Localisation and finite-size effects in graphene flakes

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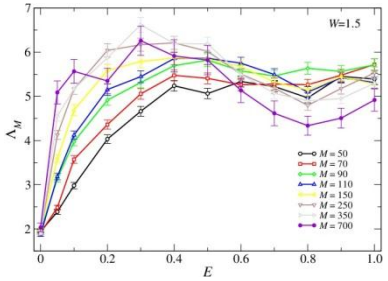
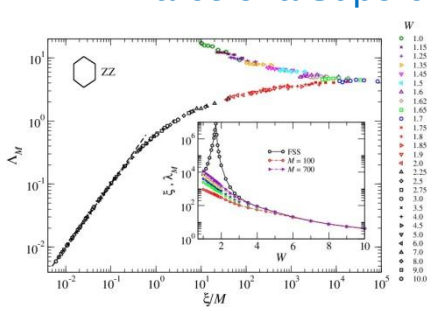
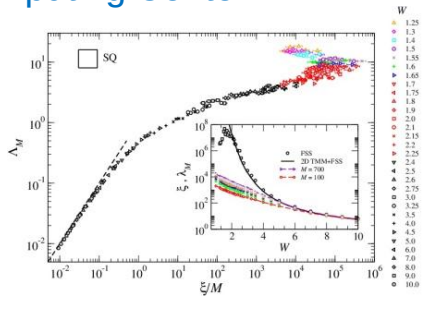
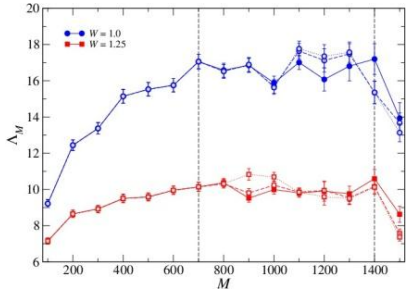








EPL 104, 17012-6 (2013)

The Anderson transition:

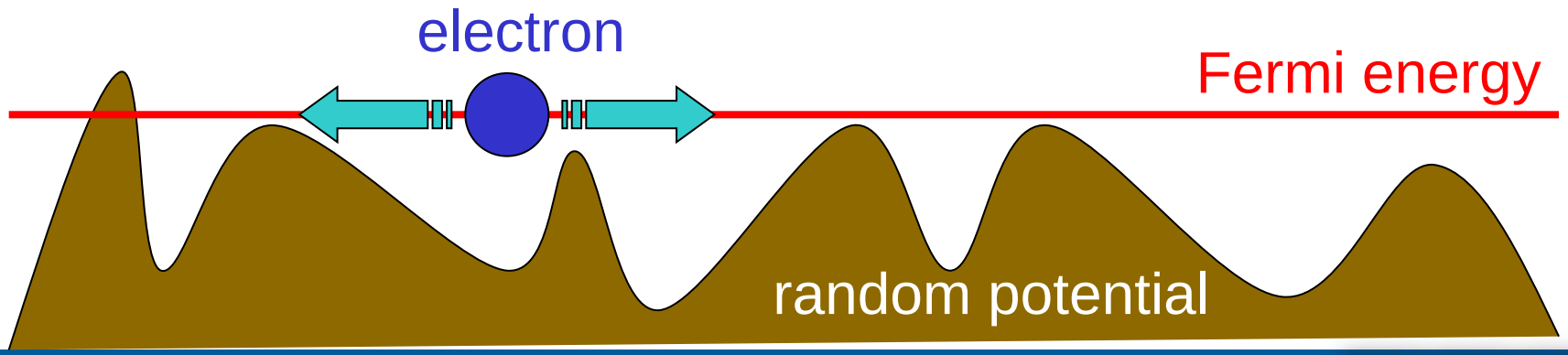
$$H\psi = E_0\psi$$

- PW Anderson 1958:

$$H = \sum_{\text{atoms } i} \varepsilon_i |i\rangle\langle i| - \sum_{\text{neighbor atoms } i,j} t_{ij} |i\rangle\langle j|$$

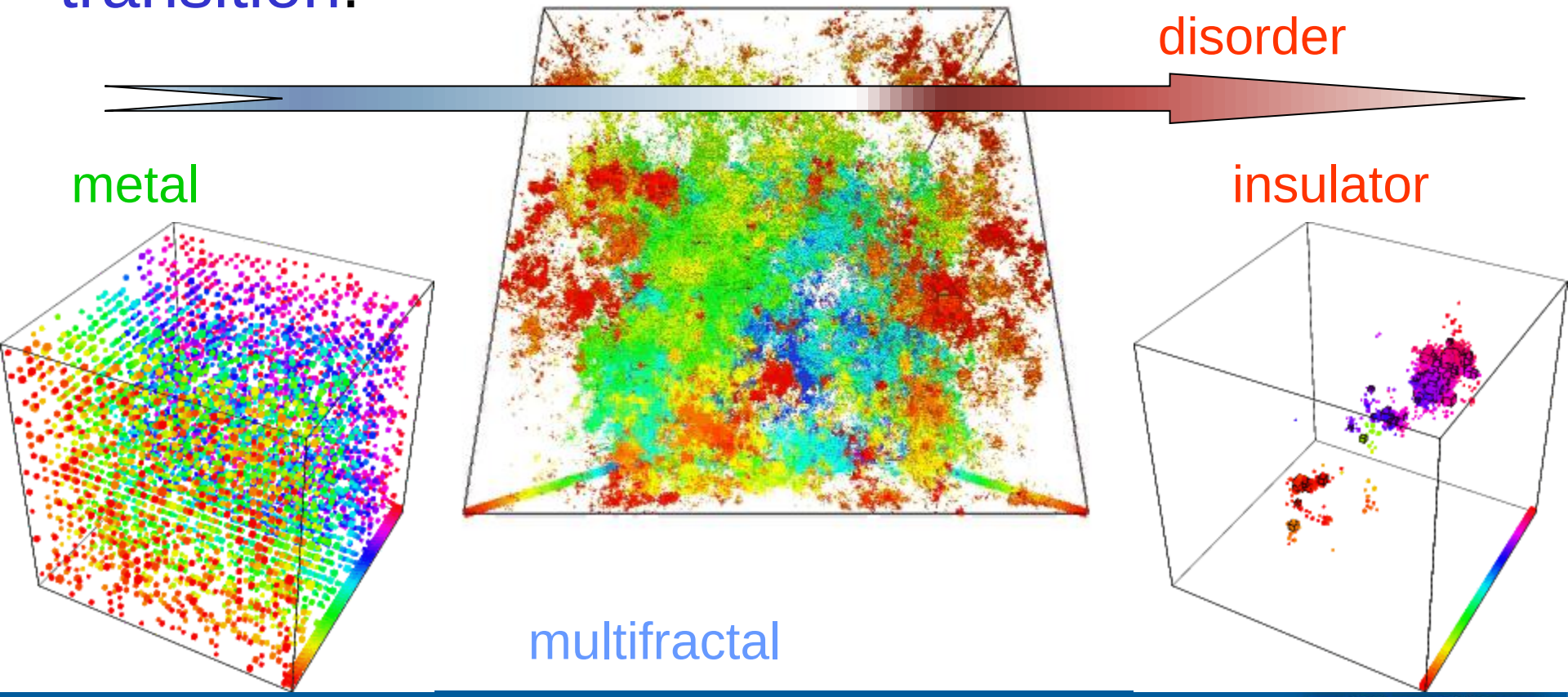
potential energy kinetic energy

localisation movement



An MIT due to disorder-induced quantum interference:

- Adding disorder to a quantum model of non-interacting electrons gives a metal-insulator transition:



Visualizing the MIT:

