From the cell equation in the Hamilton-Jacobi equations to the zero-temperature limit in one-dimensional dynamical systems.

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October 2011

Objectives

The ultimate goal of the project:
Interprete the solution of the cell equation in Hamilton-Jacobi as a ground state, that is, as a zero temperature limit of Gibbs measures.

1. The cell problem and its semidiscrete approach

$$H(x, du(x) + P) = \bar{H}(P)$$

2. The Frenkel-Kontorova model and the associated standard map

$$\inf \left\{ \sum_{k=-\infty}^{+\infty} E(x_k, x_{k+1}) \ : \ \{x_k\}_{k\in\mathbb{Z}} \ \text{ configuration } \right\}$$

3. Gibbs measures and zero-temperature phase transition

$$\mu_\beta \longrightarrow \mu_{min}, \quad \beta = T^{-1} \longrightarrow +\infty.$$

Part I

1. The cell problem and its semidiscrete approach
2. The Frenkel-Kontorova model and the associated standard map
3. Gibbs measures and zero-temperature phase transition

The cell equation for Tonelli Hamiltonian

- **Notations:** We consider an Hamiltonian $H(x,p)$, $C^2(\mathbb{T}^d \times \mathbb{R}^d)$, periodic in x, strictly convex in p and superlinear in p

$$\inf_{x\in\mathbb{T}^d, p\in\mathbb{R}^d} \partial_{pp} H(x,p) > 0, \quad \lim_{\|p\|\to+\infty} \inf_{x\in\mathbb{T}^d} \frac{H(x,p)}{\|p\|} = +\infty.$$

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- **The cell equation:** For every $P \in \mathbb{R}^d$, find a constant $\bar{H}(P)$ and a continuous periodic function $u(x)$ such that

$$H(x, Du(x) + P) = \bar{H}(P), \quad \forall\, x \in \mathbb{T}^d$$

in the viscosity sense.

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- **Viscosity subsolution:** for any x_0 and $\phi \in C^1(\mathbb{T}^d)$, if $u - \phi$ admits a local maximum at x_0, then

$$H(x_0, D\phi(x_0) + P) \leq \bar{H}(P).$$

The interest of the cell equation

- **Generating functions:** If it happens that u and $\bar{H}$ are smooth, then $S(x,P) := P\cdot x + u(x,P)$ generates a change of symplectic coordinates

$$\begin{cases} p &= \frac{\partial S}{\partial x}(x,P) \\ X &= \frac{\partial S}{\partial P}(x,P) \end{cases}, \quad \text{or} \quad \begin{cases} X &= x \\ P &= p - Du(x,P) \end{cases}$$

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- **Integrable Hamiltonian:** The new Hamiltonian becomes $H(X,P) = \bar{H}(P)$ depends only on P: it is said integrable. The new equations of motion are

$$\dot{X} = \frac{\partial \bar{H}}{\partial P}, \quad \dot{P} = -\frac{\partial \bar{H}}{\partial X} = 0.$$

The motion lives on a d-dimensional torus parametrized by a constant rotation vector $\omega(P) = \frac{\partial \bar{H}}{\partial P}$.

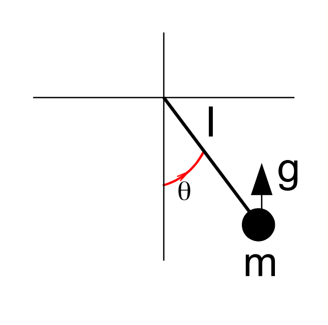
The classical main result

Theorem[Lions, Papanicolaou, Varadhan (1996)] Let $H(x,p)$ be periodic in x, $C^2(\mathbb{T}^d \times \mathbb{R}^d)$, superlinear and strictly convexe in p.
For every P, there exists a unique constant $\bar{H}(P)$ and a periodic viscosity solution $u(x)$ of

$$H(x, Du(x) + P) = \bar{H}(P), \quad \forall x \in \mathbb{T}^d.$$

The inverted pendulum example

The inverted pendulum example:



$$ml\ddot{\theta} = mg\sin\theta$$

$$x = \frac{\theta}{2\pi}$$

$$\ddot{x} = -\frac{d}{dx}V(x)$$

$$V(x) = -\frac{C}{(2\pi)^2}\left[1 - \cos(2\pi x)\right]$$

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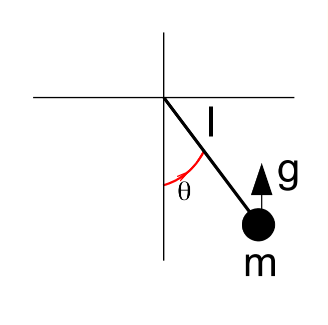

