Anderson localization in the Kohn-Sham model for disordered crystals

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Joint work with Éric Cancès and Mathieu Lewin

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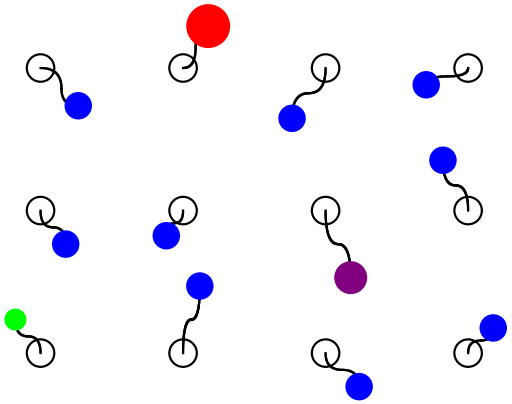
Disordered crystals

Physical system



Examples : doped semi-conductors, amorphous material, aging solids, solar cells, ...

Disordered crystals

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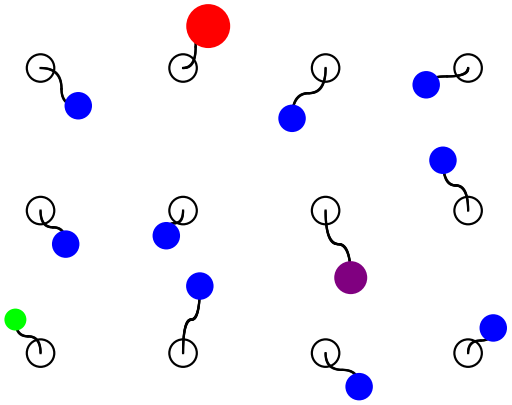

Mathematical modelling

- Classical stochastic nuclei
- Quantum disordered electrons
- Average energy per unit volume

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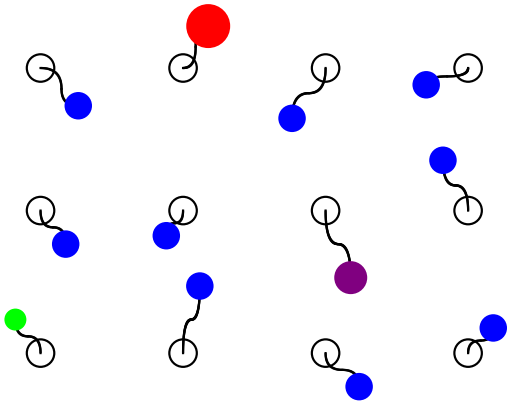

Mathematical modelling

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Examples : doped semi-conductors, amorphous material, aging solids, solar cells, ...

Objective :

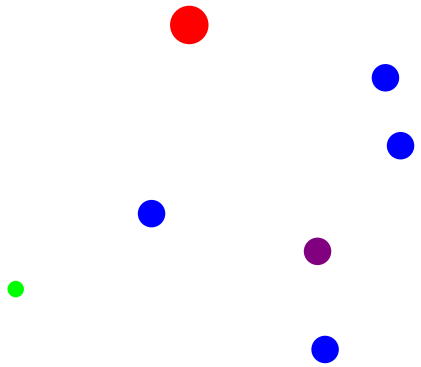
- Existence of an electronic ground state
- Properties of the ground state

Nuclei and electrons in finite systems

Born-Oppenheimer approximation

- M classical nuclei (z_k, R_k) : nuclear density μ

$$\mu = \sum_{k=1}^{M} z_k \delta_{R_k} \quad \text{or} \quad \mu = \sum_{k=1}^{M} z_k \chi(\cdot - R_k)$$



- N electrons : one-body density matrix
  $\gamma : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ in

$$\mathcal{K}_N = \{\gamma^* = \gamma,\ 0 \leq \gamma \leq 1,\ \mathrm{Tr}\,(\gamma) = N,\ \mathrm{Tr}\,(-\Delta\gamma) < \infty\}$$

