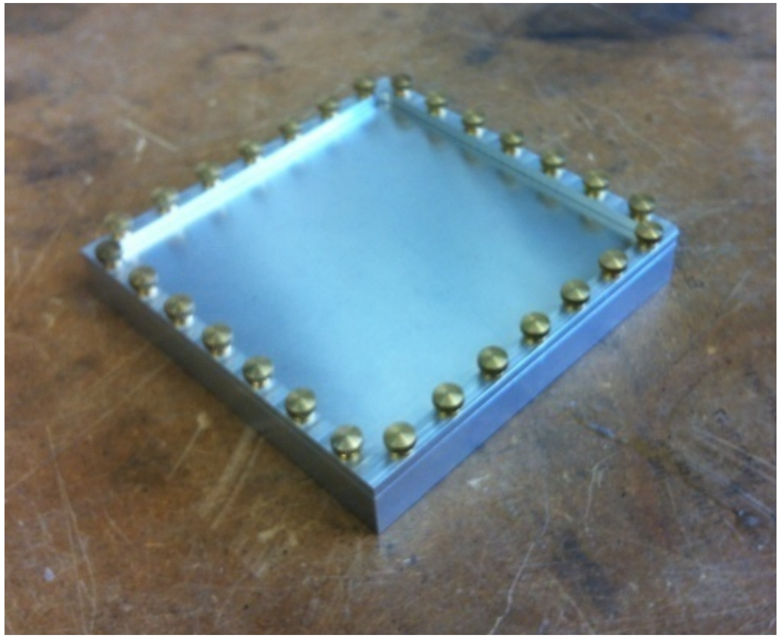
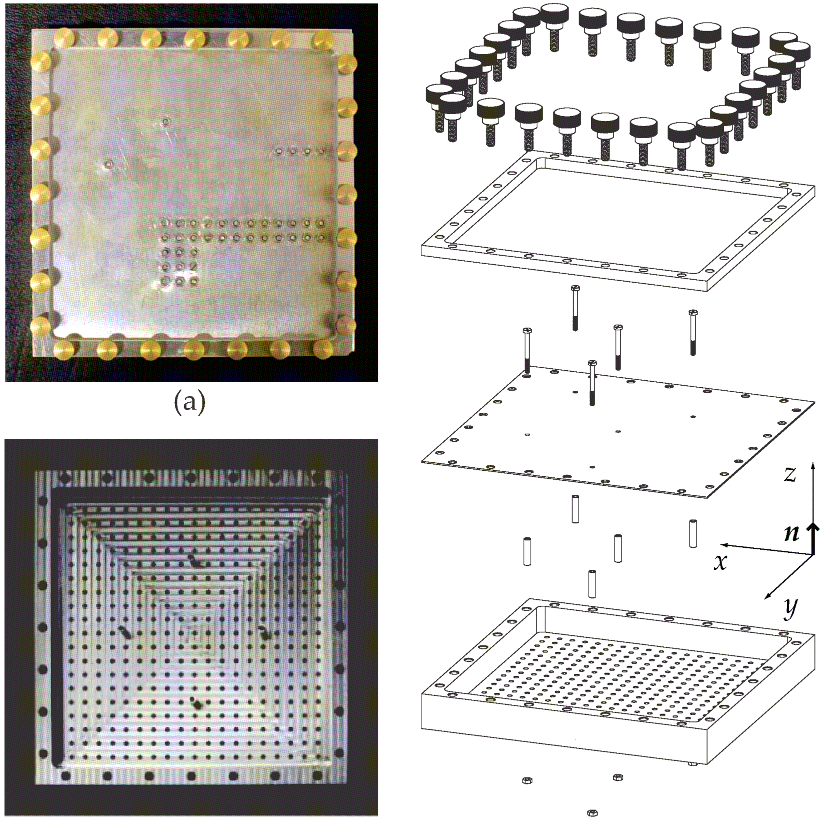


Vibrating clamped plate

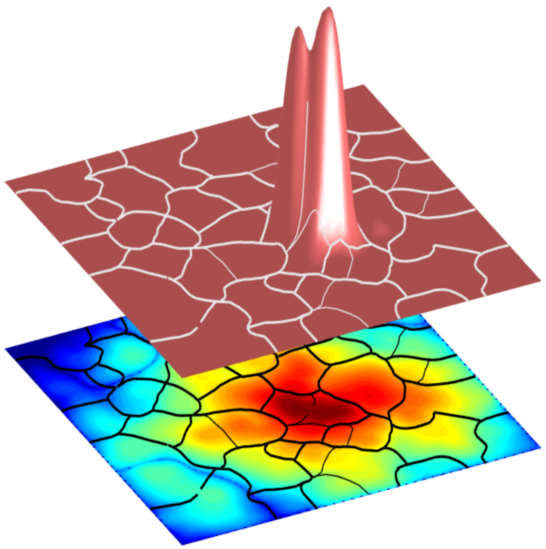


(a) (b) (c)

Question:

Find a way to predict the regions of almost independent vibrations and the frequencies of the related vibrations <u>with only static measurements</u>?

The hidden landscape of wave localization in disordered or complex structures



M. Filoche

Physique de la Matière Condensée
École Polytechnique, CNRS

Simons Collaboration Grant

http://wave.umn.edu

Séminaire DPhP CEA Saclay

November 25, 2019

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Semiconductor physics

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- **Gauthier Lefèbvre**

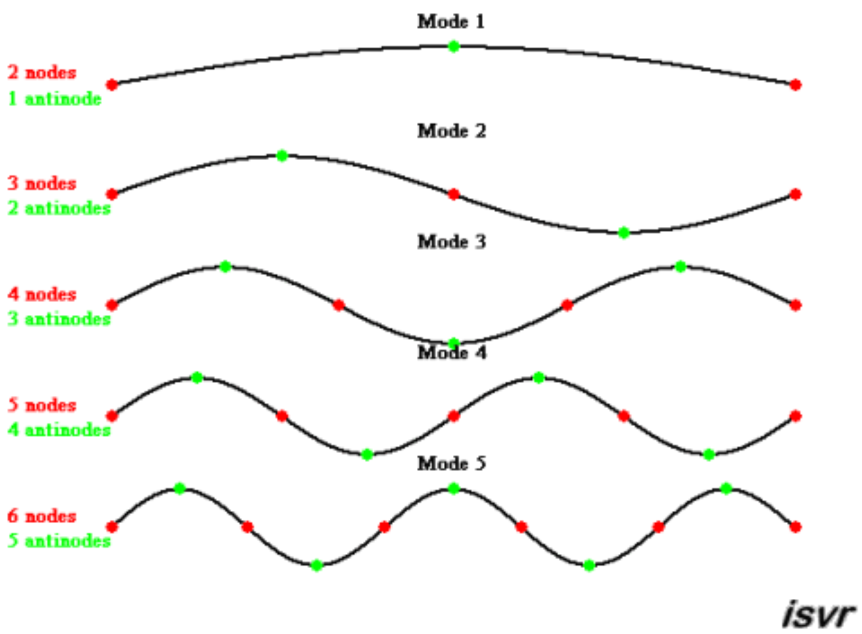
Thermal transport

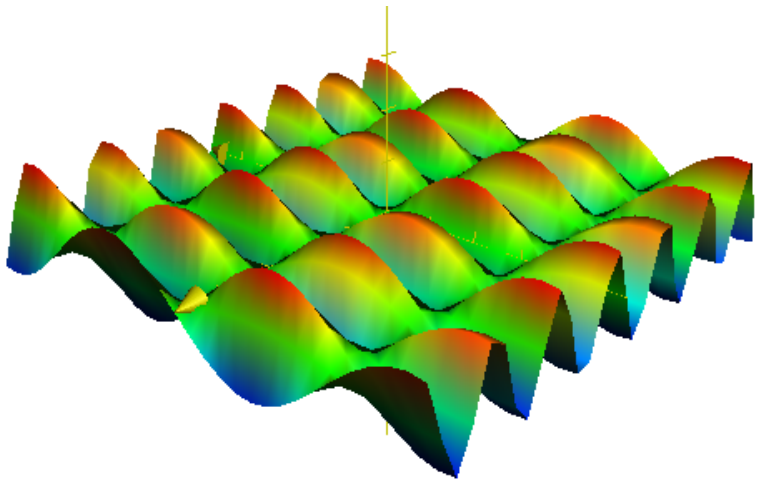
- **Yann Chalopin** (CentraleSupélec)

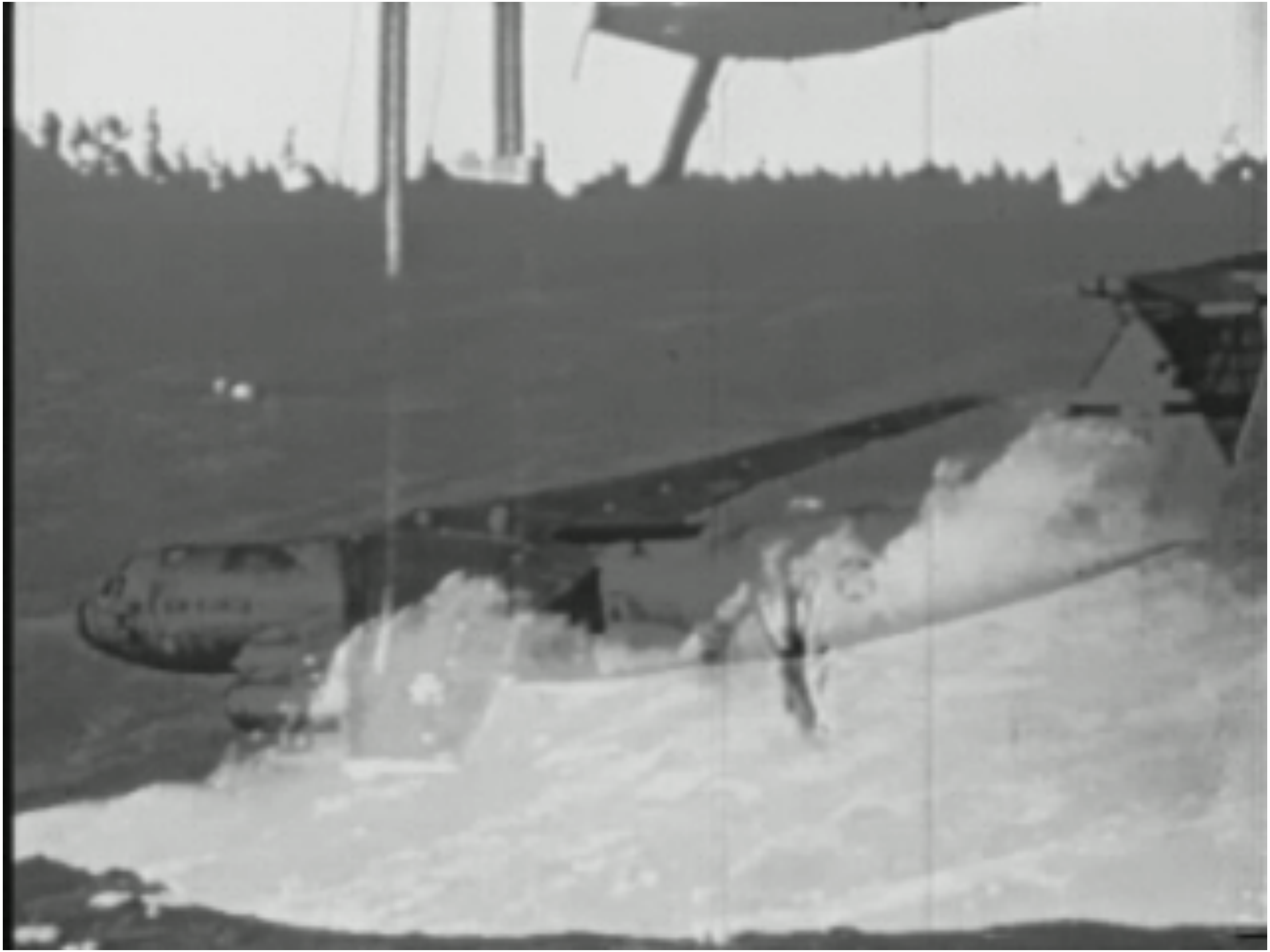
Quantum waves

Smooth geometry

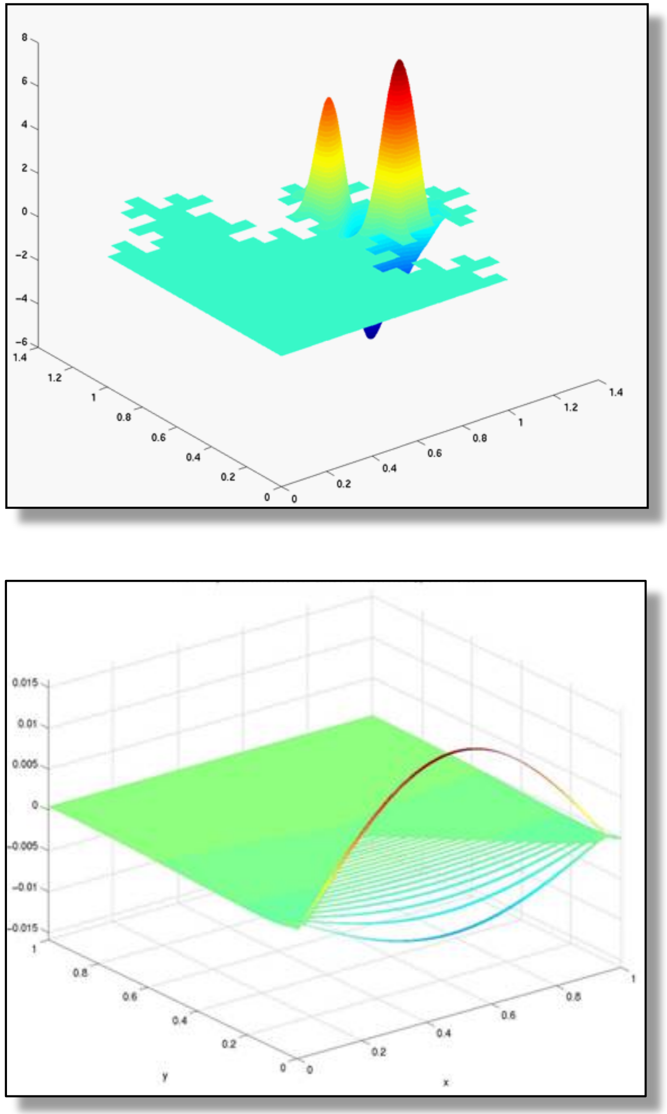
The eigenstates are (uniformly distributed) quasi-plane waves



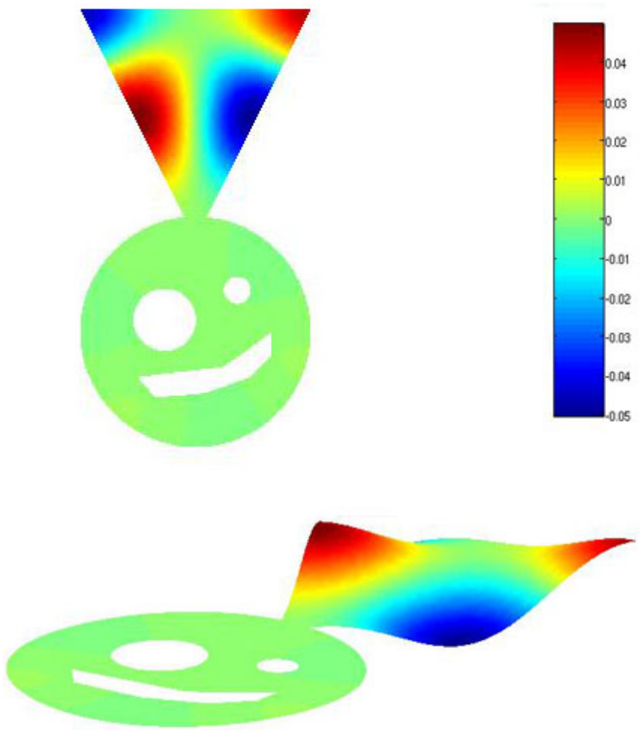




Localization by the boundary

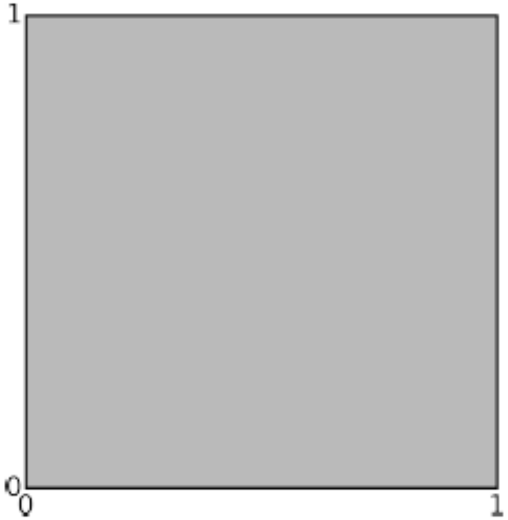


Félix et al., *J Sound Vib*, 2007



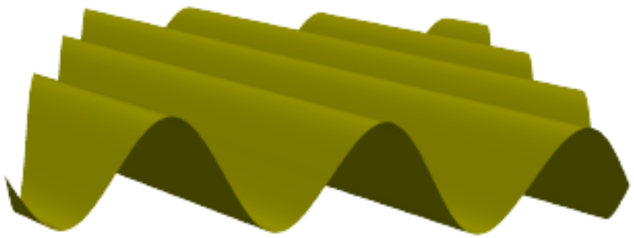
Heilman & Strichartz, *Not. Am. Math. Soc.*, 2010

“Localized eigenfunctions:
here you see them, there you don’t”

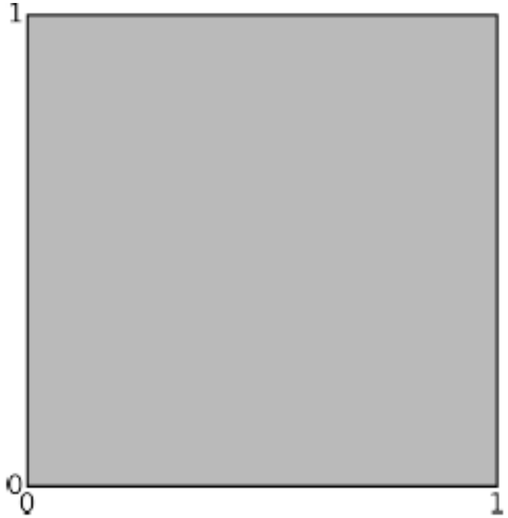


no potential

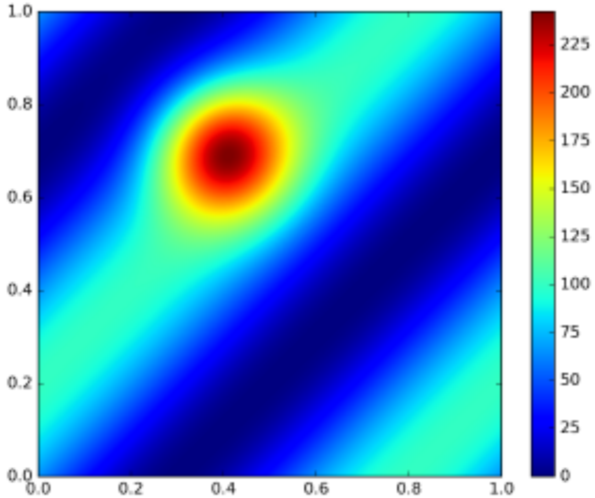
fundamental mode



57th mode

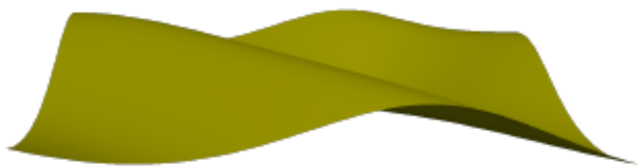


no potential

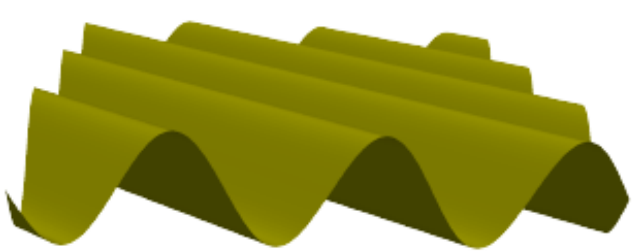


smooth potential

fundamental mode



fundamental mode



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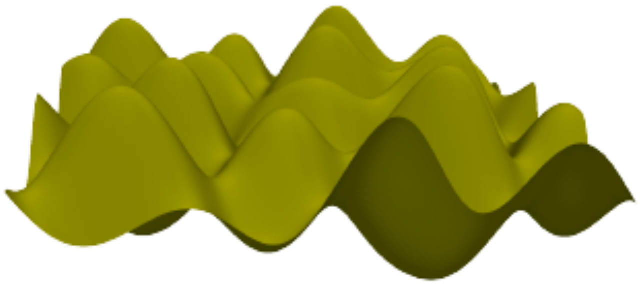

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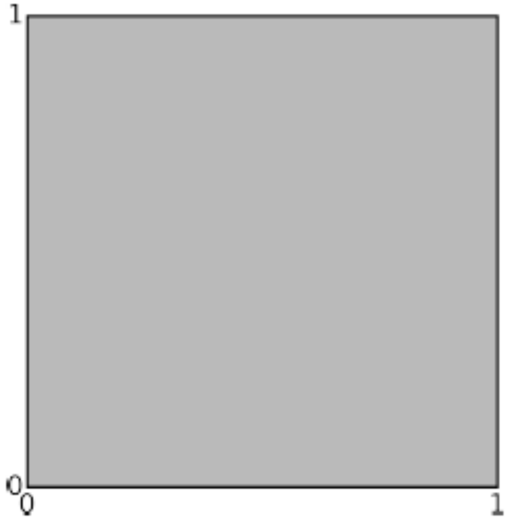
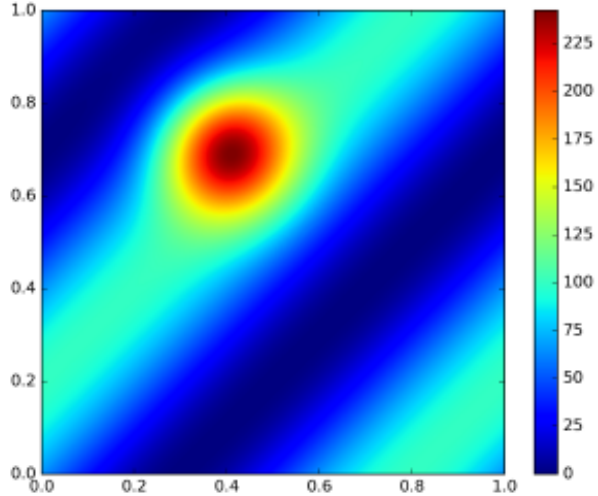
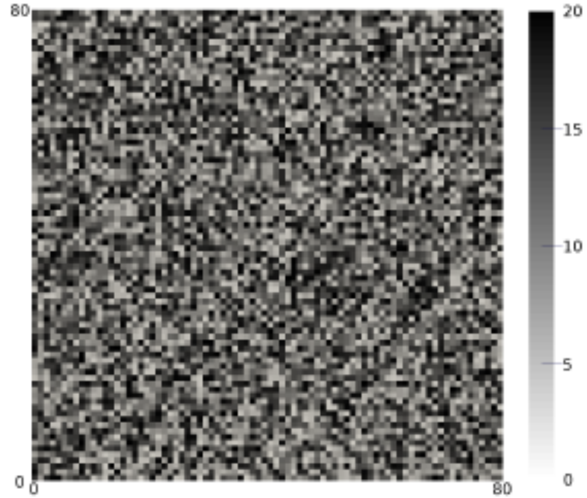


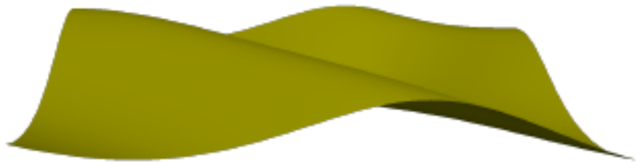
no potential



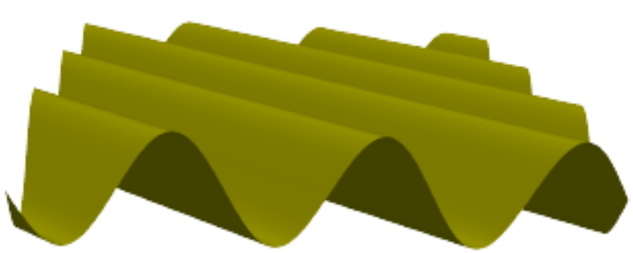
smooth potential



fundamental mode



fundamental mode



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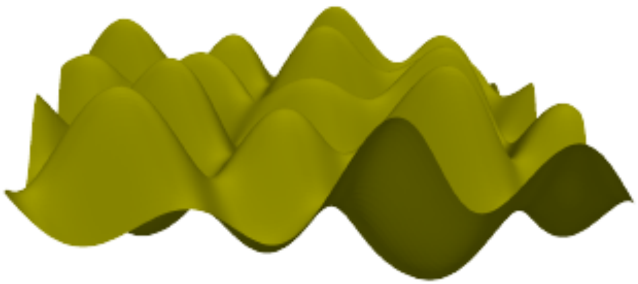

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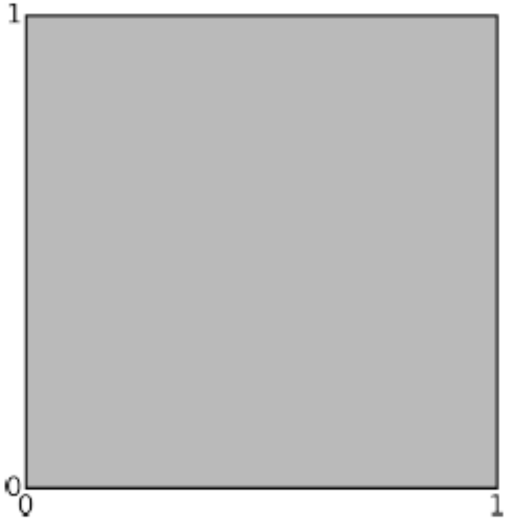
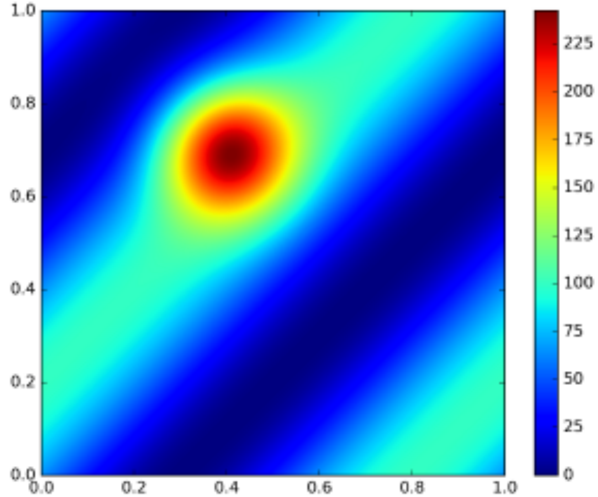
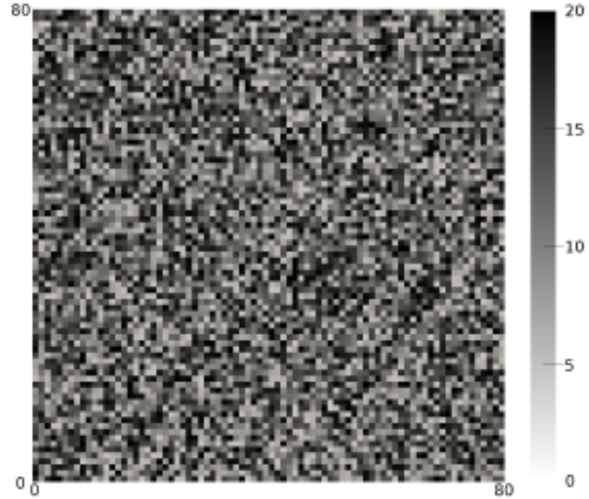


no potential



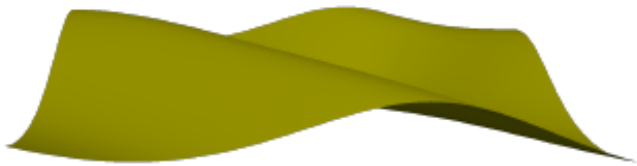
smooth potential



random potential

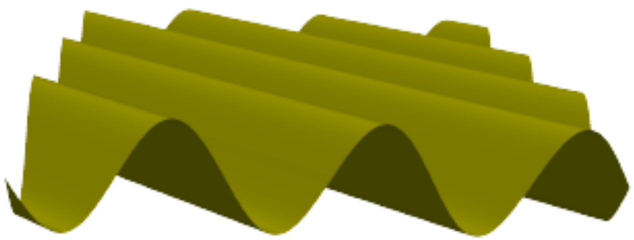
Disorder changes everything!

fundamental mode



fundamental mode

fundamental mode



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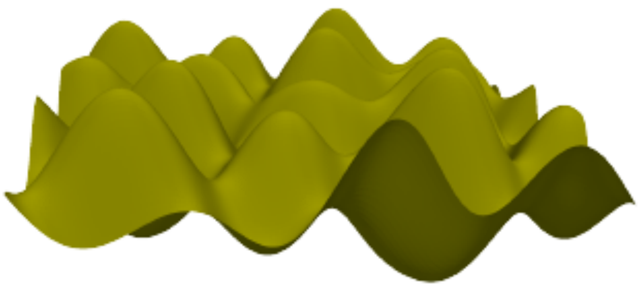
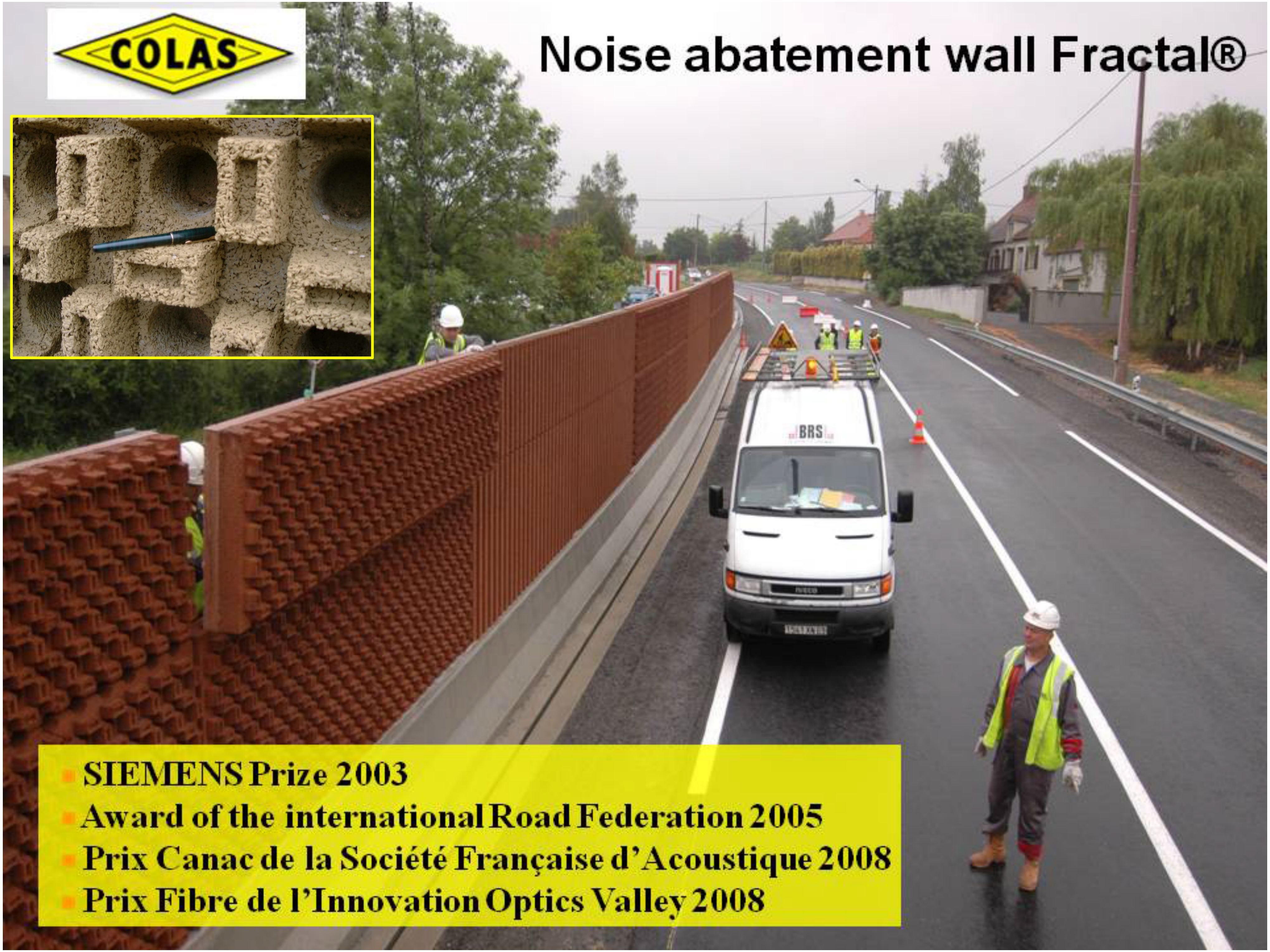


57th mode

57th mode

Noise abatement wall Fractal®



- SIEMENS Prize 2003
- Award of the international Road Federation 2005
- Prix Canac de la Société Française d'Acoustique 2008
- Prix Fibre de l'Innovation Optics Valley 2008

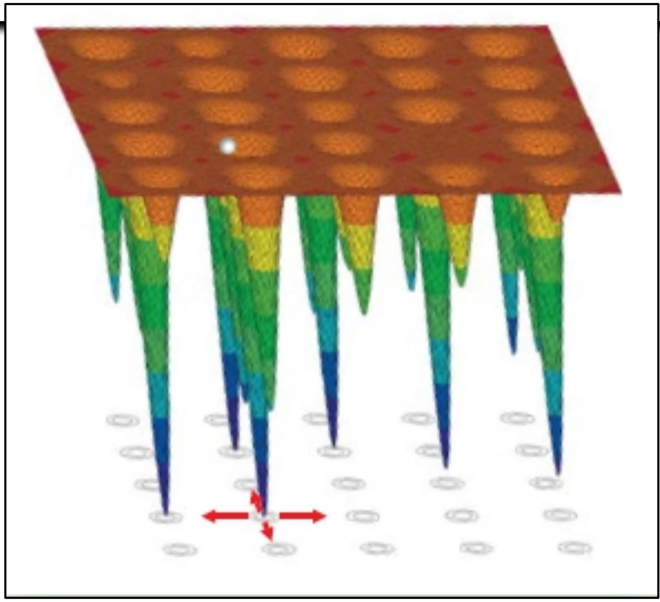
Anderson localization (1958)

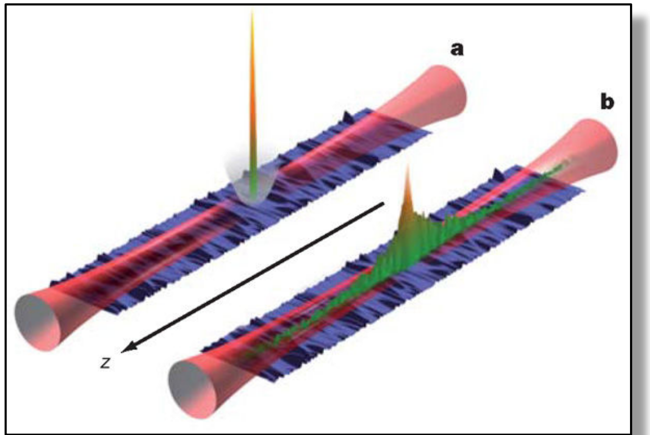
PHYSICAL REVIEW VOLUME 109, NUMBER 5 MARCH 1, 1958

Absence of Diffusion in Certain Random Lattices

P. W. Anderson
Bell Telephone Laboratories, Murray Hill, New Jersey
(Received October 10, 1957)

This paper presents a simple model for such processes as spin diffusion or conduction in the "impurity band." These processes involve transport in a lattice which is in some sense random, and in them diffusion is expected to take place via quantum jumps between localized sites. In this simple model the essential randomness is introduced by requiring the energy to vary randomly from site to site. It is shown that at low enough densities no diffusion at all can take place, and the criteria for transport to occur are given.





