Critical Exponent of the Anderson Transition using Massively Parallel Supercomputing

Keith Slevin

Graduate School of Science, Osaka University

Tomi Ohtsuki

Division of Physics, Sophia University

Anderson transition

- Critical disorder W_c
  - $W < W_c$ diffusive
  - $W > W_c$ localised
  - $W = W_c$ phase transition
- Einstein relation

$$\sigma(T=0) = \rho(E_{\mathrm{F}}) e^2 D$$

- Anderson insulator

$$\sigma = 0 \quad \rho(E_{\mathrm{F}}) \neq 0$$

- Critical phenomena

$$\xi \sim |W - W_{\mathrm{c}}|^{-\nu}$$

$$\sigma = (W_{\mathrm{c}} - W)^s \quad W < W_{\mathrm{c}}$$

- Wegner scaling relation

$$s = (d-2)\nu$$

- Universality class
  = Symmetry + Dimensionality
- Symmetry
  - Time reversal symmetry (TRS)
  - Spin rotation symmetry (SRS)
  - Particle-hole symmetry
  - Chiral symmetry

	TRS	SRS
orthogonal	○	○
unitary	✕	-
symplectic	○	✕

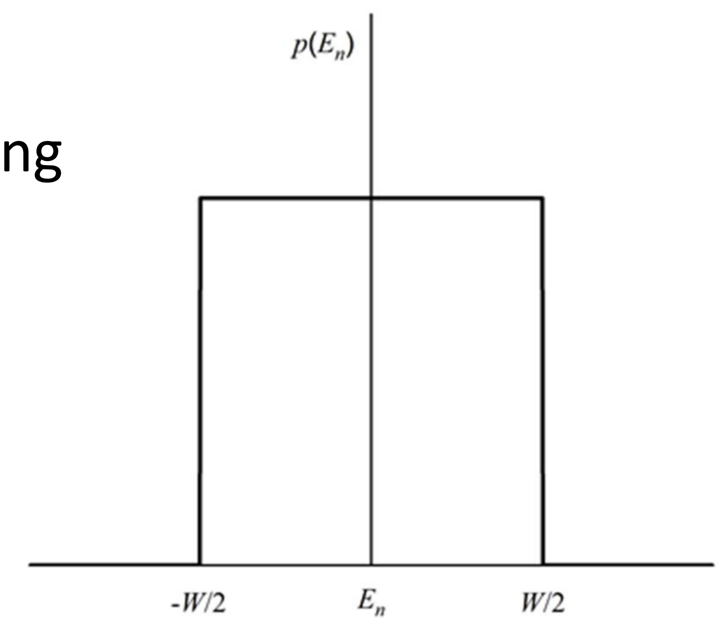
Evers, F. and A. D. Mirlin (2008). "Anderson transitions." Reviews of Modern Physics **80(4): 1355-1363.**

3D orthogonal universality class

- Anderson's model of localisation

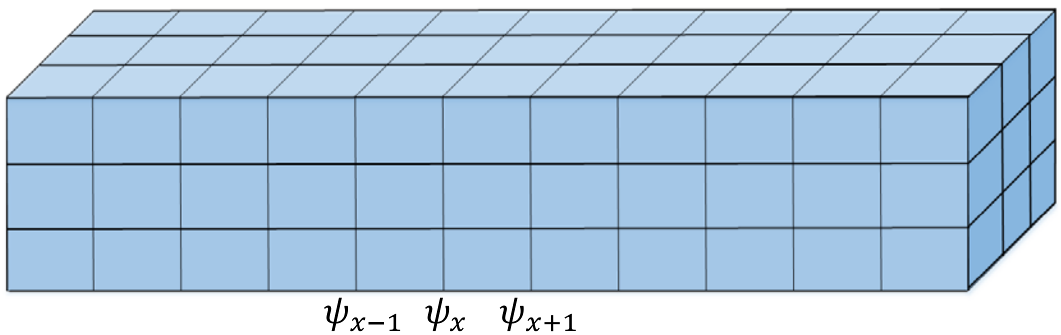
$$H = \sum_n E_n |n\rangle\langle n| - \sum_{\langle nn' \rangle} |n\rangle\langle n'|$$