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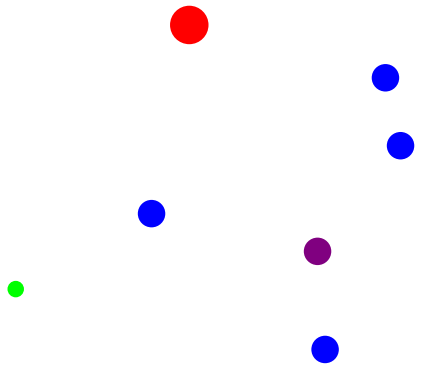

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Two types of interactions :

- long-range Coulomb interaction : $W_0(x) = \dfrac{1}{|x|}$
- short-range m-Yukawa interaction : $W_m(x) = \dfrac{e^{-m|x|}}{|x|}$

Kohn-Sham model for finite systems

Energy functional

$$\mathcal{E}_\mu(\gamma) = \frac{1}{2}\mathrm{Tr}\left(-\Delta\gamma\right) - \int_{\mathbb{R}^3\times\mathbb{R}^3} \rho_\gamma(x)\mu(y)W_m\left(x-y\right) + \frac{1}{2}\int_{\mathbb{R}^3\times\mathbb{R}^3} \rho_\gamma(x)\rho_\gamma(y)W_m\left(x-y\right)$$
$$+ E_{xc}(\rho) + U(\mu)$$

where "$\rho_\gamma(x) = \gamma(x,x)$"

Ground state

$$\gamma_0 = \arg\min\left\{\mathcal{E}_\mu(\gamma),\ \gamma \in \mathcal{K}_N\right\}$$

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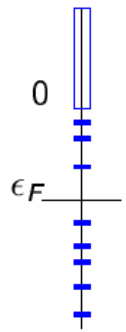
reduce Hartree Fock (rHF) model

$$E_{xc}^{rHF} = 0.$$

rHF equation (insulators and semiconductors)

$$\begin{cases} \gamma_0 = \mathbb{1}\left(H < \epsilon_F\right) \\ H = -\frac{1}{2}\Delta + V \\ -\Delta V = 4\pi\left(\rho_{\gamma_0} - \mu\right) \end{cases}$$

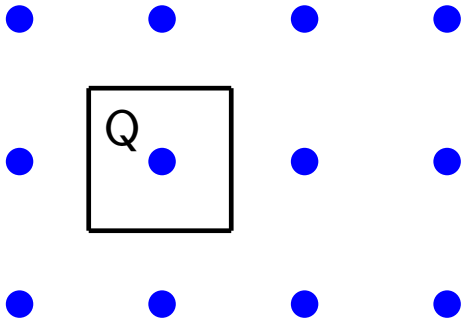


[LiSi'77] Lieb H.E. Simon B. The Hartree-Fock theory for Coulomb systems. CMP. 1977.

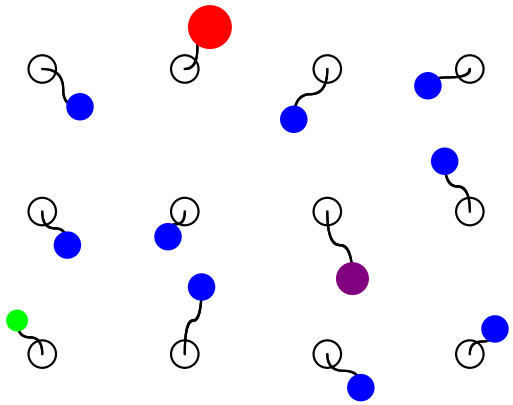
Disordered materials

Typical example

$$\mu(\omega, x) = \sum_{k \in \mathbb{Z}^d} q_k(\omega)\chi(x - k - R_k(\omega))$$



Perfect crystal



Disordered crystal

For example : (q_k) and (R_k) i.i.d bounded random variables and $\chi \in \mathcal{S}(\mathbb{R}^d)$.