Evers & Mirlin, (2008) *Rev Mod Phys*, Anderson transitions

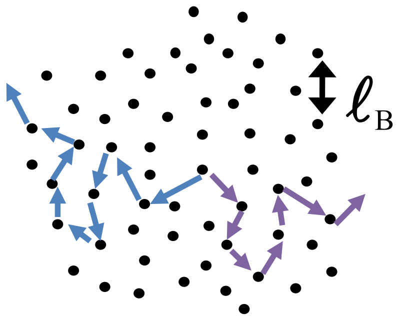
Lagendijk, van Tiggelen, Wiersma (2009), *Phys Today*, Fifty years of Anderson localization

Billy et al., (2008) Nature

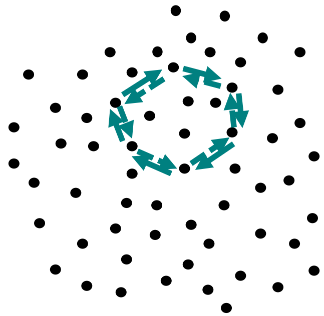
Anderson localization (1958)

P.W. Anderson, *Phys. Rev.* 1958

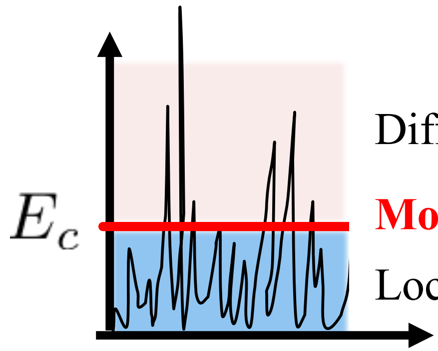
In a uniform or periodic potential, the quantum states are delocalized. Breaking the symmetry (continuous or discrete) leads to possible localization.



Diffusion in weak disorder



Localization in "extreme" disorder



In 3D, mobility edge: above, delocalized states, below, localized states.

$$\xi \propto \left(E_c - E\right)^{-\nu}$$

Localization length

$$\sigma \propto \left(E - E_c\right)^{s}$$

conductivity

Critical exponents: $s = \nu\left(d-2\right)$ (d=2, critical dimension)

The statistical approaches

- Scaling theory (renormalization) — Abrahams, Anderson, Liciardello & Ramakrishnan, *Phys. Rev. Lett.* 1979
- Random matrix theory (RMT) — Dyson, *J. Math. Phys.* 1962
- Self-consistent theory (approximate) — Vollhardt &Wolfle, *Phys. Rev. Lett.* 1980
- Interactions — Basko, Aleiner & Altshuler, *Ann. Phys.* 2006

However

- Disorder is described through its statistical properties.
- Values of the critical exponents have to be determined numerically or with approximate theories.
- The exact value of the mobility edge depends on the disorder type (correlations).
- No analytical prediction when correlations or interactions come into play.

"*Our results deviate significantly from previous theoretical estimates using an approximate, self-consistent approach of localization.*"

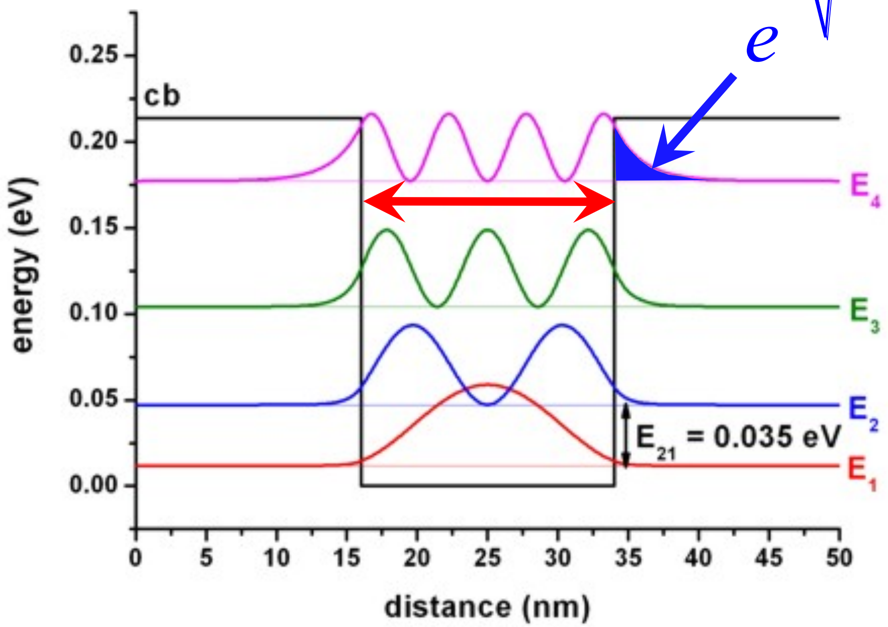
Delande & Orso, *Phys. Rev. Lett.* 2014

Particle vs. wave localization

Waves go where particles don't go

The quantum well

$$e^{-\sqrt{\frac{2m(V-E)}{\hbar^2}}\,x}$$

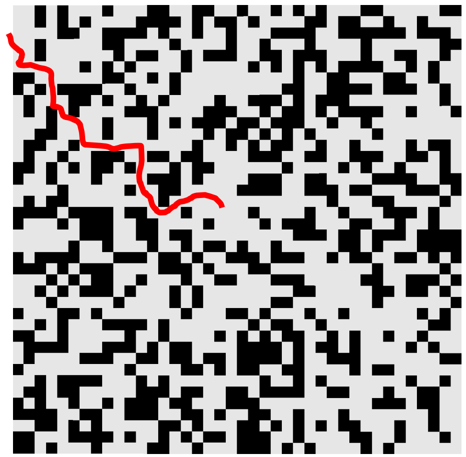


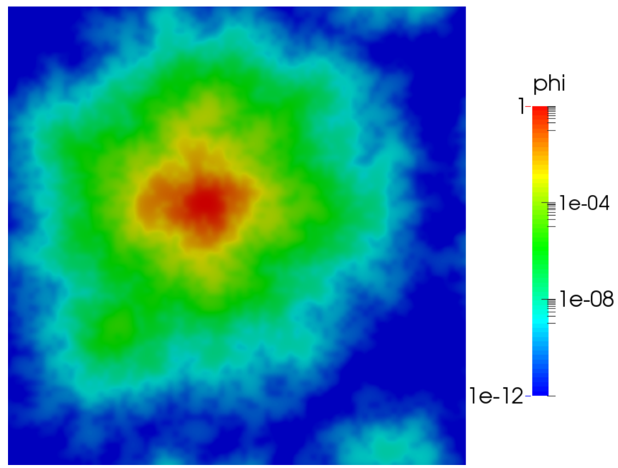
We see the classical potential

Waves see "something different"

Waves don't go where particles go

Boolean potential (60% of **0**, 40% of **1**)

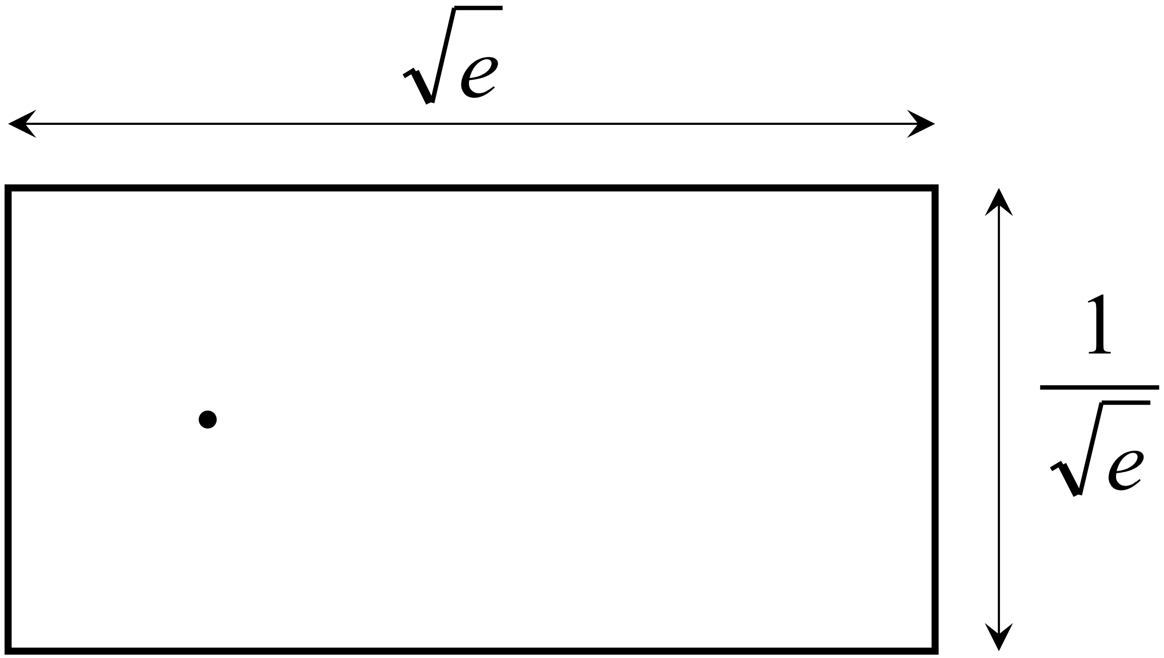




Fundamental quantum state (E>0)

The punctured clamped plate

A rectangular plate with or without an inside punctured point

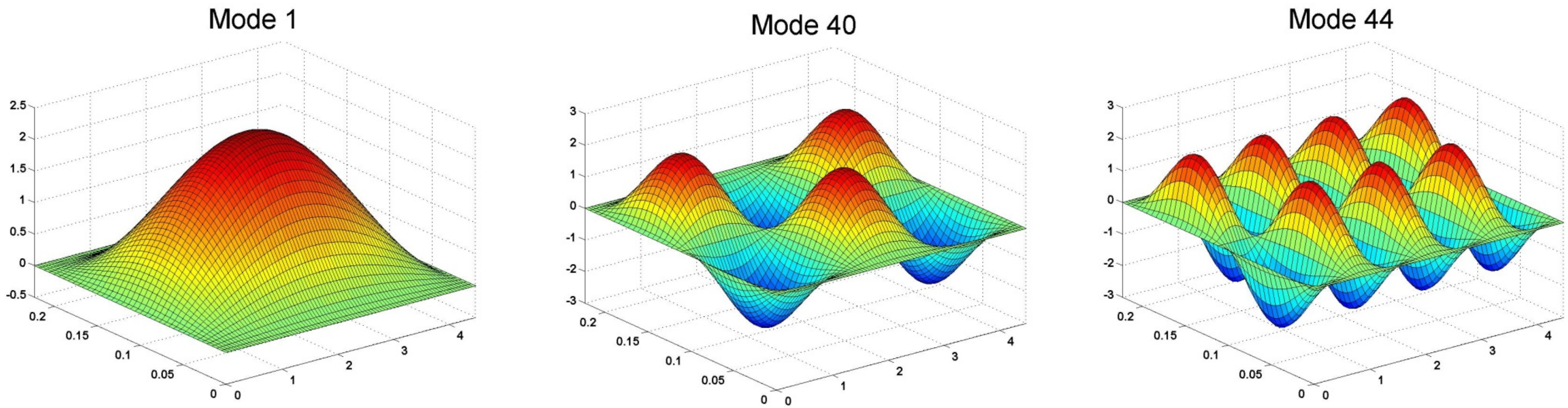


Kirchhoff-Love theory of thin vibrating plates

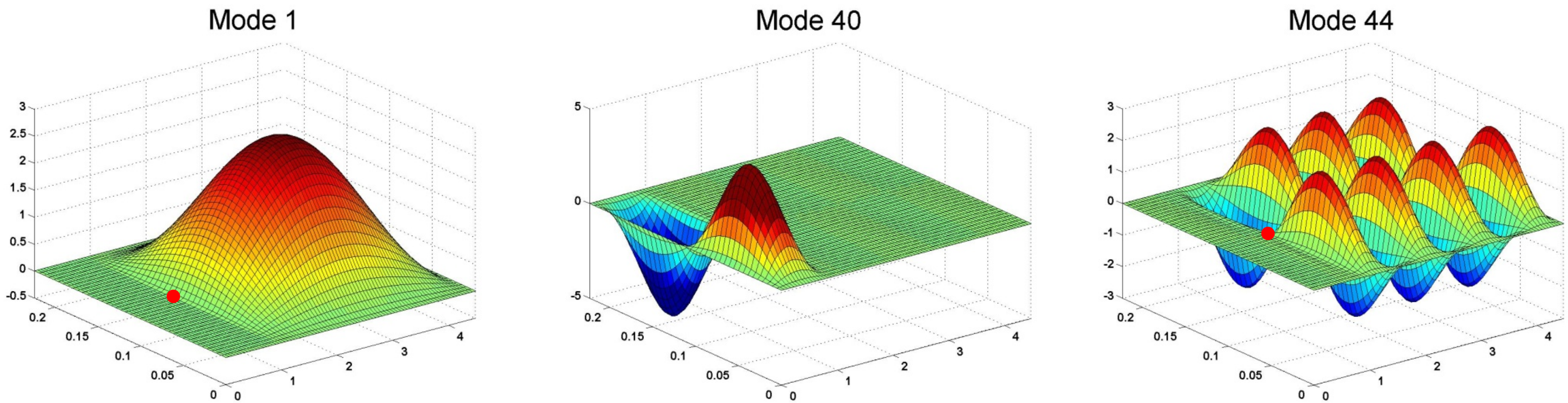
$$\Delta^2 u = \Delta\left(\Delta u\right) = \left(\partial_{x_1}^2 + \ldots + \partial_{x_n}^2\right)\left(\partial_{x_1}^2 + \ldots + \partial_{x_n}^2\right) u = \lambda^2 u$$

Localization in vibrating thin plates

Standard plate of eccentricity 20

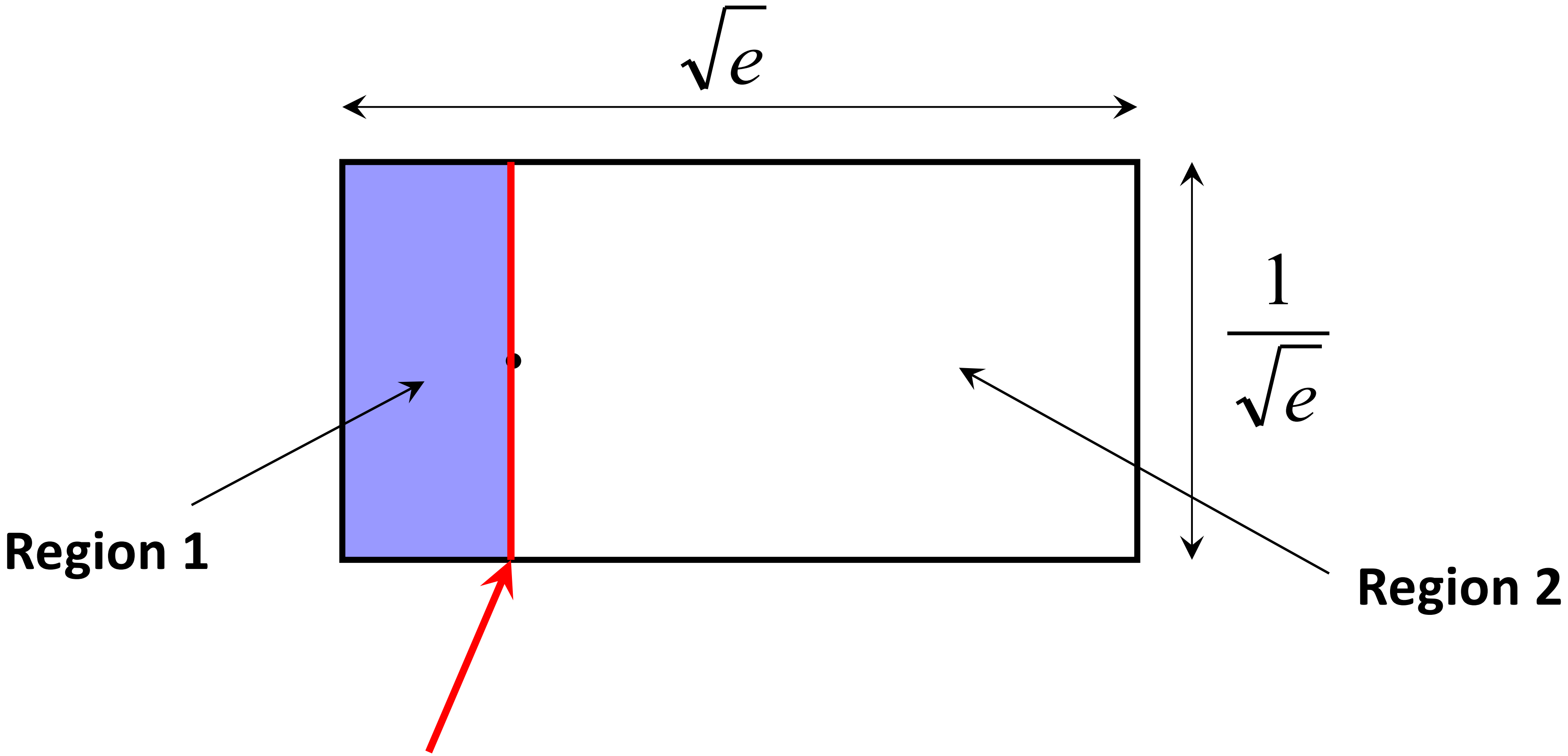


Punctured plate of eccentricity 20



MF & S. Mayboroda, PRL 2009

The punctured clamped plate



Where does this separation line come from?

What happens for any shape and any number of blocked points?

A universal approach to wave localization

L is a **wave** (elliptic) **operator** such as $-\Delta,\ \Delta^2,\ H=-\Delta+V$ of positive spectrum

$$\Delta\varphi=\frac{1}{c^2}\frac{\partial^2\varphi}{\partial t^2}$$ **acoustics, electromagnetism**

$$\Delta^2 w=-\frac{2\rho h}{D}\frac{\partial^2 w}{\partial t^2}$$ **mechanics, thin rigid plates**

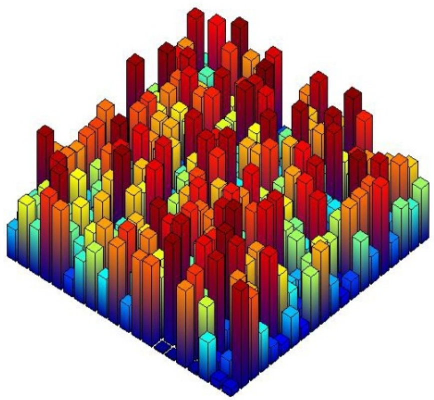
$$H\psi=\left(-\frac{\hbar^2}{2m}\Delta+V\right)\psi=i\hbar\frac{\partial\psi}{\partial t}$$ **quantum**

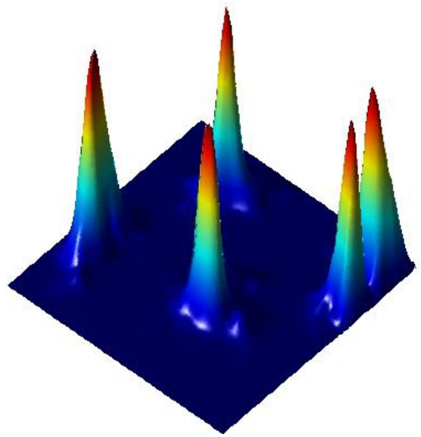
$$\boxed{L\psi=\lambda\psi}$$

$$\boxed{H\psi=E\psi}$$

Random potential $V(x,y)$

random i.i.d. variables in 20×20 cells, uniformly distributed between 0 and V_{max} (here 8000).





Quantum states

localization landscape $$\boxed{Lu=1}$$ $$(Hu=1)$$

Control of the eigenmode amplitudes

$$L\psi = \lambda\psi \quad \longrightarrow \quad \psi(\vec{r}) = \int_{\Omega} G(\vec{r},\vec{r}')\left(\lambda\psi(\vec{r}')\right)d\vec{r}'$$

$$\left|\psi(\vec{r})\right| \leq \lambda \sup_{\Omega}|\psi| \times \boxed{\int_{\Omega}\left|G(\vec{r},\vec{r}')\right|d\vec{r}'}$$

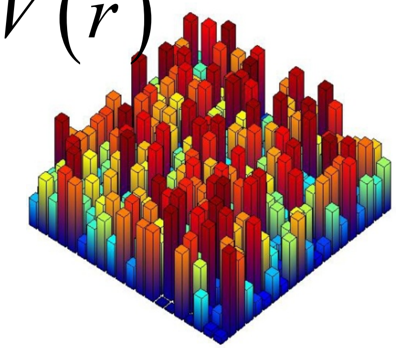
$$\boxed{\frac{\left|\psi(\vec{r})\right|}{\sup|\psi|} \leq \lambda\, u(\vec{r})}$$

Corollary: For 2nd order operators, $G(\vec{r},\vec{r}') \geq 0$

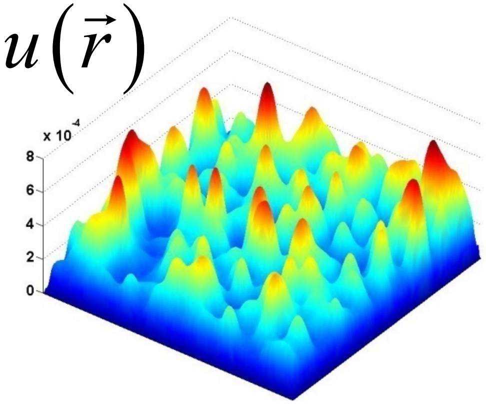
$$u(\vec{r}) = \int_{\Omega} G(\vec{r},\vec{r}')\,d\vec{r}'$$

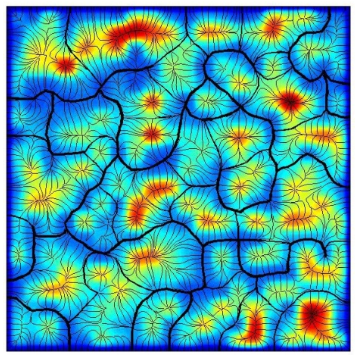
$$\boxed{Lu = 1}$$

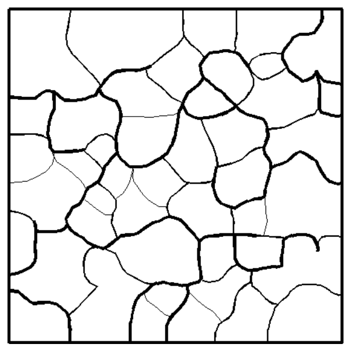
$V(\vec{r})$



$u(\vec{r})$

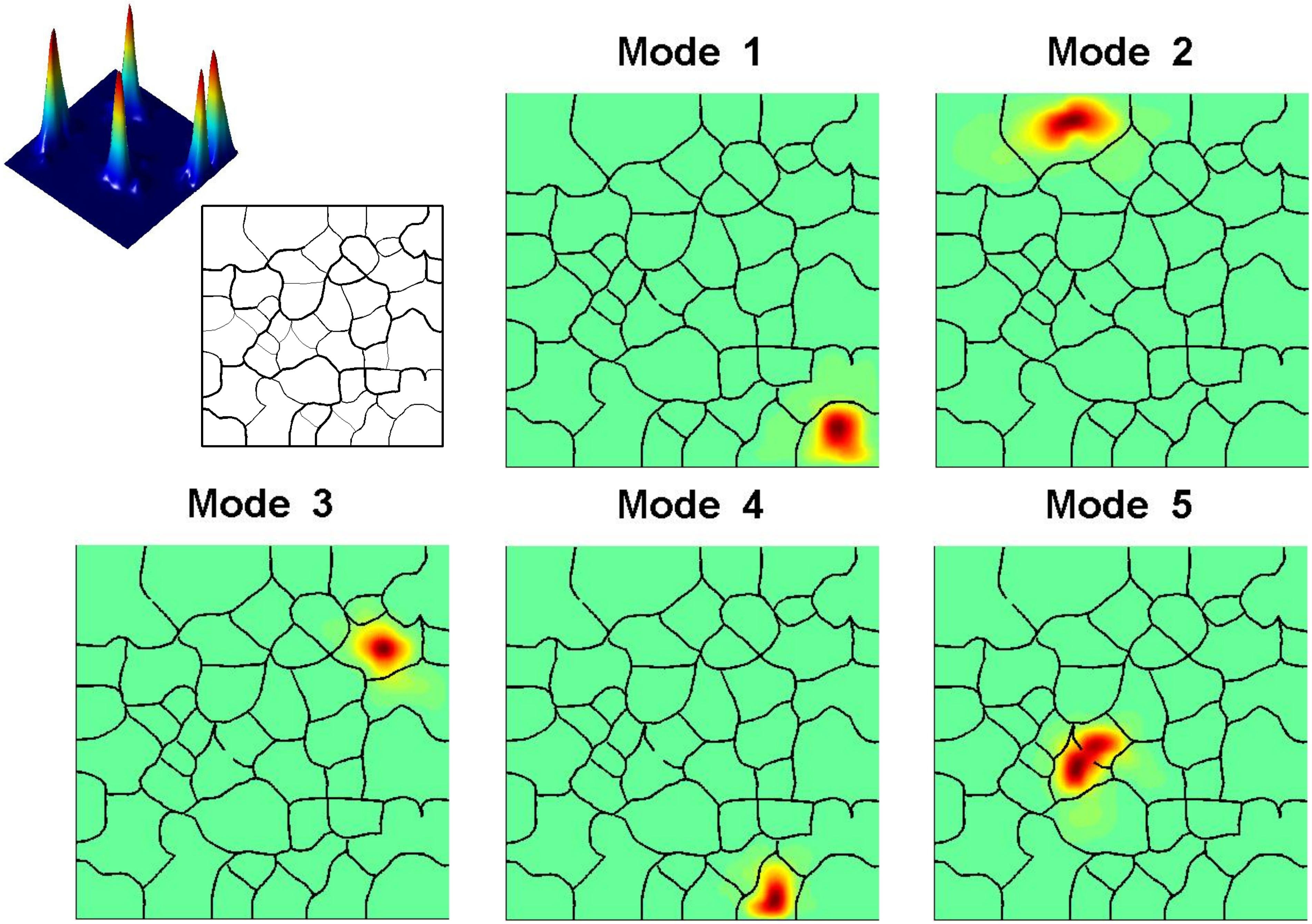




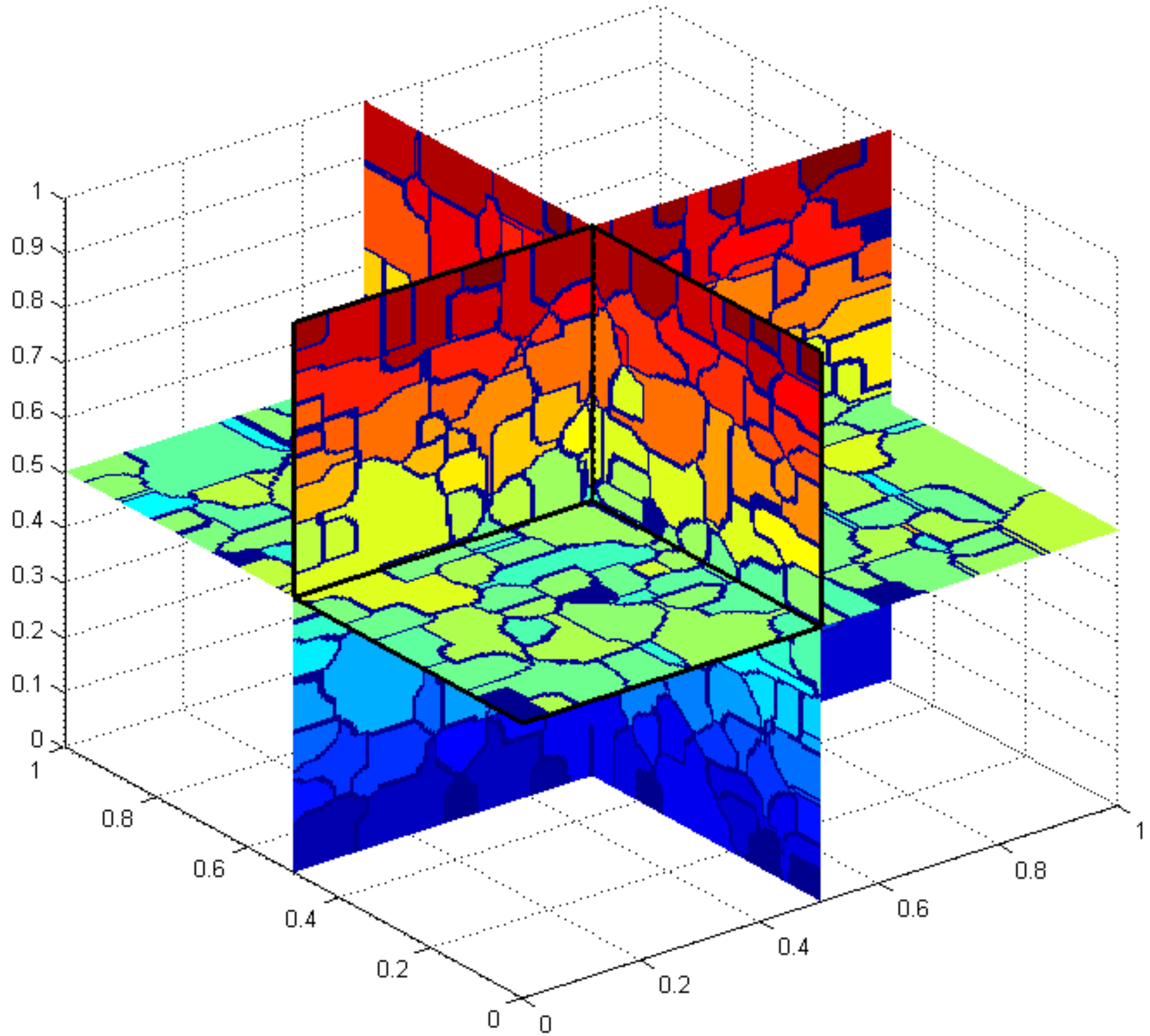


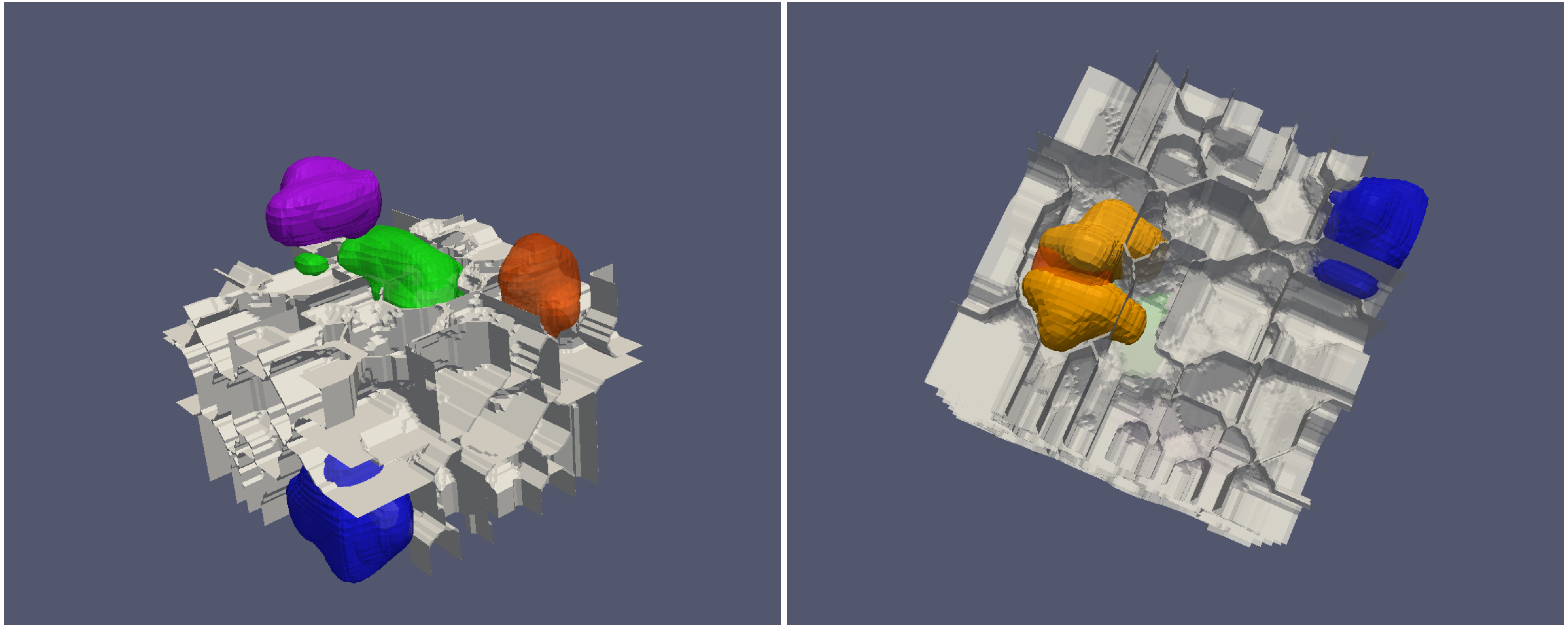
The eigenmode amplitude is "small" where *u* is "small"