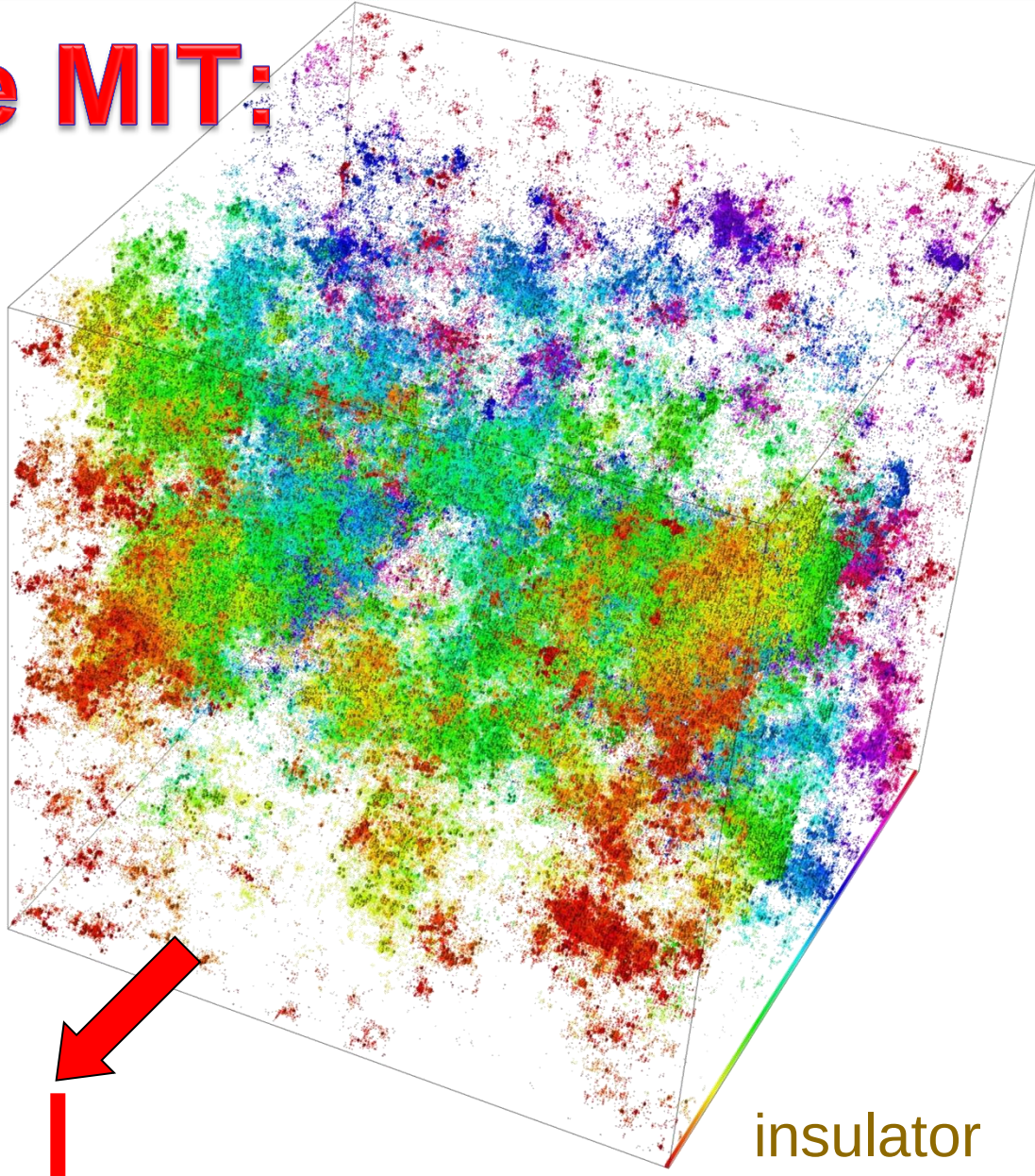
- Critical, $W=W_c$

  a **multifractal**

Calculation for a cubic system of matrix size

15,625,000 times
15,625,000

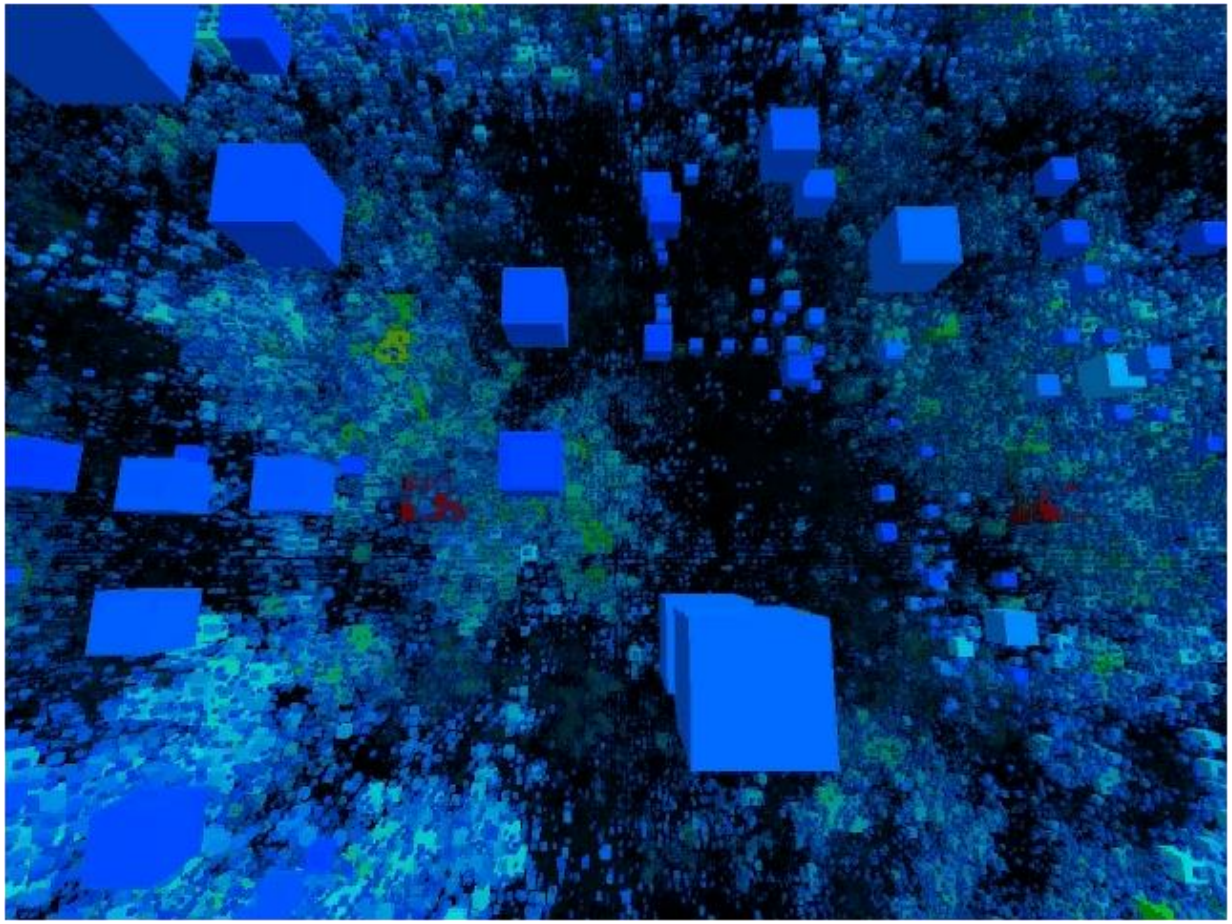
"On Large Scale Diagonalization Techniques for the Anderson Model of Localization", O. Schenk, M. Bollhöfer, R. A. Römer, accepted for publication in SIAM J. Sci. Comp., (2005); math.NA/0508111.



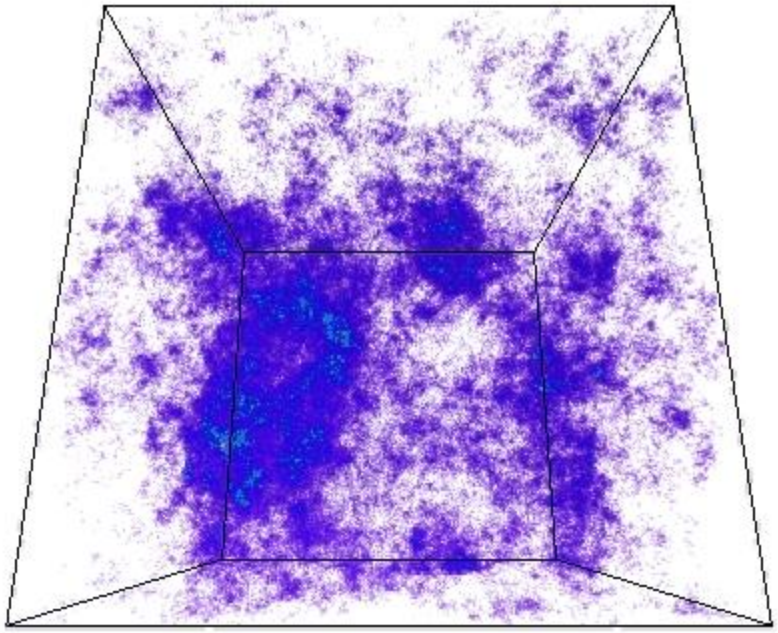
metal

insulator

Flying thru a multifractal



Flying thru a multifractal



DOS and two transitions

- metal

$W > W_c, |E| > E_c$

ψ extended

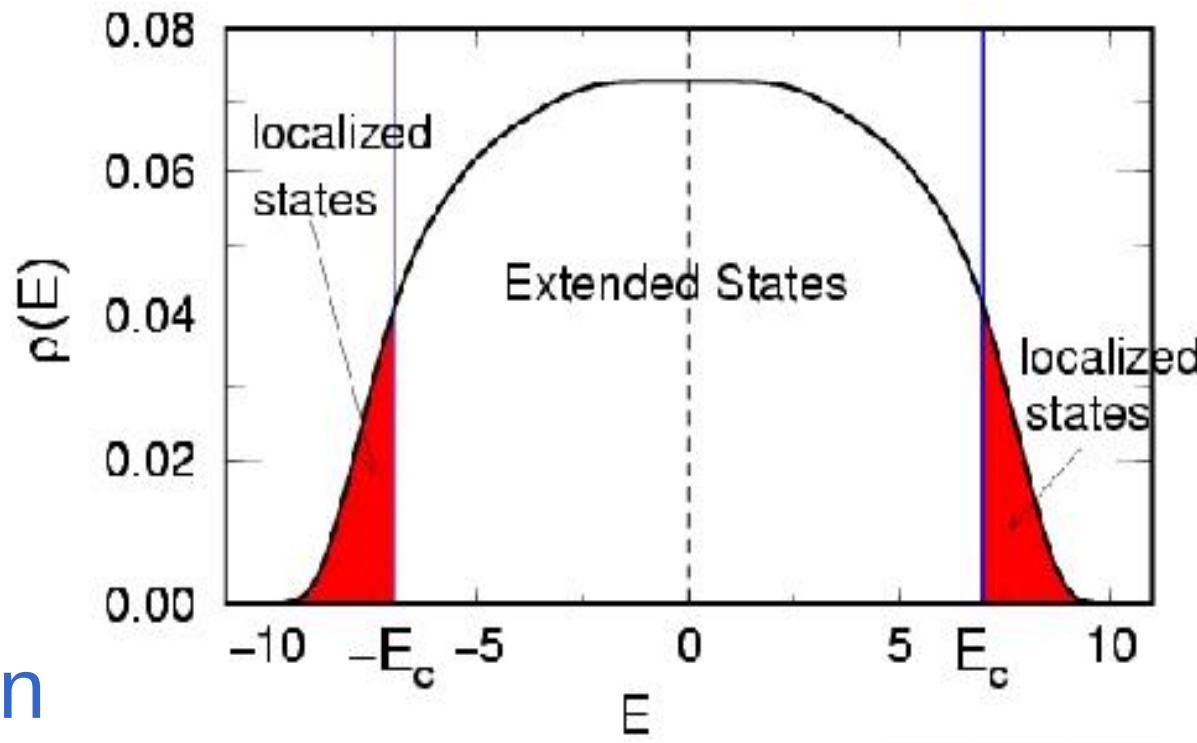
- insulator

$W < W_c, |E| < E_c$

ψ localized

- energy transition
- disorder transition

- $W = W_c, |E| = E_c$ ψ critical



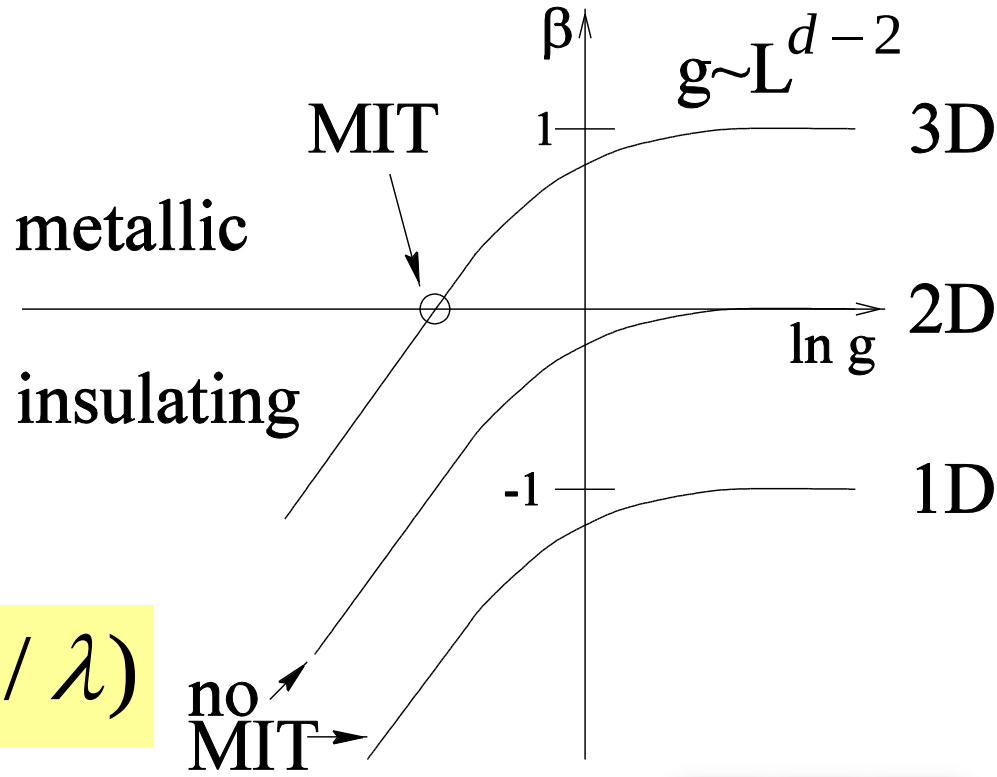
Scaling hypothesis

[Abrahams et al., PRL 42, 673 (1979)]