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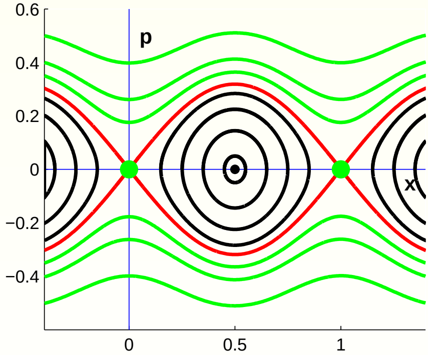
$$L(x,v) := \frac{1}{2}v^2 - V(x)$$
$$H(x,p) = \frac{1}{2}p^2 + V(x)$$
$$\frac{d}{dt}\left(\frac{\partial L}{\partial v}\right) = \frac{\partial L}{\partial x}$$

The inversted pendulum example



Phase space of the pendulum

$H(x,p)$ is constant along the flow

- black dot:
  $H(x,p) = V_{min}$,
  elliptic fixed point
- green dot:
  $H(x,p) = V_{max}$,
  hyperbolic fixed point
- red trajectories:
  $H(x,p) = V_{max}$,
  heteroclinic trajectory
- green trajectories:
  $H(x,p) > V_{max}$,
  the flow is invariant on circles, graphs over x

The inverted pendulum: the cell problem

- **The cell problem:** The viscosity solution of

$$\frac{1}{2}|Du(x) + P|^2 + V(x) = \bar{H}(P)$$

is explicit and for any P: $u(x)$ and $\bar{H}$ are unique.

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- **If $\mathbf{0} \le \mathbf{P} \le \mathbf{P}_*$:** $\bar{H}(P)=V_{max}$

$$\begin{cases} u(x) = -Px + \int_0^x \sqrt{2(V_{max}-V(s))}\;\epsilon(s)\,ds \\ \text{if } 0 \le x \le x_*(P), \quad \epsilon(x)=+1 \\ \text{if } x_*(P) \le x \le 1, \quad \epsilon(x)=-1 \end{cases}$$

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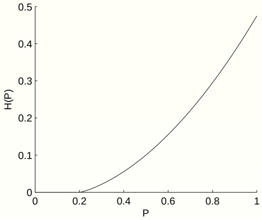
- **If $\mathbf{P} > \mathbf{P}_*$:** $\bar{H}(P) > V_{max}$ is smooth

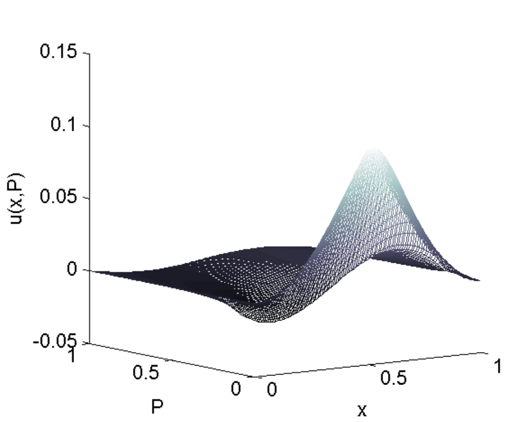
$$u(x) = -Px + \int_0^x \sqrt{2(\bar{H}(P)-V(s))}\,ds$$

The inversed pendulum: the cell problem

The viscosity solution of $H(x, Du(x) + P) = \bar{H}(P)$



the effective Hamiltonian $\bar{H}(P)$



the viscosity solution $u(x, P)$

A semidiscrete cell equation

- **An approximate cell problem:** (Hamilton-Jacobi-Belman) There exists a unique periodic viscosity solution $u_\epsilon(x)$ of

$$\epsilon u_\epsilon(x) + H(x, Du_\epsilon(x) + P) = 0, \quad \forall\ x \in \mathbb{R}^d$$