General case

- A probability space $(\Omega, \mathcal{F}, \mathcal{P})$.
- An ergodic group action $\tau = (\tau_k)_{k\in\mathbb{Z}^d}$ of $\mathbb{Z}^d$ on $(\Omega, \mathcal{F}, \mathcal{P})$, i.e.
- A function $f : \Omega \times \mathbb{R}^d \to \mathbb{C}$ is stationary if $\forall k \in \mathbb{Z}^d$, a.s. and a.e.

$$f(\tau_k(\omega), x) = f(\omega, k + x).$$

- We assume that

$$\mu \text{ is stationary} \qquad \text{and} \qquad \mu \in L^1(\Omega, L^1_{\mathrm{loc}}(\mathbb{R}^3))$$

Electronic states

- Ergodic density matrices $(\gamma(\omega))_{\omega\in\Omega}$

$$\gamma(\omega)^* = \gamma(\omega), \quad 0 \leq \gamma(\omega) \leq 1, \quad \gamma(\tau_k(\omega))(x,y) = \gamma(\omega)(x+k, y+k) \quad \text{a.s..}$$

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- Number of electrons per unit volume

$$\underline{\mathrm{Tr}}\ (\gamma) := \mathbb{E}\left(\mathrm{Tr}\left(\mathbb{1}_Q \gamma \mathbb{1}_Q\right)\right) = \mathbb{E}\left(\int_Q \rho_\gamma(\cdot, x)\, dx\right)$$

- Kinetic energy per unit volume

$$\frac{1}{2}\underline{\mathrm{Tr}}\ (-\Delta\gamma) := \sum_{j=1}^{3} \mathbb{E}\left(\mathrm{Tr}\left(\mathbb{1}_Q P_j \gamma P_j \mathbb{1}_Q\right)\right)$$

- Interaction energy per unit volume of a charge distribution f

$$\frac{1}{2} D_m(f,f) = \frac{1}{2}\mathbb{E}\left(\int_Q \int_{\mathbb{R}^3} f(\cdot, x) W_m(x-y) f(\cdot, y)\right)$$

The rHF model for stochastic systems

Set of admissible density matrices

$$\mathcal{K}_\mu = \Big\{ \gamma \text{ is an ergodic density matrix, } \underline{\mathrm{Tr}}\,(-\Delta\gamma) < \infty, \\ \underline{\mathrm{Tr}}\,(\gamma) = \mathbb{E}\left(\int_Q \mu\right),\ D_m(\rho_\gamma - \mu, \rho_\gamma - \mu) < \infty \Big\}$$

Average energy per unit volume

$$\mathcal{E}_\mu(\gamma) = \frac{1}{2}\underline{\mathrm{Tr}}\,(-\Delta\gamma) + \frac{1}{2} D_m\left(\rho_\gamma - \mu, \rho_\gamma - \mu\right)$$

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Theorem (CLL'13)

For $m \geq 0$, $\mathcal{E}_\mu$ admits a minimizer on $\mathcal{K}_\mu$.

[CLL'13] E.Cancès, S.L., M.Lewin, J. math. pures appl.

Properties of the ground state

Theorem (CLL'13)

For $m > 0$ and $\mu \in L^\infty(\Omega \times \mathbb{R}^3)$, $\mathcal{E}_\mu$ admits a unique minimizer on $\mathcal{K}_\mu$, which the solution of the self-consistent equation

$$\begin{cases} \gamma(\omega) = \mathbb{1}\left(H(\omega) \leq \epsilon_F\right) \\ H(\omega) = -\frac{1}{2}\Delta + V(\omega, \cdot) \qquad \text{a.s.} \\ -\Delta V(\omega, \cdot) + m^2 V(\omega, \cdot) = 4\pi\left(\rho_{\gamma(\omega)} - \mu(\omega, \cdot)\right) \end{cases}$$

Anderson localisation

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$$H = -\frac{1}{2}\Delta + V$$

with

$$V(\omega) = \sum_{k\in\mathbb{Z}} q_k(\omega)V_1(x) + (1 - q_k(\omega))V_2(x)$$

and $q_k \sim \mathcal{B}(p)$

  - if $p \in \{0, 1\}$: no localization
  - if $p \notin \{0, 1\}$: there is Anderson localization at all energies (DSS'02, GK'13)

[DSS'02] D. Damanik, R. Sims, G. Stolz, Duke Math. J.
[GK'13] F. Germinet, A. Klein, J. Euro. Math. Soc.

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- KS model : $H = -\frac{1}{2}\Delta + V$ solution of the rHF equation. Is there localization ? ?