- conductance $g(L)$
- beta-function

$$\beta = \frac{d \ln g}{d \ln L}$$

$$g_{\text{metal}}(L) \sim L^{d-2}$$



- no MIT in 1D,2D with

$$g_{\text{insulator}}(L) \sim \exp(-L/\lambda)$$

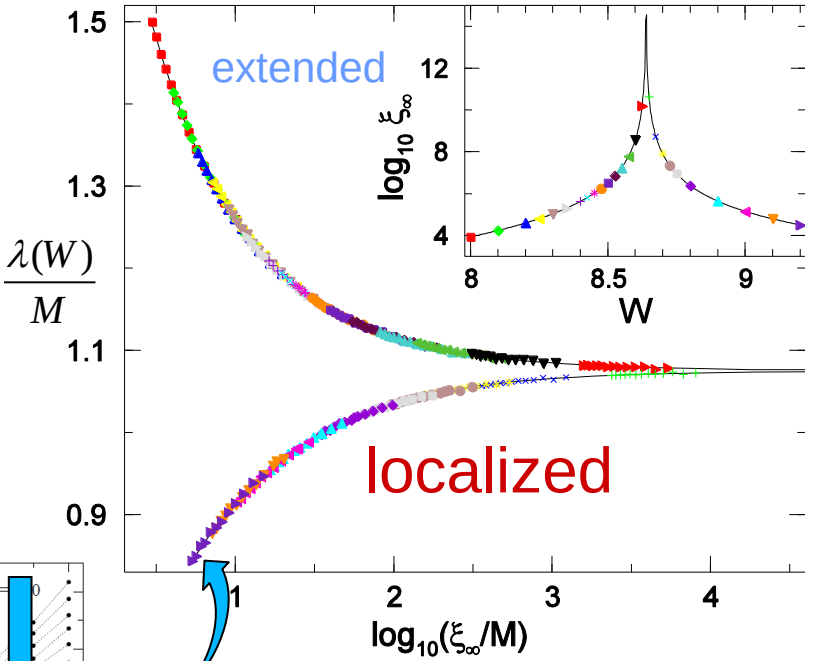
Scaling functions

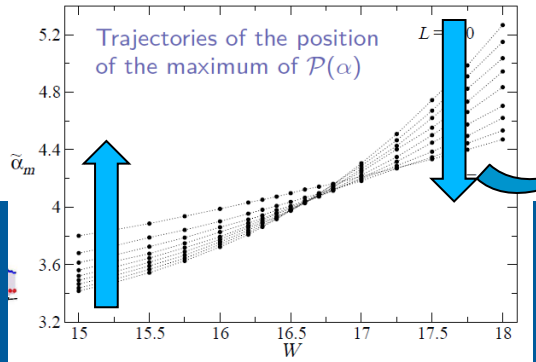
$$\frac{\lambda(W)}{L} = f\left(\xi(W)/L\right)$$

- all data collapse onto a single curve
- two branches indicate
  extended
  localized behaviour

$$\xi \propto |W - W_c|^{-\nu}$$

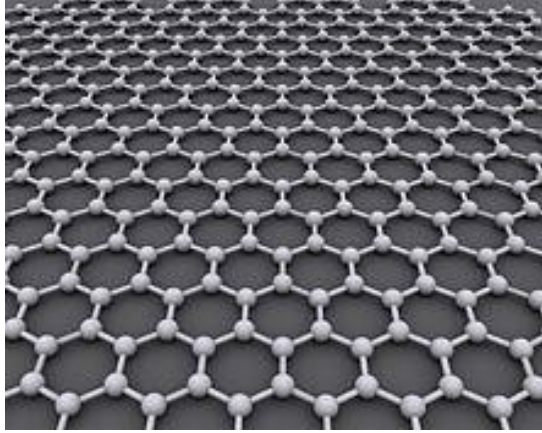
$$\xi \propto |E - E_c|^{-\nu}$$



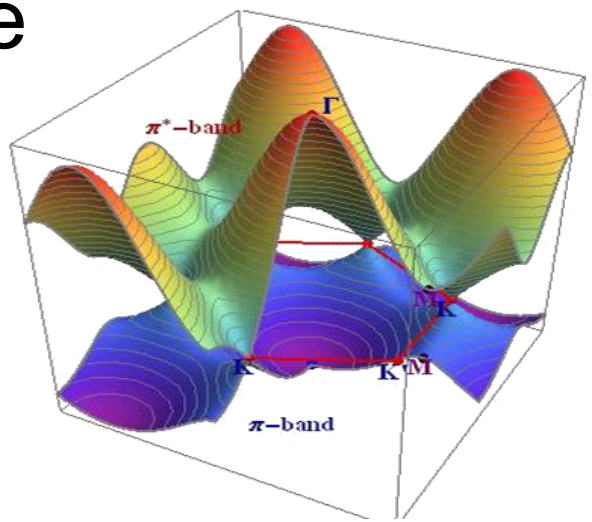


[F. Milde, RAR, M. Schreiber, V. Uski, Eur. Phys. J. B 15, 685-690 (2000).

Graphene (2D)



- allotrope of carbon (like graphite, diamond)
- Dirac-like cone at 6 points in Brilluoin zone, only 2 inequivalent ones, K and K' (hexagonal lattice is bipartite)
- Dirac cone implies ballistic transport, i.e. novel electronic properties.

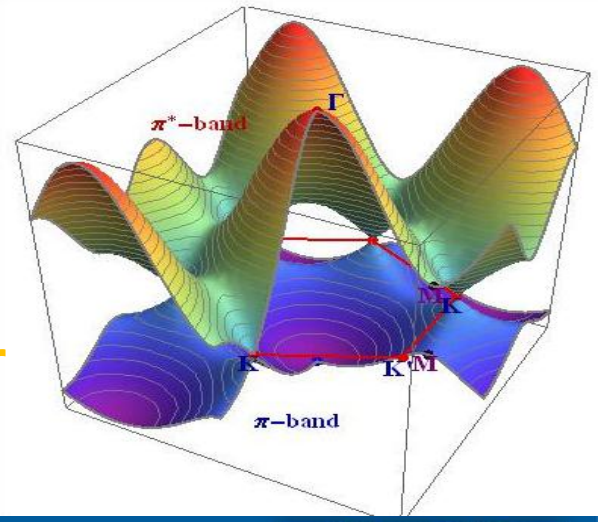


Graphene is 2D and hence localized

- E. McCann, K. Kechedzhi, V. I. Fal'ko, H. Suzuura, T. Ando, and B. L. Altshuler, PR L 97, 146805 (2006); I. L. Aleiner and K. B. Efetov, PRL 97, 236801 (2006); A. Altland, PRL. 97, 236802 (2006); Bardarson J. H., Tworzydło J., Brouwer P. W. and Beenakker C. W. J. 2007 PRL 99 106801 + ….

- G **with inter-valley** scattering due to disorder is **localized** in the large system limit:
  - **uncorrelated** Anderson on-site disorder

- G **without inter-valley** scattering is **not:**
  - **Smooth (**correlated) disorder



Graphene is 2D and hence localized

for inter-valley scattering

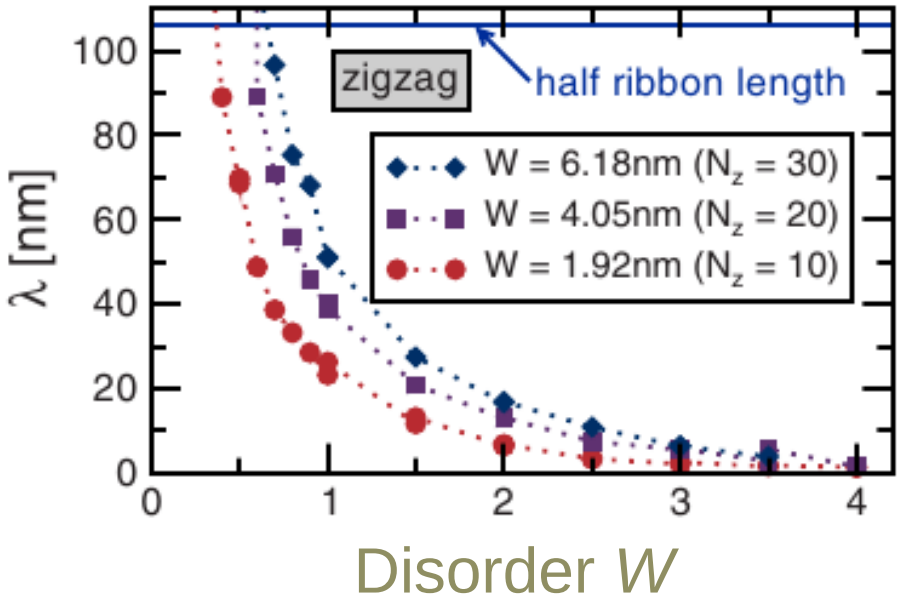
- Much num. evidence of localization in G since

Schreiber M. and Ottomeier M. 1992 J. Phys.: Condens. Matter 4 1959

$$W \geq 2$$

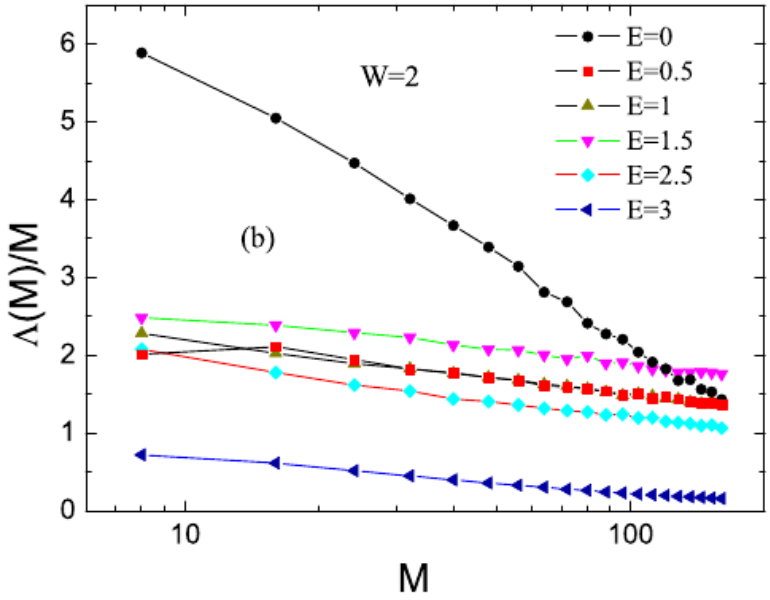
PRB 79, 235116 (2009)

Graphene nanoribbons. Local density of states. Time evolution wavefunction



PRB 76, 214204 (2009)

Bulk disorder. Anderson localization of states at E=0 and away.