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- **The value function:** (of an infinite horizon problem)

$$u_\epsilon(x) = u_\epsilon(x, P) = \inf \Big\{ \int_{-\infty}^{0} \Big[L(\gamma, \dot\gamma) - P \cdot \dot\gamma \Big] e^{-\epsilon|s|}\, ds \ : \\ \gamma \in AC(]-\infty, 0], \mathbb{R}^d),\ \gamma(0) = x \Big\}$$

where $L(x, v) = \sup\{p \cdot v - H(x, p) \ : \ p \in \mathbb{R}^d\}$ is the Legendre transform of $H(x, p)$

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- **Theorem:** [Lions, Papanicolau, Varadhan] For some subsequence of ϵ, uniformly in x

$$\epsilon u_\epsilon(x) \to -\bar{H}(P), \quad u_\epsilon(x) - \min u_\epsilon \to u(x)$$

A semidiscrete cell equation

- **The semidiscrete HJB equation:** Let $\tau > 0$ be a time step. Take $t_{-k} = -\tau k$, k=1,2,... and piececewise affine trajectories

$$u_{\epsilon,\tau}(x) = \inf\Big\{ \sum_{k=1}^{+\infty} \tau \Big[L(x_{-k}, v_{-k}) - P \cdot v_{-k}\Big](1 - \epsilon\tau)^{k-1} \ : \\ v_{-k} \in \mathbb{R}^d,\ x_{-k+1} = x_{-k} + \tau v_{-k},\ x_0 = x \Big\}$$

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- **Theorem:** [Falcone, Rorro, 2006] Remember $H(x,p)$ is C^2-smooth and strictly convex and superlinear in p, then, for some constant C,

$$\sup_{x \in \mathbb{R}^d} |u_{\epsilon,\tau}(x) - u_\epsilon(x)| \leq C \frac{\tau}{\epsilon}$$

A semidiscrete cell equation

- **The semidiscrete dynamical programming principal:** The discrete value function $u(x) = u_{\epsilon,\tau}$ satisfies

$$\epsilon u(x) + \sup_{v\in\mathbb{R}^d} \left\{ (1-\epsilon\tau)\frac{u(x)-u(x-\tau v)}{\tau} - L(x-\tau v, v) + P\cdot v \right\} = 0$$

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(which is very close, as $\tau \to 0$, to)

$$\epsilon u_\epsilon(x) + \sup_{v \in \mathbb{R}^d} \{ Du_\epsilon(x) \cdot v - L(x, v) + P \cdot v \} = 0$$

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- **versus a semidiscrete cell equation:**

$$-\tau\bar{H}(P) + \sup_{v\in\mathbb{R}^d} \left\{ u_\tau(x) - u_\tau(x-\tau v) - \tau L(x-\tau v, v) + \tau P\cdot v \right\} = 0$$

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(which can be written as)

$$E_\tau(x,y) := \tau L(x, \frac{y-x}{\tau}) - P\cdot(y-x), \quad \bar{E}_\tau(P) = -\tau\bar{H}(P)$$

$$u_\tau(x) + \bar{E}_\tau(P) = \inf_{x'\in\mathbb{T}^d} \{ u_\tau(x') + E_\tau(x', x) \}$$

A semidiscrete cell equation

Partial Result: Assume $H(x,p)$ periodic in x, $C^2(\mathbb{T}^d \times \mathbb{R}^d)$, strictly convex and superlinear in p. Assume (some growth control at infinity of L)

$$\lim_{R \to +\infty} \frac{\inf_{|v| \geq R, x \in \mathbb{T}^d} \ L(x,v)/|v|}{\sup_{|v| \leq R, x \in \mathbb{T}^d} \ \|D^2 L(x,v)\|} = +\infty$$

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for some subsequence (τ) converges

$$\begin{cases} \tau^{-1}\bar{E}_\tau \longrightarrow -\bar{H}(P) \\ u_\tau(x) \longrightarrow u(x) \quad \text{uniformly in } x \\ H(x, Du(x)+P) = \bar{H}(P) \quad \text{in the viscosity sense} \end{cases}$$

A semidiscrete cell equation

Conclusion of part I:

- The discrete cell equation with two unknowns $(\bar{E}, u)$ is of the form

$$\begin{cases} u(x) + \bar{E} = \min_{x'} \{u(x') + E(x', x)\}, \quad u(x) \text{ periodic in } x, \\ E(x', x) = E(x' + 1, x + 1), \\ E(x', x) \text{ is strictly convex, superlinear in } |x - x'| \end{cases}$$

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- In the special case of the inverted pendulum

$$E_\tau(x,y) = \frac{1}{2\tau}|y-x|^2 + \frac{\tau C}{(2\pi)^2}\Big(1 - \cos(2\pi x)\Big) - P(y-x)$$

numerically: for $\tau = 0.1, \quad \tau^{-1}\bar{E}_\tau \simeq \bar{H}(P)$ up to 10^{-4}

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- The optimal backward trajectory $(x_{-k})_{k \geq 0}$

$$u(x_{-k}) + \bar{E} = u(x_{-k-1}) + E(x_{-k-1}, x_{-k})$$

  can be interpreted as the ground configuration of the Frenkel-Kontorova model, that is as the configuration with the lowest energy or as the temperature tends to zero.