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- Partial results by D'18

[DSS'02] D. Damanik, R. Sims, G. Stolz, Duke Math. J.
[GK'13] F. Germinet, A. Klein, J. Euro. Math. Soc.
[D'18] R. Ducatez, Journal of Spectral Theory

Settings

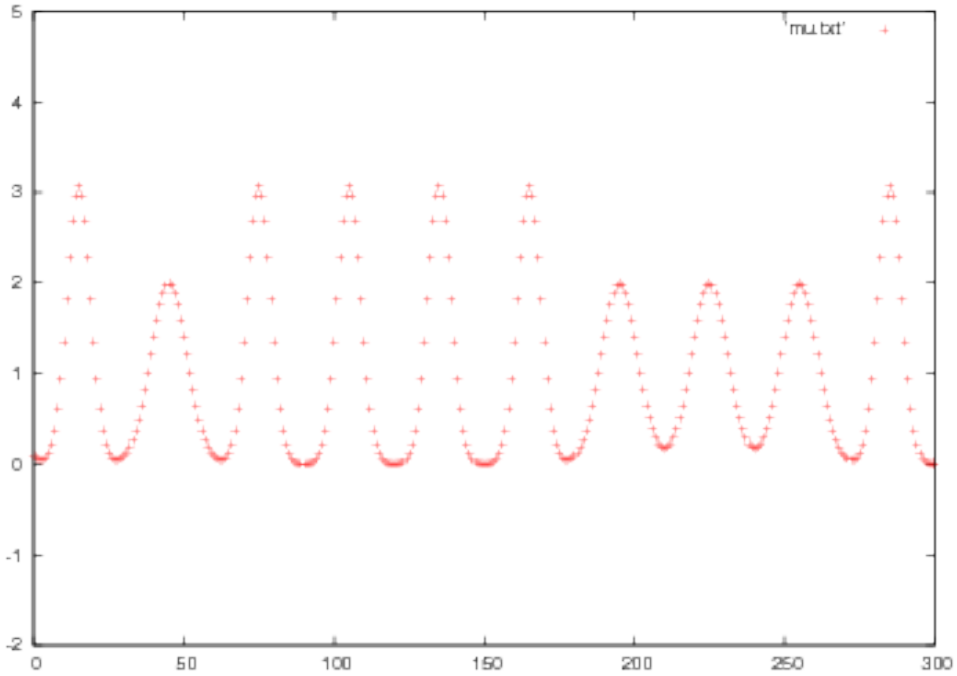
One dimensional stochastic alloy

$$\mu(\omega, x) = \sum_{k\in\mathbb{Z}} q_k(\omega)\mu_1(x-k) + (1-q_k(\omega))\mu_2(x-k),$$

$$q_k \sim \mathcal{B}(p)$$

$$\mu_1(x) = \frac{1}{\sqrt{0,02\pi}} \exp\left(-\frac{\left(x-\frac{1}{2}\right)^2}{0,02}\right)$$