Disorder-induced (Anderson) localization



3D valley network in a random potential

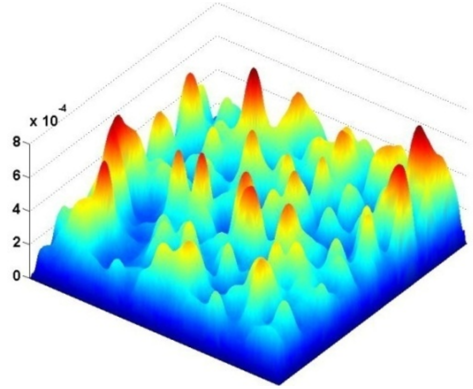




Simulations by Douglas Arnold, Univ. of Minnesota

$W \equiv 1/u$ acts as an effective confining potential

$$H\psi = \left[-\Delta + V(x)\right]\psi = E\psi$$



Transformation: $\psi \equiv u \times \varphi$

$$\boxed{-\frac{1}{u^2} div\left(u^2 \nabla \varphi\right) + \frac{1}{u}\varphi = E\varphi}$$

$\boxed{W \equiv \frac{1}{u}}$ acts as an **effective potential** for the “reduced” wavefunction

General identity

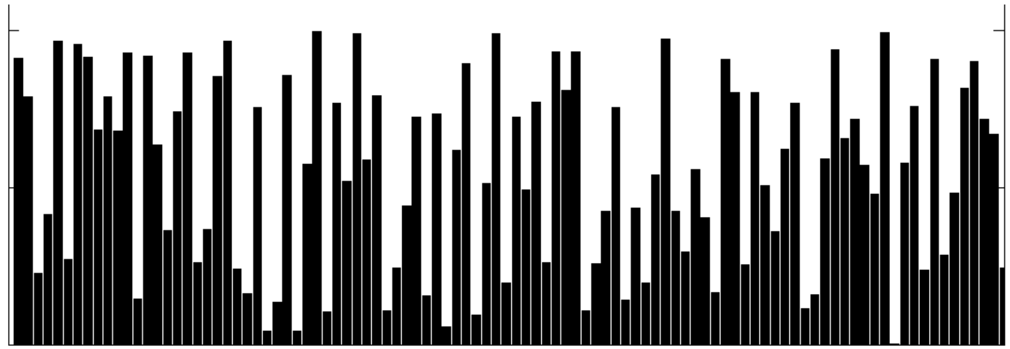
$$\boxed{\langle \psi | H | \psi \rangle = \langle \nabla \psi | \nabla \psi \rangle + \langle \psi | V | \psi \rangle = \left\langle u \nabla \left(\frac{\psi}{u}\right) \middle| u \nabla \left(\frac{\psi}{u}\right) \right\rangle + \left\langle \psi \middle| \frac{1}{u} \middle| \psi \right\rangle}$$

reduced kinetic energy

effective potential energy

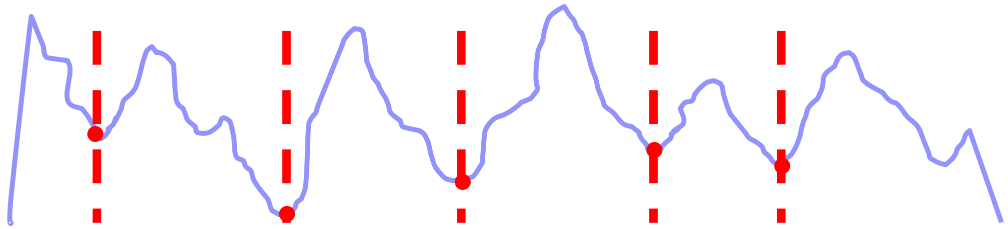
The effective confining potential

$$V$$



$$H\,u = 1$$

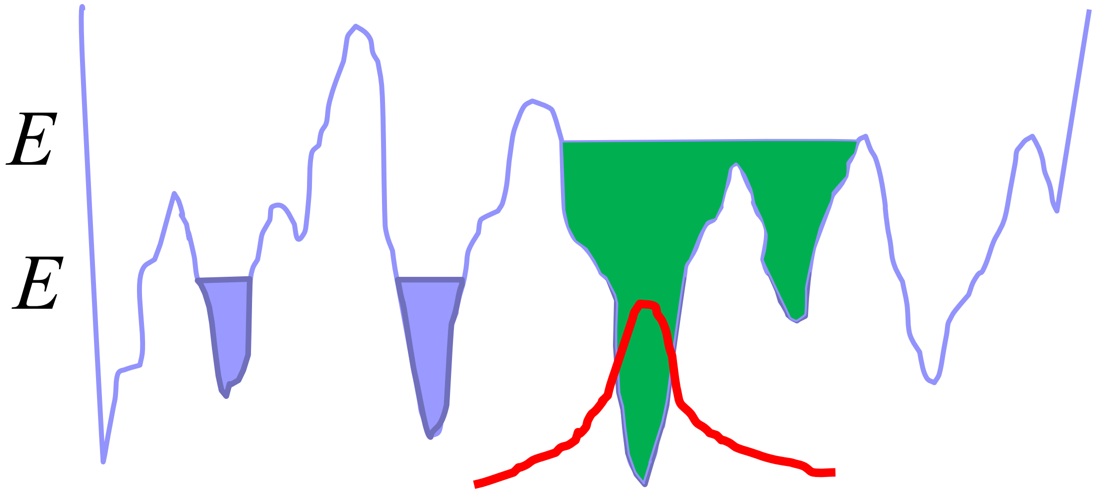
$$u$$



$$|\psi| \le E\,u$$

$$\psi = u \times \varphi$$

$$\frac{1}{u}$$

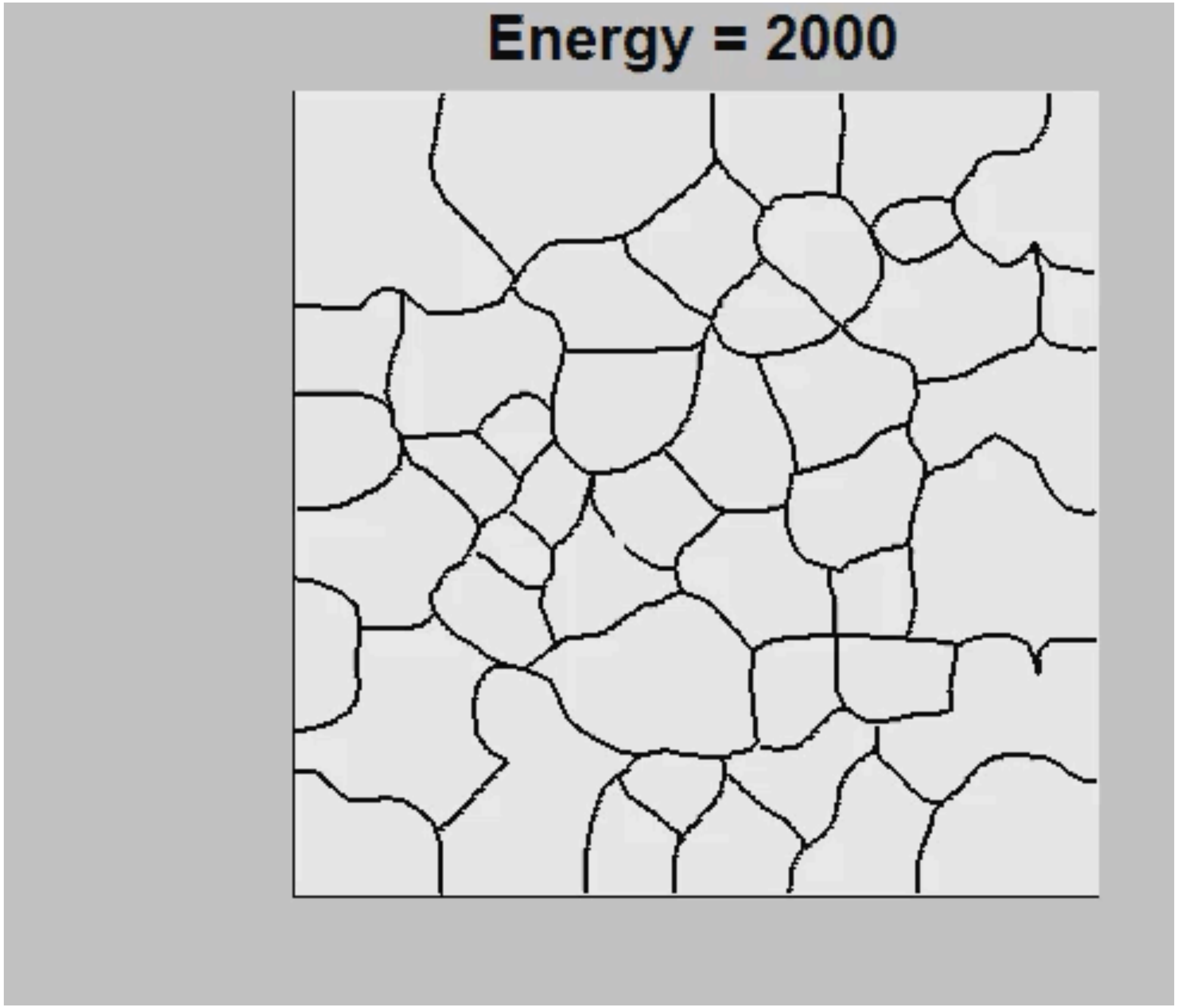


Transition to delocalized states at higher energy

$$\frac{|\psi(x)|}{\sup|\psi|} \le \lambda\, u(x)$$

Meaningful only if

$$u(x) < \lambda^{-1} \equiv E^{-1}$$

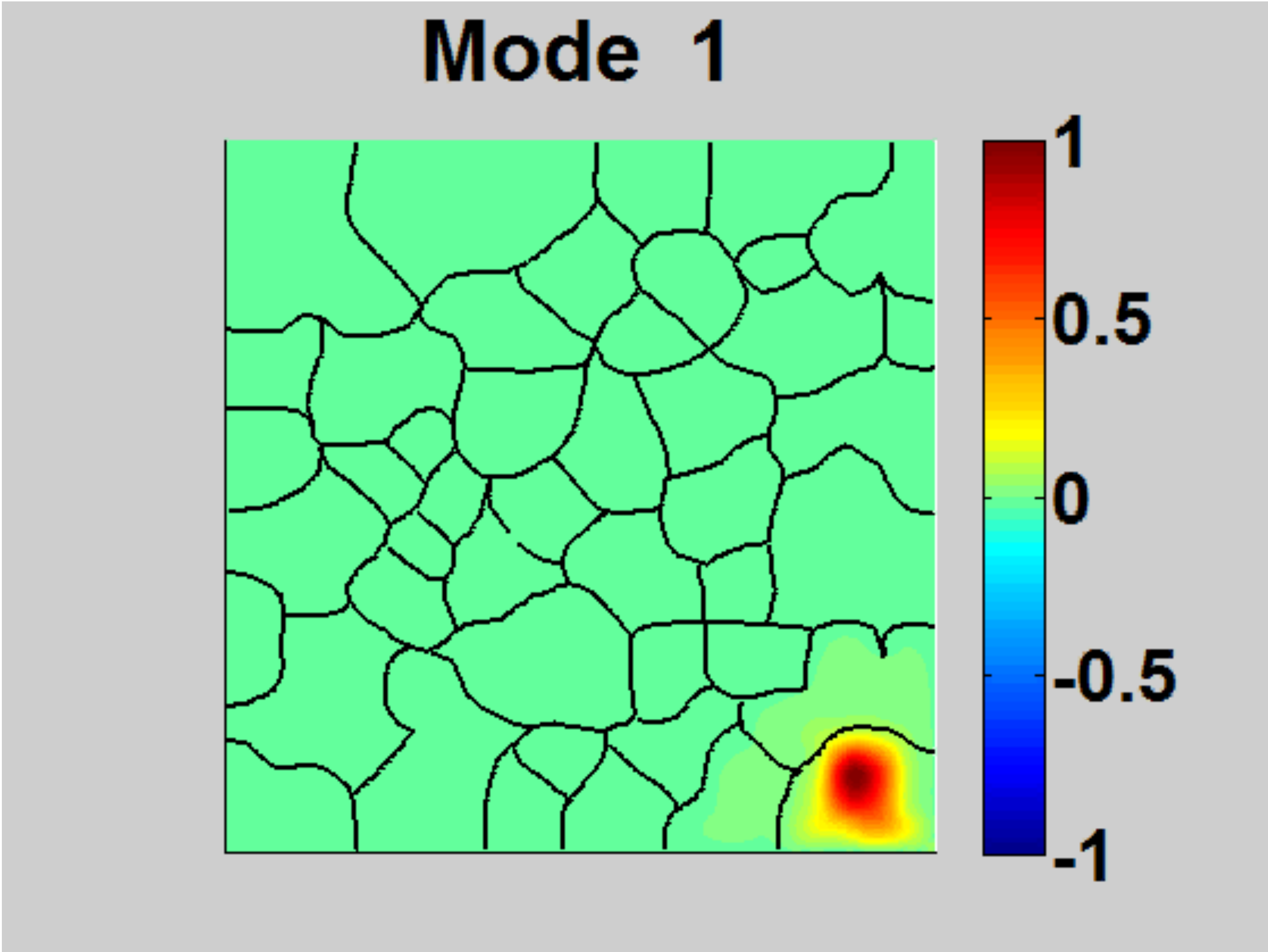


Transition to delocalized states at higher energy

$$\frac{|\psi(x)|}{\sup|\psi|} \leq \lambda u(x)$$

Meaningful only if

$$u(x) < \lambda^{-1} \equiv E^{-1}$$

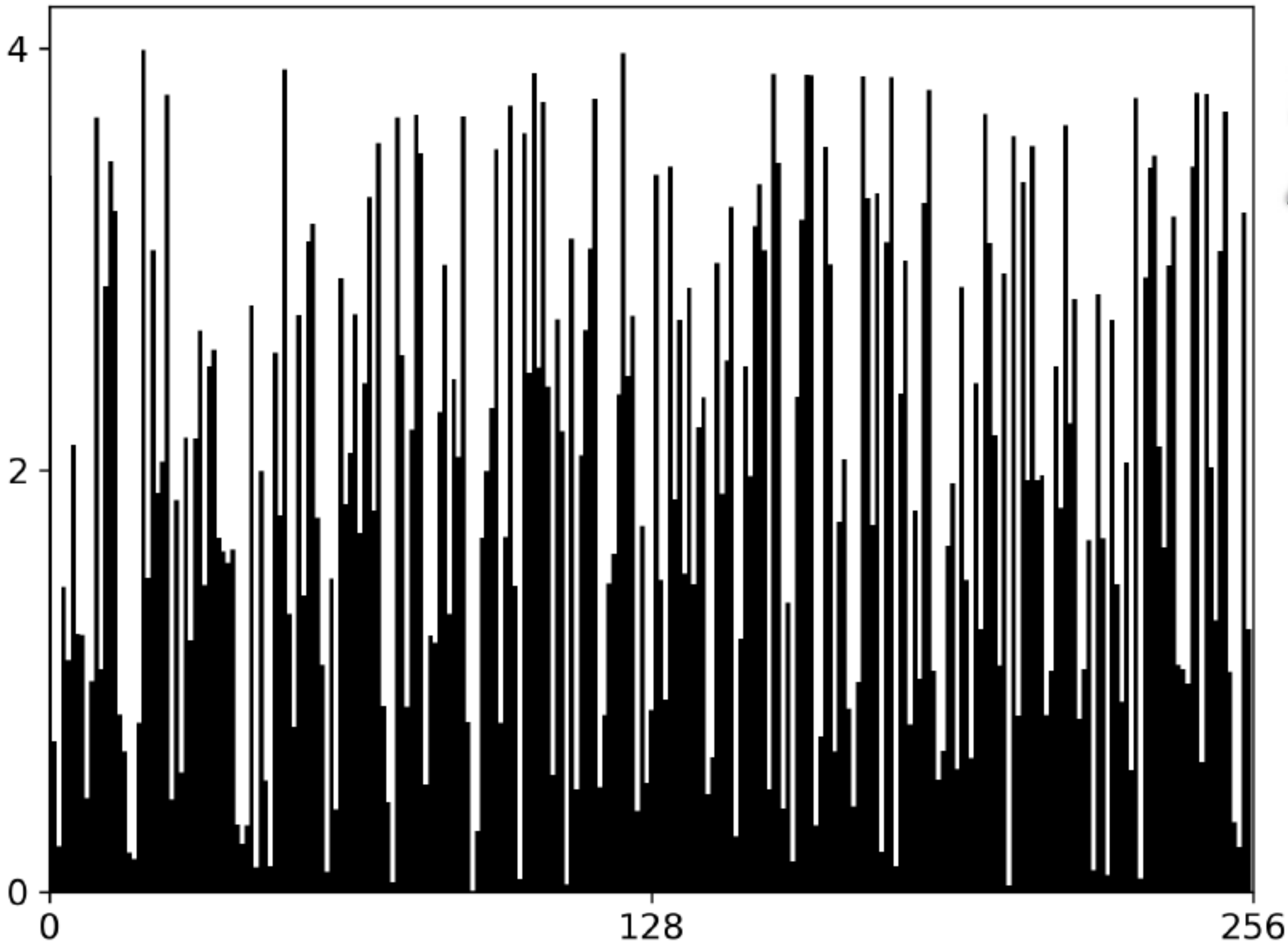


MF and S. Mayboroda, PNAS 2012

Where is Waldo?

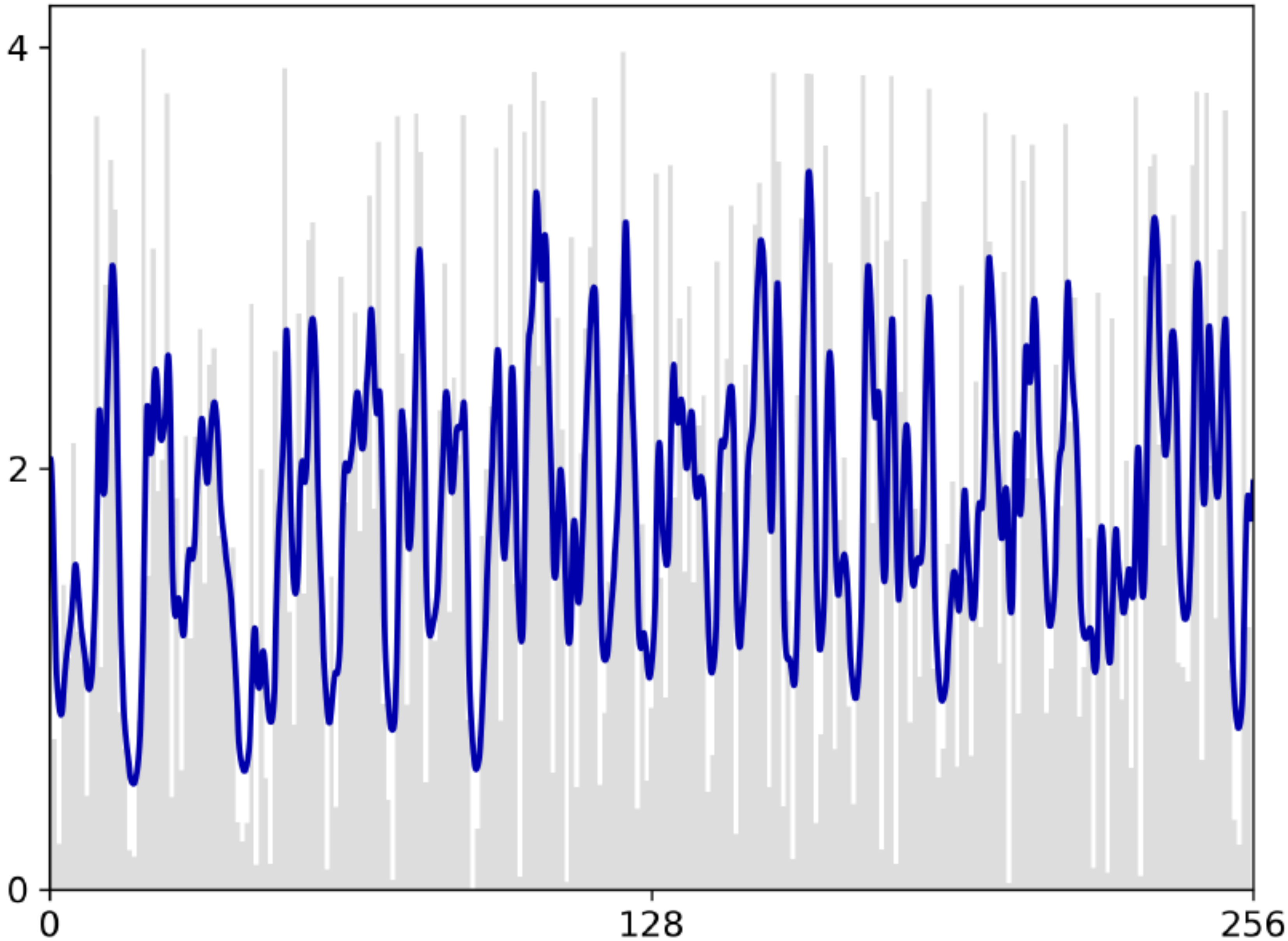
Where's Waldo?   Eigenfunction prediction in 1D

start from the potential



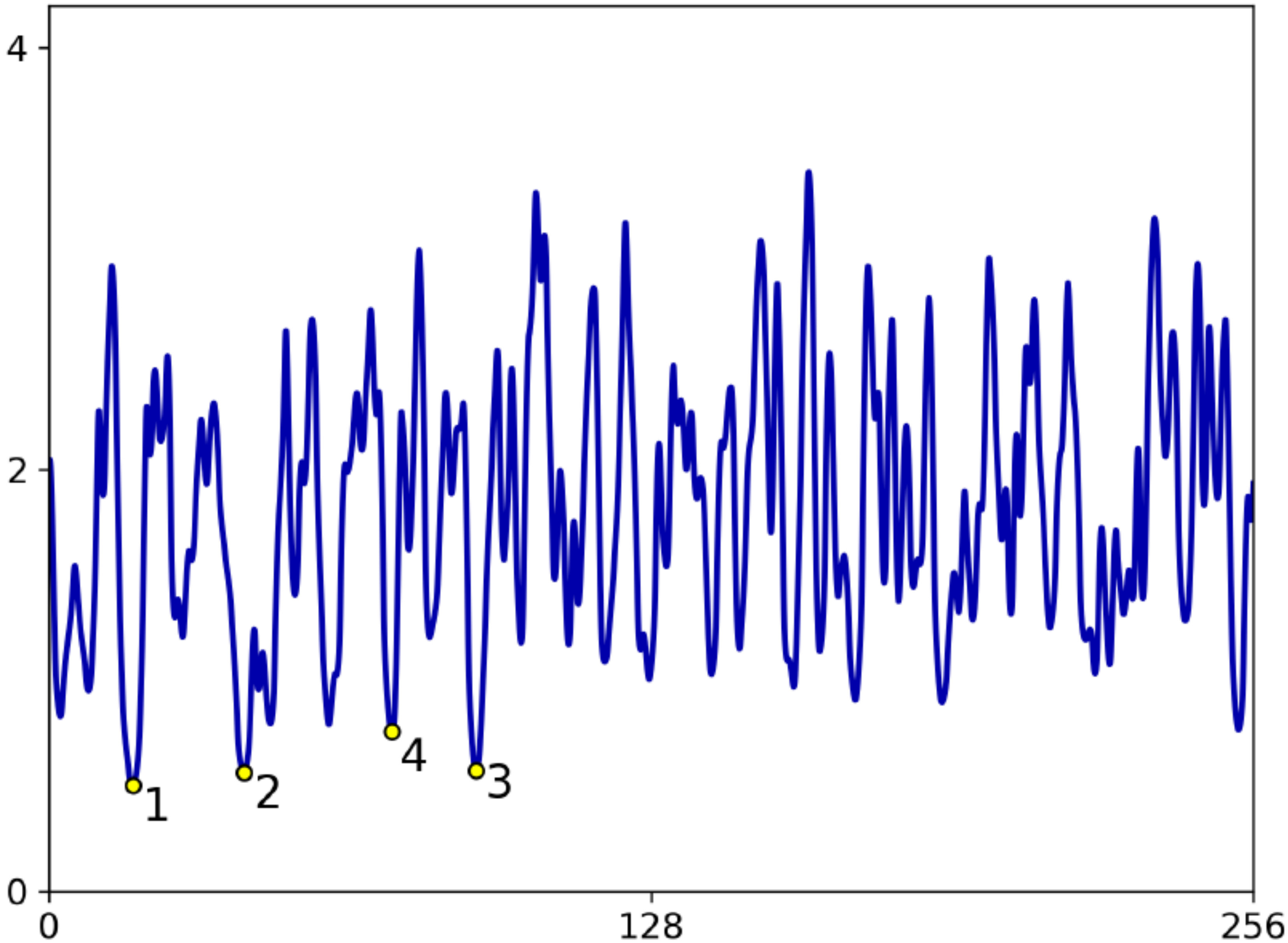
Where's Waldo? Eigenfunction prediction in 1D

solve landscape equation and take reciprocal to get effective potential



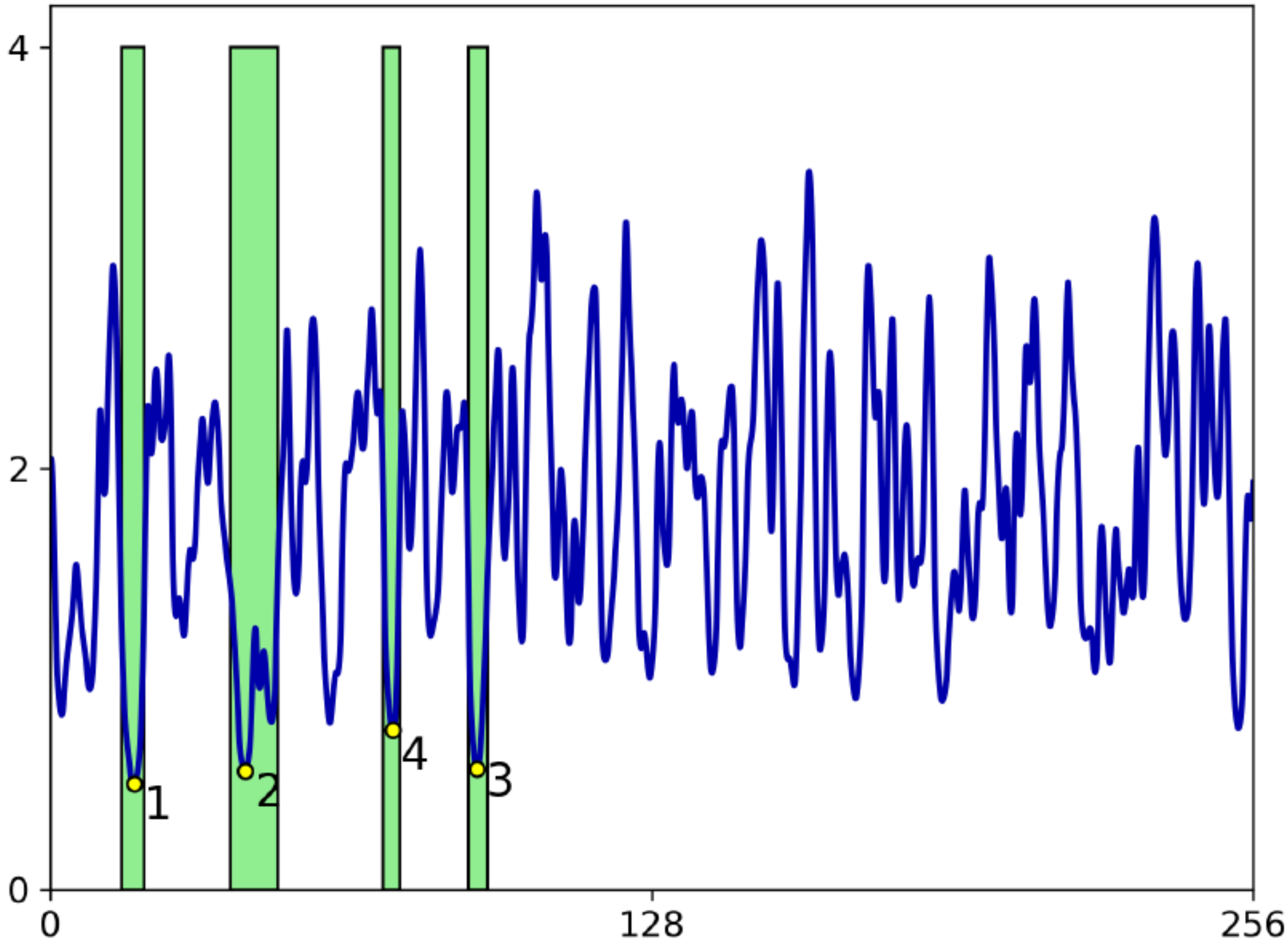
Where's Waldo? Eigenfunction prediction in 1D

find deepest local minima x_i



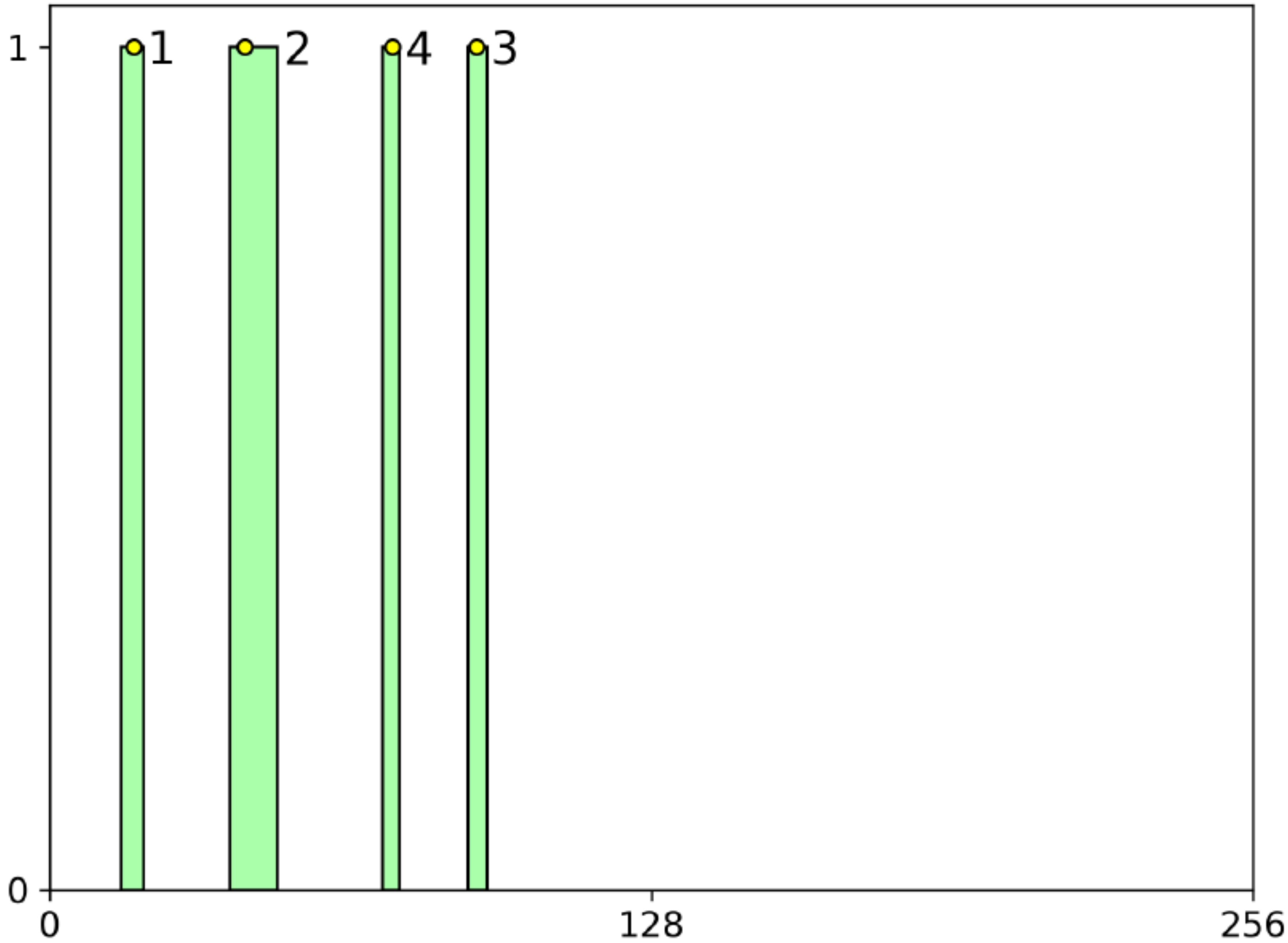
Where's Waldo? Eigenfunction prediction in 1D