Part II

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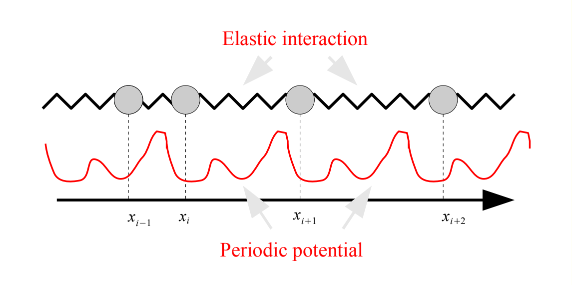
2. The Frenkel-Kontorova model and the associated standard map
3. Gibbs measures and zero-temperature phase transition

The Frenkel-Kontorova model

- **The physical model:** The model describes the set of configurations of a chain of atoms at equilibrium



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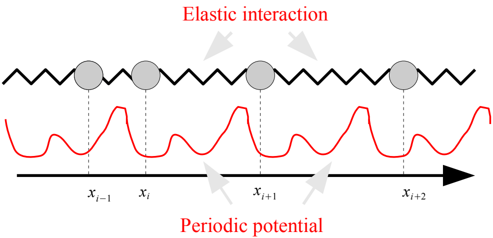

- **The original 1D-FK:** $x_i \in \mathbb{R}$

$$E_{\lambda,K}(x,y) = W_\lambda(x,y) + KV(x),$$

$$W_\lambda(x,y) = \frac{1}{2}|y-x-\lambda|^2 - \frac{1}{2}\lambda^2, \quad V(x) = \frac{1}{(2\pi)^2}\Big(1-\cos(2\pi x)\Big)$$

$$E_{\lambda,K}(x,y) = E_{0,K}(x,y) - \lambda(y-x).$$

Minimizing configurations

- **Question:** Define a notion of configuration $\underline{x} := (x_k)_{k\in\mathbb{Z}}$ with the smallest total energy

$$E_{tot}(\underline{x}) := \sum_{k=-\infty}^{+\infty} E(x_k, x_{k+1}) \leq E_{tot}(\underline{y}), \quad \forall\, \underline{y} = (y_k)_{k\in\mathbb{Z}} \quad ?$$

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- **Minimizing configuration:** $\underline{x} := (\ldots, x_{-1}, x_0, x_1, \ldots)$ such that

$$\begin{cases} E(x_m, x_{m+1}, \ldots, x_n) := \sum_{k=m}^{n-1} E(x_k, x_{k+1}) \\ E(x_m, \ldots, x_n) \leq E(y_m, \ldots, y_n) \\ \forall\ \underline{y} \text{ configuration} \quad \text{s.t.} \quad y_m = x_m \text{ and } y_n = x_n \end{cases}$$

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- **Problem:** Let $E_\lambda(x,y) := E(x,y) - \lambda \cdot (y - x)$ then

$$(x_k)_{k\in\mathbb{Z}} \text{ is minimizing for } E \iff (x_k)_{k\in\mathbb{Z}} \text{ is minimizing for } E_\lambda$$

the minimizing-configuration notion does not enough distinguish these configurations.

The effective potential

- **Effective potential:** [Chou-Griffiths, 1986] A C^0 periodic function $u(x)$ such that there exists a constant $\bar{E}$ solution of the problem

$$\begin{cases} u(y) + \bar{E} = \min_x \{u(x) + E(x,y)\}, & \forall\ y \quad \text{(backward)} \\ u(x) + \bar{E} = \max_y \{u(y) - E(x,y)\}, & \forall\ x \quad \text{(forward)} \end{cases}$$

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Remark: this is exactly the previous discrete cell equation: u plays the role of a discrete viscosity solution (sometimes called calibrated solution or corrector)

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  Remark: this is exactly the previous discrete cell equation: u plays the role of a discrete viscosity solution (sometimes called calibrated solution or corrector)

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- Does an effective potential exist ?