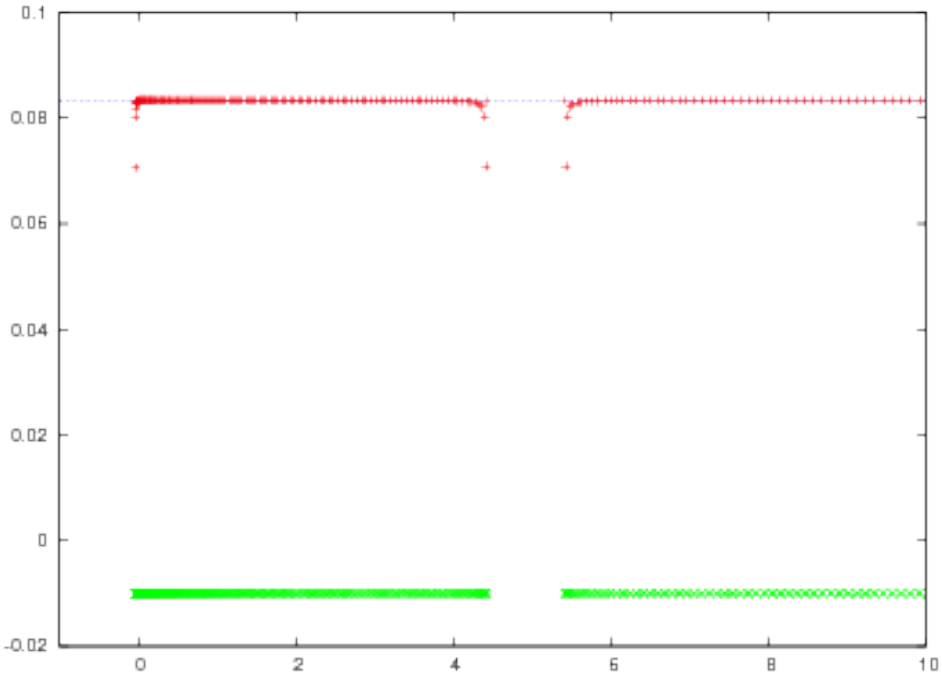
$$\mu_2(x) = 1 - \cos(2\pi x).$$



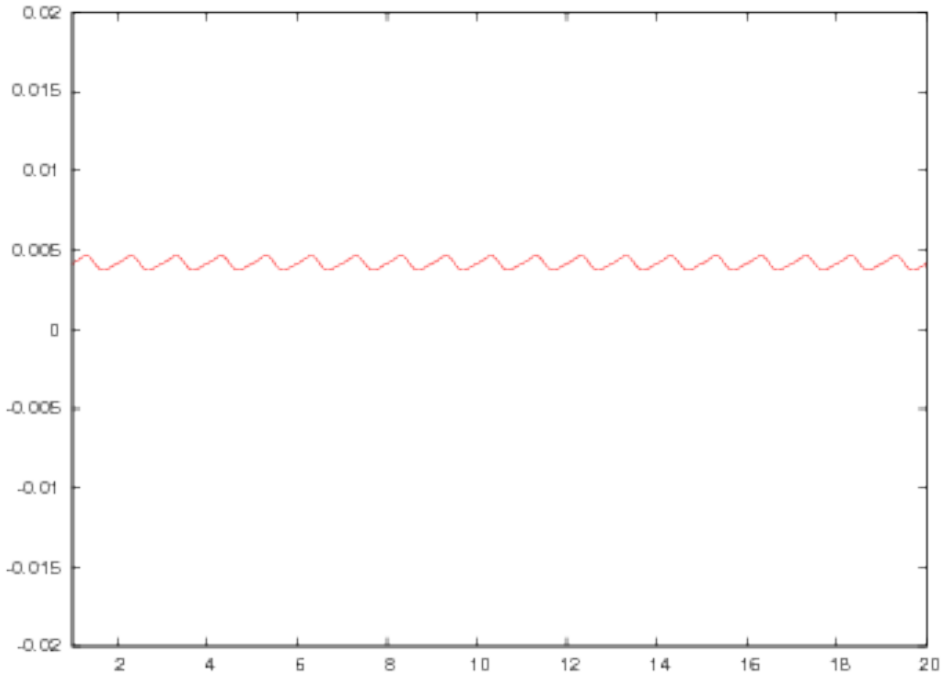
Numerical characterization : variance criterion

$$v_L(\psi) = \int_0^L x^2 \left|\psi(x)\right|^2 - \left(\int_0^L x \left|\psi(x)\right|^2\right)^2$$

Linear model (p=0)