  - cubic lattice
  - $|n\rangle$ orbital localised on site n
  - unit nearest neighbour hopping (sets unit of energy)
  - random orbital energies E_n



Transfer matrix

- Bar divided into layers (labelled by *x*)



- Rewrite time independent Schrödinger equation as transfer matrix equation

$$h_x\psi_x - \psi_{x+1} - \psi_{x-1} = E\psi_x$$

$$\begin{pmatrix} \psi_{x+1} \\ -\psi_x \end{pmatrix} = \begin{pmatrix} h_x - E & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \psi_x \\ -\psi_{x-1} \end{pmatrix} = M_x \begin{pmatrix} \psi_x \\ -\psi_{x-1} \end{pmatrix}$$

Transfer matrix method

- Single very long quasi-1D sample

$$L \times L \times L_x \qquad\qquad L_x \gg L$$

- Length typically $10^6 \sim 10^7$

Oseledec's theorem

- Product of transfer matrices

$$M = M_{L_x} \cdots M_1$$

- Following limiting matrix exists

$$\Omega = \lim_{L_x \to \infty} \frac{\ln M^T M}{2L_x}$$

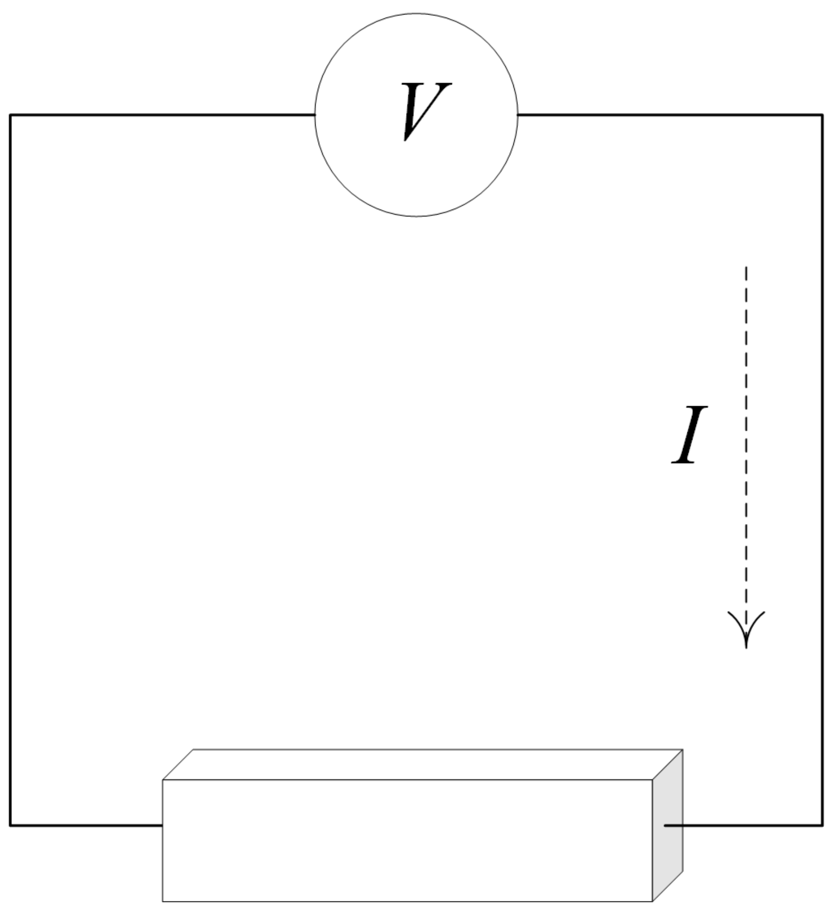
  - matrix depends on sequence but eigenvalues do not