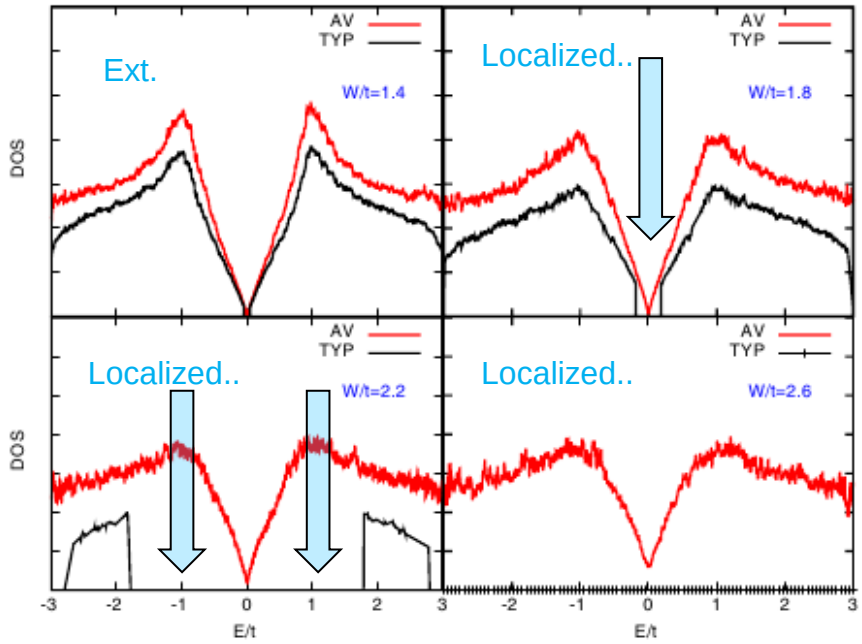


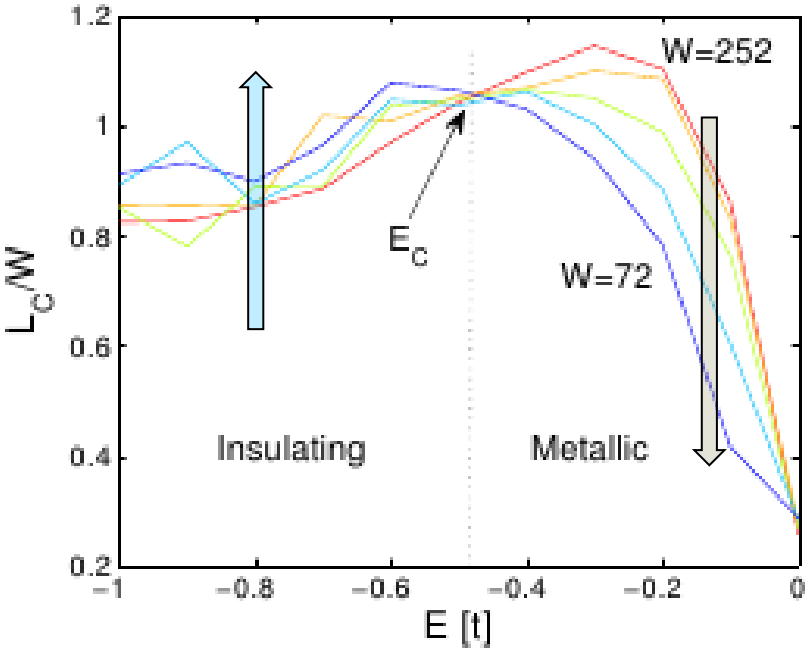
But G is special around E=0 and hence new things could happen (?)

for inter-valley scattering

- Amini M., Jafari S. A. and Shahbazi F. 2009 *EPL* **87** 37002: typ. DOS, mobility edge
- Amanatidis I. and Evangelou S. N. 2009 *Phys. Rev. B* **79** 205420: level spacing, PR, ballistic transport
- Song Y., Song H. and Feng S. 2011 *J. Phys.: Condens. Matter* **23** 205501: typ. DOS, PR, MIT
- Barrios-Vargas J. E. and Naumis G. G. 2012 *J. Phys.: Condens. Matter* **24** 255305: PR, critical WF (power-law)
- Amanatidis H., Kleftogiannis I., Katsanos D. and Evangelou S. 2013 arXiv:1302.2470: level spacing, critical $P(s)$
- Hilke M. 2009 arXiv:0912.0769: GFM, MIT?

But G is special around E=0 and hence new things could happen (?)





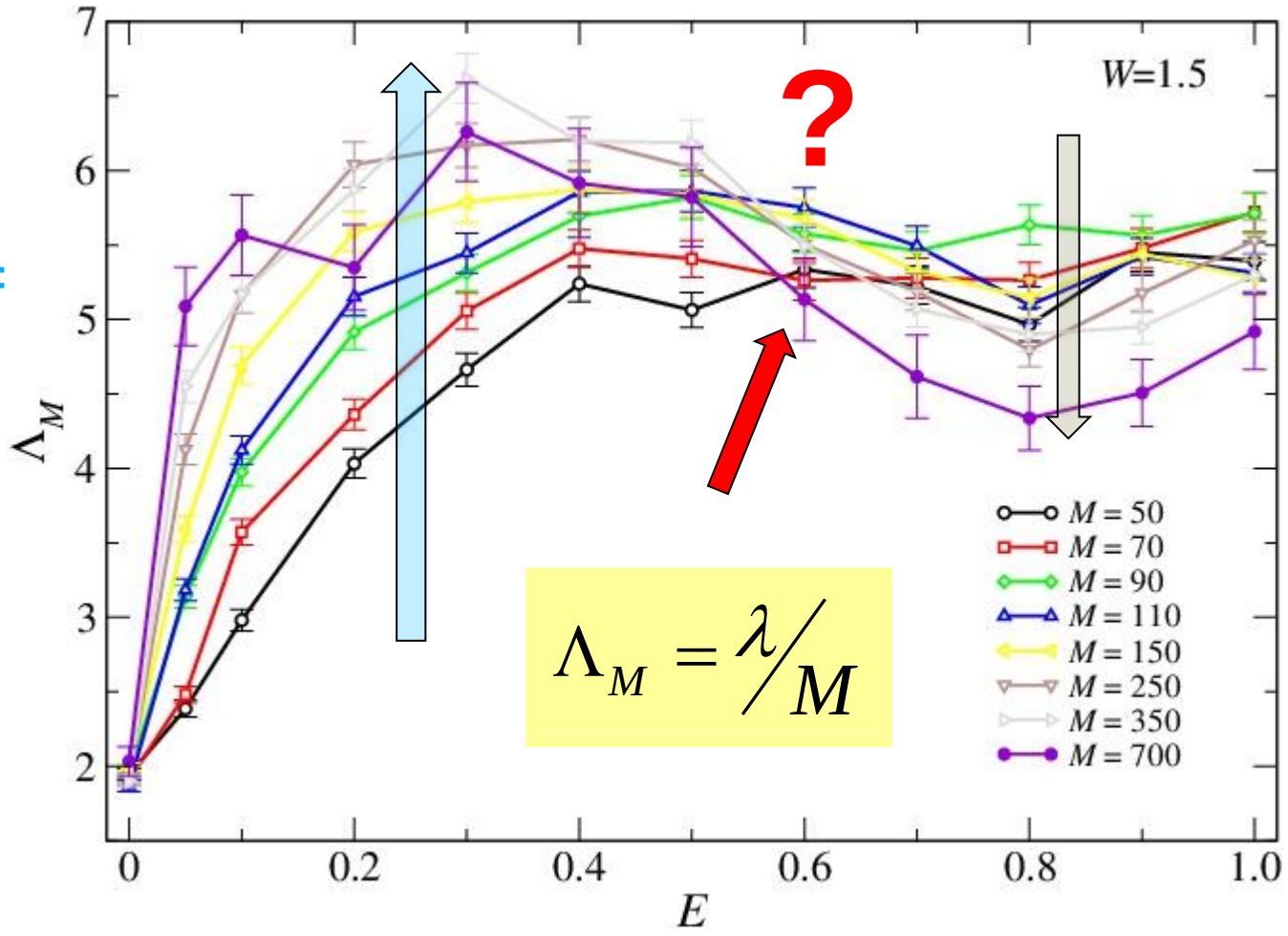
EPL 87, 37002 (2009)
Kernel polynomial method. Distinguish a mobility edge and $W_c = 2.5 \pm 0.5$

arXiv:0912.0769v1 (2009)
Iterative Green's function technique. Metallic to insulating transition a $E_c = 0.5$ and $W_c = 2.0$

Let's see: our code, our numerics (TMM)

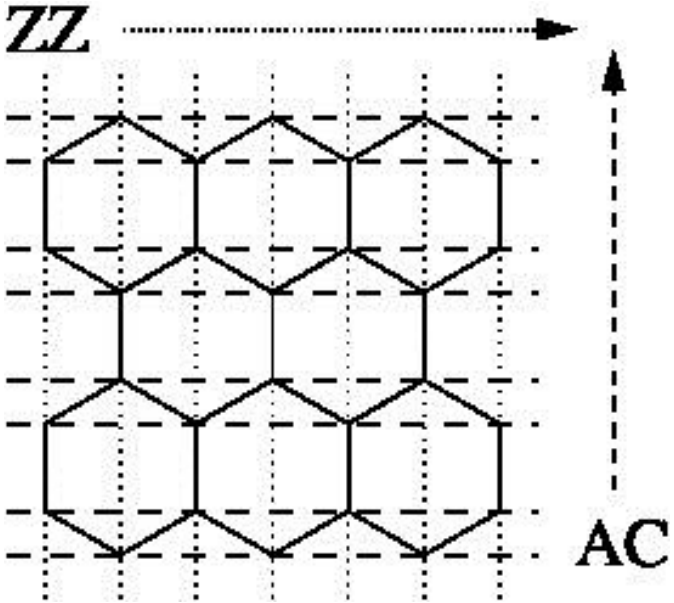
for inter-valley scattering

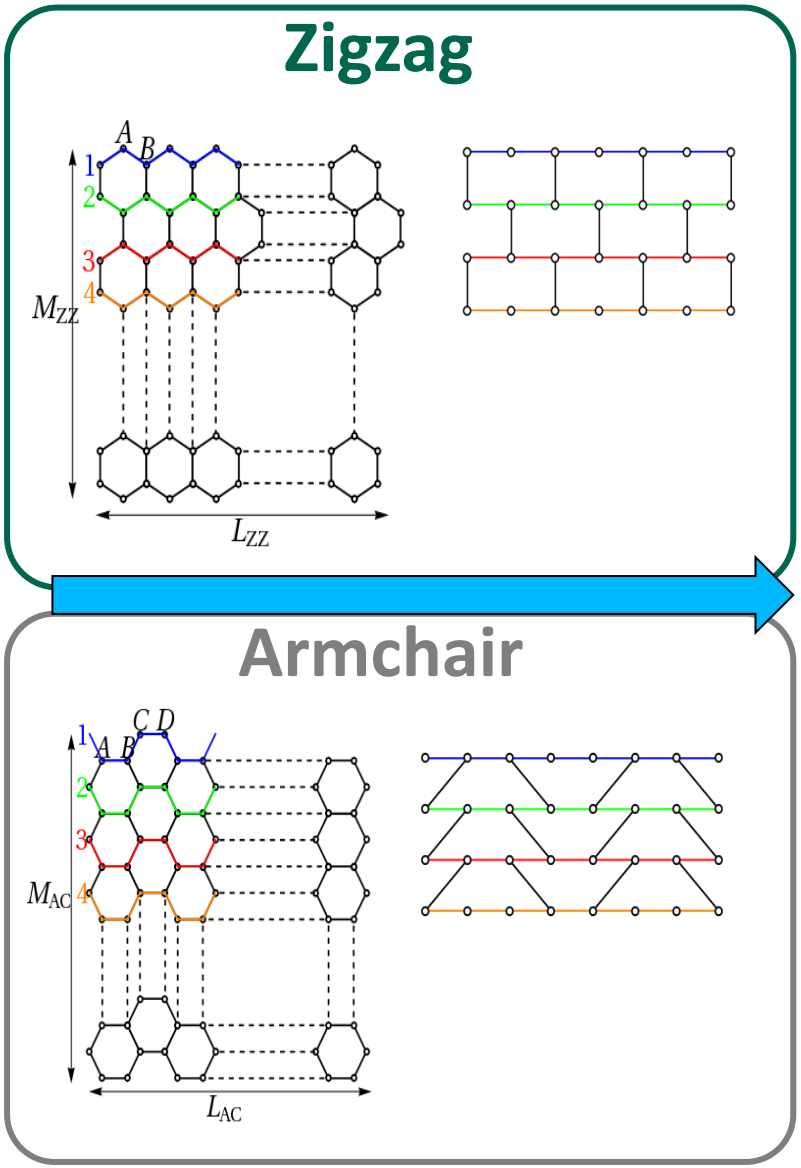
- Up to M=700 we can reproduce existence of 2 regimes
- But, no clear crossing point!