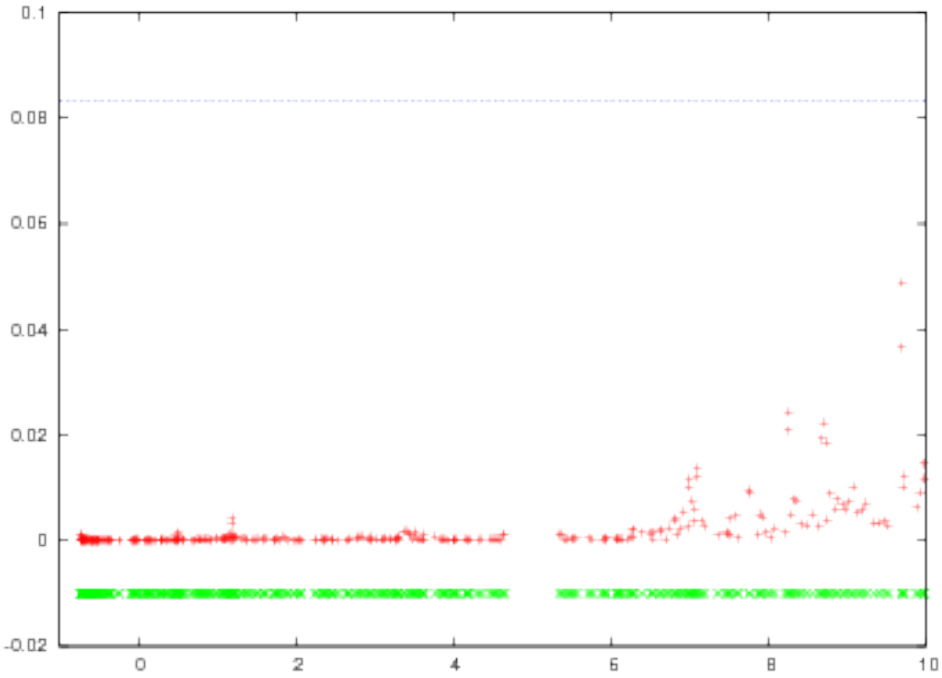


Variance corresponding to each eigenvalue



Eigenfunction corresponding to the first eigenvalue

Linear model (p=0.5)