$$\gamma_1 > \cdots \gamma_N, -\gamma_N > \cdots - \gamma_1$$

  - smallest positive Lyapunov exponent

$$\gamma = \gamma_N$$

Two-terminal conductance



$$I = GV$$

$$G = \frac{e^2}{h} g$$

$$g_{\text{typical}} \sim \exp\left(-2\gamma_N L_x\right)$$

Transfer Matrix Method

- Assume

$$L_x = lq$$

- Initial matrix

$$Q_0$$

- Estimates of Lyapunov exponents

$$\tilde{\gamma}_i = \frac{1}{l}\sum_{j=1}^{l} \ln\left(R_j\right)_{i,i}$$

  - Result depends only on L_x

$$\begin{aligned}
QR &= MQ_0 \\
&= M_{L_x} \cdots M_1 Q_0 \\
&= M_{L_x} \cdots M_{q+1} \underbrace{M_q \cdots M_1 Q_0}_{Q_1 R_1} \\
&= M_{L_x} \cdots M_{q+1} Q_1 R_1 \\
&= M_{L_x} \cdots M_{2q+1} Q_2 R_2 R_1 \\
&\vdots \\
&= Q_l R_l \cdots R_1
\end{aligned}$$

Pichard, J. L. and G. Sarma (1981). Journal of Physics C: Solid State Physics 14: L127. MacKinnon, A. and B. Kramer (1981). Physical Review Letters 47: 1546.
Slevin, K. and T. Ohtsuki (2014). New Journal of Physics 16: 015012.

Scaling for quasi-1D

- Estimates of Lyapunov exponents

$$\tilde{\gamma}_i = \frac{1}{l}\sum_{j=1}^{l} \ln\left(R_j\right)_{i,i}$$

- Scaling law

$$\left\langle \tilde{\gamma}_N \right\rangle L_x = f\left(\frac{L_x}{\xi}, \frac{L}{\xi}, \frac{L}{\xi}\right)$$

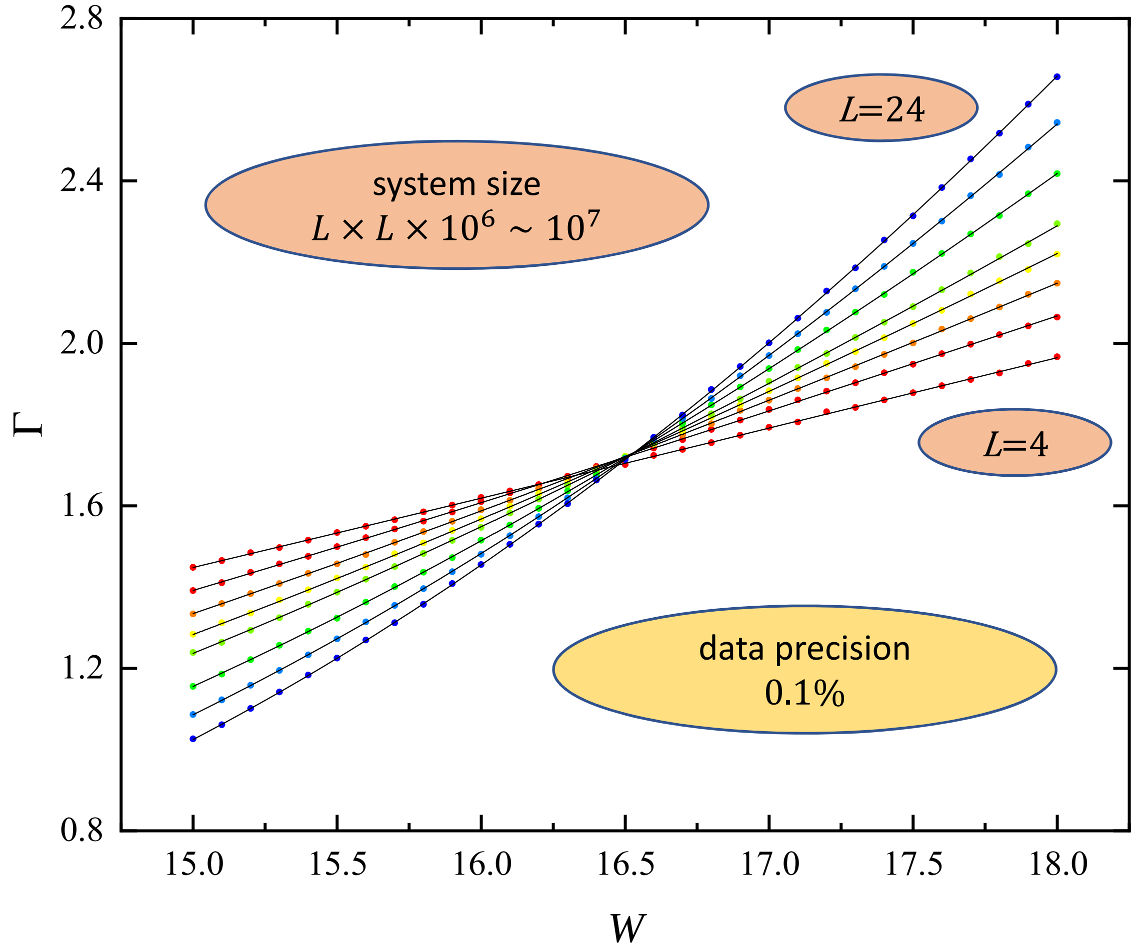
- Limit $L_x \to \infty$
  - For sufficiently long sample r.h.s. $\propto L_x$