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$$u_n \longrightarrow u_{n+1} := \frac{u_n + T_-[u_n]}{2} - \min\left(\frac{u_n + T_-[u_n]}{2}\right)$$

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What about the converse ?

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Theorem: [Aubry, Mather, 1983, 1989, ...] Assume $d = 1$, $E(x, y)$ is $C^2(\mathbb{R} \times \mathbb{R})$, periodic, superlinear and satisfies the twist condition

$$E(x+1, y+1) = E(x, y), \quad \lim_{|y-x| \to +\infty} \frac{E(x, y)}{|y-x|} = +\infty, \quad \frac{\partial^2 E}{\partial x \partial y} < 0.$$

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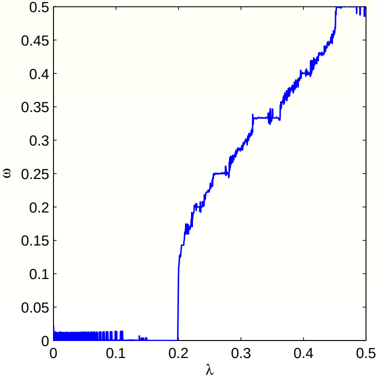
- If $\omega \in \mathbb{Q}$ then $\Lambda(\omega) := \{\lambda \text{ s.t. } \omega = -\frac{d\bar{E}}{d\lambda}(\lambda)\}$ has non empty interior. If $\omega \notin \mathbb{Q}$, $\mathrm{int}(\Lambda(\omega)) = \emptyset$.

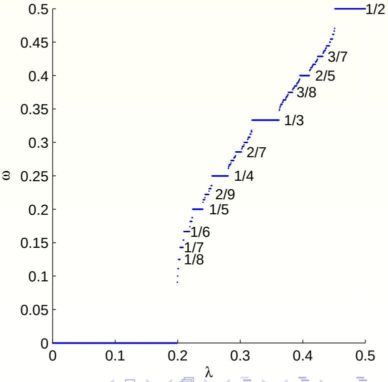
The Devil's staircase

Phase locking at rational rotation number:

$$E_{\lambda,K}(x,y) = \frac{1}{2}|y-x|^2 - \lambda(y-x) + \frac{K}{(2\pi)^2}\Big(1-\cos(2\pi x)\Big)$$

$$K=3, \quad \omega = -\frac{\partial \bar{E}}{\partial \lambda}(\lambda, K)$$





The phase transition in (λ, K)

Phase transition with respect to K:

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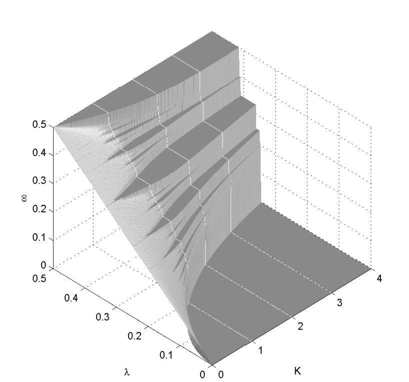

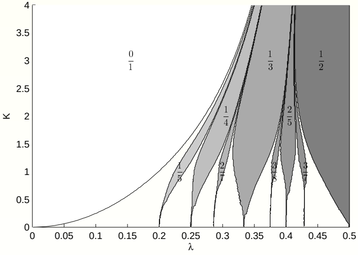

The Frenkel-Kontorova model

Conclusion of part II:

- The periodic cell problem and the Frenkel-Kontorova model are related by the two energies

$$\begin{cases} H_{P,C}(x,p) = \frac{1}{2}|p+P|^2 - \frac{C}{(2\pi)^2}\big(1-\cos(2\pi x)\big) \\ E_{\lambda,K}(x,y) = \frac{1}{2}|y-x|^2 - \lambda(y-x) + \frac{K}{(2\pi)^2}\big(1-\cos(2\pi x)\big) \end{cases}$$

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- Let τ be a small parameter and $\lambda = \tau P$ and $K = \tau^2 C$, then

$$\begin{cases} H_{P,C}(x, Du(x)+P) = \bar{H}(P,C) \\ u_\tau(x) + \bar{E}(\lambda,K) = \min_{x'}\{u_\tau(x') + E_{\lambda,K}(x',x)\} \\ -\frac{1}{\tau^2}\bar{E}(\tau P, \tau^2 K) \longrightarrow \bar{H}(P,C), \quad \frac{1}{\tau}u_\tau(x) \longrightarrow u(x) \end{cases}$$

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- Moreover the optimal trajectories can be understood as ground configurations, that is, as configurations with the lowest energy. They can also be understood as probability states describing the system at zero temperature.