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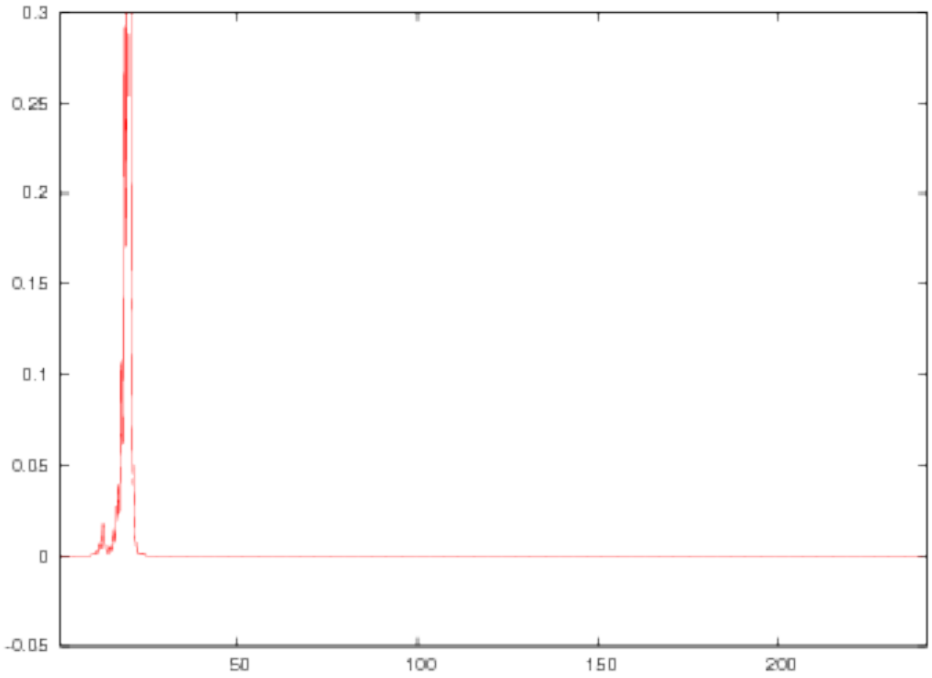
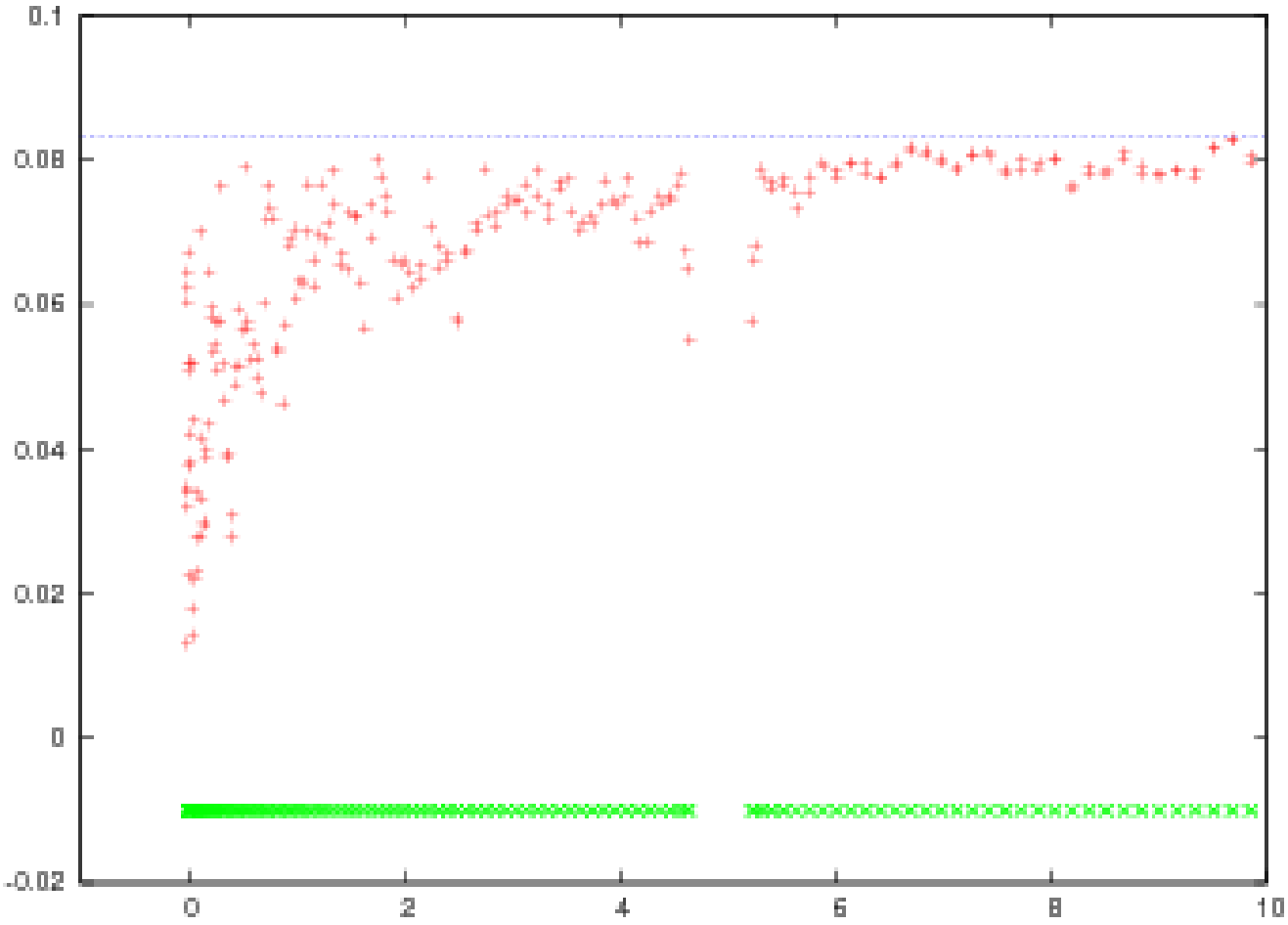