$$\left\langle \tilde{\gamma}_N \right\rangle L_x = \frac{L_x}{\xi}\, \tilde{f}\left(\frac{L}{\xi}\right)$$

$$\boxed{\Gamma = \gamma_N L = f_{\mathrm{Q1D}}\left(\frac{L}{\xi}\right)}$$

(box distributed random potential)

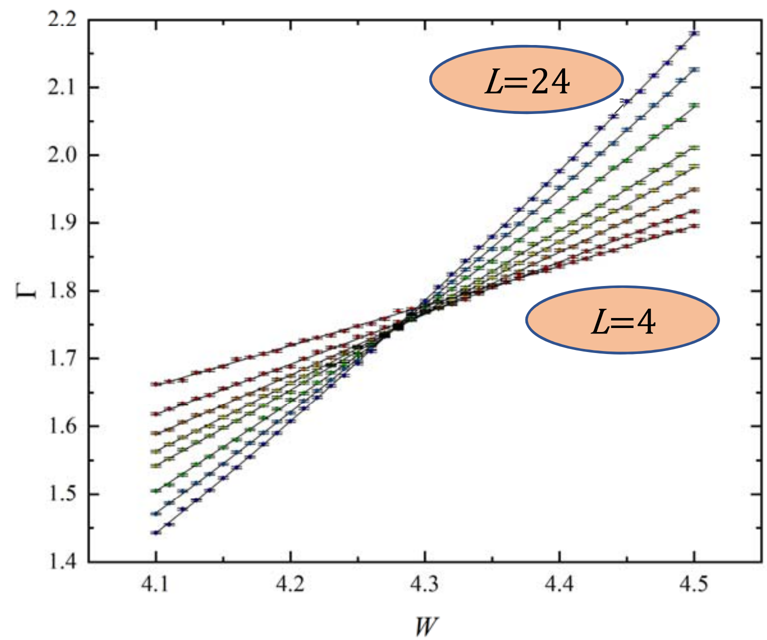
Quasi-1D data

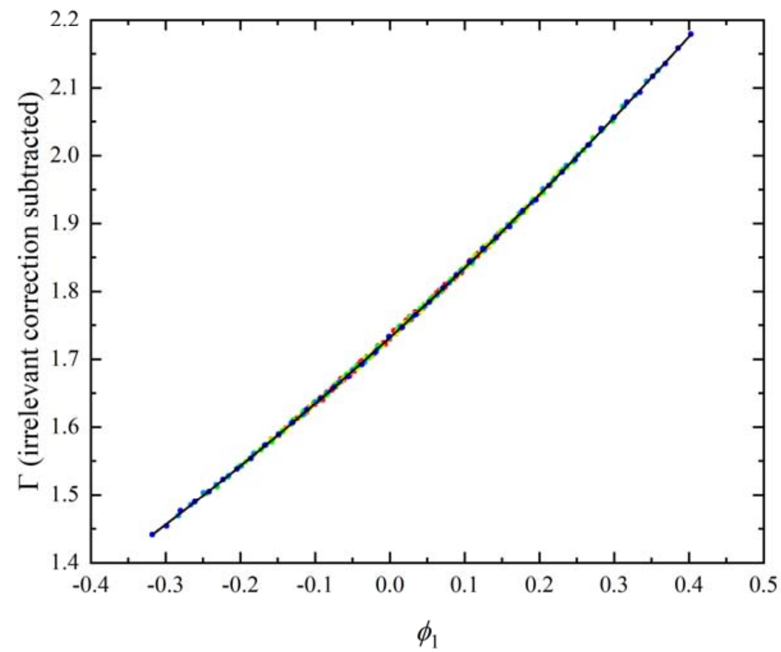


Slevin, K. and T. Ohtsuki (2014). New Journal of Physics 16: 015012.

(Cauchy distributed random potential)

Finite size scaling





$\Gamma = F\left(\phi_1, \phi_2\right)$ $\quad w = W - W_c$ $\quad \phi_i = u_i\left(w\right) L^{\alpha_i}$ $\quad \nu = \dfrac{1}{\alpha_1} > 0$ $\quad y = \dfrac{1}{\alpha_2} < 0$ $\quad F = \sum_{j_1=0}^{n_1} \sum_{j_2=0}^{n_i} a_{j_1, j_2} \phi_1^{j_1} \phi_2^{j_i}$ $\quad u_i\left(w\right) = \sum_{j=0}^{m_i} b_{i,j} w^j$

irrelevant correction

non-linearity

Huckestein, B. (1994). Physical Review Letters 72: 1080. Slevin, K. and T. Ohtsuki (1999). Physical Review Letters 82: 382.
Slevin, K. and T. Ohtsuki (2014). New Journal of Physics 16: 015012.

Finite size scaling

Goodness of fit probability

Table 3. The range of data, the orders of the expansions, the total number of data and the value of χ^2_{min} obtained in the finite size scaling analysis. For the box distribution the energy $E = 1$, and for the normal and Cauchy distributions $E = 0$.