TMM for flakes of G

- Standard TMM for squares
- Needs adjusting for ZZ and AC via connectivity matrices *C*





TMM setup (in 1D)

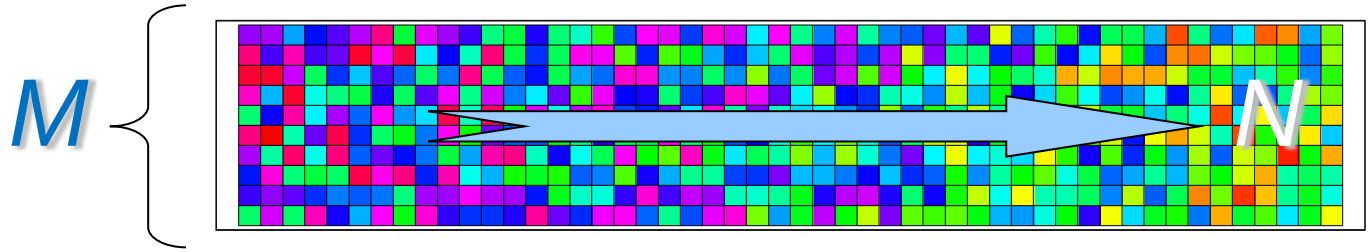
$$H\psi = E\psi \Leftrightarrow \psi_{n+1} = (\varepsilon_n - E)\psi_n - \psi_{n-1}$$

$$\psi = \sum \psi_n |n\rangle$$

$$H\psi = E\psi \Leftrightarrow T_2(n) = \begin{pmatrix} \varepsilon_n - E & -1 \\ 1 & 0 \end{pmatrix}$$

$$\begin{pmatrix} \psi(N) \\ \psi(N-1) \end{pmatrix} = \underbrace{T_2(N) \cdot T_2(N-1) \cdots T_2(1)}_{Q_2(N)} \begin{pmatrix} \psi(1) \\ \psi(0) \end{pmatrix}$$

TMM setup (in Q1D)



$$H\psi = E\psi \Leftrightarrow T_M(n) = \begin{pmatrix} \Delta_M + \boldsymbol{\varepsilon}(n) - E\mathbf{1} & -\mathbf{1} \\ \mathbf{1} & 0 \end{pmatrix}$$

Δ_M: transverse discrete hopping, $\varepsilon(n) = diag\left(\varepsilon_{n,1}, \ldots, \varepsilon_{n,L}\right)$

$$\begin{pmatrix} \boldsymbol{\psi}_M(M) \\ \boldsymbol{\psi}_M(M-1) \end{pmatrix} = \underbrace{T_M(M) \cdot T_M(M-1) \cdots T_M}_{Q_M(M)}(1) \begin{pmatrix} \boldsymbol{\psi}_M(1) \\ \boldsymbol{\psi}_M(0) \end{pmatrix}$$

Computing the localization length

- Solve for eigenvalues of *Q(M)*

$$\left[U^{\dagger} Q\, QU\right]^{\frac{1}{2N}} \xrightarrow{N\to\infty} \mathrm{diag}\left(e^{\gamma_1}, e^{\gamma_2}, \ldots, e^{\gamma_M}, e^{-\gamma_M}, \ldots, e^{-\gamma_1}\right)$$

- Making use of the symplectic structure

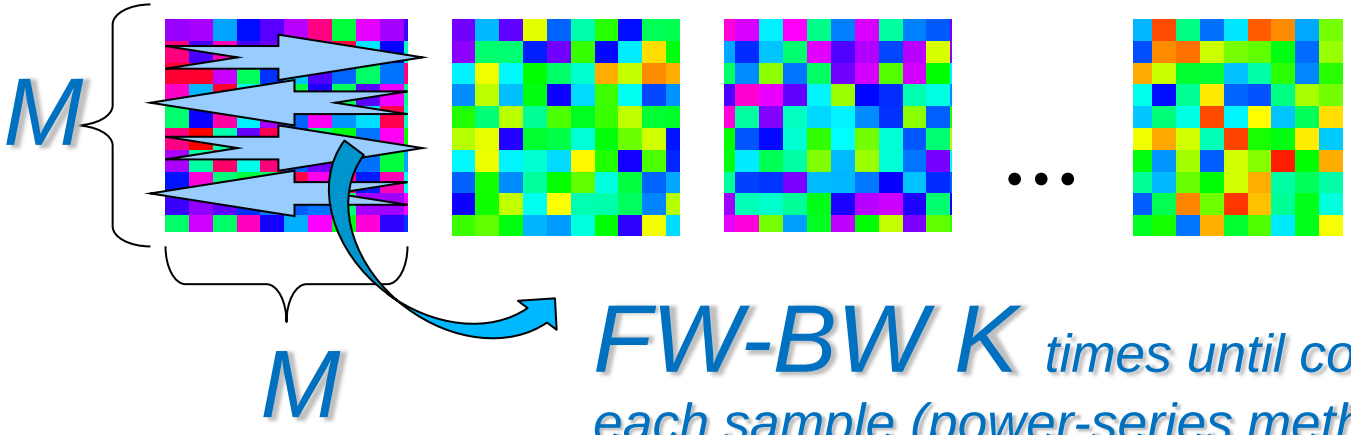
$$T^{\dagger}(n) J T(n) = J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

- To obtain the localization length

$$\lambda = \frac{1}{\gamma_{\min}} = \frac{1}{\gamma_M}$$

Assumes self-averging: one long sample is like averaging over many short samples

TMM setup for flakes: FW/BW-TMM



FW-BW K times until convergence for each sample (power-series method, exact!)

$$\left[U_M^{\text{嗆}}\left(Q_M Q_M\right)^K U_M\right]^{\frac{1}{2KM}} \xrightarrow{K\to\infty} \operatorname{diag}\left(e^{\gamma_1}, e^{\gamma_2}, \ldots, e^{\gamma_M}, e^{-\gamma_M}, \ldots, e^{-\gamma_1}\right)$$

- **FW/BW-TMM allows to compute estimate of decay for each sample**
- **Does not rely on self-averaging**
- **Averaging Lyapunov exponents over samples gives**
- **Variance of $\langle \lambda_M \rangle_K$ distribution gives accuracy**

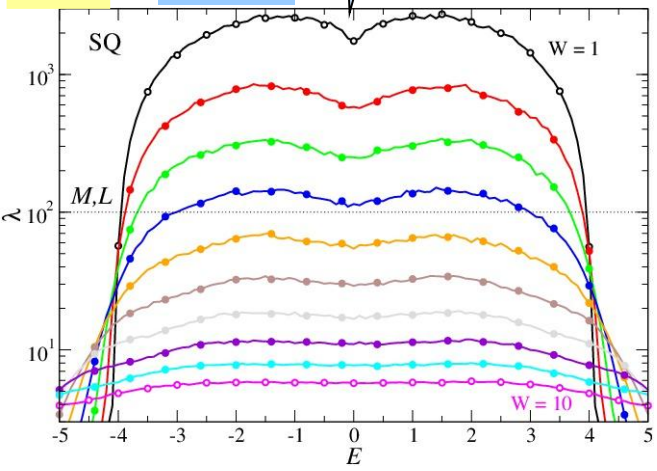
$$\langle \lambda_M \rangle_K = \frac{1}{\langle \gamma_{\min,M} \rangle_K}$$