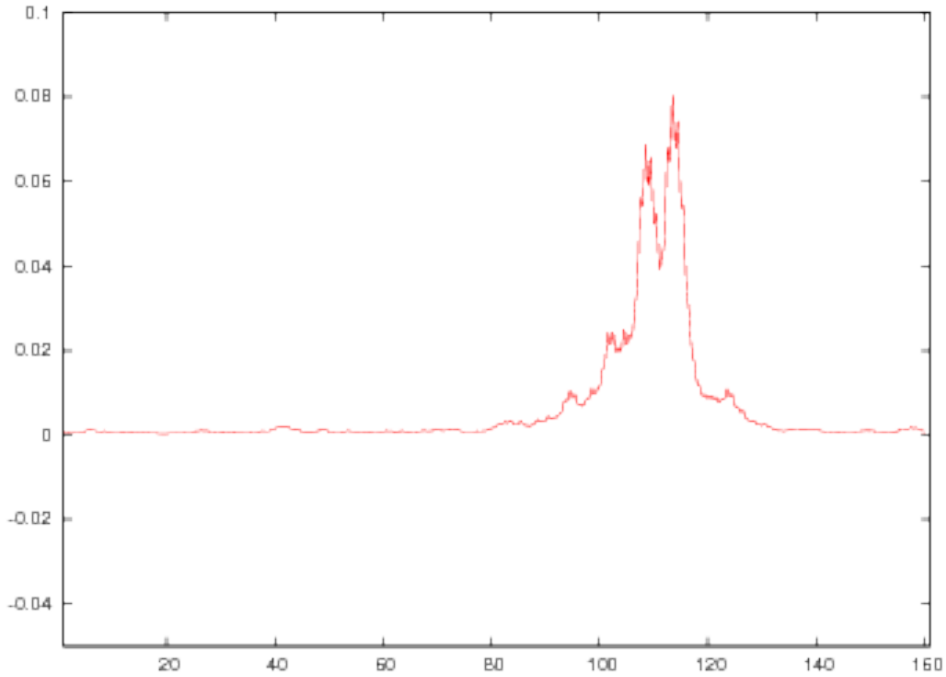
Eigenfunction corresponding to the first eigenvalue

rHF model (p=0.5)



Variance corresponding to each eigenvalue

Eigenfunctions in the rHF model (p=0.5)



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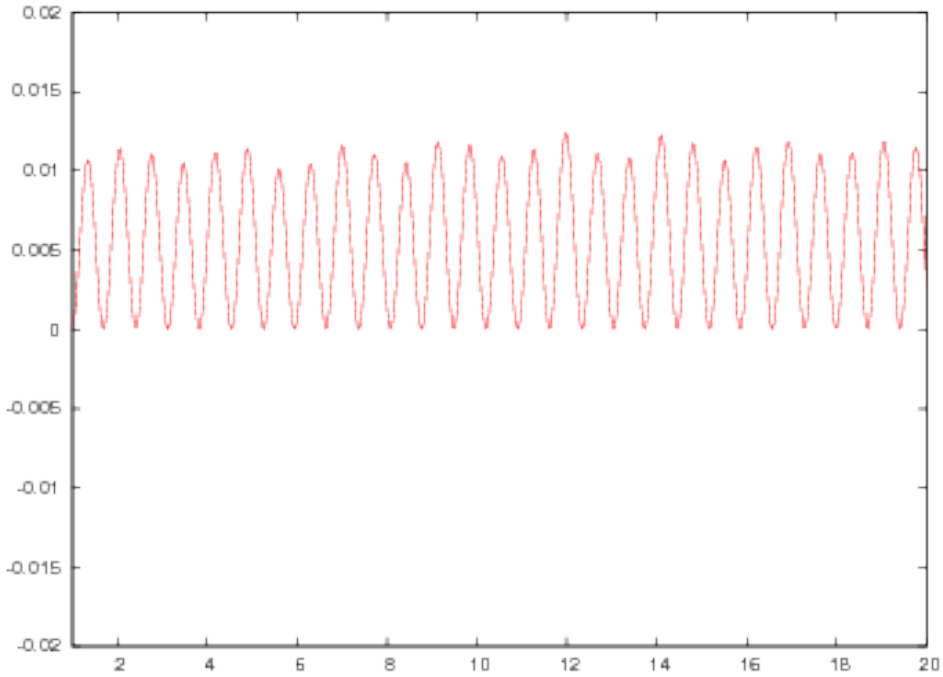

Eigenfunction corresponding to the last eigenvalue

Conclusions and perspectives

Conclusions

- A variational model for stochastic systems with Coulomb and Yukawa interactions
- Existence of a ground state
- Numerical study of Anderson localization

Perspectives

- Derive the rHF equation for Coulomb interacting systems
- Study the spectral properties of the mean-field Hamiltonian (localization, transport, ...)
- Extend to other models (ex : HF, KS with xc)