$p(W_i)$	W	L	Orders of expansions	Details of fit
Box	[15, 18]	$\geqslant 4$	$m_1 = 2, m_2 = 2, n_1 = 3, n_2 = 1$	$N_{\mathrm{D}} = 248, \chi^2_{\mathrm{min}} = 239$
Normal	[5.75, 6.55]	$\geqslant 4$	$m_1 = 2, m_2 = 1, n_1 = 3, n_2 = 1$	$N_{\mathrm{D}} = 328, \chi^2_{\mathrm{min}} = 317$
Cauchy	[4.1, 4.5]	$\geqslant 4$	$m_1 = 2, m_2 = 1, n_1 = 2, n_2 = 1$	$N_{\mathrm{D}} = 328, \chi^2_{\mathrm{min}} = 318$
Box	[15, 18]	$\geqslant 12$	$m_1 = 2, n_1 = 3$	$N_{\mathrm{D}} = 124, \chi^2_{\mathrm{min}} = 112$
Normal	[5.75, 6.55]	$\geqslant 12$	$m_1 = 2, n_1 = 3$	$N_{\mathrm{D}} = 164, \chi^2_{\mathrm{min}} = 158$

Stability of fit

Table 4. The results of the finite size scaling analyses. Details of the simulations are given in the corresponding row of table 3.

$p(W_i)$	W_c	Γ_c	ν	y
Box	16.536[.531, .543]	1.7339[.7314, .7371]	1.576[.562, .582]	−3.3[−3.9, −2.8]
Normal	6.1467[.1450, .1498]	1.7371[.7351, .7411]	1.566[.549, .576]	−3.1[−4.0, −2.1]
Cauchy	4.2707[.2680, .2731]	1.7318[.7266, .7360]	1.576[.546, .594]	−2.0[−2.4, −1.7]
Box	16.532[.526, .538]	1.7316[.7286, .7345]	1.577[.568, .586]	Not applicable
Normal	6.1463[.1441, .1483]	1.7364[.7340, .7388]	1.571[.560, .583]	Not applicable

