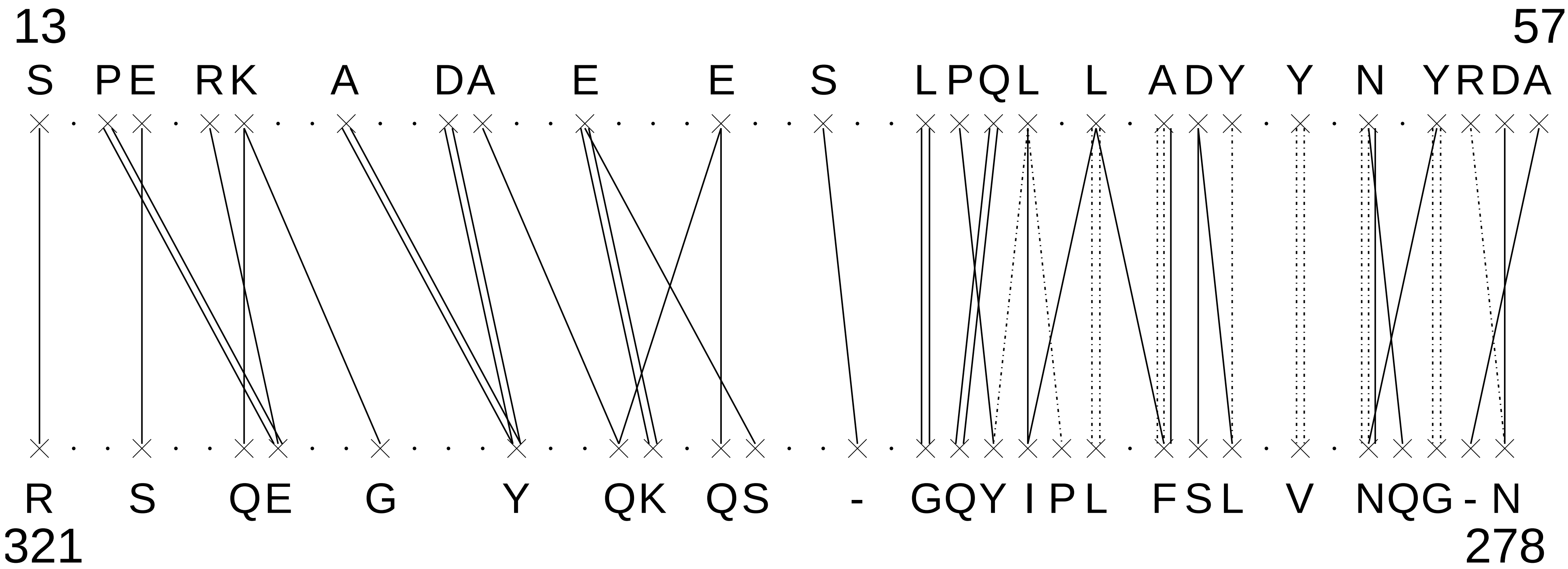
similar geometry → similar graph

graph topology → geometric constraints

α, β structures

comparison with programs of int. prediction





trimeric membrane protein 1ek9

Tutoring

Supervision of the “tesi di laurea” of A. Nigro, Dipartimento di Fisica, Università di Milano: *Integrals of motion in the two dimensional Ising model and lattice-conformal dictionary*, 2005.

Supervision of the Master 2 internship of J. Zrimi, student of Physique Chimie, Faculté des Sciences et Techniques de Guéliz, Marrakech, 2010.

Supervision of the Master 1 internship of M. Chevalier, Bioinformatique et modélisation, Lyon, 2010.

Supervision of students from the local IUT (Informatique, Mesures Physiques), licence 2, 2009, 2010.

Teaching

Mathematical methods for physics (2008-2010)
Quantum mechanics (2008)
Statistical field theory (2007)
Short course of bioinformatics (2010)

Research projects

- Turing machines: adaptation to more general “performance landscapes”; investigations around the maintain and the evolution of sexual reproduction

- Oligomeric proteins: characterization of the Gemini graphs; use of molecular dynamics tools