to minima associate connected component of sublevel set $W(x) < 2W_{\min}$



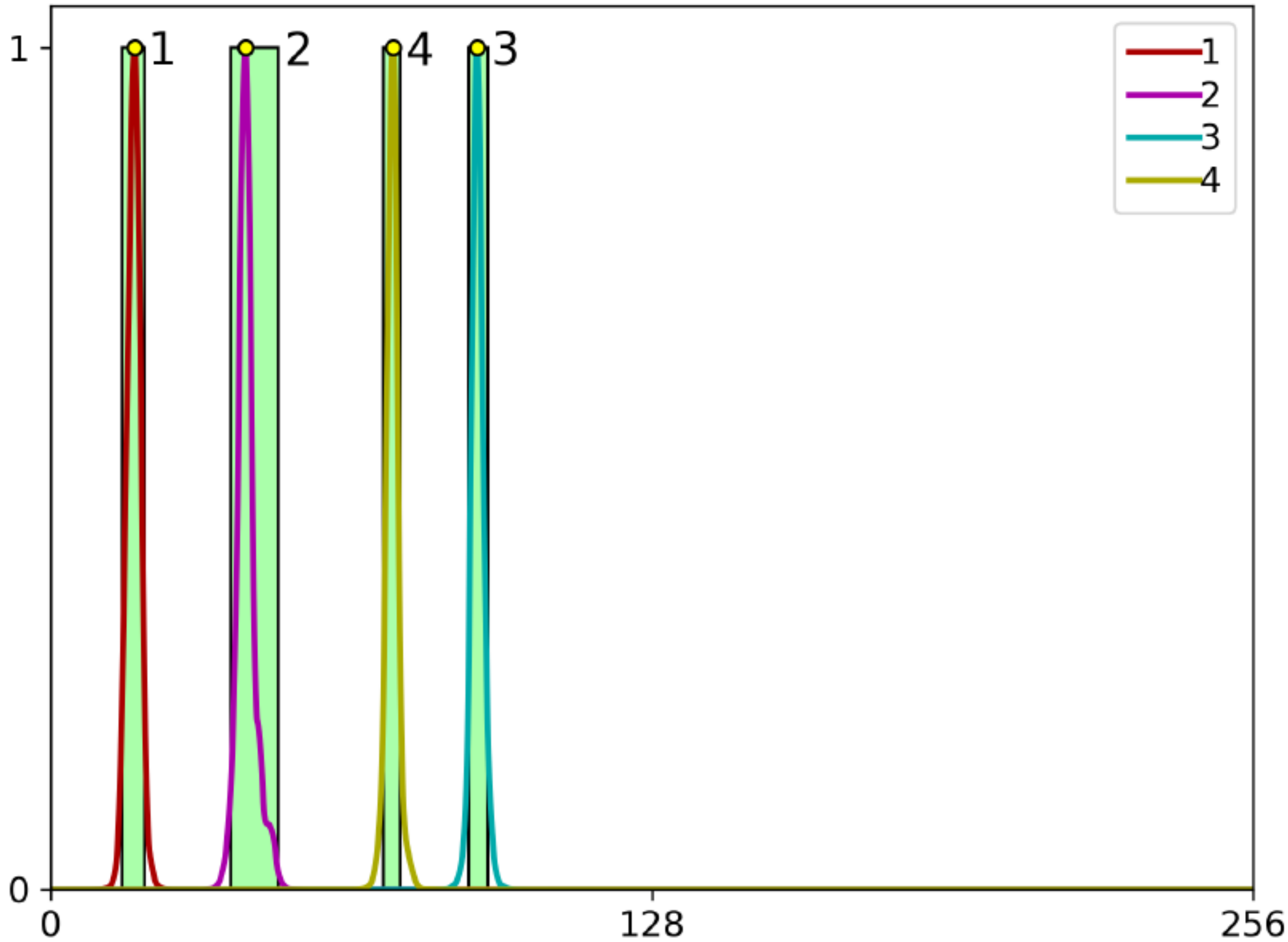
Where's Waldo? Eigenfunction prediction in 1D

eigenmode predictions



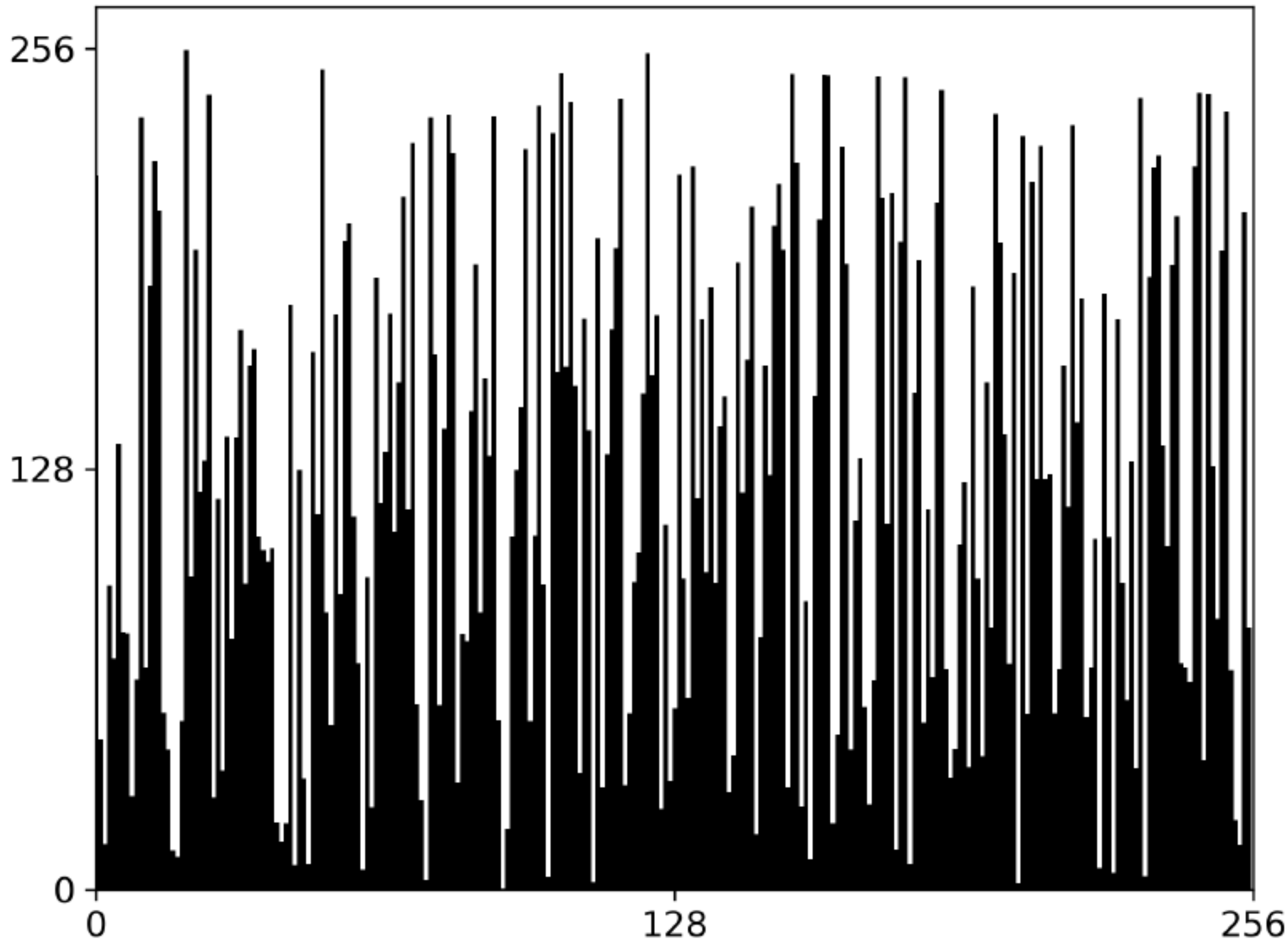
Where's Waldo? Eigenfunction prediction in 1D

true eigenmodes versus predictions



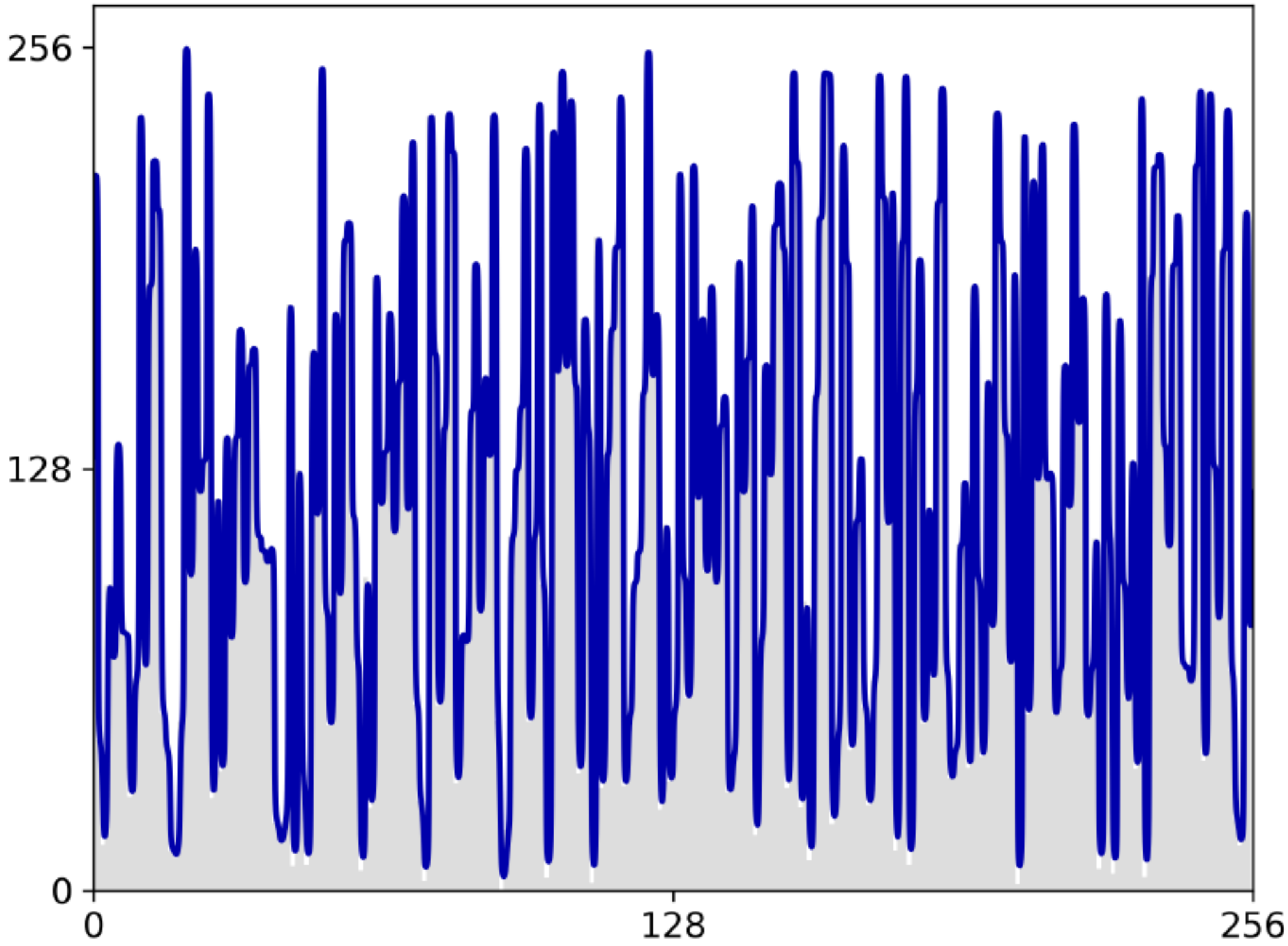
Increasing the amplitude of the potential

Increase V by a factor of 64 and do it again.



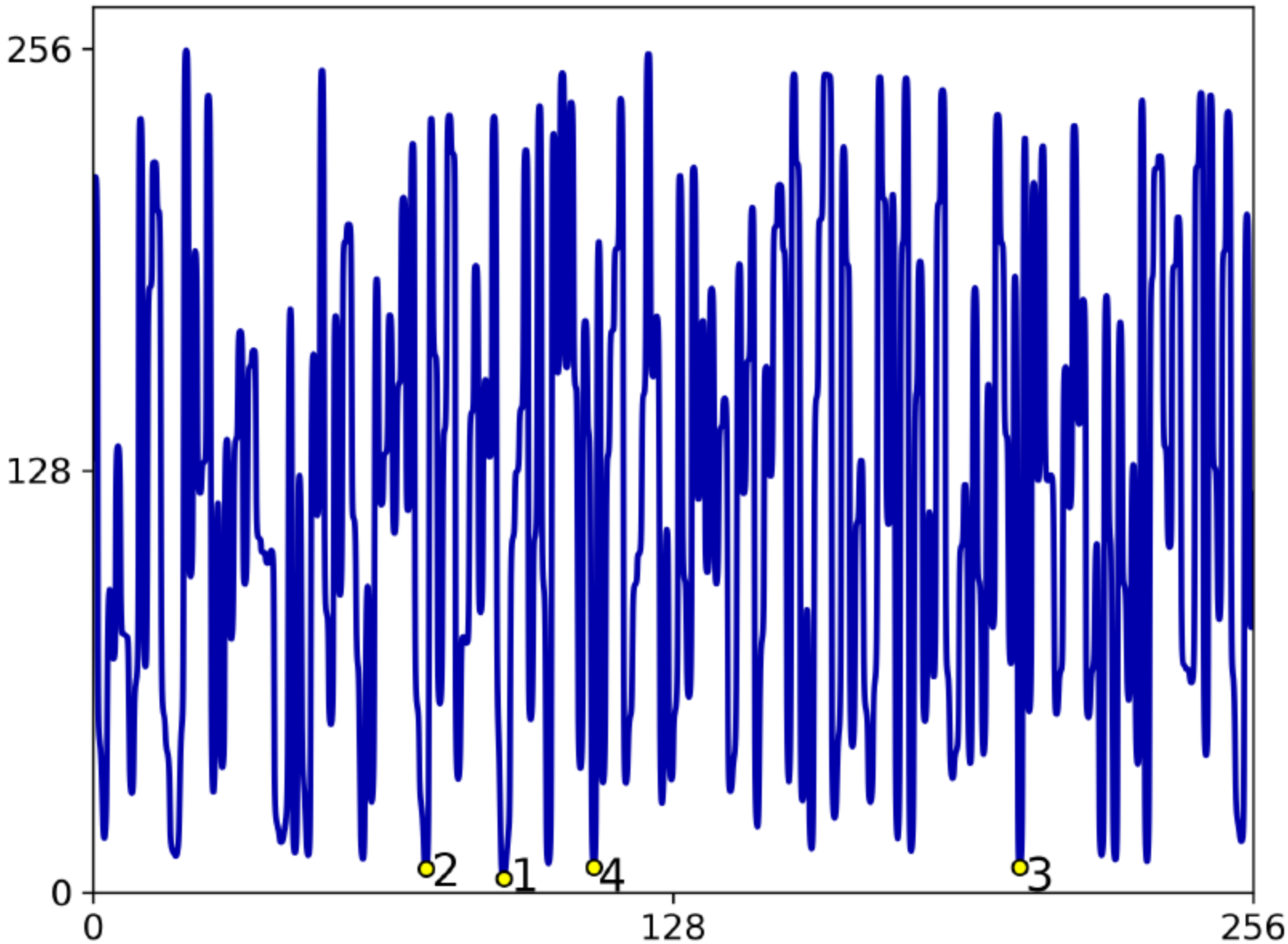
Increasing the amplitude of the potential

the effective potential is very different



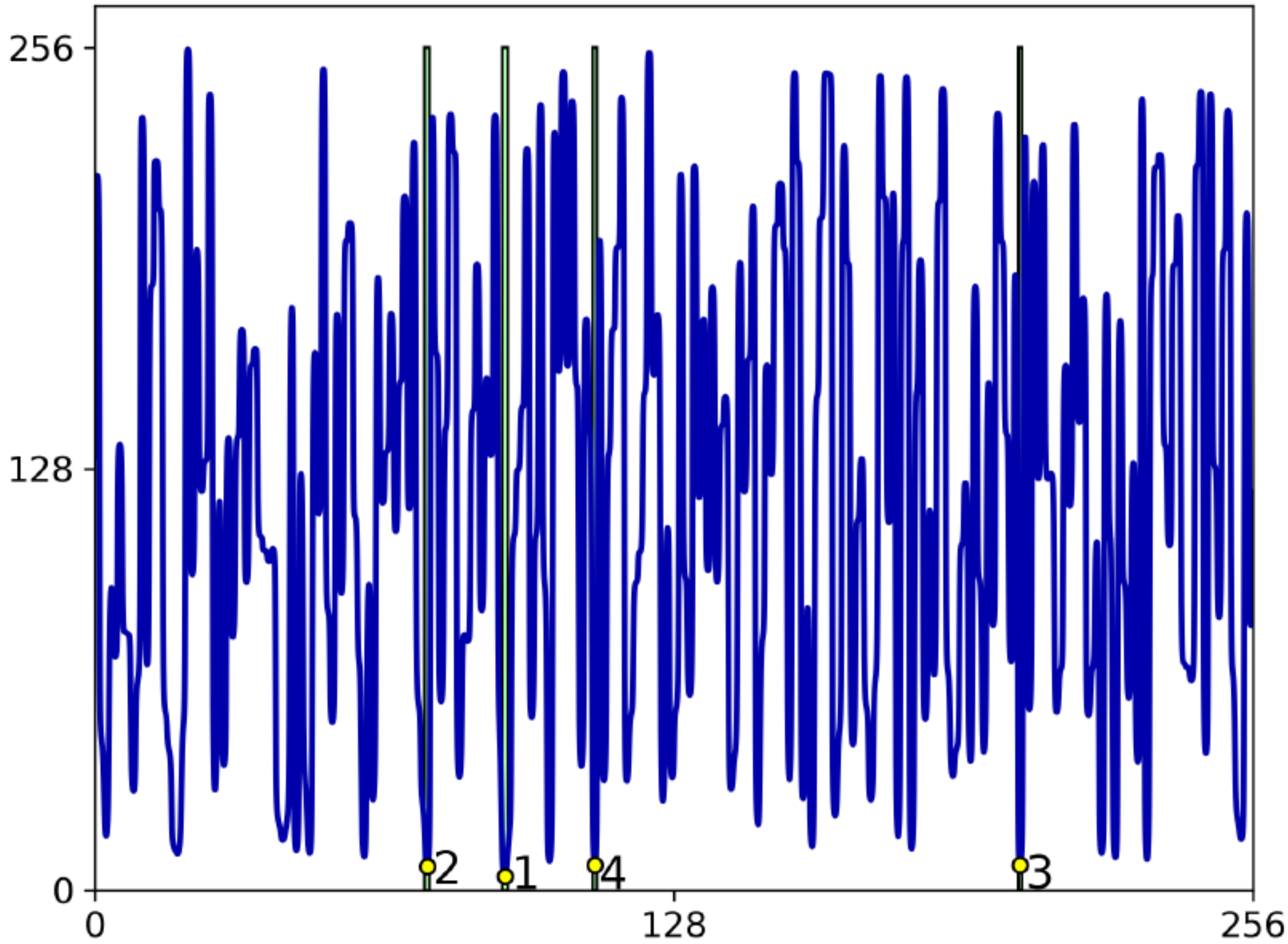
Increasing the amplitude of the potential

find deepest local minima x_i



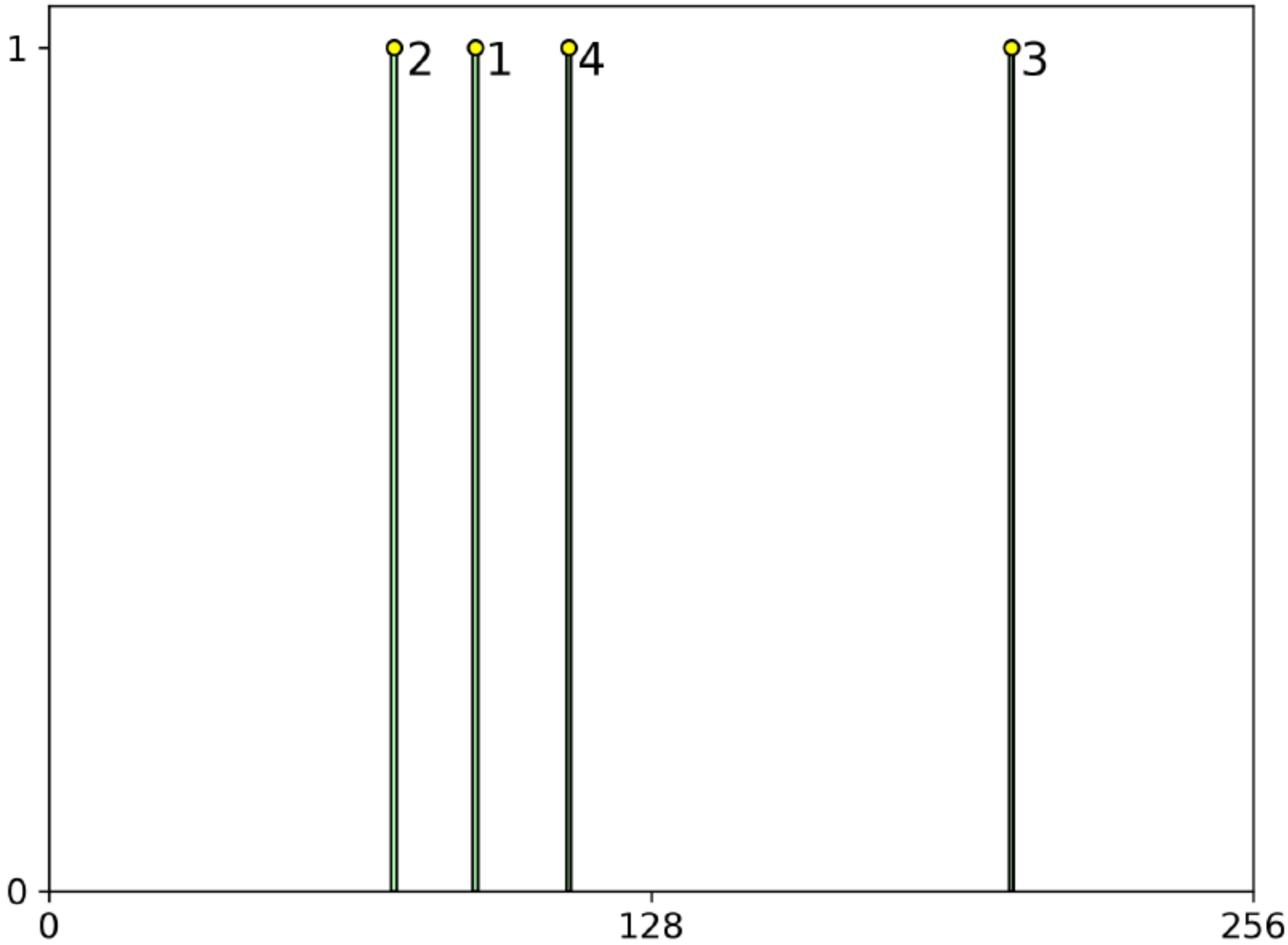
Increasing the amplitude of the potential

to minima associate connected component of sublevel set $W(x) < 2W_{\min}$



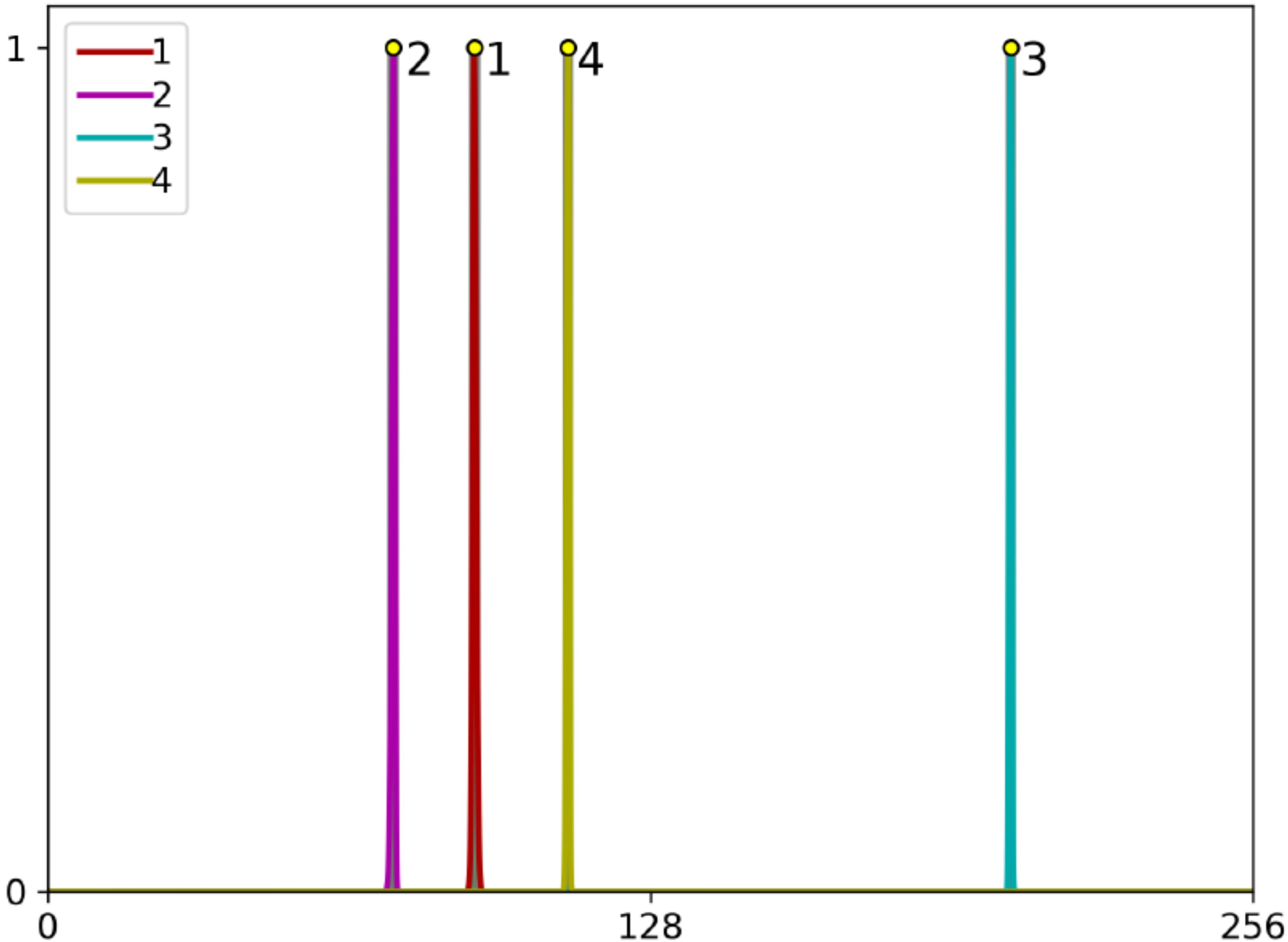
Increasing the amplitude of the potential

eigenmode predictions



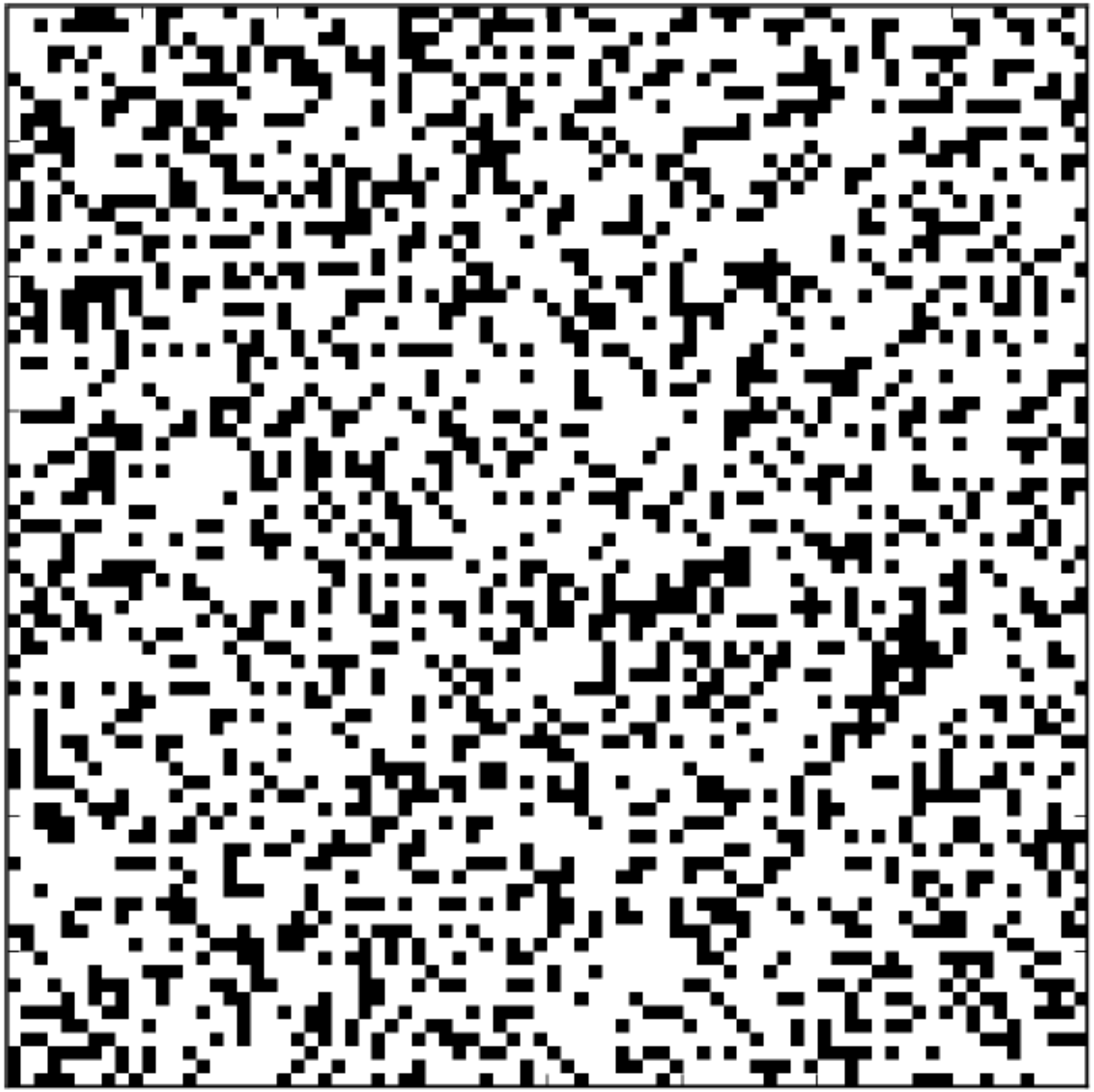
Increasing the amplitude of the potential

And they capture the true eigenfunctions perfectly again!