Monte Carlo simulation of synthetic datasets

Goodness of fit probability

N = number of data

M = number of parameters

Degrees of freedom

$$\nu = N - M$$

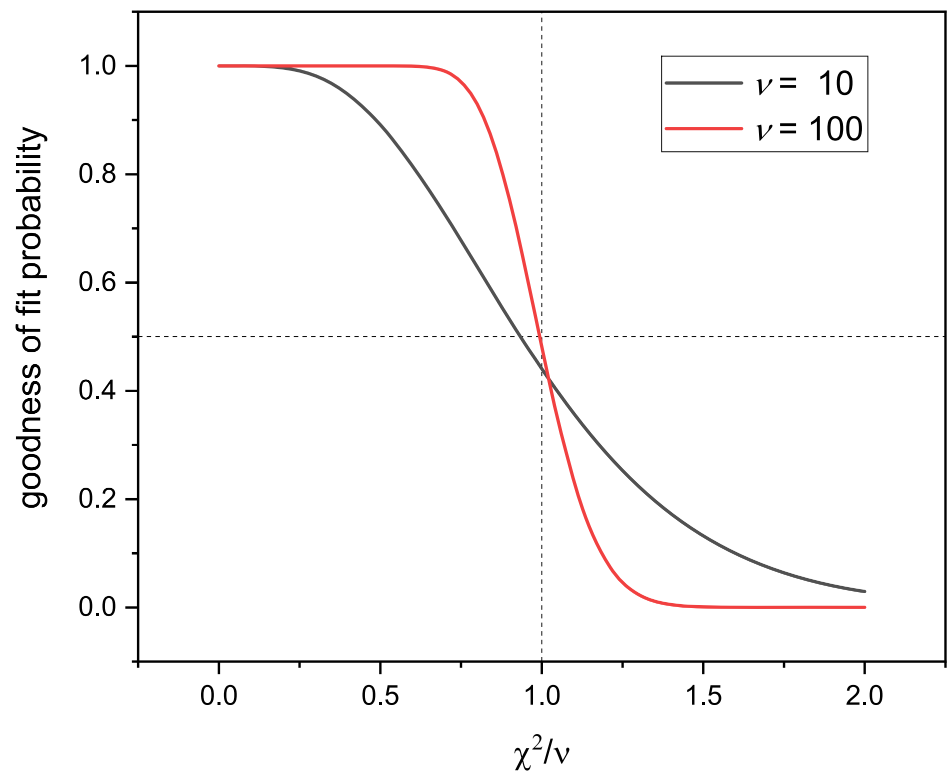
Goodness of fit probability

$$P = 1 - Q$$

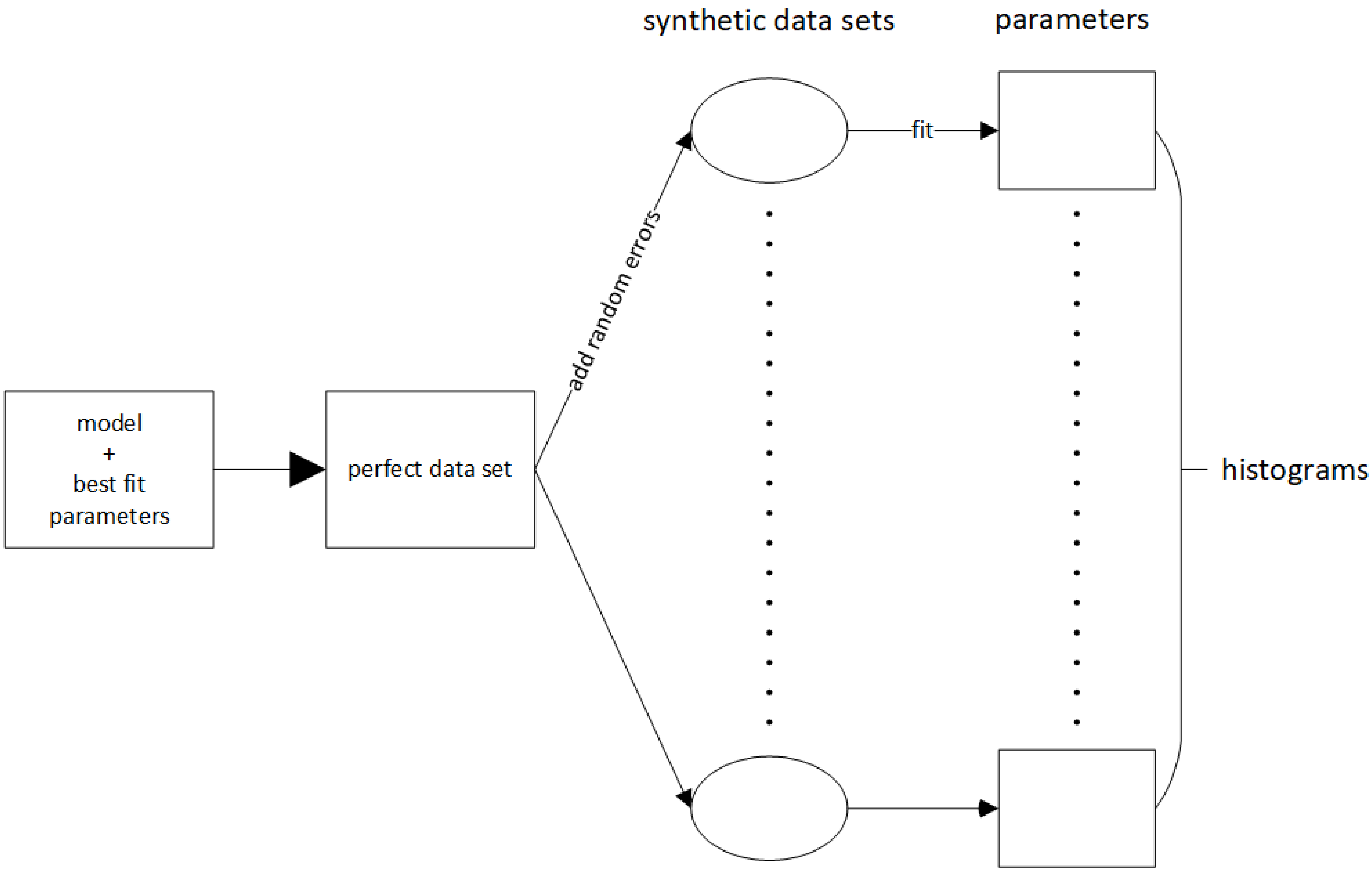
$$Q = \int_{\chi^2}^{\infty} p(\chi^2; \mathrm{DOF})\, d\chi^2$$

$$p(\chi^2; \upsilon) = \frac{(\chi^2)^{(\upsilon-2)/2} \exp(-\chi^2/2)}{2^{\upsilon/2}\,\Gamma(\upsilon/2)}$$