Part III

1. The cell problem and its semidiscrete approach
2. The Frenkel-Kontorova model and the associated standard map
3. Gibbs measures and zero-temperature phase transition

Sub-shift of finite type

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Gibbs measures / ground configurations

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Theorem: (easy results for general Hölder $\boldsymbol{E : \Sigma_G^+ \to \mathbb{R}}$)
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$$\bar{E} = \int E\,d\mu_{min}, \quad \mathrm{Ent}(\mu_{min}) = \mathrm{Ent}(\Sigma_G^+), \quad \mathrm{supp}(\mu_{min}) \subset \mathrm{G.C.}$$

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$$\exp\Big(-\beta[u_\beta(x) + \bar{E}_\beta]\Big) = \sum_{x' \,:\, \sigma(x')=x} \exp\Big(-\beta[u_\beta(x') + E(x')]\Big)$$

- any accumulation point of u_β is an effective potential

Finite-range potential

Theorem: for finite-range interactions $E(x) = E(x_0, x_1)$:

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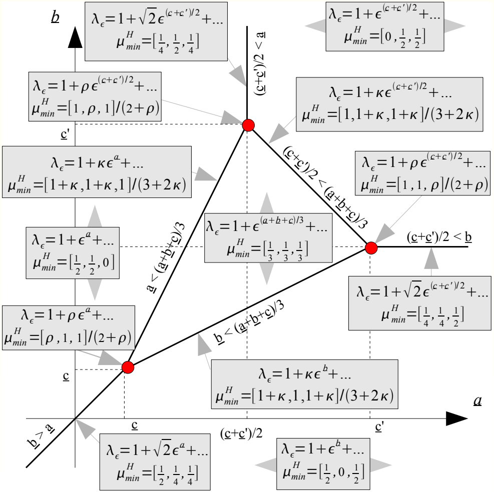
- (E. Garibaldi, Ph. Thieullen) There exists a formal algorithm which describes μ_{min} with respect to the initial data $E(x, y)$
- The existence of $\bar{E}$ and μ_{min} are related to a problem of singular matrices: let

$$M_\beta := \left[e^{-\beta E(x,y)}\right]_{x,y \in S}$$

$$L_\beta M_\beta = \lambda_\beta L_\beta, \quad M_\beta R_\beta = \lambda_\beta R_\beta, \quad \sum_x L_\beta(x) R_\beta(x) = 1$$

then $\lambda_\beta = e^{-\beta \bar{E}_\beta} \sim \lambda_0 e^{-\beta \bar{E}}$ and $L_\beta(x) R_\beta(x) \to \mu_{min}(x)$

Gibbs measures and phase transition



$$S = \{1,2,3\}$$

$$M_\beta = \begin{bmatrix} 1 & e^{-\beta a} & e^{-\beta b} \\ e^{-\beta a} & 1 & e^{-\beta c} \\ e^{-\beta b} & e^{-\beta c'} & 1 \end{bmatrix}$$

$$a, b, c, c' > 0 \quad c > c'$$

$$\mu_{min} = c_1\delta_1 + c_2\delta_2 + c_3\delta_3$$

$$\delta_i = \text{ Dirac measure at}$$

$$(\dots, i, i, i, \dots)$$

$$\rho^2 - \rho - 1 = 0$$

$$\kappa^3 - \kappa - 1 = 0$$

Gibbs measures and phase transition

Conclusion: A possible research program

- Develop a thermodynamical formalism for the the cell problem without passing to the fully discretized model (finite-range sub-shift of finite type)

Gibbs measures and phase transition

Conclusion: A possible research program

- Develop a thermodynamical formalism for the the cell problem without passing to the fully discretized model (finite-range sub-shift of finite type)
- Use the fast technics developped in MCMC (Markov chain Monte Carlo) method to obtain numerically the effective Hamiltonian $\bar{H}(P)$ and the viscosity solutions $u(x)$ as limits of quantities at equilibrium when the system is freezing