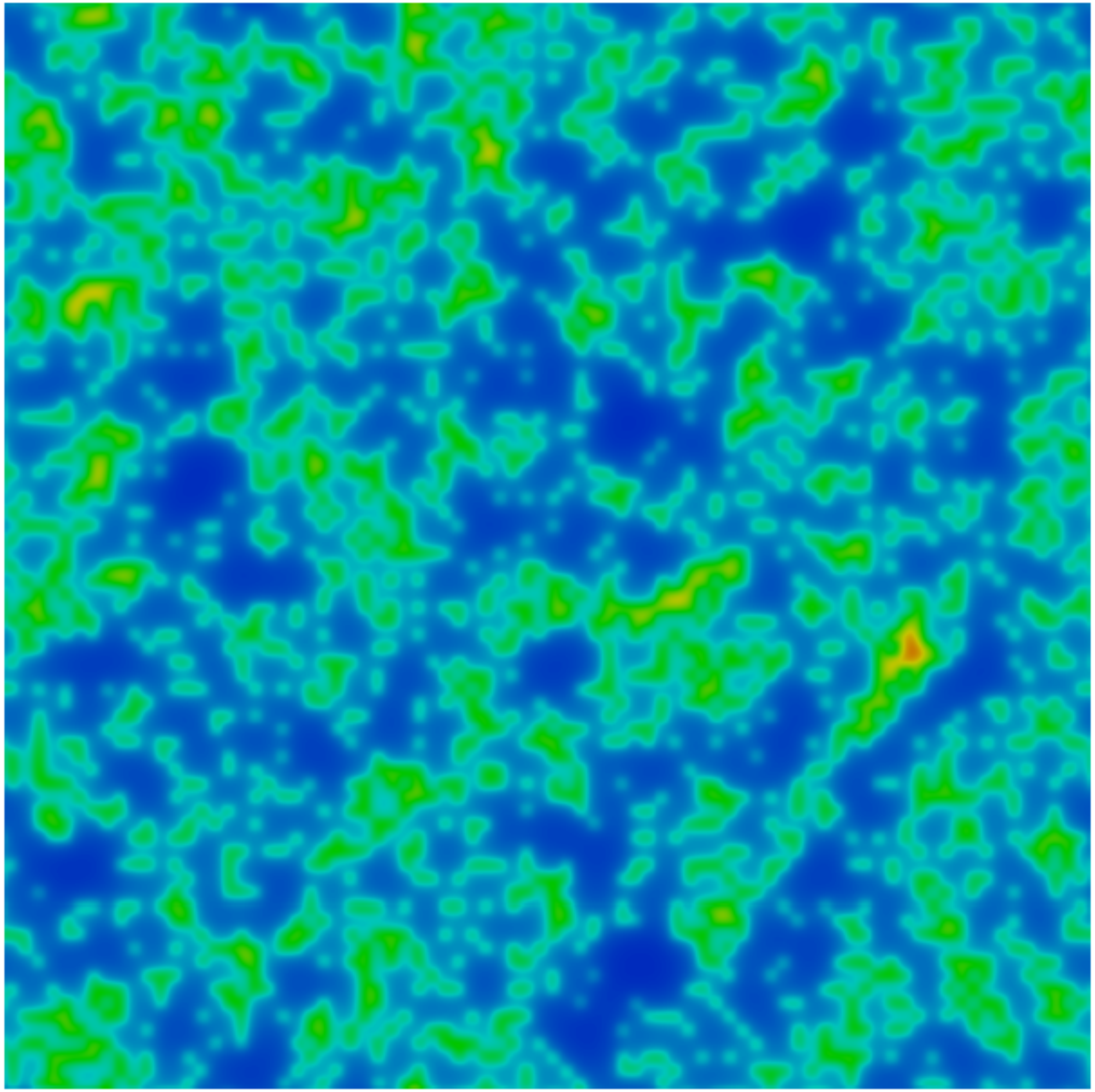
Eigenfunction prediction in 2D

80×80 Bernoulli potential



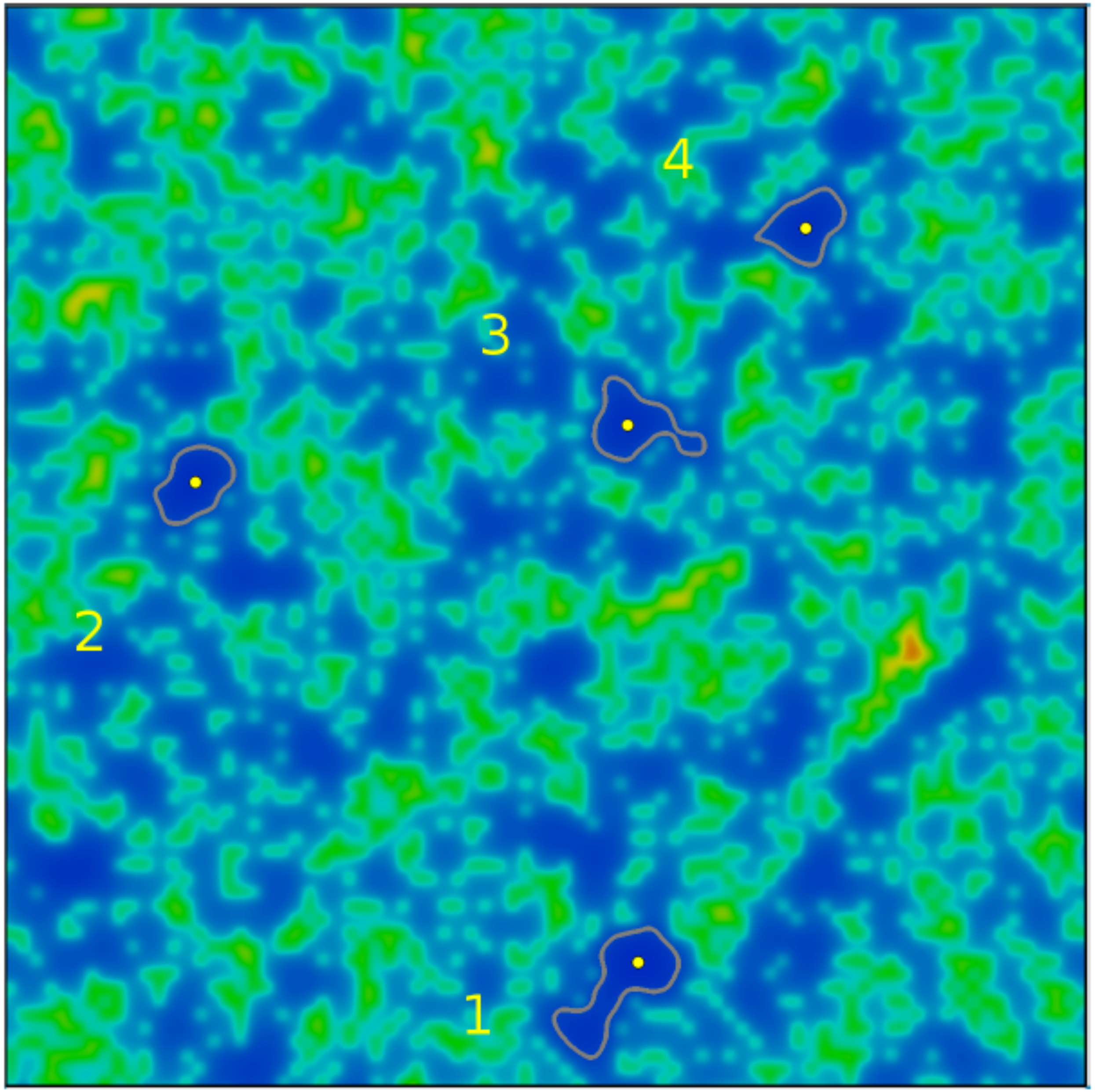
Eigenfunction prediction in 2D

effective potential



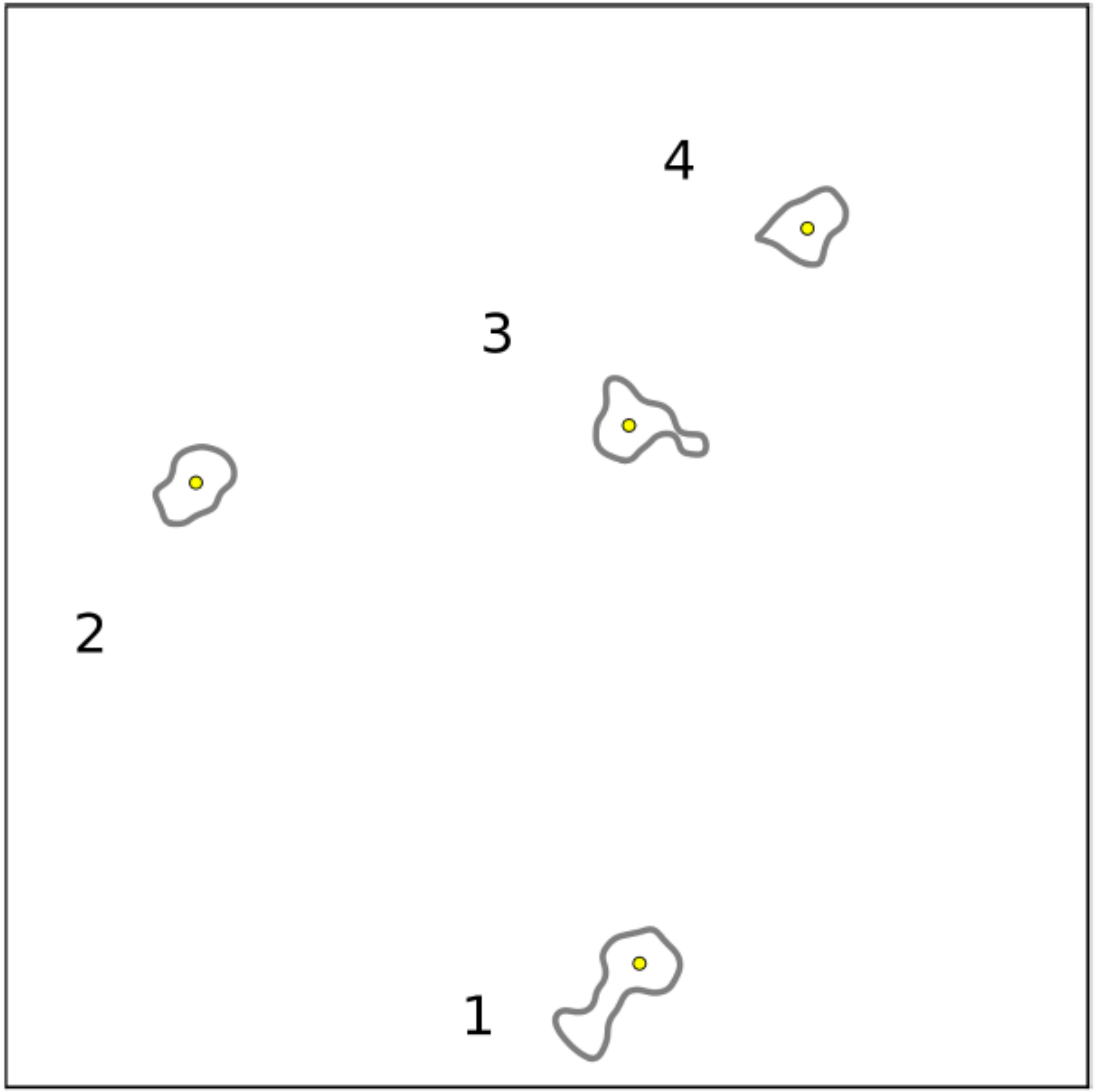
Eigenfunction prediction in 2D

local minima and sublevel sets



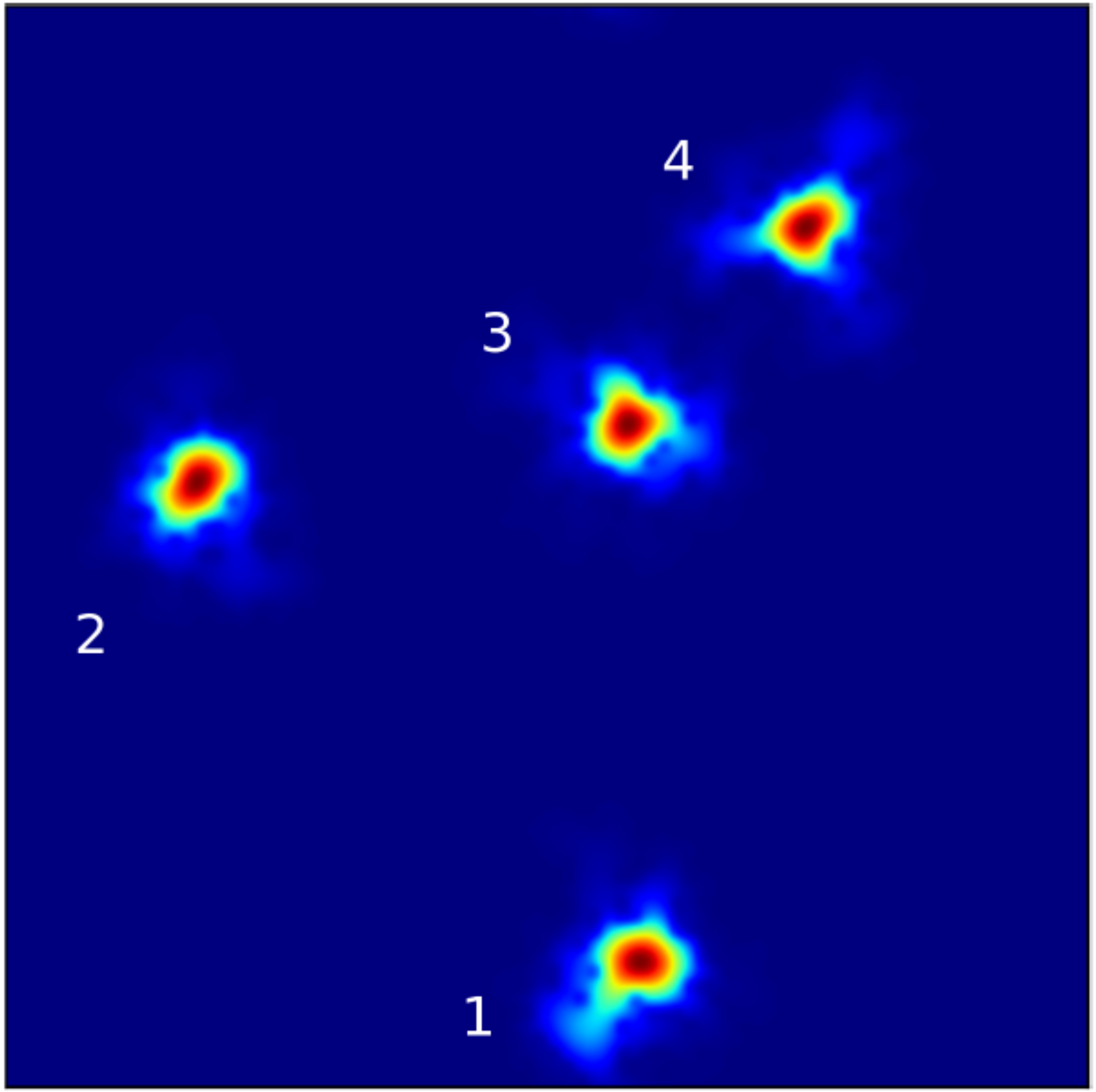
Eigenfunction prediction in 2D

eigenfunction predictions



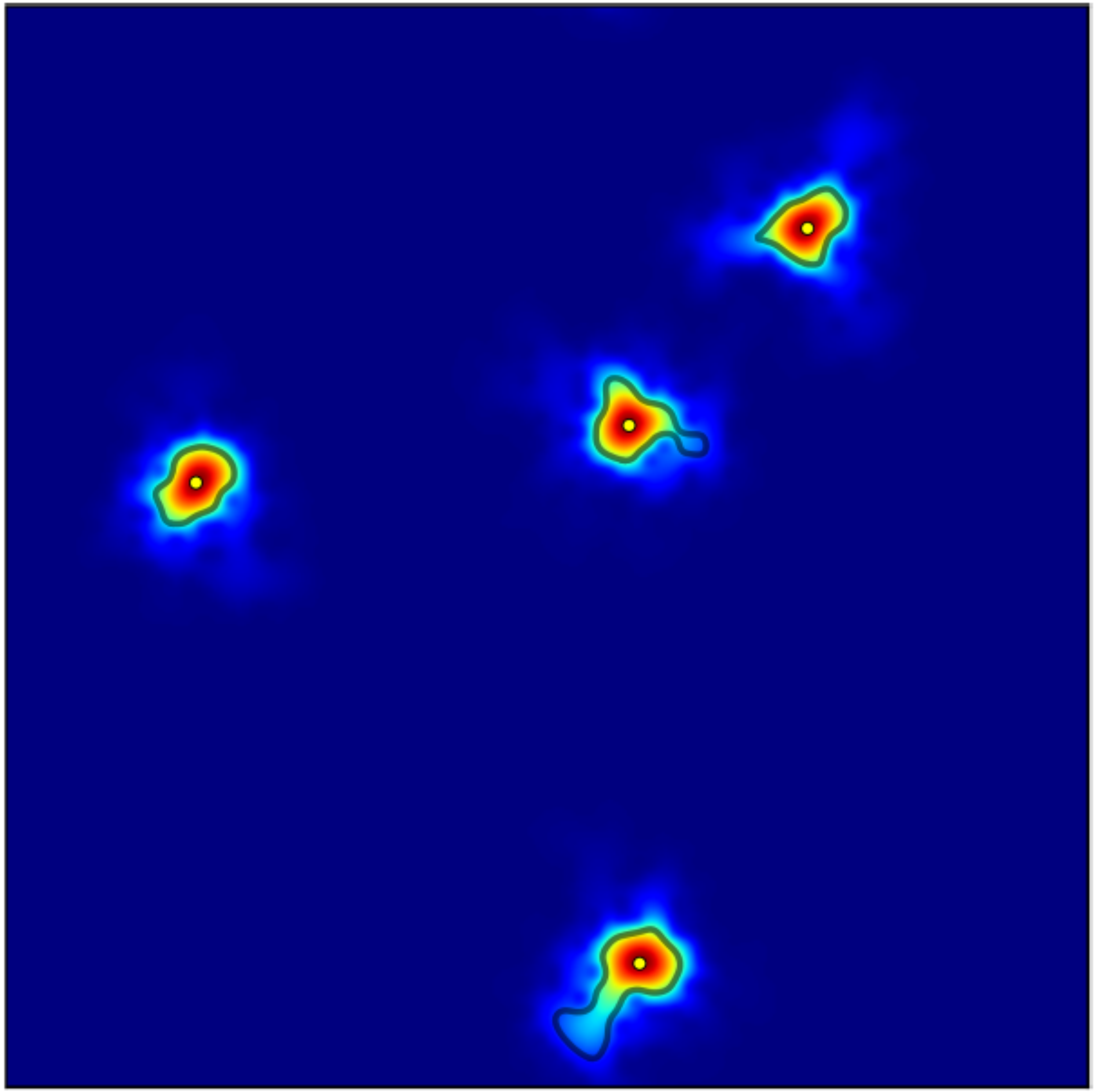
Eigenfunction prediction in 2D

true eigenfunctions



Eigenfunction prediction in 2D

predicted versus true eigenfunctions

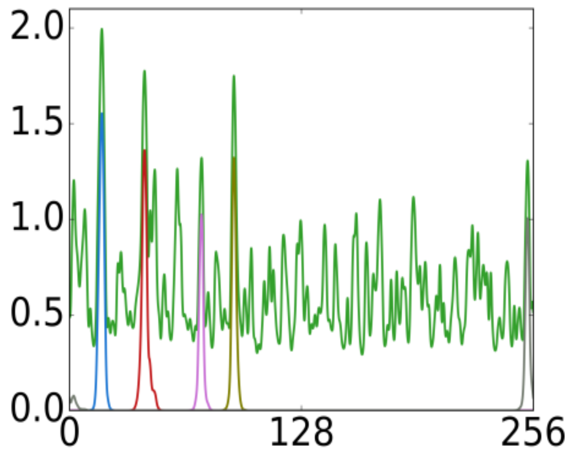


Properties of the localization landscape

u predicts the fundamental energy and quantum state inside each region

Fundamental state in each region

$$\boxed{\psi_0^{(m)} \approx \frac{u}{\|u\|}}$$

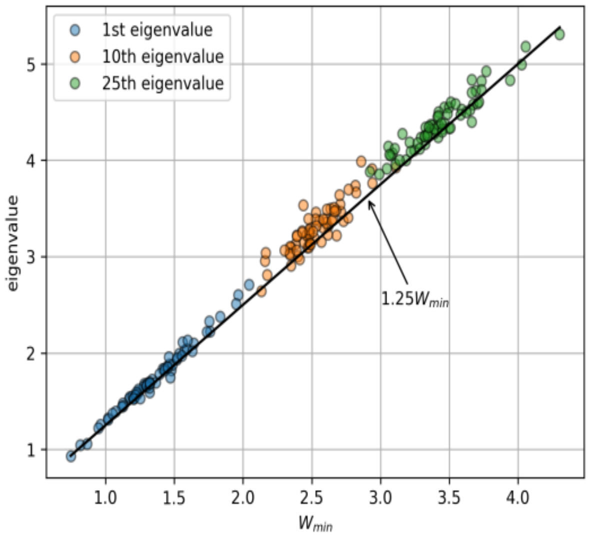


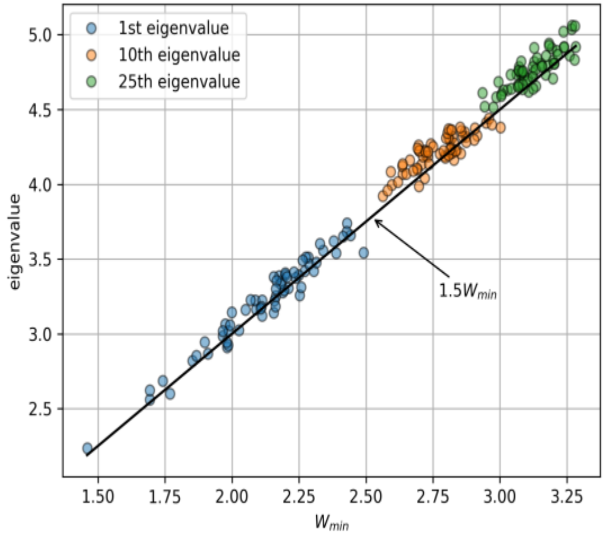
$$\langle \psi | H | \psi \rangle = \langle \nabla \psi | \nabla \psi \rangle + \langle \psi | V | \psi \rangle = \left\langle u \nabla\left(\frac{\psi}{u}\right) \middle| u \nabla\left(\frac{\psi}{u}\right) \right\rangle + \left\langle \psi \middle| \frac{1}{u} \middle| \psi \right\rangle$$

Fundamental energy

$$E_0^{(m)} \approx \frac{\left\langle u \middle| \frac{1}{u} \middle| u \right\rangle}{\|u\|^2} = \frac{\iiint_{\Omega_m} u(\vec{r})\, d^3 r}{\iiint_{\Omega_m} u^2(\vec{r})\, d^3 r}$$

$$E_0^{(m)} \approx \left(1 + \frac{d}{4}\right) \min\left(\frac{1}{u}\right)$$

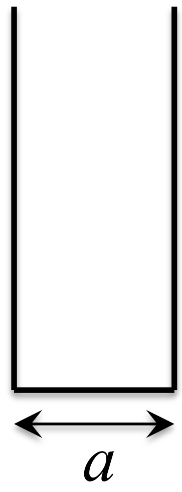




Arnold *et al.*, SIAM J Comput Sci (2019)

Properties of the localization landscape

A paradigm: the infinite quantum well



$$\hat{H} = -\frac{\partial^2}{\partial x^2}$$

Fundamental mode $$\psi_0(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right)$$

$$E_0 = \frac{\hbar^2 k^2}{2m} = \frac{\pi^2}{a^2}$$

Localization landscape $$u(x) = \frac{1}{2} x (a - x)$$

$$\left(1 + \frac{d}{4}\right)\left(\frac{1}{u}\right)_{\min} = 1.25 \times \frac{8}{a^2} = \frac{10}{a^2}$$

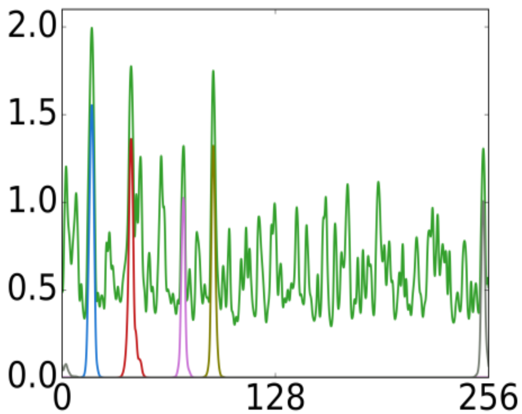
Fraction of the effective potential energy $$\frac{1}{E_0} \int_0^a \frac{2}{a} \sin^2\left(\frac{\pi x}{a}\right) \frac{2dx}{x(a-x)} \approx 96.2\%$$

Properties of the localization landscape

u predicts the fundamental energy and quantum state inside each region

Fundamental state in each region

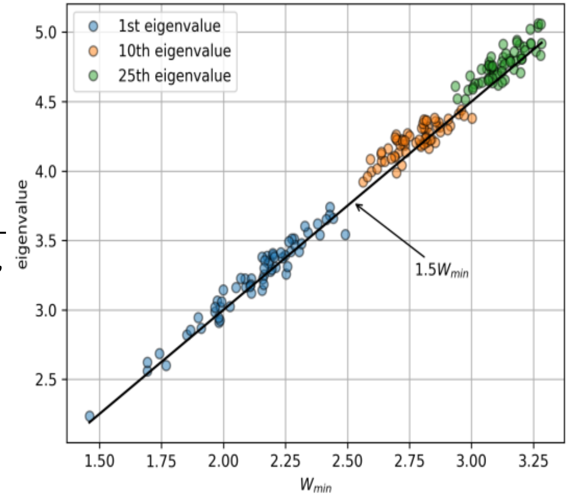
$$\boxed{\psi_0^{(m)} \approx \frac{u}{\|u\|}}$$



Fundamental energy

$$E_0^{(m)} \approx \frac{\left\langle u \middle| \frac{1}{u} \middle| u \right\rangle}{\|u\|^2} = \frac{\iiint_{\Omega_m} u(\vec{r})\, d^3r}{\iiint_{\Omega_m} u^2(\vec{r})\, d^3r}$$

$$E_0^{(m)} \approx \left(1 + \frac{d}{4}\right) \min\left(\frac{1}{u}\right)$$



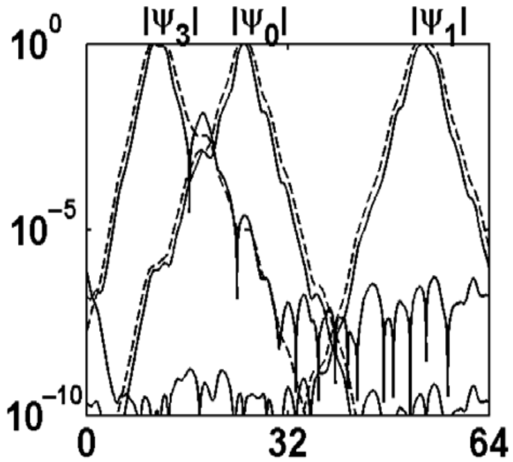
Arnold *et al.*, SIAM J Comput Sci (2019)

1/u accounts for the decay of the quantum state outside its localization region

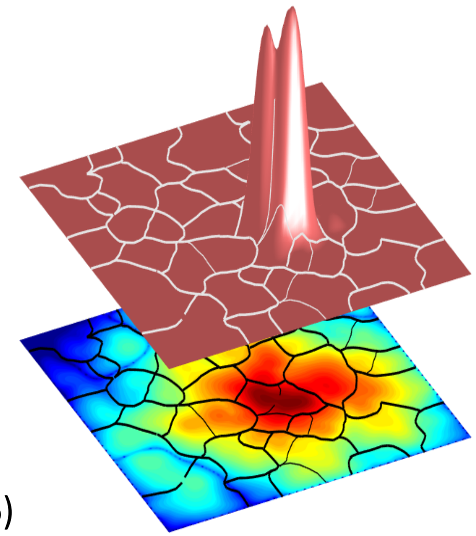
$$\rho_{W,E}(\vec{r}_1, \vec{r}_2) = \inf_{\text{paths}} \left(\int_{\vec{r}_1}^{\vec{r}_2} \sqrt{\frac{2m}{\hbar^2} \left(W(s) - E\right)_+}\, ds \right)$$

$$\left|\psi(\vec{r})\right| \prec e^{-\rho_{W,E}(\vec{0}, \vec{r})}$$

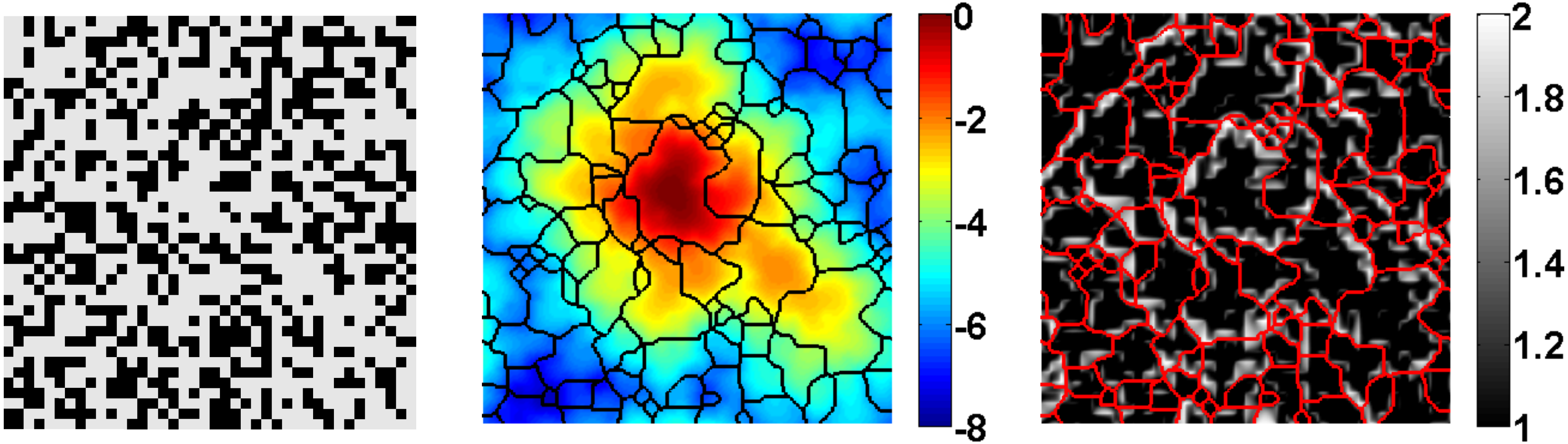
Tunneling through the barriers of W=1/u



Arnold *et al.*, *PRL* **116**, 056602 (2016)



2D binary Anderson model

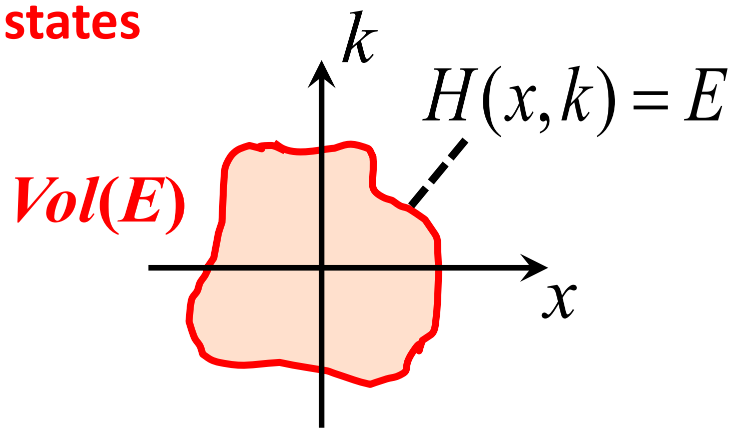


$$\boxed{\frac{\log\left(\left|\nabla\psi\right|\right)}{\left|\psi\right|}}$$

Arnold et al., PRL (2016)

Properties of the localization landscape

$1/u$ provides an accurate estimate of the density of states



Uncertainty principle: $\Delta x\, \Delta k \approx 2\pi$

Counting eigenvalues below *E* ⬌ Counting volume in phase space

Weyl's law

$$\boxed{IDOS(E) \equiv \#\{E_j \le E\} \approx \frac{Vol(E)}{(2\pi)^d} = \frac{1}{(2\pi)^d} \iint_{H(x,k)\le E} dx\, dk}$$

Modified law:

$$\boxed{IDOS(E) \approx \frac{1}{(2\pi)^d} \iint_{\frac{\hbar^2 k^2}{2m}+\frac{1}{u(\vec{r}')}} d^d k\, d^d r = \frac{\omega_d}{(2\pi)^d}\left(\frac{2m}{\hbar^2}\right)^{\frac{d}{2}} \int_\Omega \left(E - \frac{1}{u(\vec{r})}\right)^{\frac{d}{2}} d^d r}$$