Results for SQ, ZZ and AC

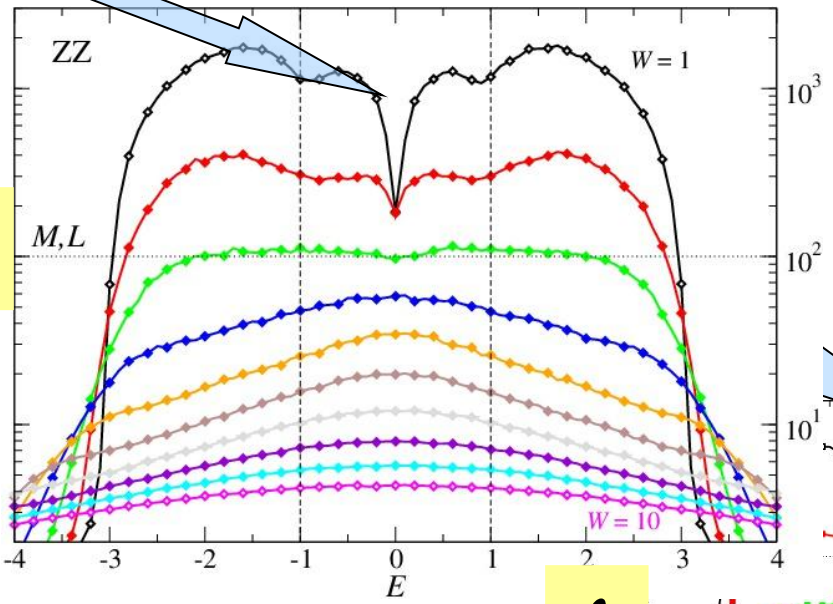
$$W = 1, 2, \ldots, 10$$

$$M = 100$$

λ SQ



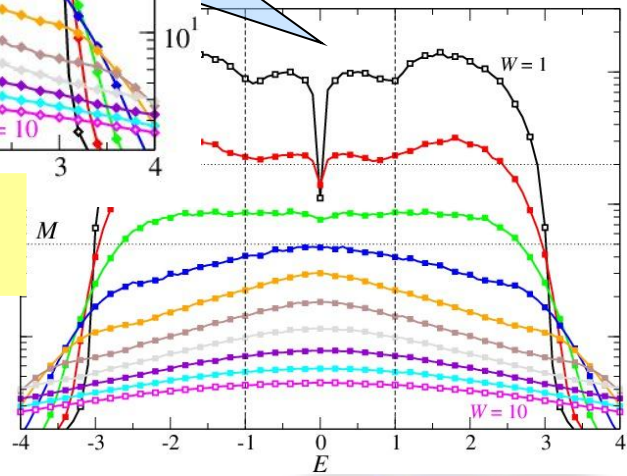
λ



ZZ

AC

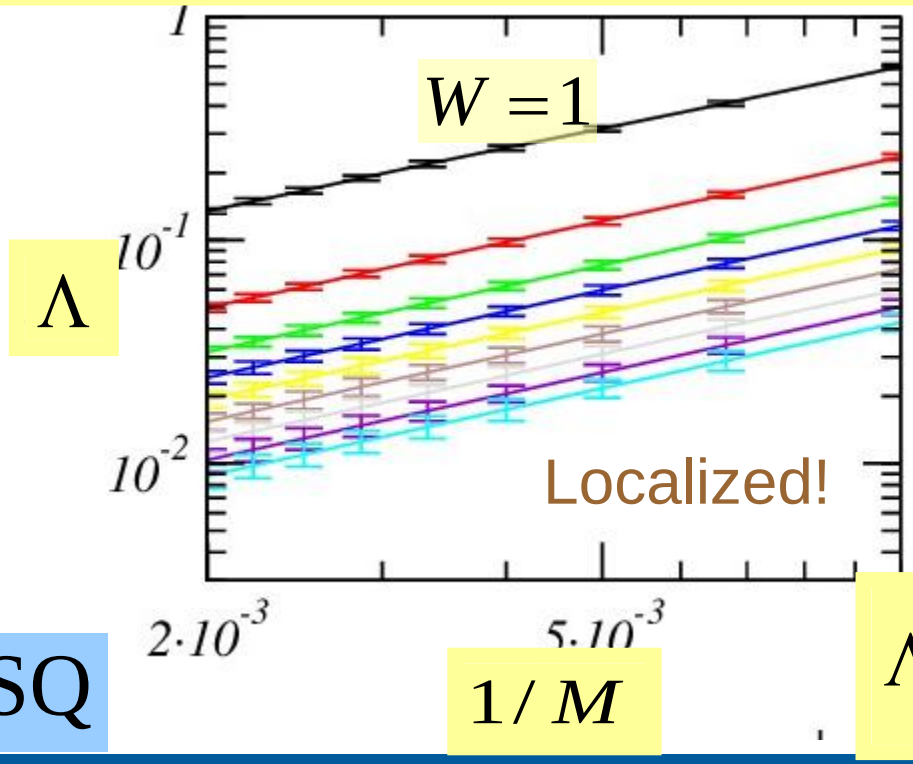
λ



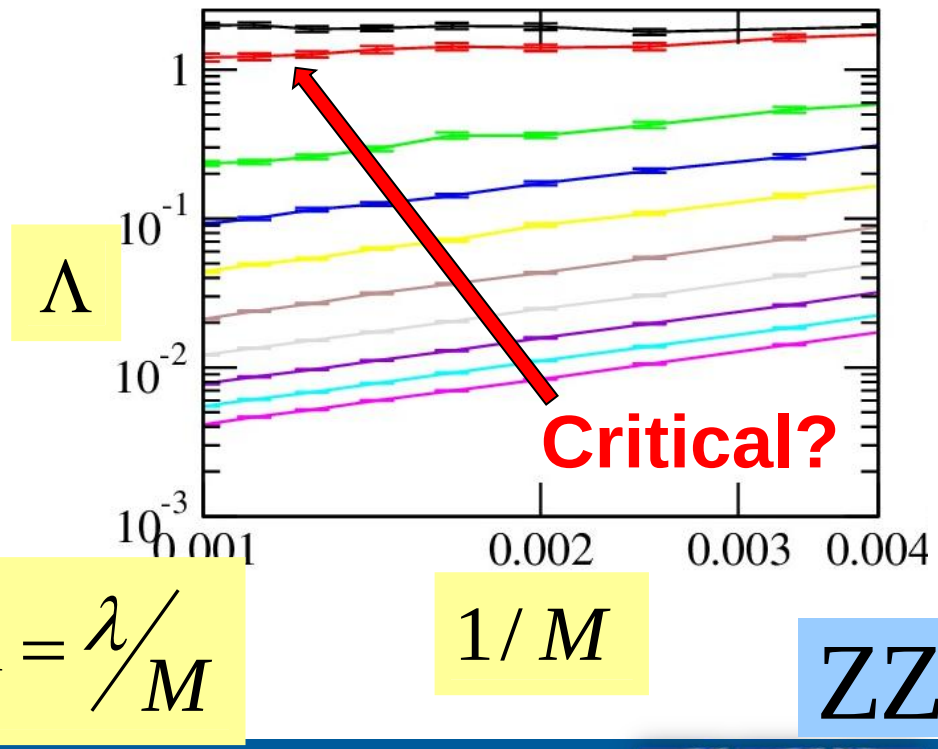
Changing the system width to larger flakes

$$W = 1, 2, \ldots, 10$$

$$M = 50, 70, 90, 110, 150, 200, 250, 350, 700$$



SQ



ZZ

$$\Lambda = \lambda / M$$

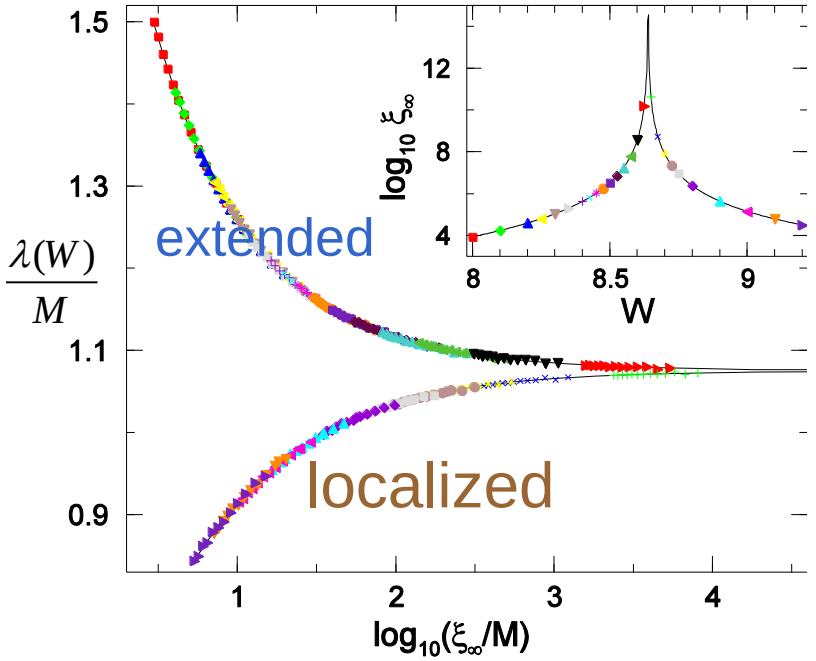
$E = 0.25$

Finite-size scaling

$$\frac{\lambda(W)}{L} = f\left(\xi(W)/L\right)$$

- all data collapse onto a single curve
- two branches indicate
  extended
  localized behaviour

$$\xi \propto |W - W_c|^{-\nu} \qquad \xi \propto |E - E_c|^{-\nu}$$



[F. Milde, RAR, M. Schreiber, V. Uski, Eur. Phys. J. B 15, 685-690 (2000)]

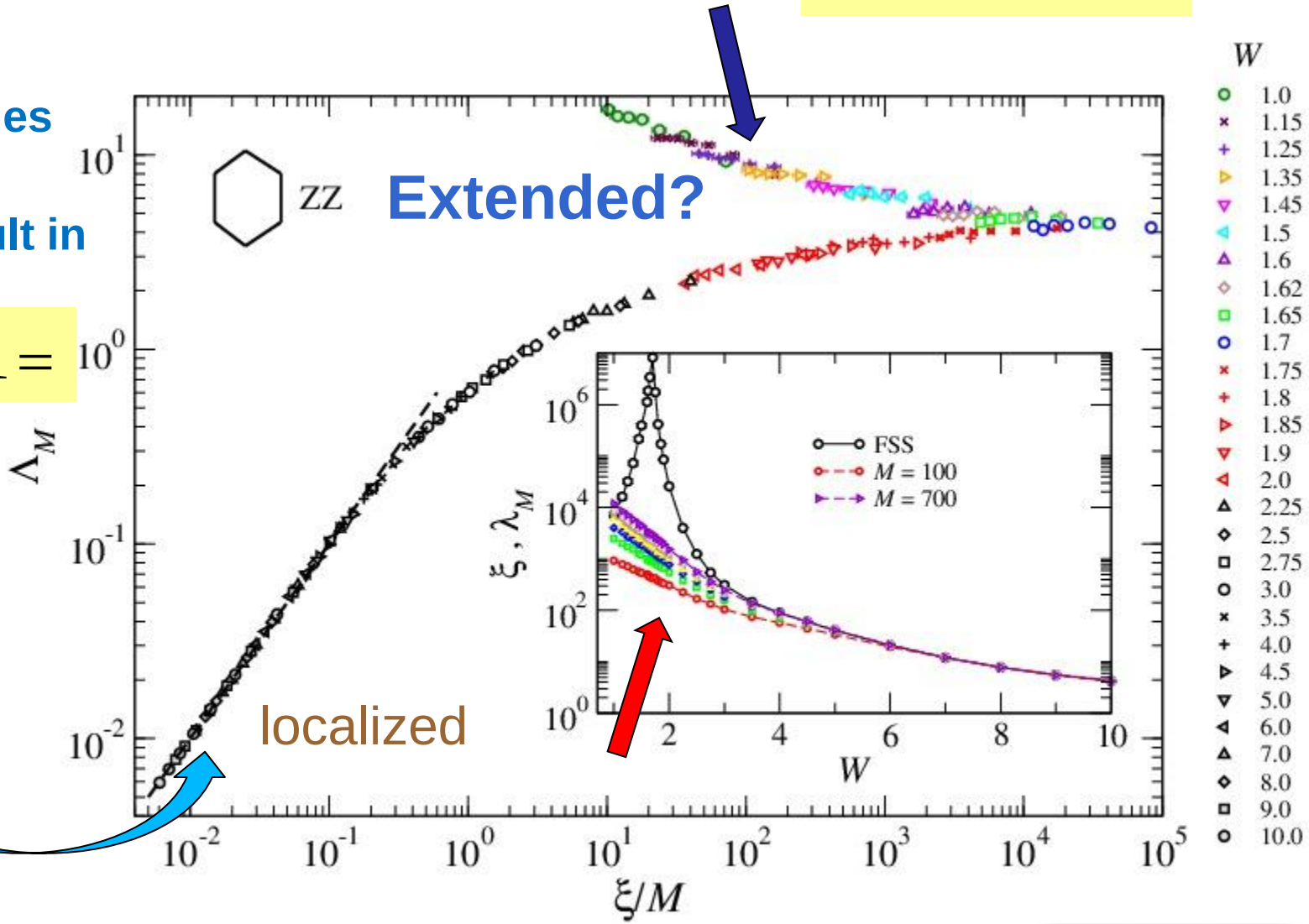
FSS in ZZ-G

$M \leq 700$

- Two branches in ZZ-G!
- Similar result in AC-G

$1 =$

$\Lambda \propto 1/M$



FSS in a square lattice

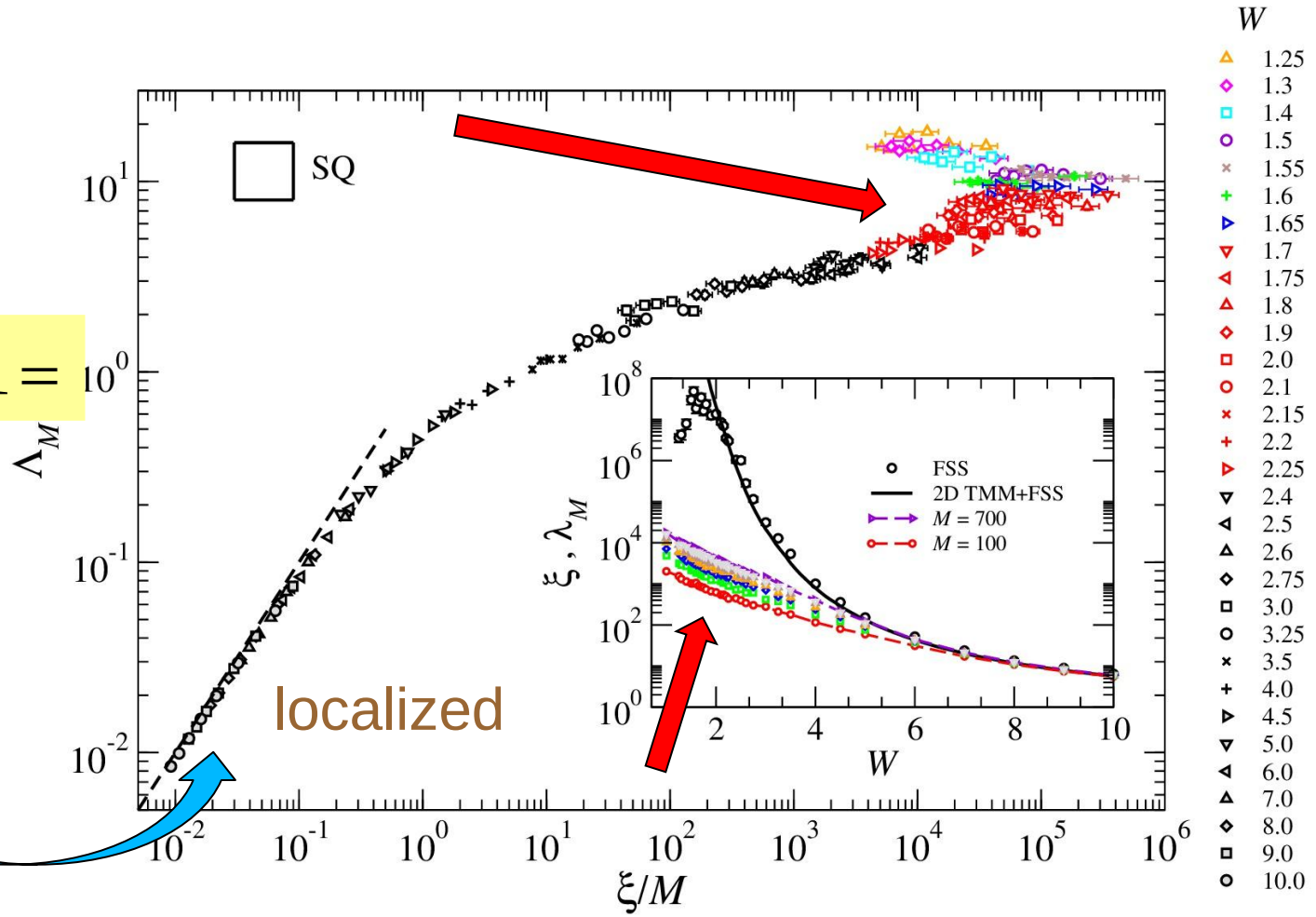
$M \leq 700$

- ?

But we know from scaling theory that all states are localized in 2d square lattices!

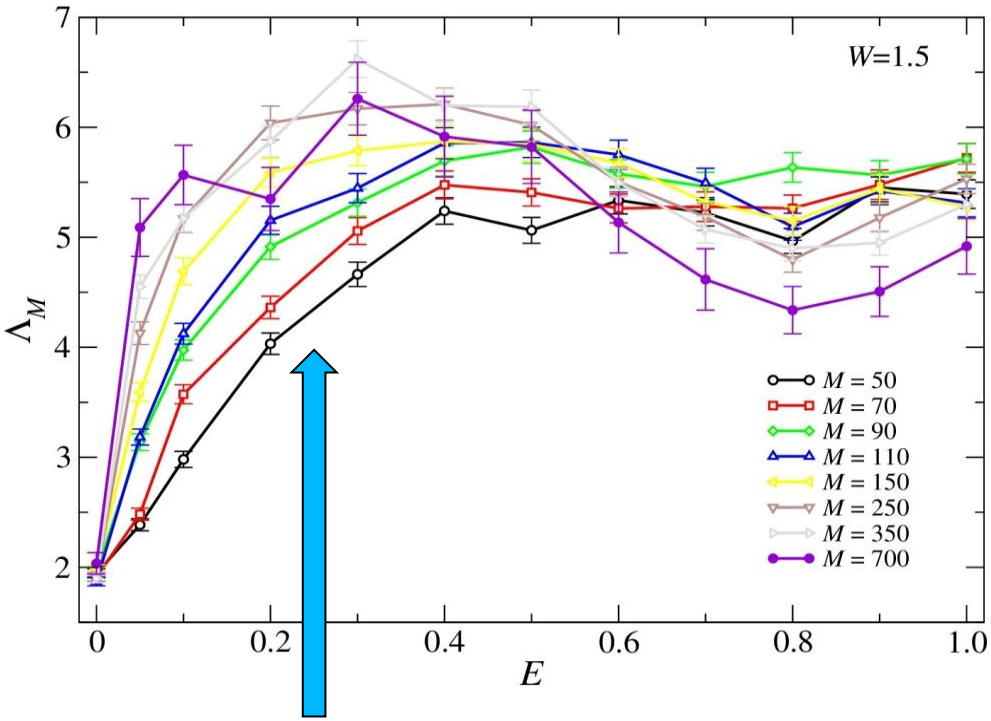
$1 =$

$\Lambda \propto 1/M$



Strategy:

- We select two weak disorders at suitable energy and then increase the system size as much as possible while keeping the number of samples high enough (low variance)



$$E = 0.25$$

$$W = 1.25 \text{ and } 1.5$$

Results for small *M*

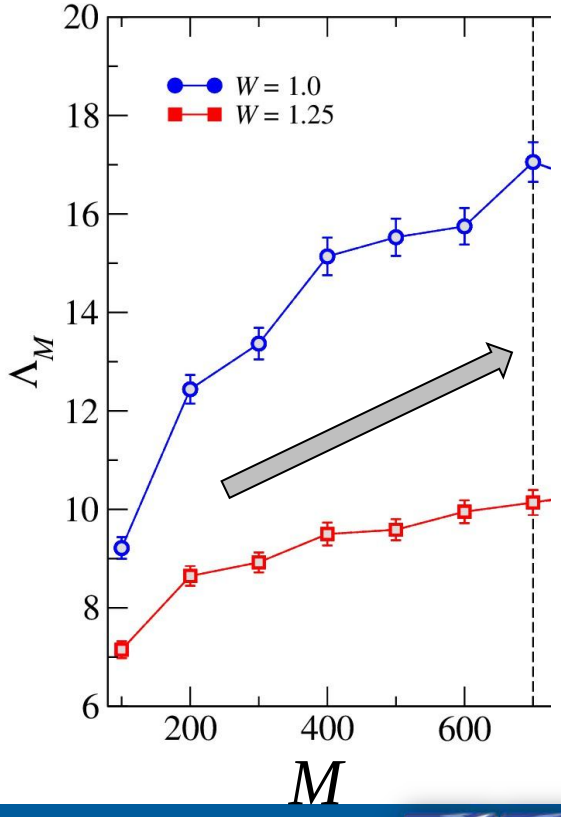
- Reduced localization length increases with *M* up to

$$M = 700$$

This is consistent with extended behaviour

- Days for each data point to compute, >1000 samples for each point

$$W = 1.25, 1.5$$

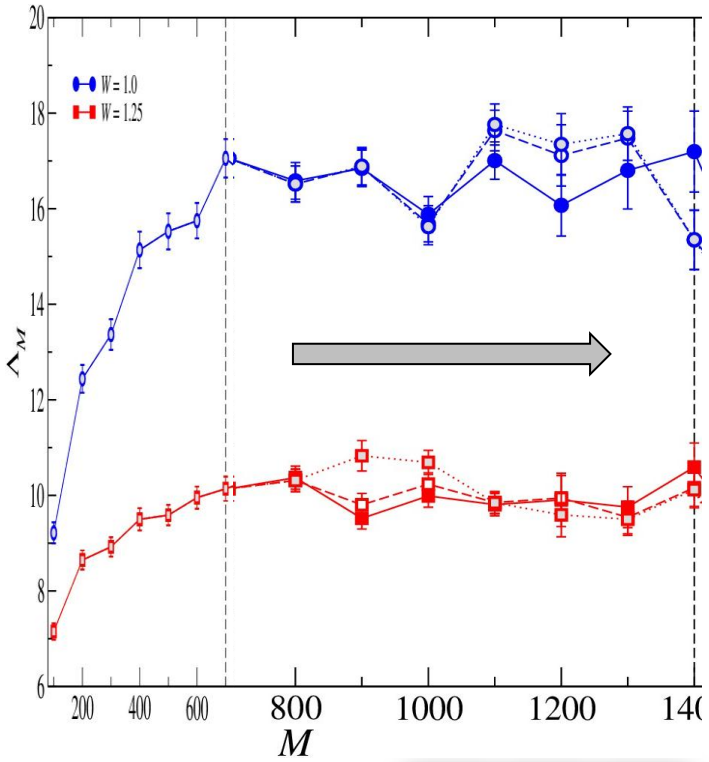


Results for medium *M*

- Reduced localization lengths constant with *M* in the range

$$M = 700, \ldots, 1400$$

$$W = 1.25, 1.5$$



This is consistent with extended behaviour

- Weeks for each data point to compute, >1000 samples for each point

Results for large *M*

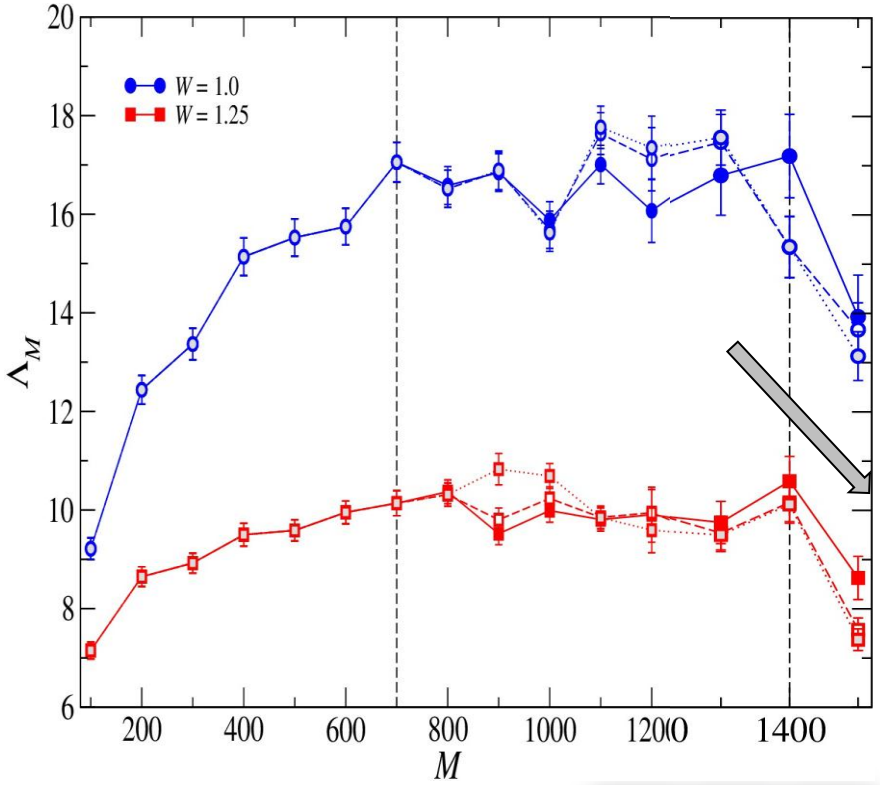
- Reduced localization lengths decreases with *M* for