Arnold et al., Phys. Rev. Lett., 2016

5. $1/u$ provides an accurate estimate of the density of states

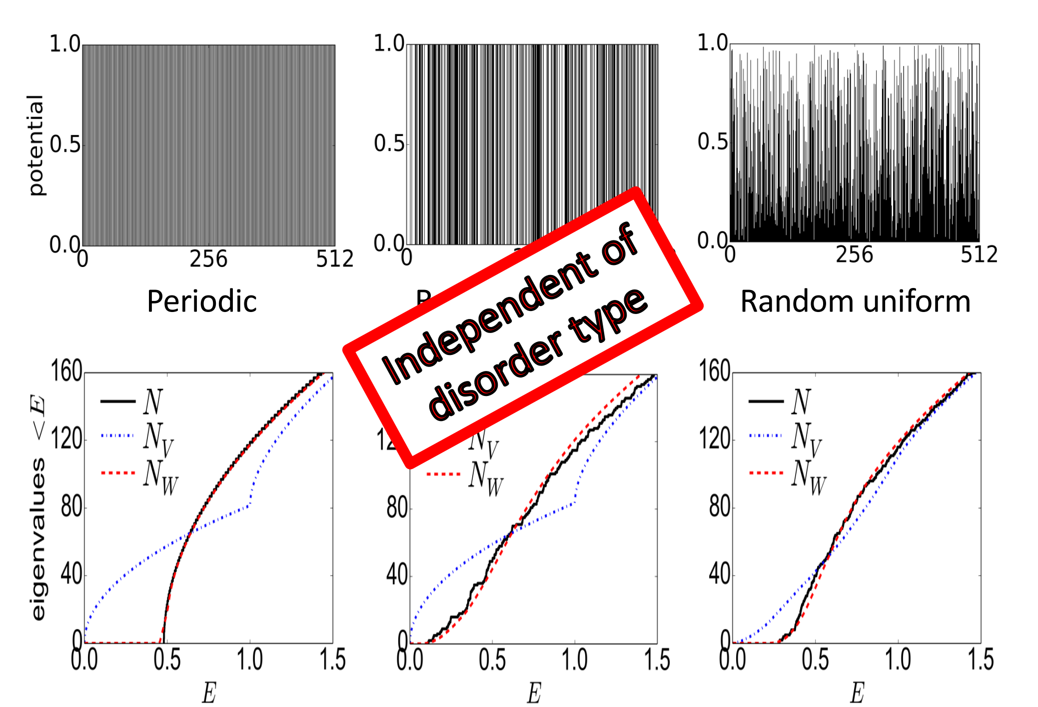
Weyl's law

$$IDOS(E) \approx \frac{1}{(2\pi)^d} \iint_{H(x,k)\leq E} d^d r \, d^d k$$

Homogeneous medium

$$IDOS(E) \propto (E - E_c)^{d/2}$$

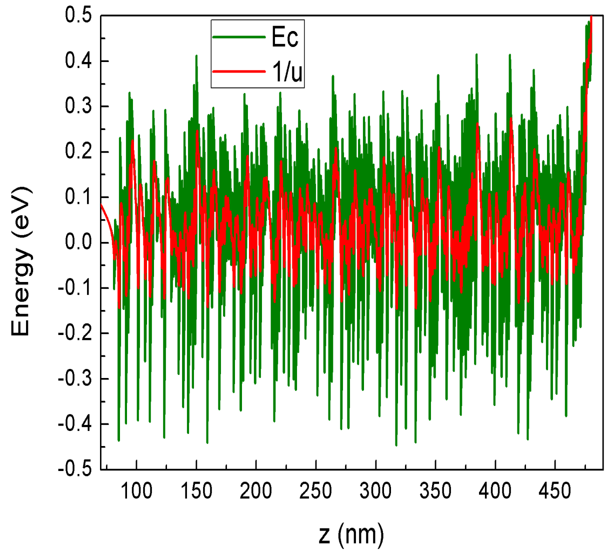
$$DOS(E) \propto (E - E_c)^{d/2 - 1}$$

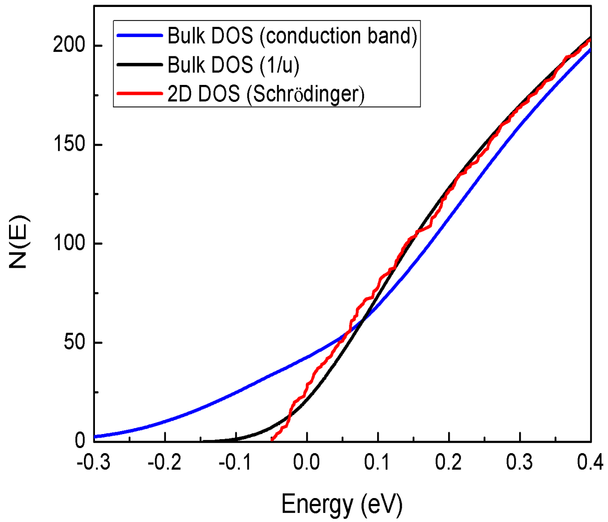


N = actual IDOS (computed from the Schrödinger equation)
N_V = IDOS classically obtained using the original potential V
N_W = IDOS obtained using W=1/u

Arnold *et al.*, *PRL* **116**, 056602 (2016)

200-pairs superlattice





MF *et al.*, *PRB* **95**, 144204 (2017)

7. Quantum transport in disordered medium (hopping)

Electron-phonon coupling

$$H_{ep} = \sum_q a_j^+ a_i b_q^\eta (-i\eta c_q \langle \psi_j | e^{(-i\eta \vec{q}.\vec{r})} | \psi_i \rangle)$$

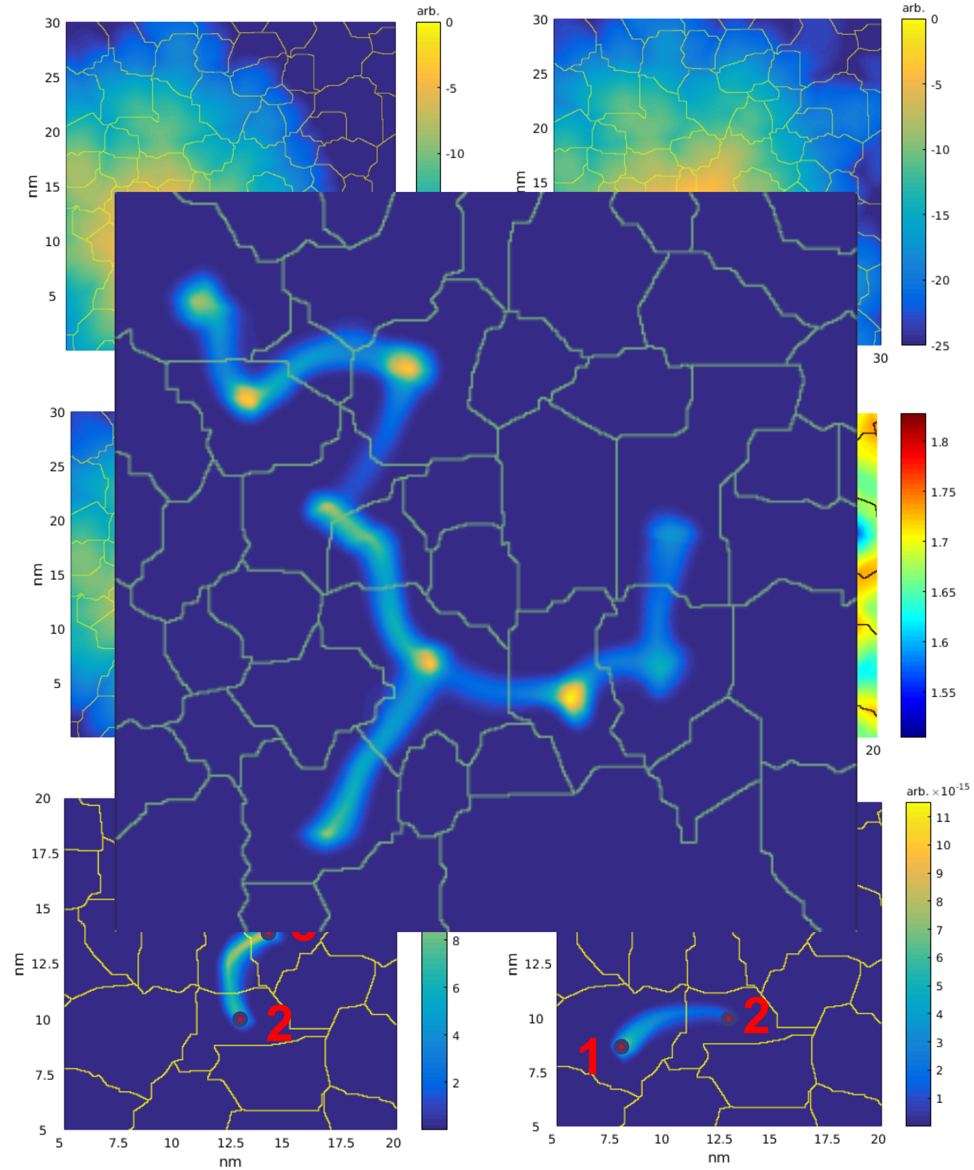
first order:

$$\left\langle \psi_1 \middle| e^{-i\vec{q}\cdot\vec{r}} \middle| \psi_2 \right\rangle \approx \iiint e^{-\rho_1(\vec{r})} e^{-i\vec{q}\cdot\vec{r}} e^{-\rho_2(\vec{r})} d^3r$$

$$= \iiint e^{-i\vec{q}\cdot\vec{r}} e^{-(\rho_1(\vec{r})+\rho_2(\vec{r}))} d^3r$$

The integrand remains significantly large only along a path that minimizes simultaneously both $\rho_1(\vec{r})$ and $\rho_2(\vec{r})$.

The main interaction path can be read on the *1/u* map (through the saddle points of the effective potential)



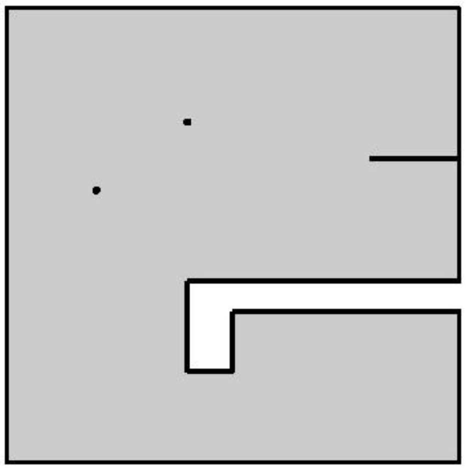
PhD thesis Jean-Marie Lentali

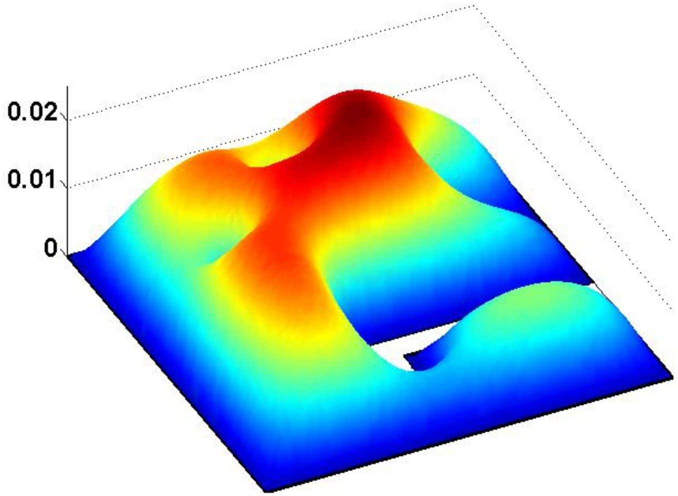
Mechanical vibrations

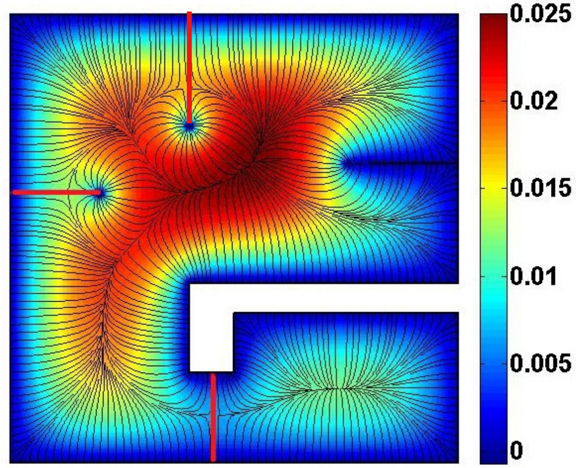
The landscape in a “complex” membrane or plate

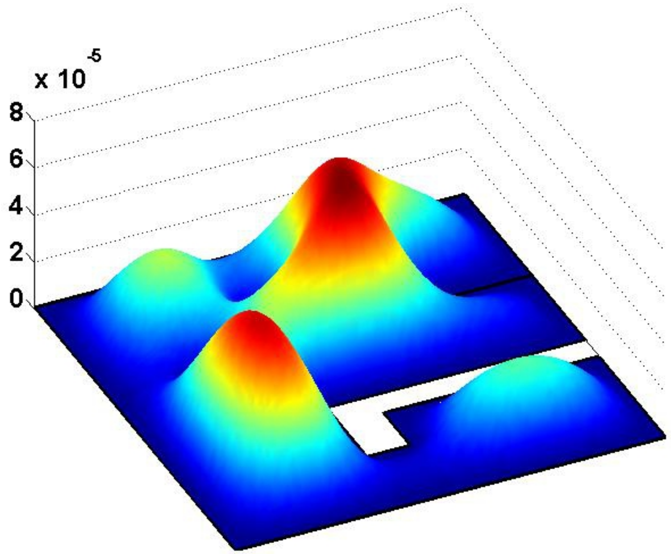
Laplacian

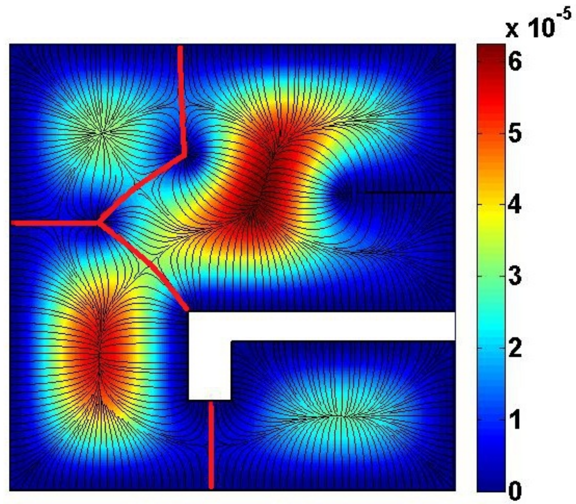
$$\Delta u = 1$$











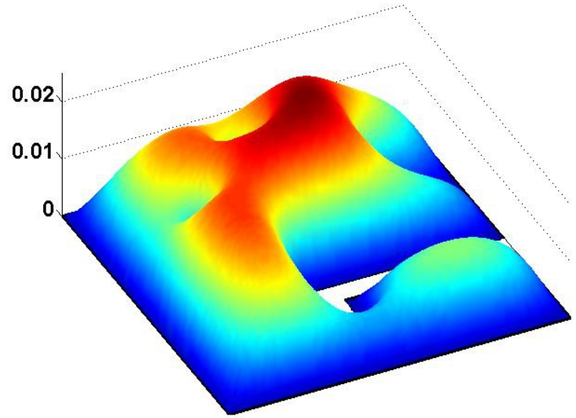
biLaplacian

$$\Delta\left(\Delta u\right) = 1$$

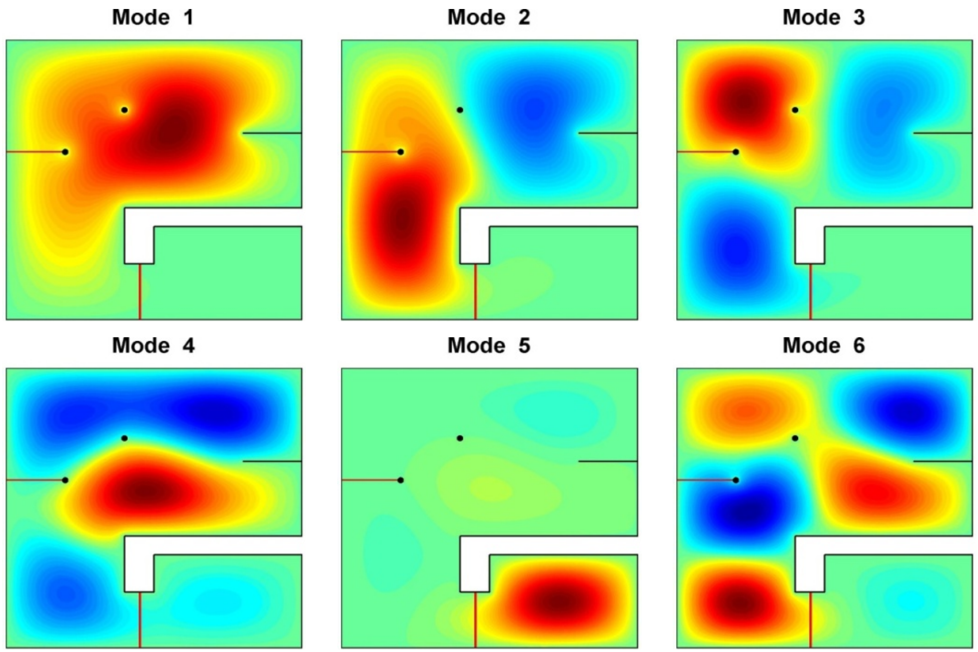
MF & S. Mayboroda., PNAS 2012

The landscape in a “complex” membrane or plate

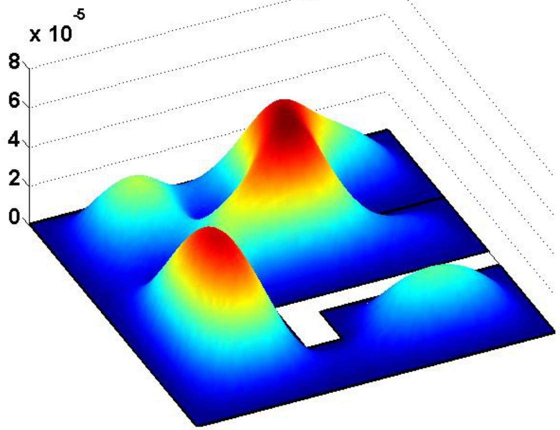
Laplacian



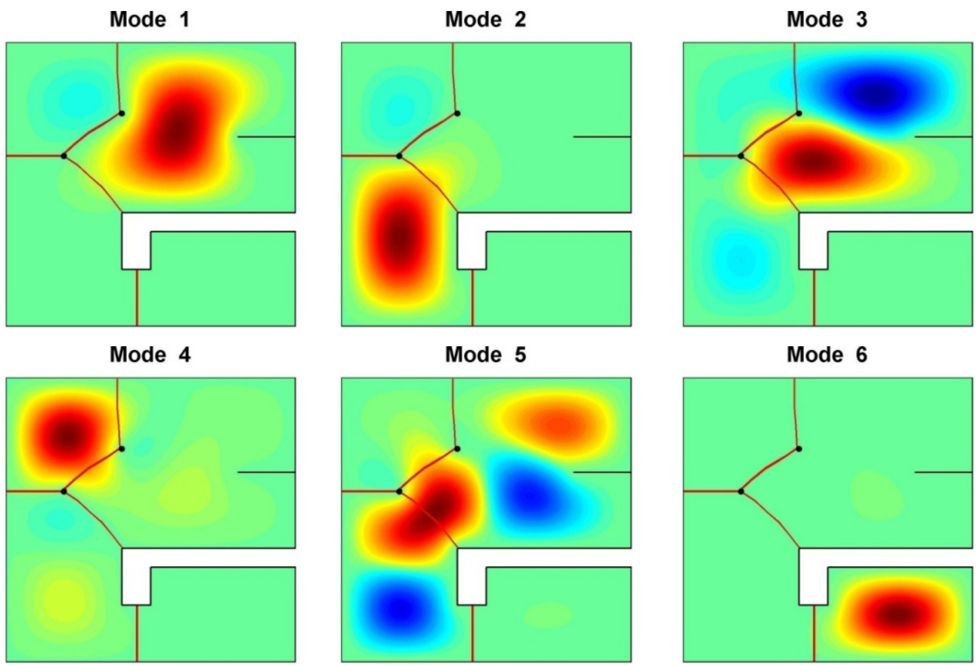
Landscape $u(x)$



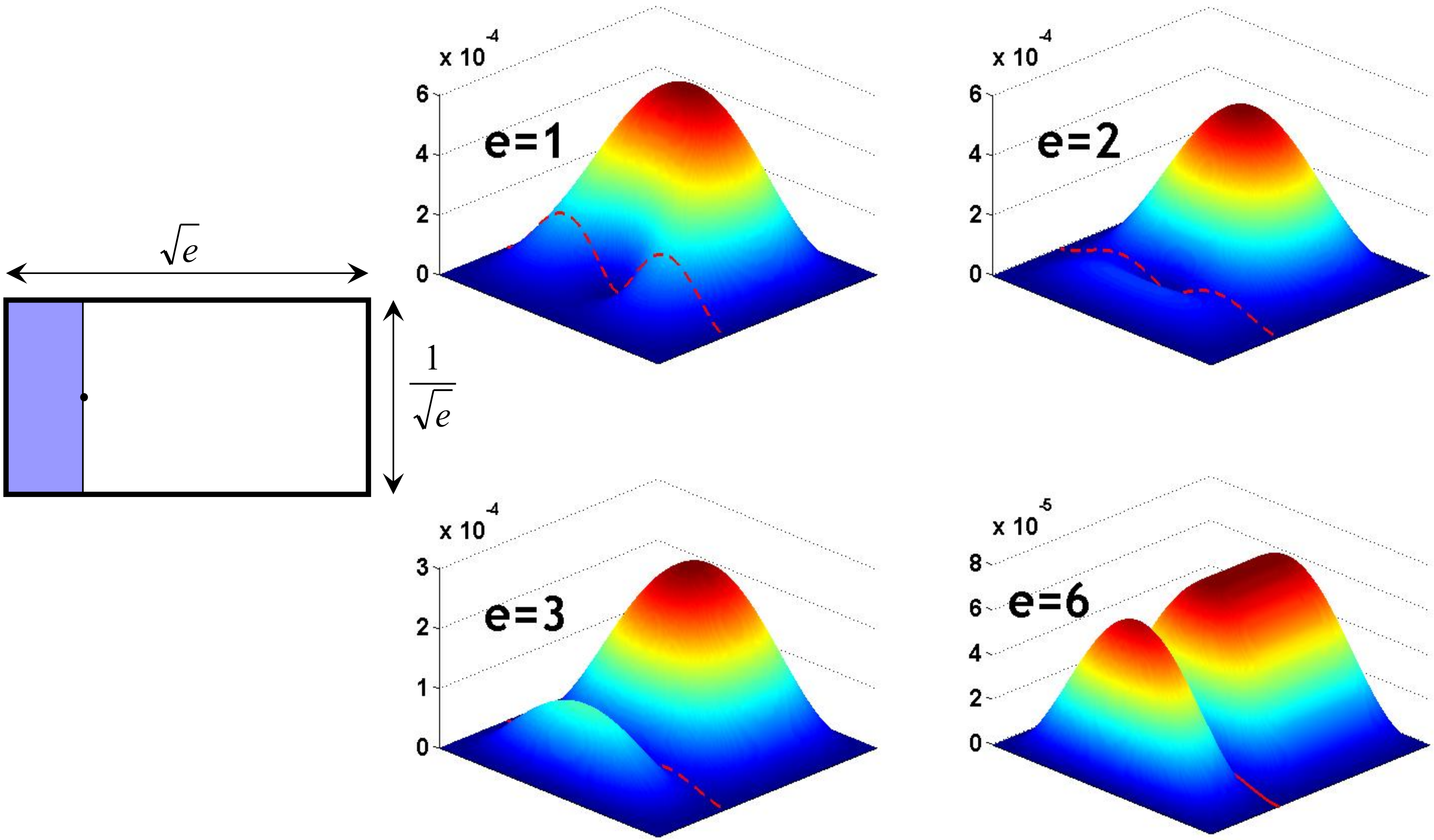
biLaplacian



Landscape $u(x)$

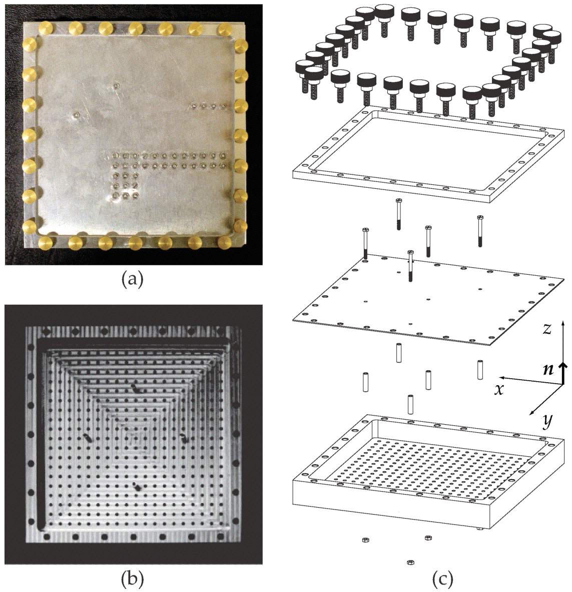


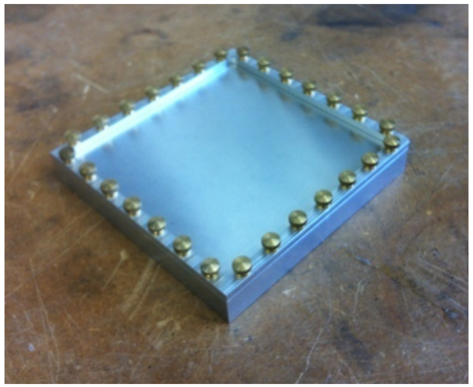
The landscape in the clamped plate



Mechanical vibrations: thin plates

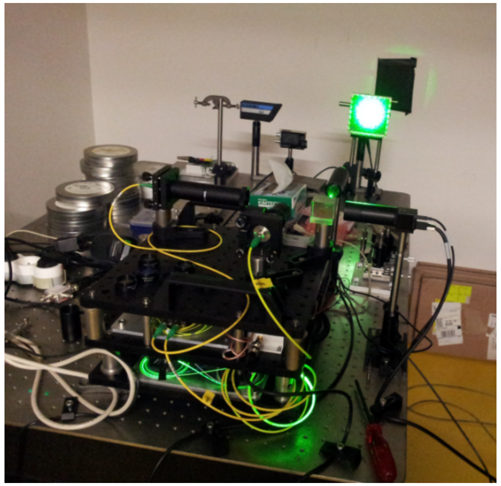
Thin plate of Duraluminium

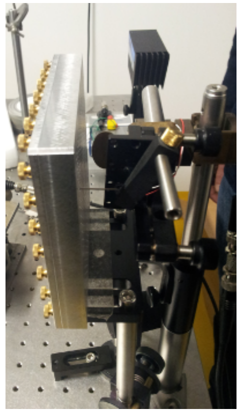




10 cm × 10 cm, 0.5 mm thick

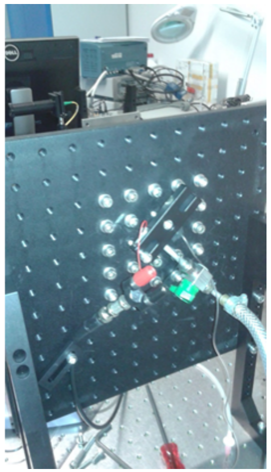
Experiments performed at Institut Langevin





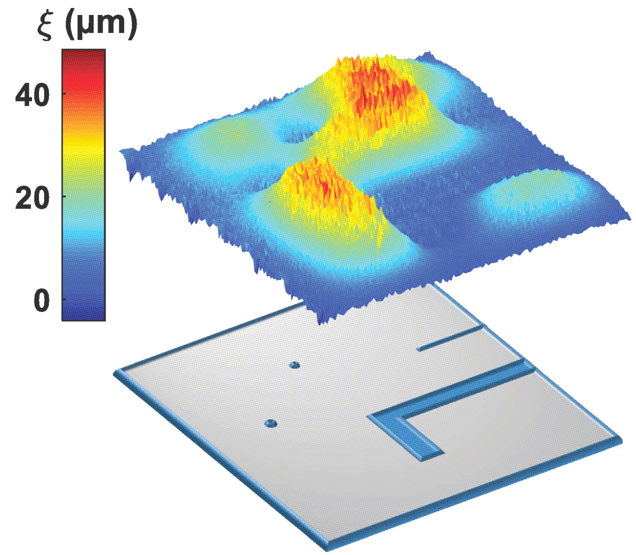
P. Sebbah,
M. Atlan
F. Feppon,
A. Labbé,
C. Gillot,
A. Garelli,
M. Ernoult,
M. Dubois,
G. Lefebvre,
A. Gondel,

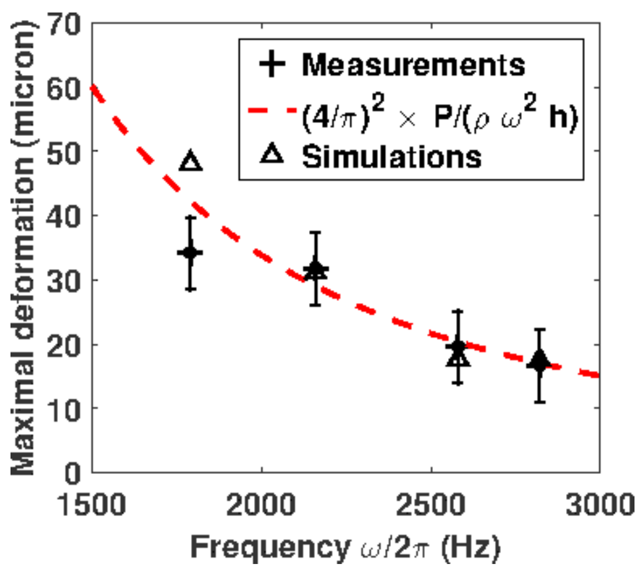
Optical heterodyne holographic interferometer

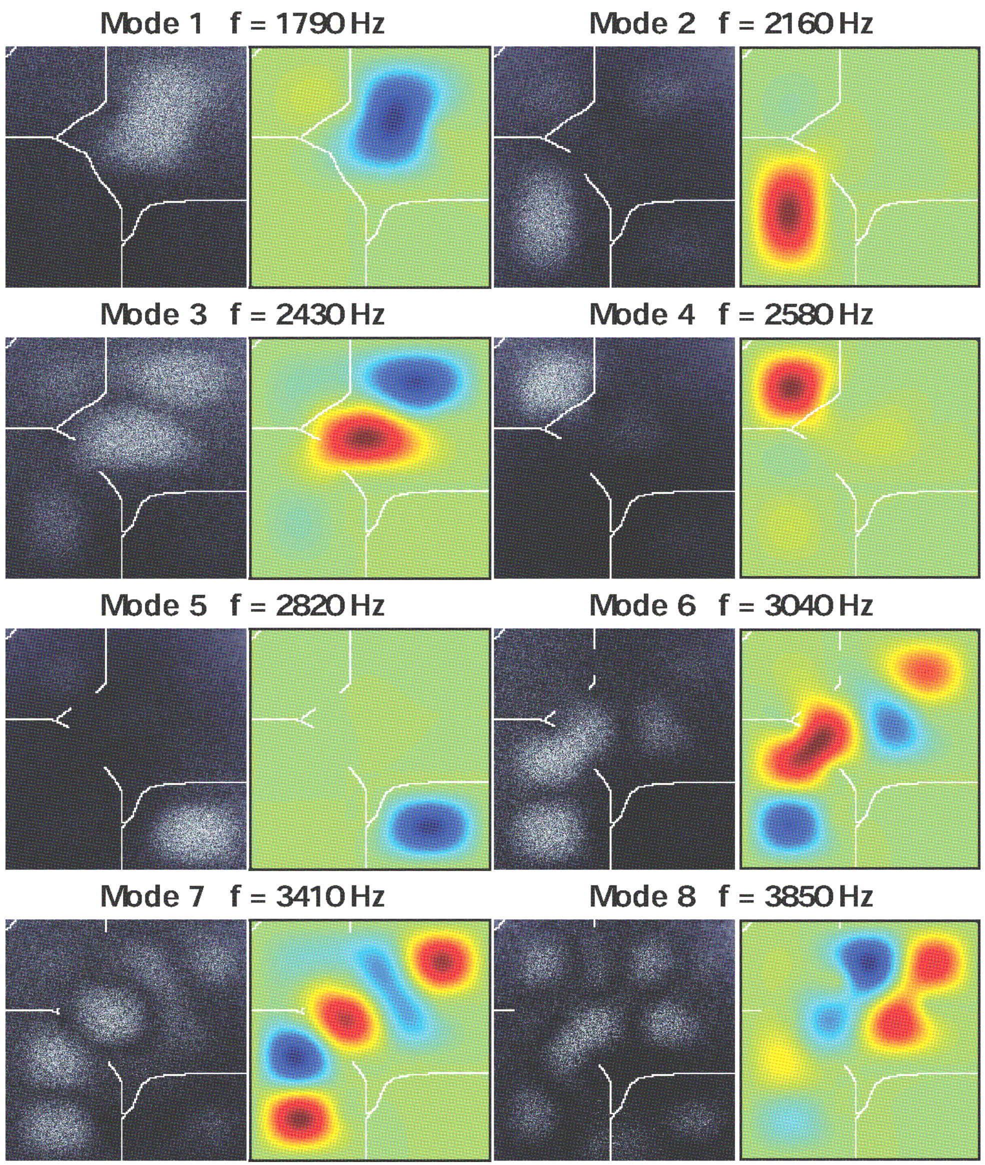


static deformation

Mechanical vibrations: thin plates





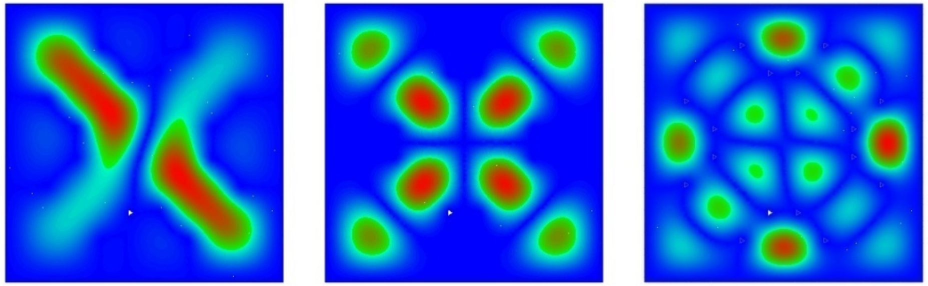


Lefèbvre et al., PRL 2016

The inverse problem: “localization design”

Sensitivity of the solution

Simulations / Experiments



2952 Hz 3807 Hz 5595 Hz

2950 Hz 3730 Hz 5540 Hz

The Simons collaboration: WAVE (http://wave.umn.edu)

Douglas Arnold
(Univ. of Minnesota)

Alain Aspect
(IOGS)

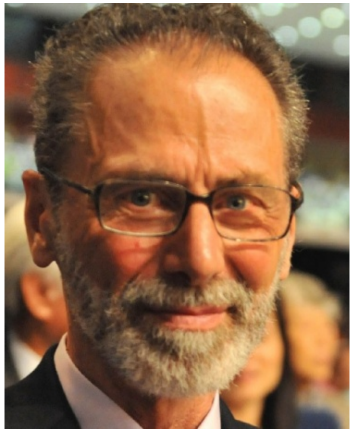
Guy David
(Univ. Paris Sud)

David Jerison
(MIT)

Marcel Filoche
(Ecole Polytechnique)

Richard Friend
(Univ. of Cambridge)

Svitlana Mayboroda
(Univ. of Minnesota)



Yves Meyer
(ENS Paris Saclay)

Jim Speck
(UCSB)

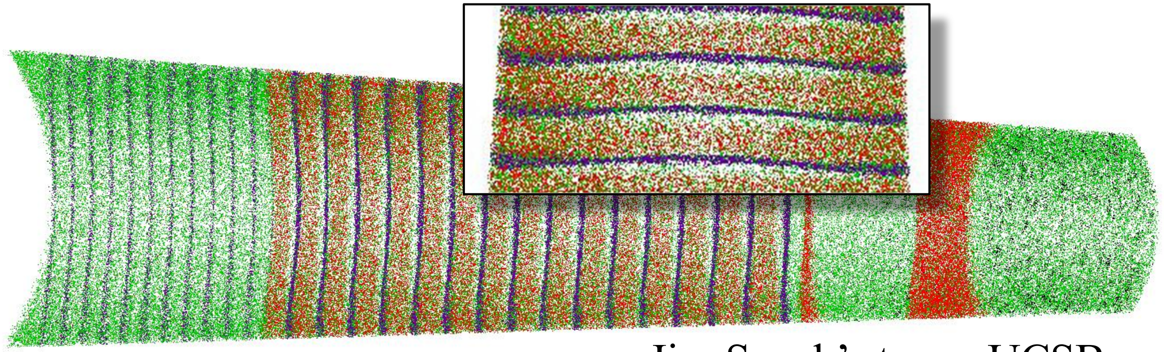
Claude Weisbuch
(UCSB/
Ecole Polytechnique)

Disordered semiconductors

Disorder at the nanometer scale: semiconductors

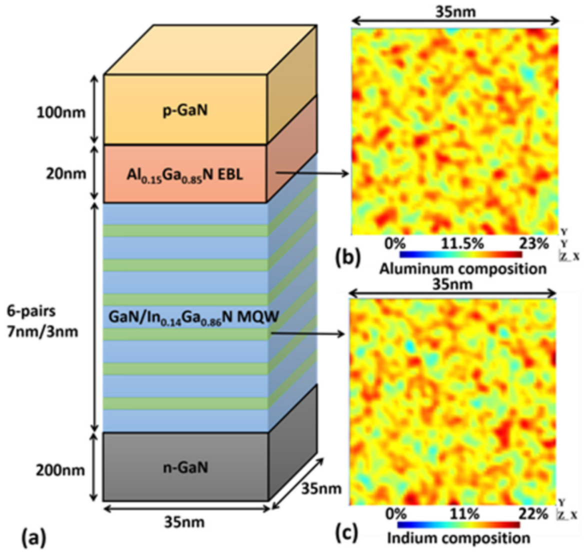
Atom Probe Tomography imaging atomic composition

60 million atoms positioned



Jim Speck's team, UCSB

LED structure and landscape computations



Li *et al.*, *Phys. Rev. B*. 2017

Computing at the nanometer scale

$E_{c,v}(\vec{r})$

Band edges

Schrödinger equation

$$-\frac{\hbar^2}{2m_{e,h}}\Delta\psi_{i,j} + E_{c,v}(\vec{r})\psi_{i,j} = E_{i,j}\psi_{i,j}$$

Quantum states

$\{\psi_{i,j}, E_{i,j}\}$

$$\left(-\frac{\hbar^2}{2m_e}\Delta + E_{c,v}(\vec{r})\right)u_{c,v} = 1$$

Localization landscapes

$$n(\vec{r}) = \sum_i |\psi_i|^2 n_i$$

$$E_c(\vec{r}) = -e\varphi(\vec{r}) + \delta E_c(\vec{r})$$

$$E_v(\vec{r}) = e\varphi(\vec{r}) + \delta E_v(\vec{r})$$

Poisson equation

Electrostatic potential

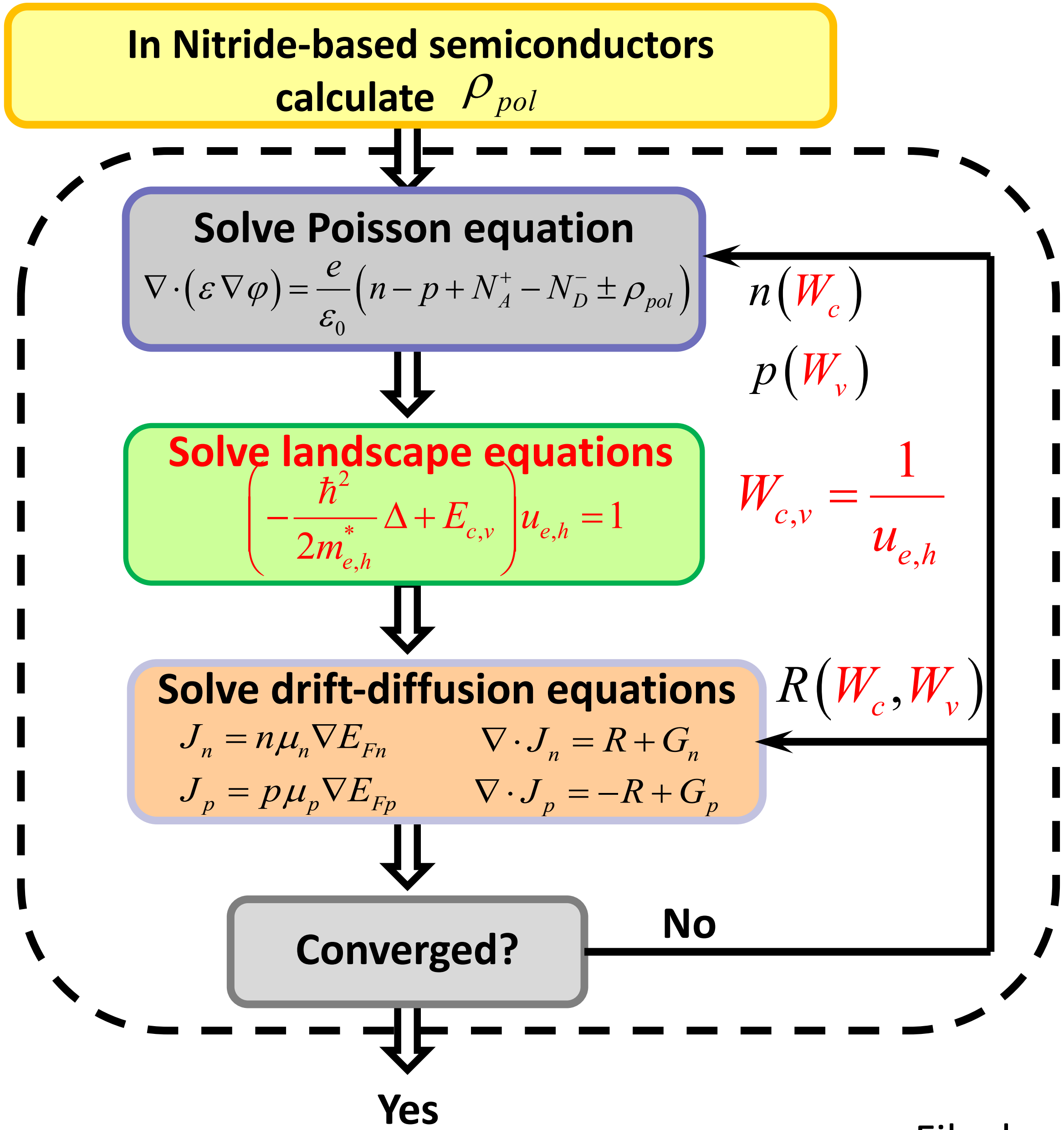
$\varphi(\vec{r})$

$$div\left(\varepsilon_r(\vec{r})\vec{\nabla}\varphi\right) = \frac{q}{\varepsilon_0}\left(n - p + N_A^+ - N_D^-\right)$$

Carrier densities

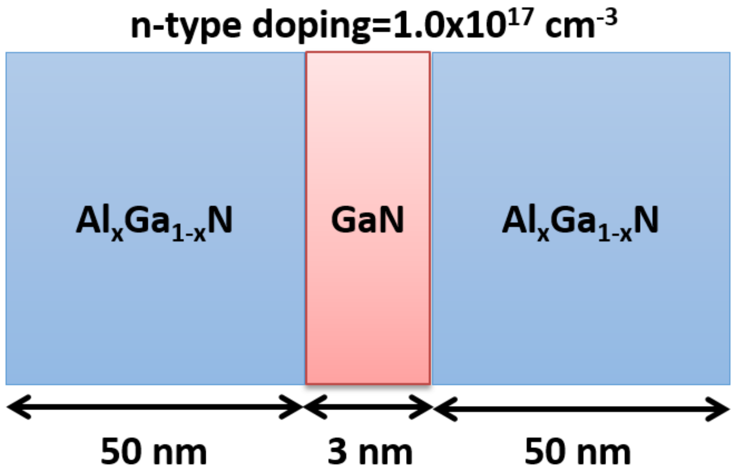
$n(\vec{r}), p(\vec{r})$

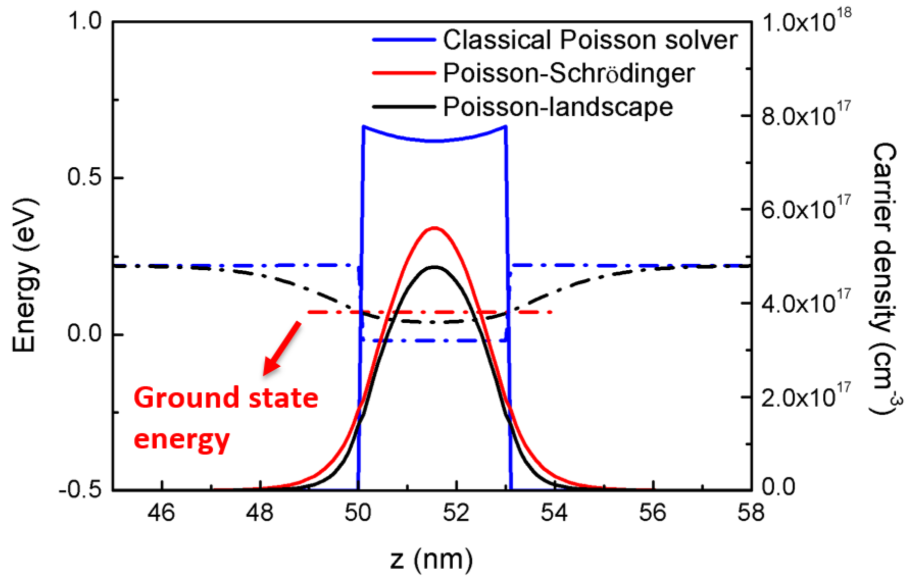
The new self-consistent scheme



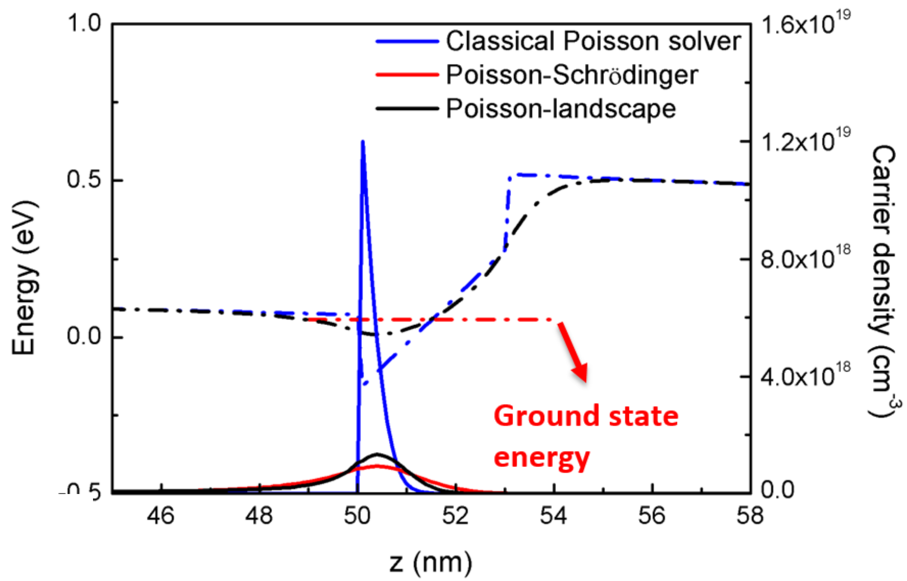
Filoche et al., *PRB* 2017

Carrier distribution in one quantum well

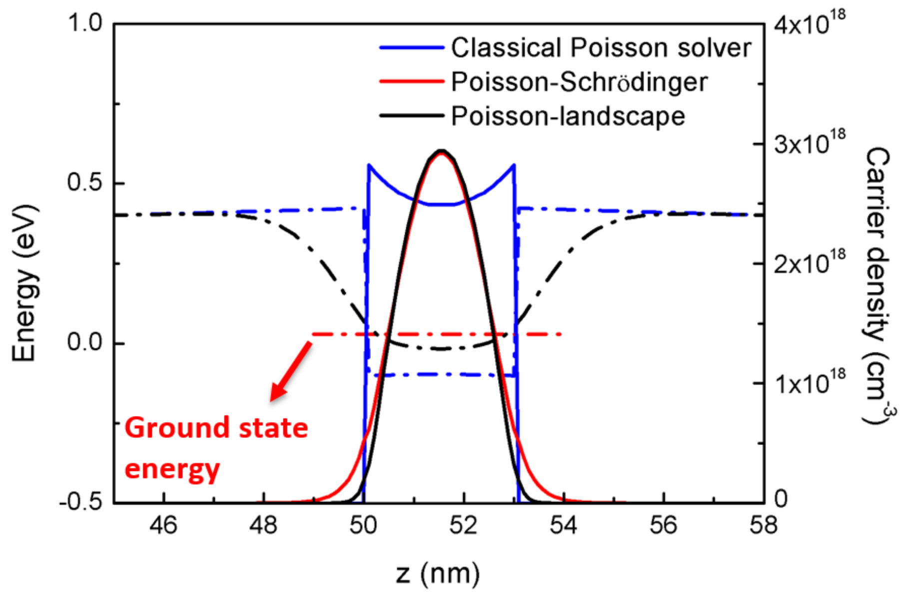




m-plane, x=0.2

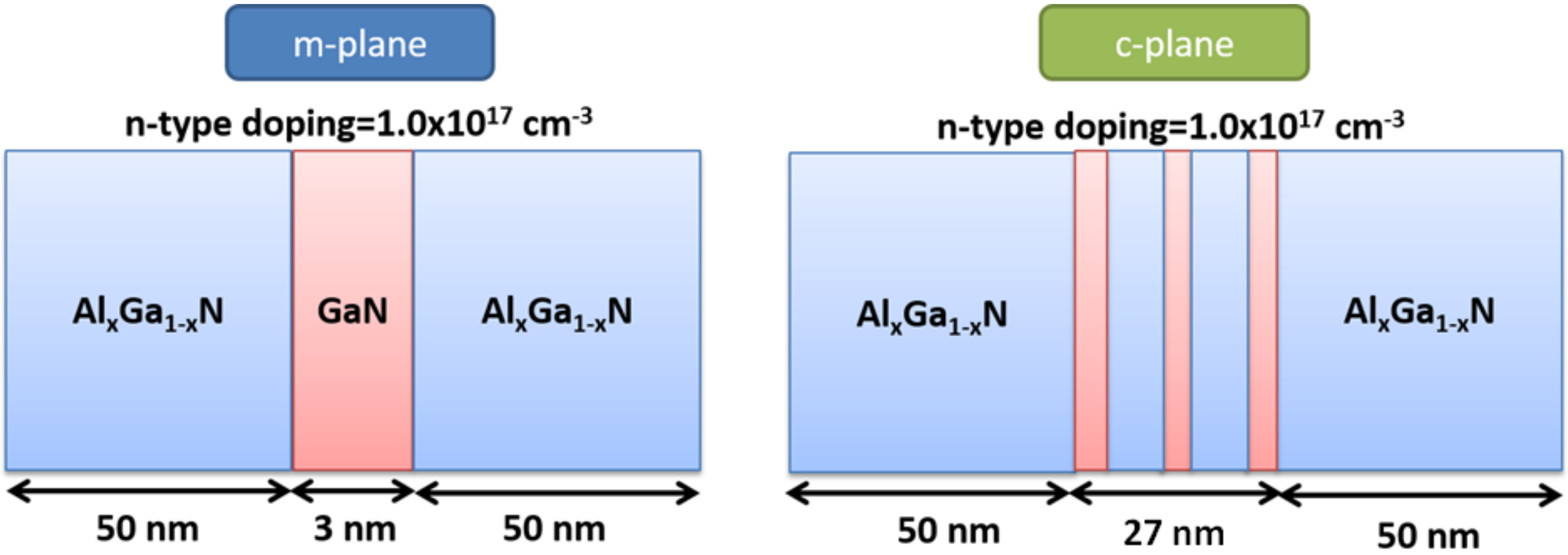


c-plane, x=0.2

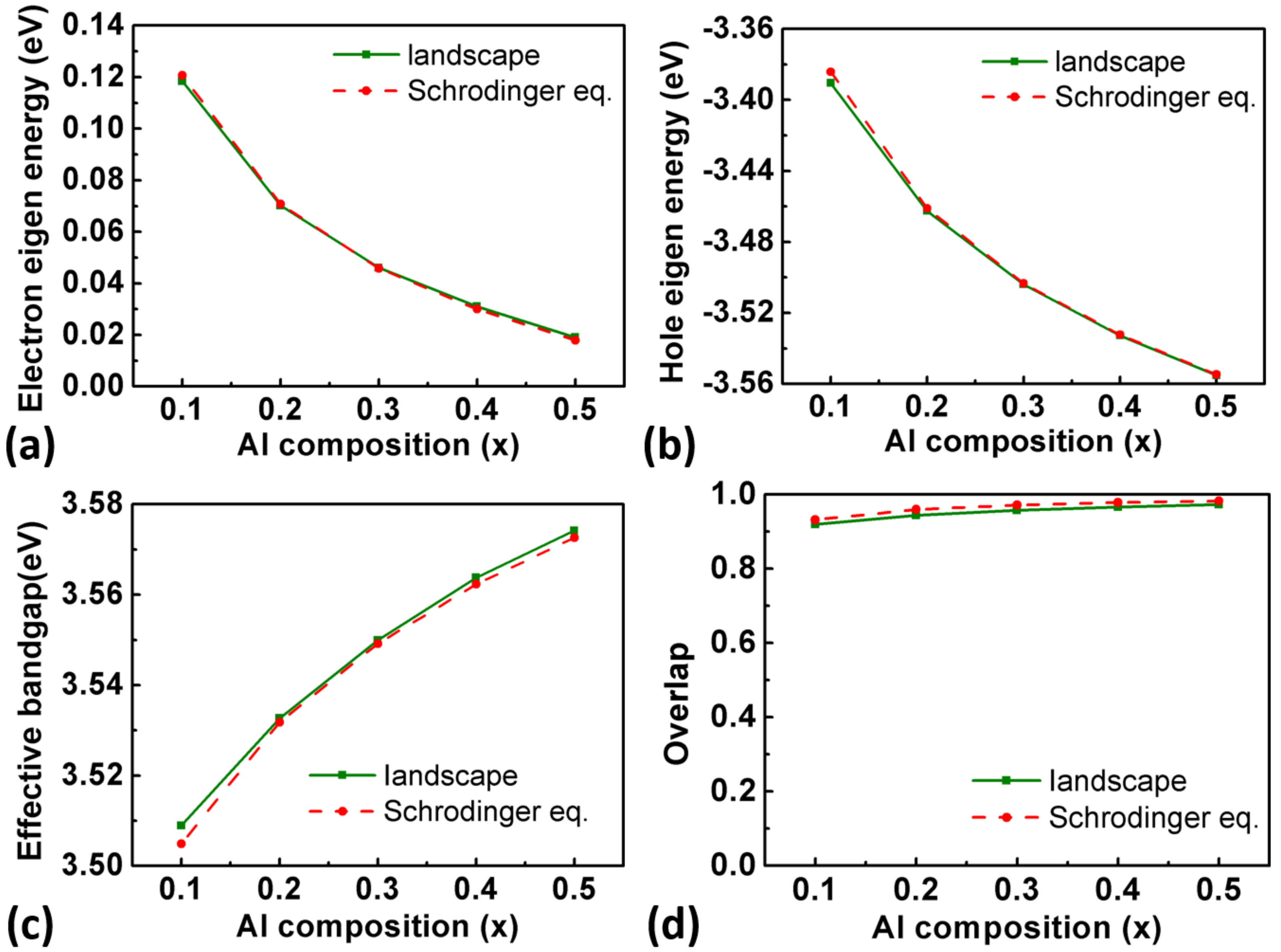


m-plane, x=0.4

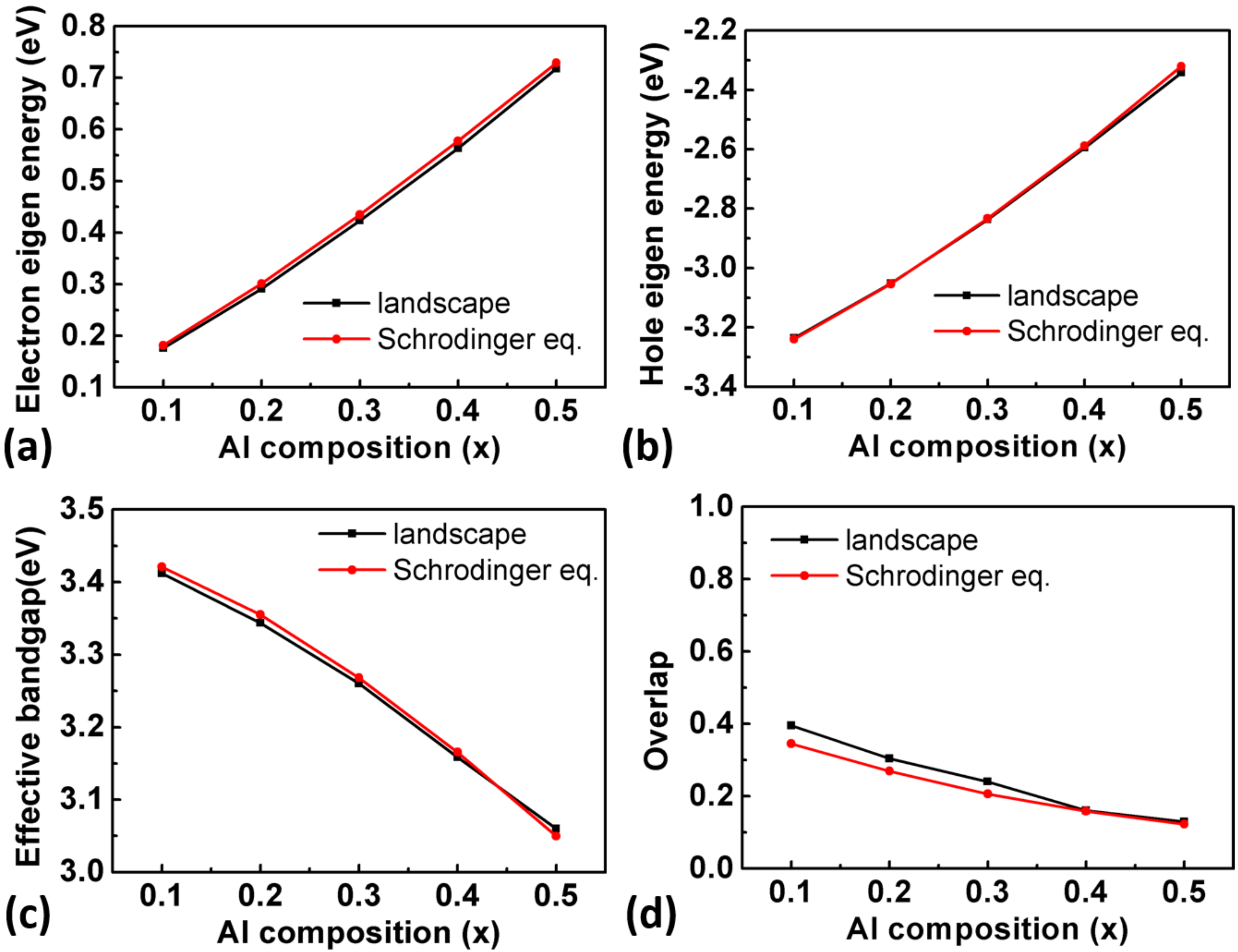
m-plane and c-plane quantum well structures



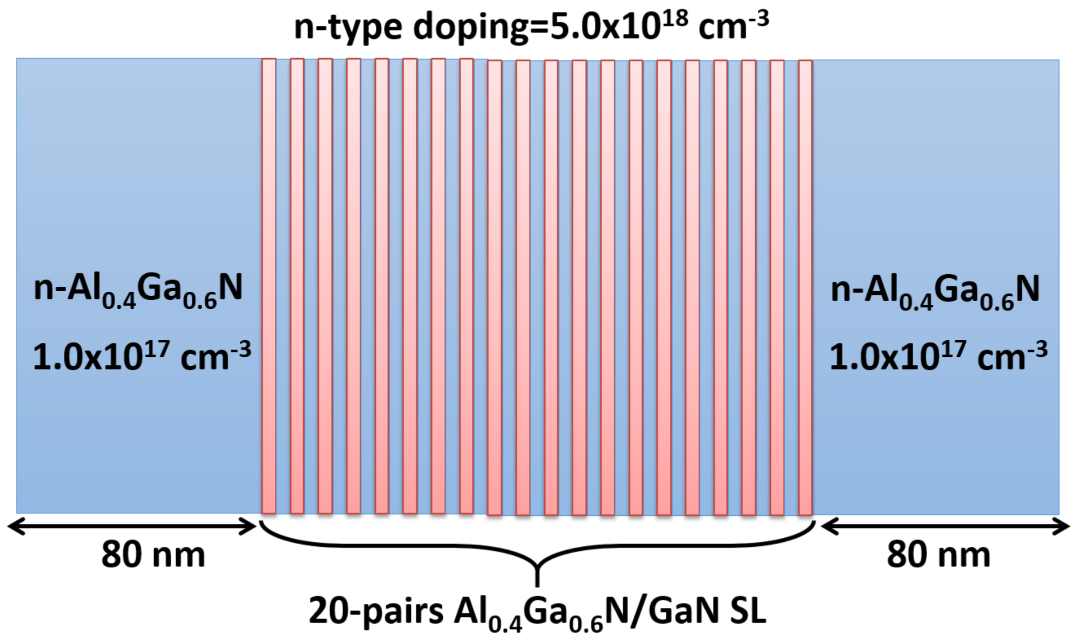
Fundamental energies and overlap (1 QW, m-plane)

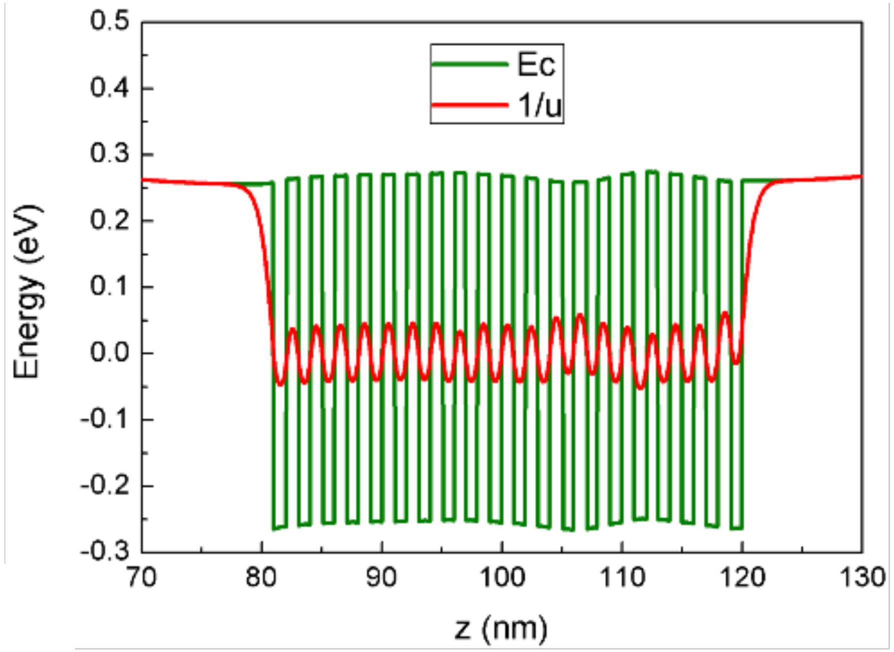


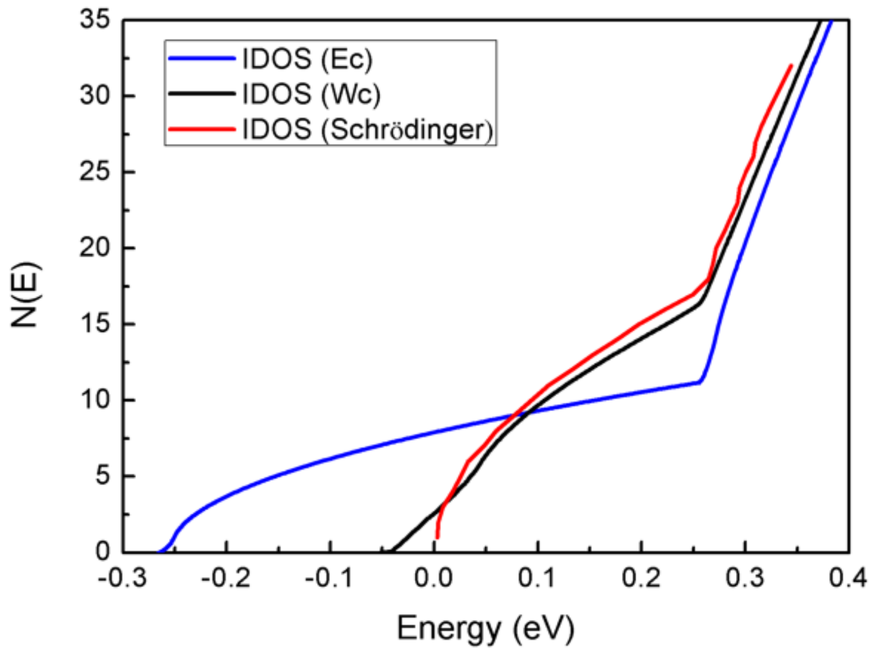
Fundamental energies and overlap (3 QW, c-plane)