$$M \geq 1400$$

$$W = 1.25, 1.5$$

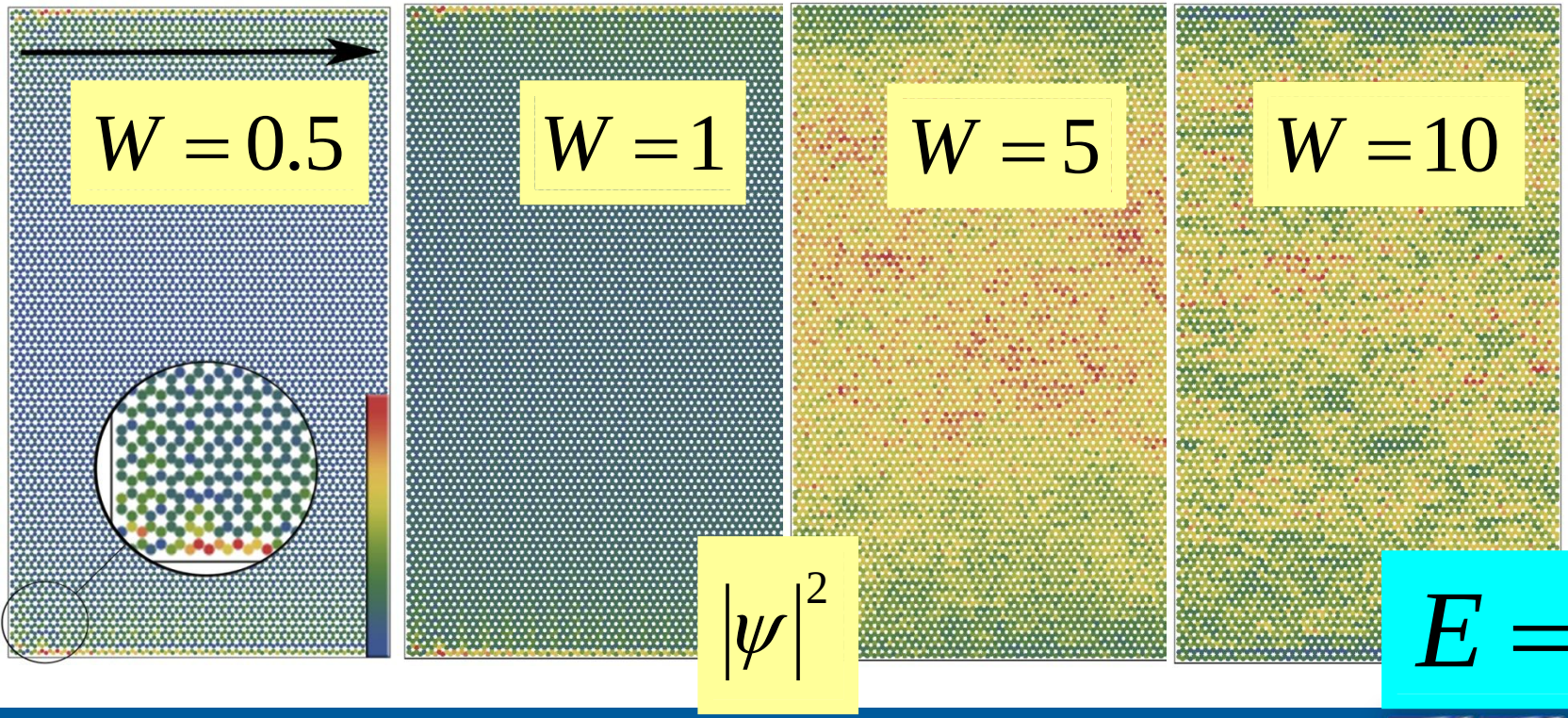
This is consistent with extended behaviour

- Months for each data point to compute, >100 samples for each point



FW/BW-TMM produces wave functions

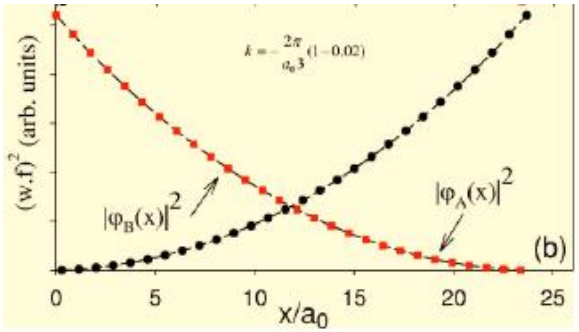
- Converged transport “eigenstates” show crossover from edge state to bulk

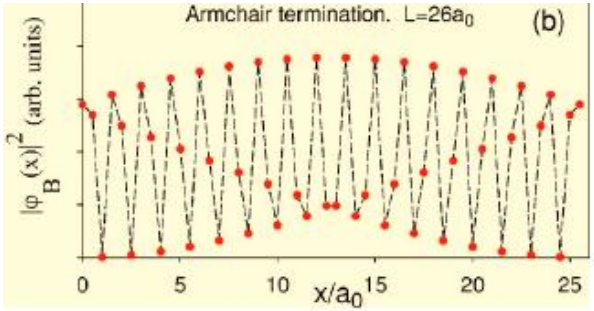


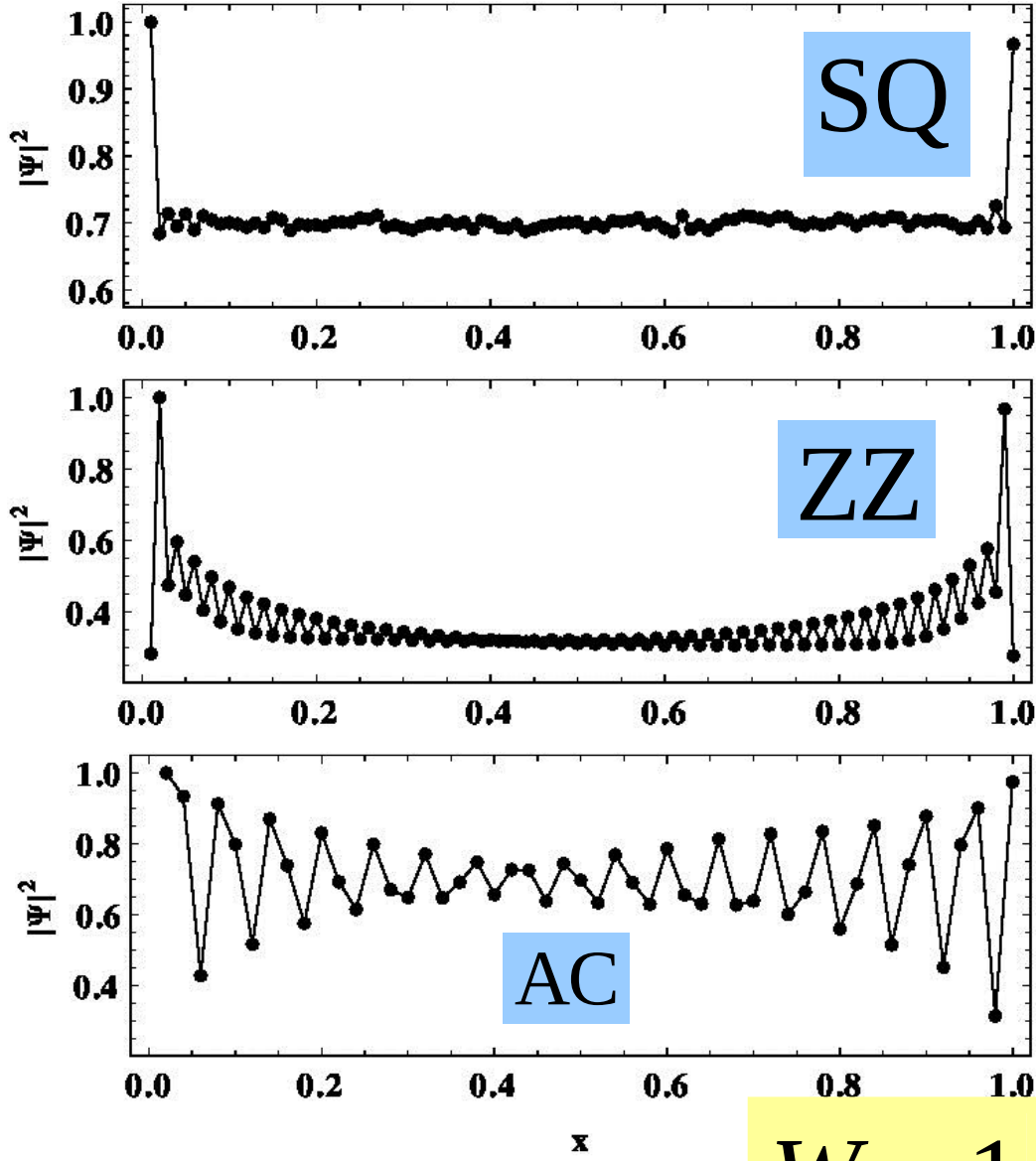
Edge channels

- for clean G:

PRB 73, 235411 (2006)







$W = 0$

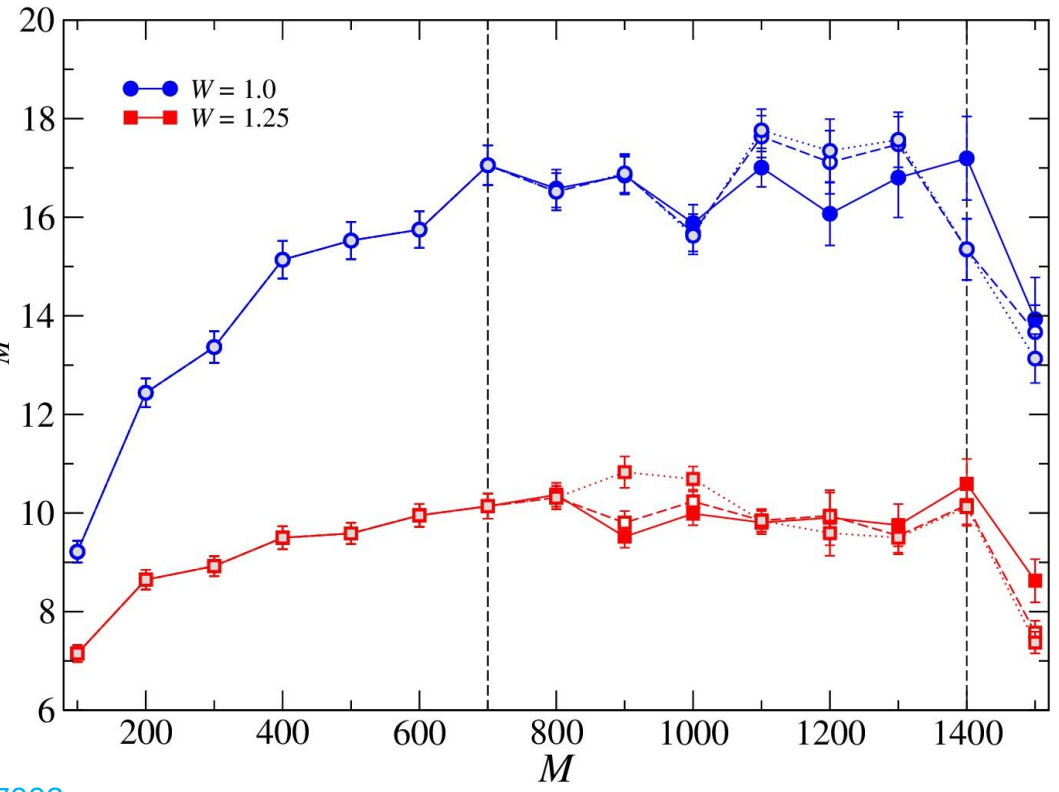
$W = 1$

Conclusions

for inter-valley scattering

- Graphene, ZZ and AC, supports localized states close to Dirac point for weak disorder

- Localization lengths can become very large (>213nm for 0.142nm C-C sp2)
- Can explain discrepancy in the literature



Schleede J., Schubert G. and Fehske H. 2010 *EPL* **90** 17002;
Lee K. L., Grémaud B., Miniatura C. and Delande D. 2013 Phys. Rev. B 87 144202

Thank you for your attention!

Disordered Quantum Systems

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