Periodic superlattices

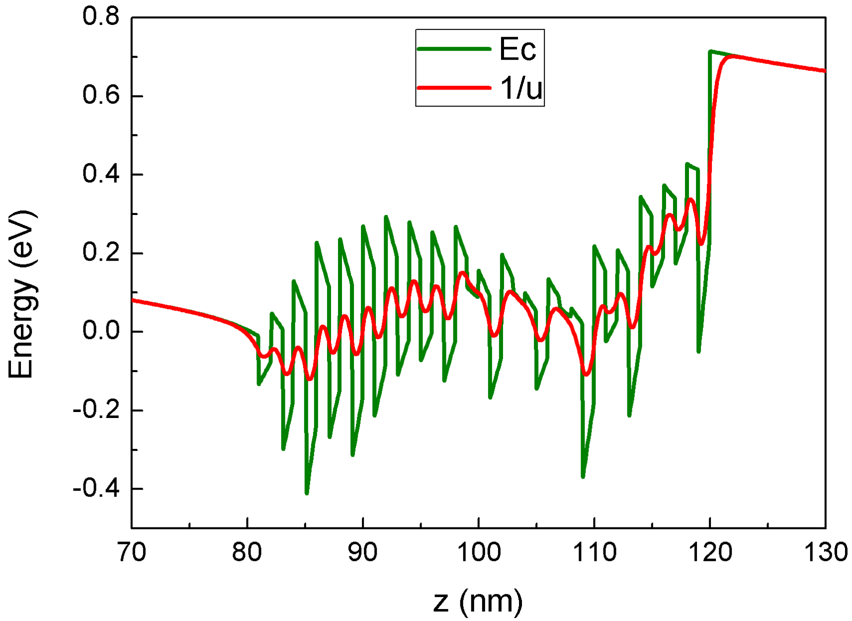


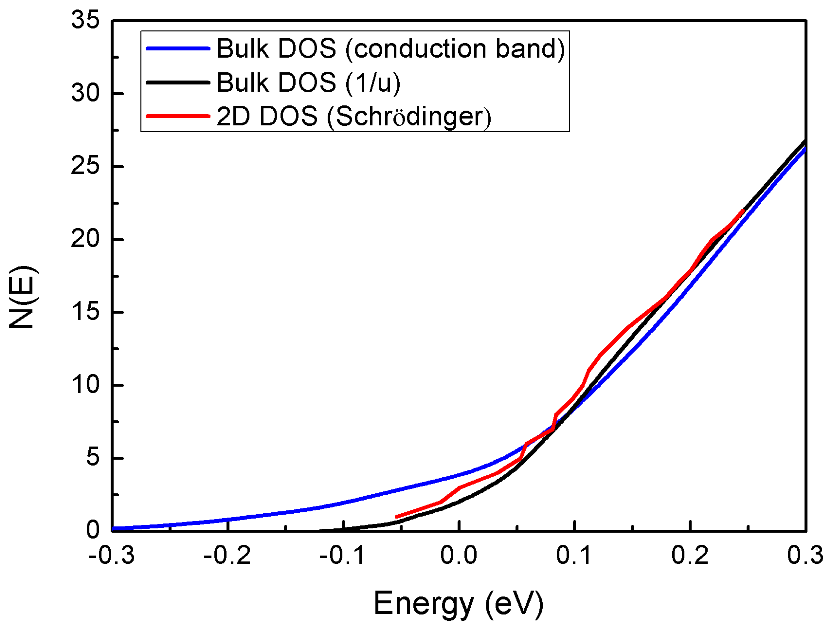




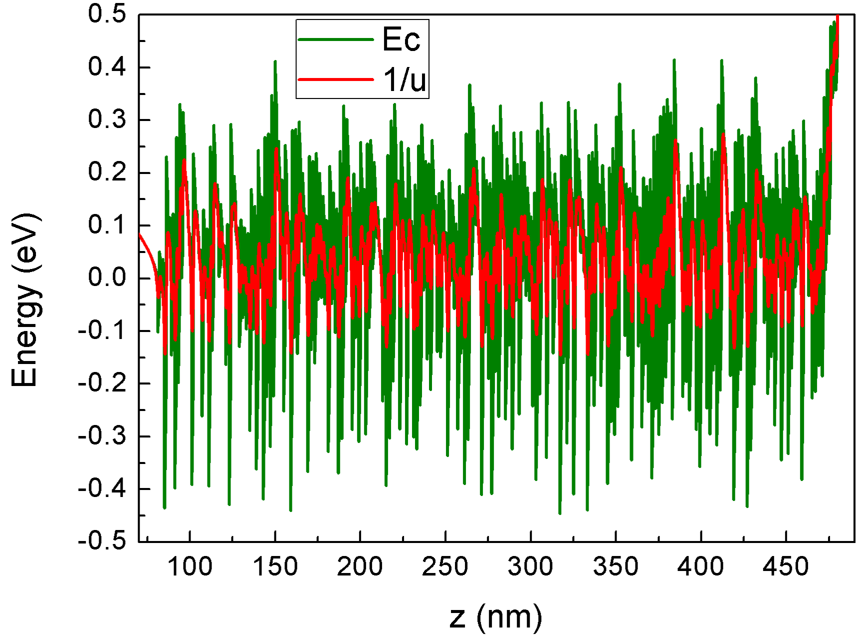
Disordered superlattices

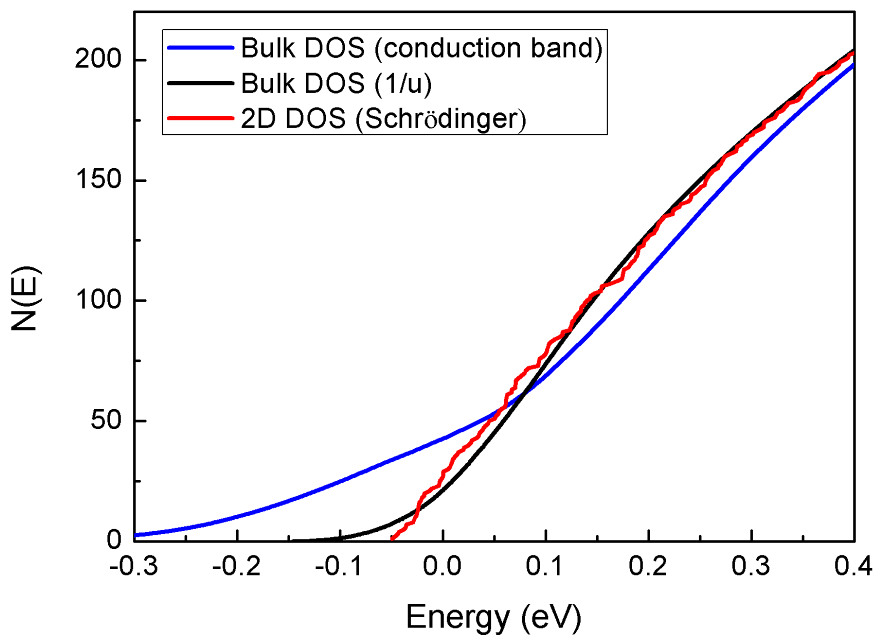
20-pairs SL



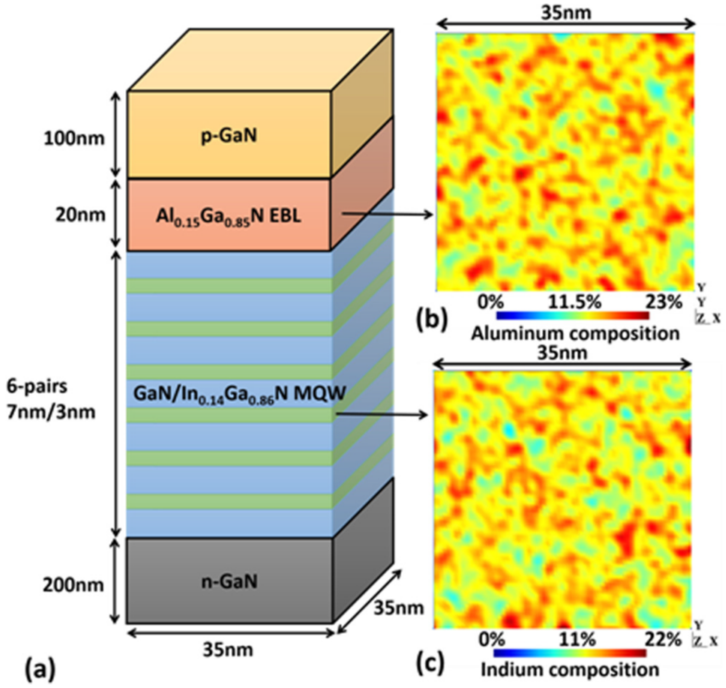


200-pairs SL





Large-scale numerical simulations



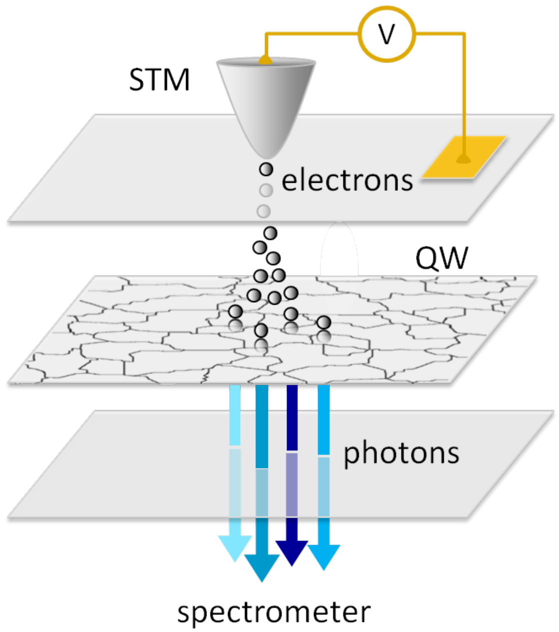
Li et al., *Phys. Rev. B* 2017

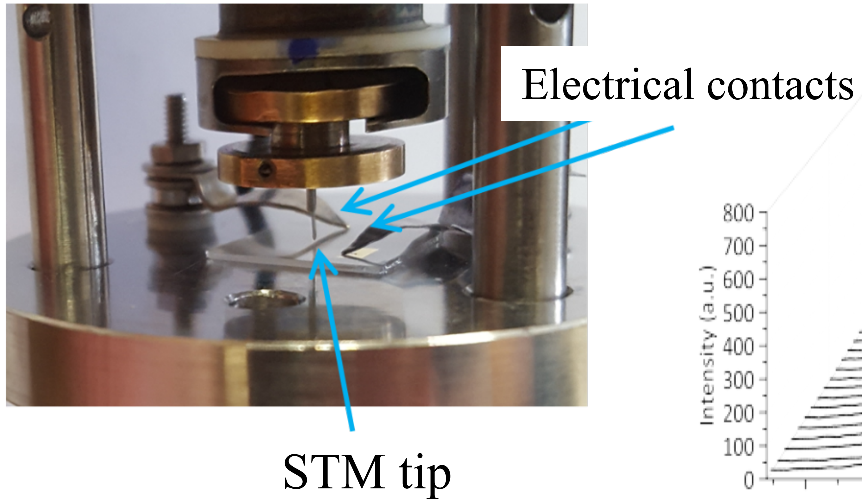
C. Weisbuch Yuh-Renn Wu S. Nakamura

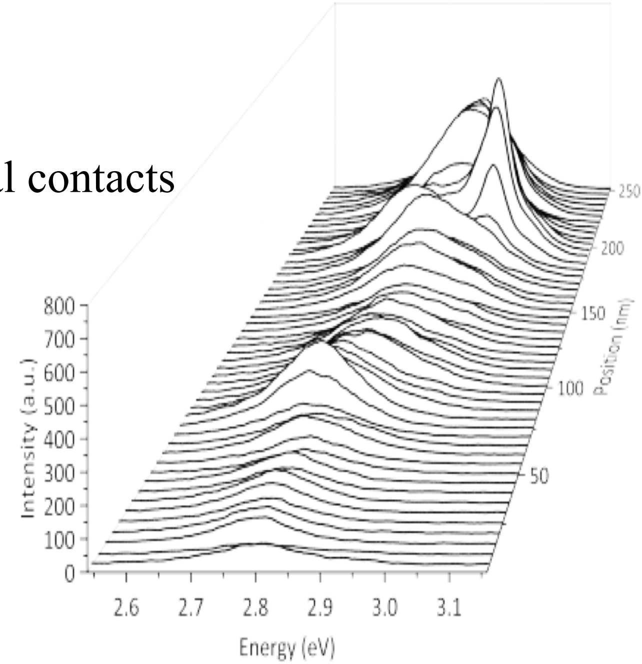
	Node number (matrix size)	Computation time (s)
Poisson	428 655	25
Drift diffusion	428 655	50
Localization landscape	428 655	50
Schrödinger	428 655	63 650
Refs. [14,62]	1 500 000	60 000
Ref. [20]	328 000	7500
Ref. [21]	100 000	24 000

With the landscape, large-scale numerical simulations accounting for quantum effects on the entire structure are now **feasible**!

We observe the landscape at the nanometer scale!

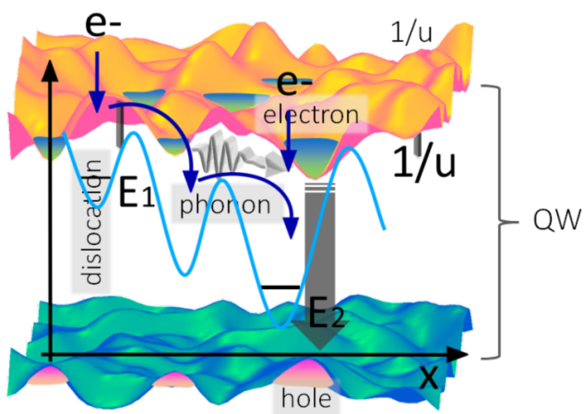


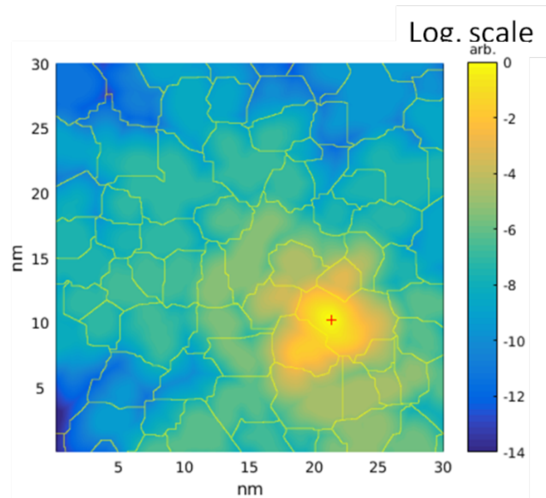




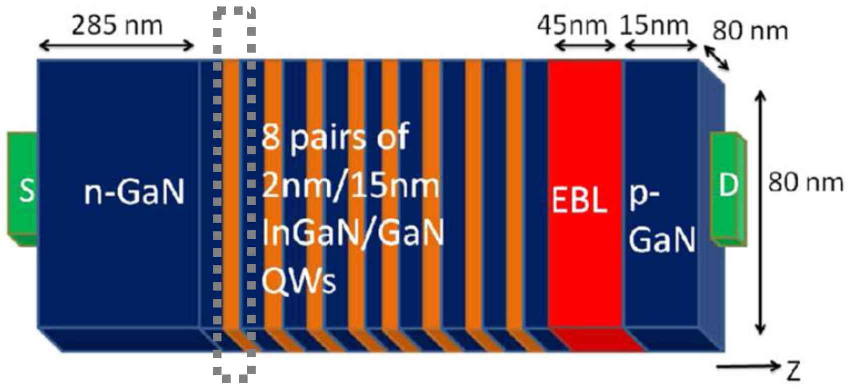
Hahn *et al.*, *PRB* **98**, 045305 (2018)

Luminescence spectra show the transitions between localized states

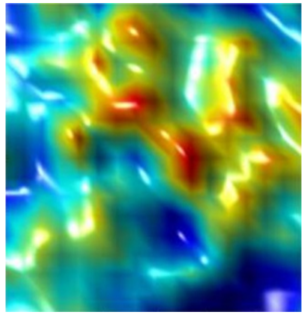




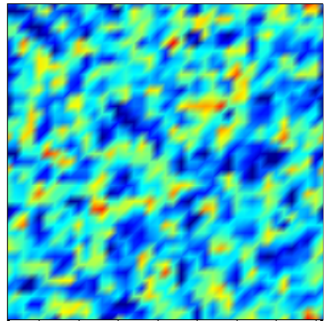
Localization in GaN-based Multi-Quantum Well Light Emitting Diodes



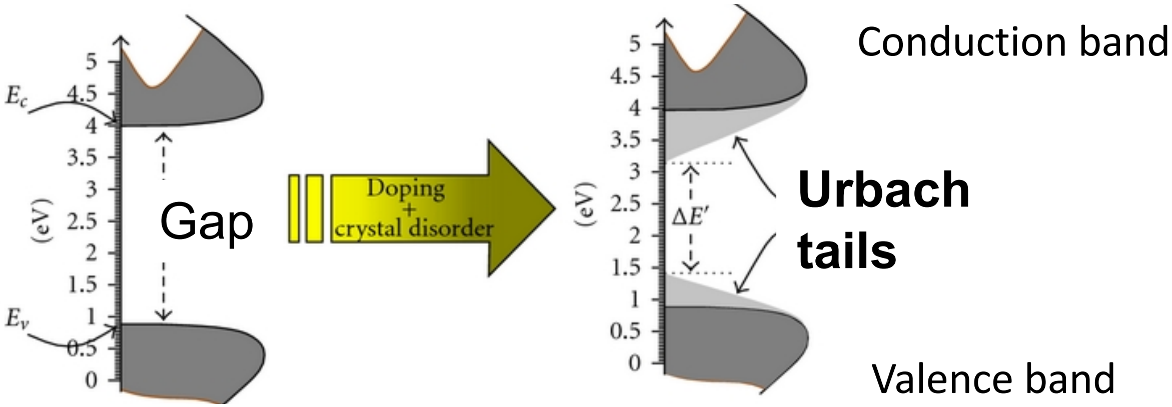
Indium map



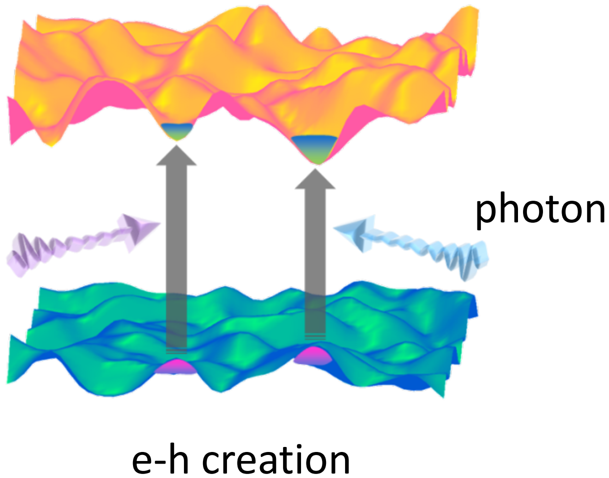
E_c map



Characterizing disorder in InGaN layers by absorption

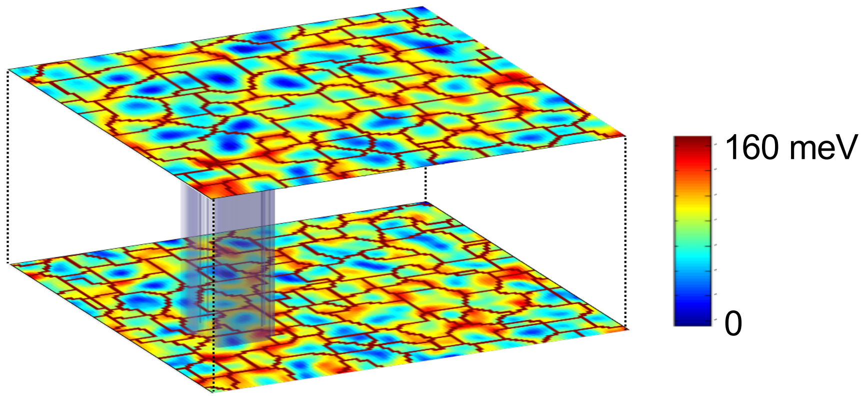


Absorption process

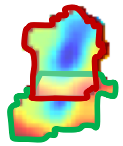


Quantum well absorption in InGaN with random alloy fluctuations

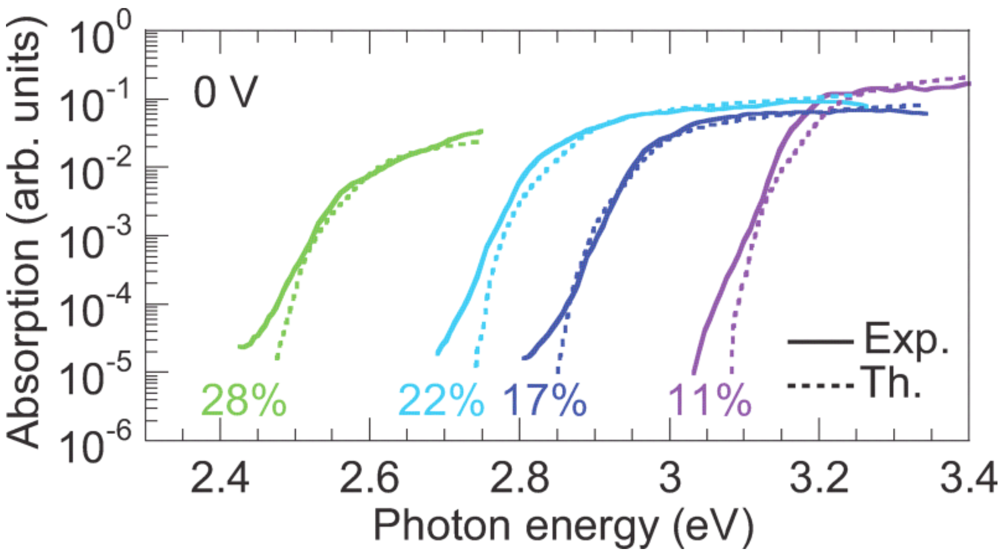
2D cut plane for 3D landscape in QW



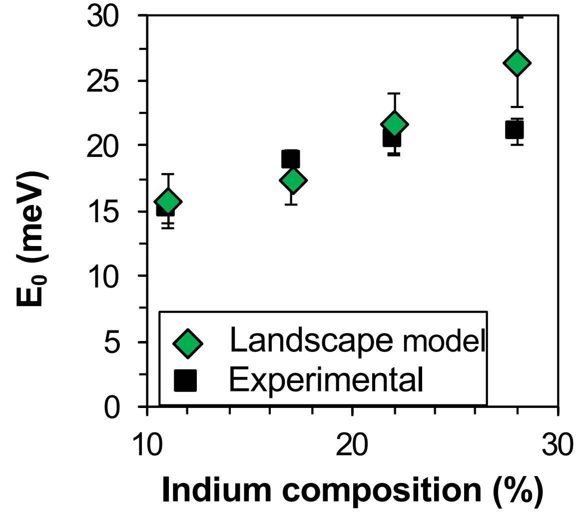
Overlap of regions of $1/u_c$ and $1/u_v$



Classical transport model cannot compute overlap!



Slope comparison

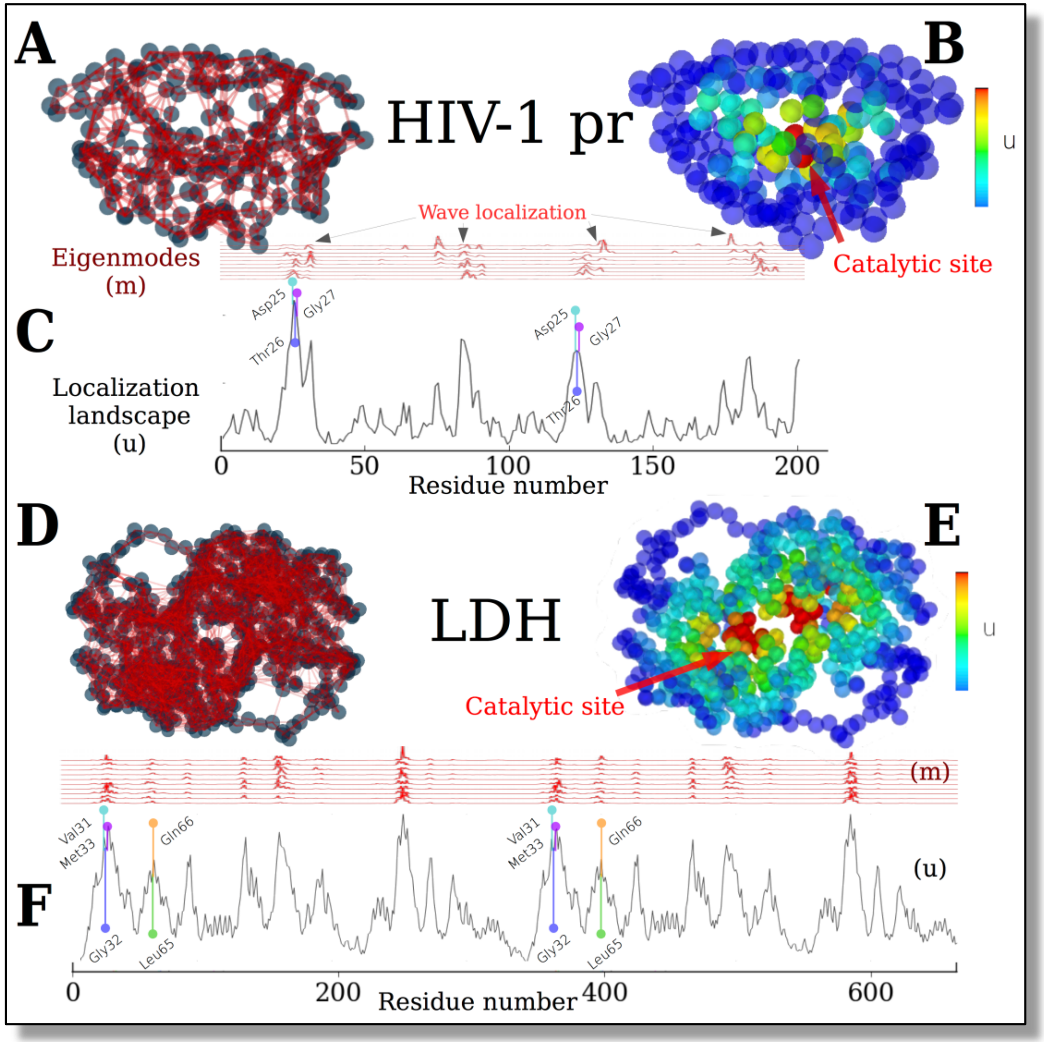


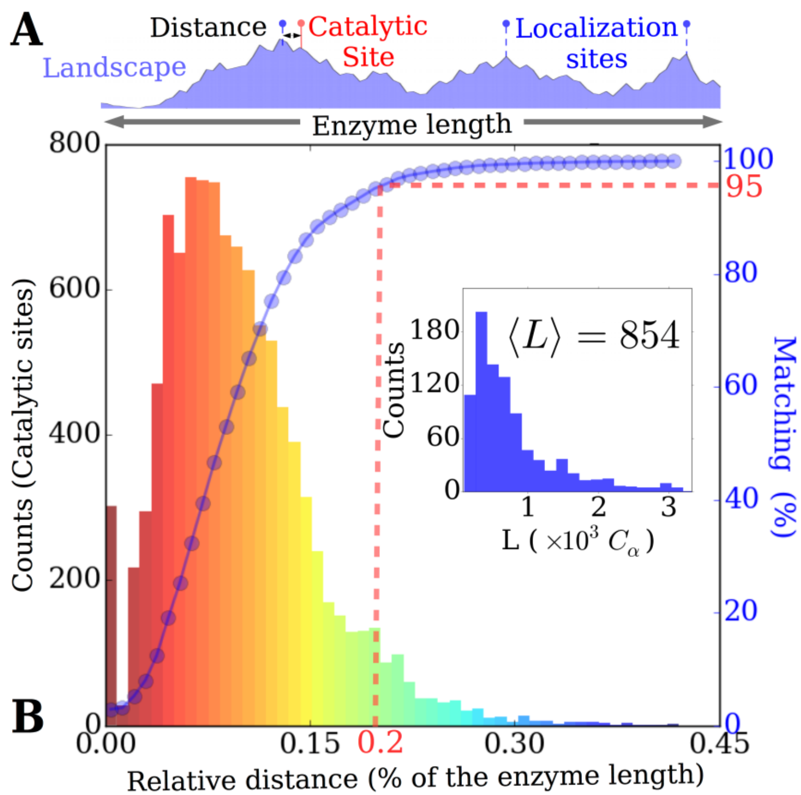
Piccardo et al., *PRB* 2017

Li et al., *PRB* 2017

Enzyme proficiency

Enzyme catalytic sites are hot-spots of localized vibrations





Chalopin et al., submitted

Localization landscape for Dirac fermions

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[2] *Institute of Theoretical Physics, Warsaw University, Hoża 69, 00–681 Warsaw, Poland*

(Dated: November 2019)

In the theory of Anderson localization, a landscape function predicts where wave functions localize in a disordered medium, without requiring the solution of an eigenvalue problem. It is known how to construct the localization landscape for the scalar wave equation in a random potential, or equivalently for the Schrödinger equation of spinless electrons. Here we generalize the concept to the Dirac equation, which includes the effects of spin-orbit coupling and allows to study quantum localization in graphene or in topological insulators and superconductors. The landscape function $u(\boldsymbol{r})$ is defined on a lattice as a solution of the differential equation $\overline{H}\,u(\boldsymbol{r})=1$, where $\overline{H}$ is the Ostrowsky comparison matrix of the Dirac Hamiltonian. Random Hamiltonians with the same (positive definite) comparison matrix have localized states at the same positions, defining an equivalence class for Anderson localization. This provides for a mapping between the Hermitian and non-Hermitian Anderson model.

Introduction — The localization landscape is a new tool in the study of Anderson localization, pioneered in 2012 by Filoche and Mayboroda [1], which has since stimulated much computational and conceptual progress [2–10]. The "landscape" of a Hamiltonian H is a function $u(\boldsymbol{r})$ that provides an upper bound for eigenstates ψ at energy $E>0$:

$$|\psi(\boldsymbol{r})|/|\psi|_{\max} \leq E\,u(\boldsymbol{r}),\;\; |\psi|_{\max} = \max_{\boldsymbol{r}}|\psi(\boldsymbol{r})|. \tag{1}$$

This inequality implies that a localized state is confined to spatial regions where $u \gtrsim 1/E$. Extensive numerical simulations [8] confirm the expectation that higher and higher peaks in u identify the location of states at smaller and smaller E.

Such a predictive power would be unremarkable for particles confined to potential wells (deeper and deeper wells trap particles at lower and lower energies). But Anderson localization happens because of wave interference in a random "white noise" potential, and inspection of the potential landscape $V(\boldsymbol{r})$ gives no information on the localization landscape $u(\boldsymbol{r})$.

Filoche and Mayboroda considered the localization of scalar waves, or equivalently of spinless electrons, governed by the Schrödinger Hamiltonian $H=-\nabla^2+V$. They used the maximum principle for elliptic partial differential equations to derive [1] that the inequality (1) holds if $V>0$ and u is the solution of

$$[-\nabla^2+V(\boldsymbol{r})]u(\boldsymbol{r})=1. \tag{2}$$

Our objective here is to generalize this to spinful electrons, to include the effects of spin-orbit coupling and study localization of Dirac fermions.

Construction of the landscape function — Our key innovation is to use Ostrowski's comparison matrix [11–14] as a general framework for the construction of a localization landscape on a lattice. By definition, the comparison

In our context the index $n=1,2,\ldots$ labels both the discrete space coordinates as well as any internal (spinor) degrees of freedom. The comparison theorem [11] states that if the comparison matrix is positive-definite, then [15]

$$|H^{-1}| \leq \overline{H}^{\,-1}, \tag{4}$$

where both the absolute value and the inequality is taken elementwise.

We apply Eq. (4) to an eigenstate Ψ of H at energy E,

$$\begin{aligned}|E^{-1}\Psi_n| &= |(H^{-1}\Psi)_n| \leq \textstyle\sum_m \big|(H^{-1})_{nm}\big||\Psi_m| \\ &\leq |\Psi|_{\max}\textstyle\sum_m \big(\overline{H}^{\,-1}\big)_{nm},\end{aligned} \tag{5}$$

with $|\Psi|_{\max}=\max_n|\Psi_n|$. We thus arrive at the desired inequality

$$|\Psi_n|/|\Psi|_{\max} \leq |E|\textstyle\sum_m \big(\overline{H}^{\,-1}\big)_{nm} \equiv |E|\,u_n. \tag{6}$$

The elements u_n of the landscape function are determined by a set of linear equations with coefficients given by the comparison matrix:

$$\overline{H}\,u=1 \Leftrightarrow \textstyle\sum_m \overline{H}_{nm}u_m=1,\;\; n=1,2,\ldots N. \tag{7}$$

As a sanity check, we make contact with the original landscape function [1] for the Schrödinger Hamiltonian $H_{\rm S}=p^2/2m+V$, with $V>0$. The Laplacian is discretized in terms of nearest-neighbor hoppings on a lattice. For each dimension

$$\begin{aligned}&p^2 \mapsto (\hbar/a)^2(2-2\cos ka) \Rightarrow \\ &(H_{\rm S})_{nm} = t_0(2\delta_{nm}-\delta_{n-1,m}-\delta_{n+1,m})+V_n\delta_{nm},\end{aligned} \tag{8}$$

with lattice constant a and hopping matrix element $t_0=\hbar^2/2ma^2$. The comparison matrix $\overline{H}_{\rm S}$ is equal to $H_{\rm S}$ and is positive-definite, so that Eq. (7) is a discretized version of the original landscape equation $H_{\rm S}u=1$ [1, 16].

Conclusions

- One mathematical object, the **localization landscape**, contains most of the information about the localization of stationary states in complex or **disordered** systems. It is obtained by solving **one single linear problem**:

$$\boxed{Lu = 1}$$

- It predicts the localization **subregions**, the localization **energies**, and the transition towards more extended states.

- The landscape also approximates the shape of the **fundamental eigenfunction** in each localization region.

- **W=1/u** can be understood as an **effective confining potential** that is experienced by the eigenstates.

- This new potential can be used to compute the **density of states** and assess the **long range decay** of the states.

- Quantum **transport** (hopping) is currently under study.

Challenges

- **Theory**: proving mathematically the $1/u$-Weyl's law, the quality of the approximation.
  - Anderson localization (high energy modes) at lower dimension
  - handling complex operator (magnetic), vector waves (electromagnetic), interactions (landscape in higher dimension)
  - Quantum transport
- **Cold atoms**:
  - Spectral functions, prediction of the **mobility edge**
- **Nitride-based semiconductors**:
  - **Green gap**, **Droop**, design
- **Organic semiconductors**:
  - Coulomb interaction, model efficiently the **dynamics of scales**.
- **Proteins**:
  - proving the **chemical role** of phonon localization.
- **Electromagnetic waves**:
  - Localization near band gaps, “quantum simulator”

Open Post-doc position now!

marcel.filoche@polytechnique.fr

Aim: **Modeling and numerical simulation of quantum transport in disordered semiconductors (GaN-based) using the landscape theory**

Team: Physique de la Matière Condensée, Ecole Polytechnique

Skills:

- Wave equations
- Statistical physics – semiconductor physics
- Applied Mathematics. Partial Differential Equations
- Programming (C, C++, Fortran, Matlab)
- Scientific writing

Collaborations:

- University of California at Santa Barbara
- National Taiwan University
- Université de Genève
- University of Minnesota