Or directly from histogram



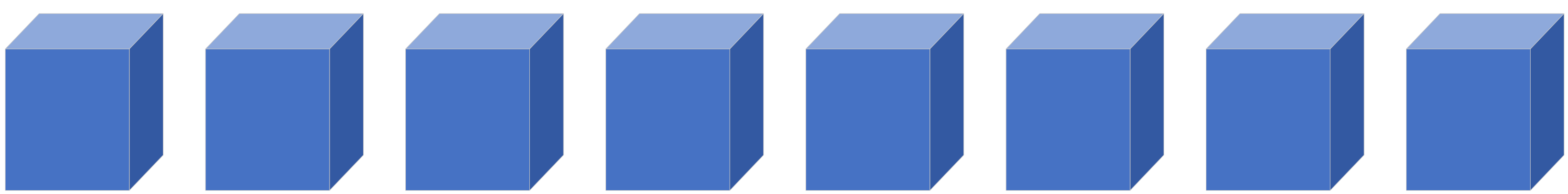
Error bars


synthetic data sets
parameters
fit
add random errors
model
+
best fit
parameters
perfect data set
histograms

Parallelization

- Single very long quasi-1D sample
  - serial – runs on one node

- Average over ensemble of cubes
  - parallel – distribute over nodes using MPI



Scaling for cubes

$$QR = MQ_0 = M_L \cdots M_1 Q_0$$

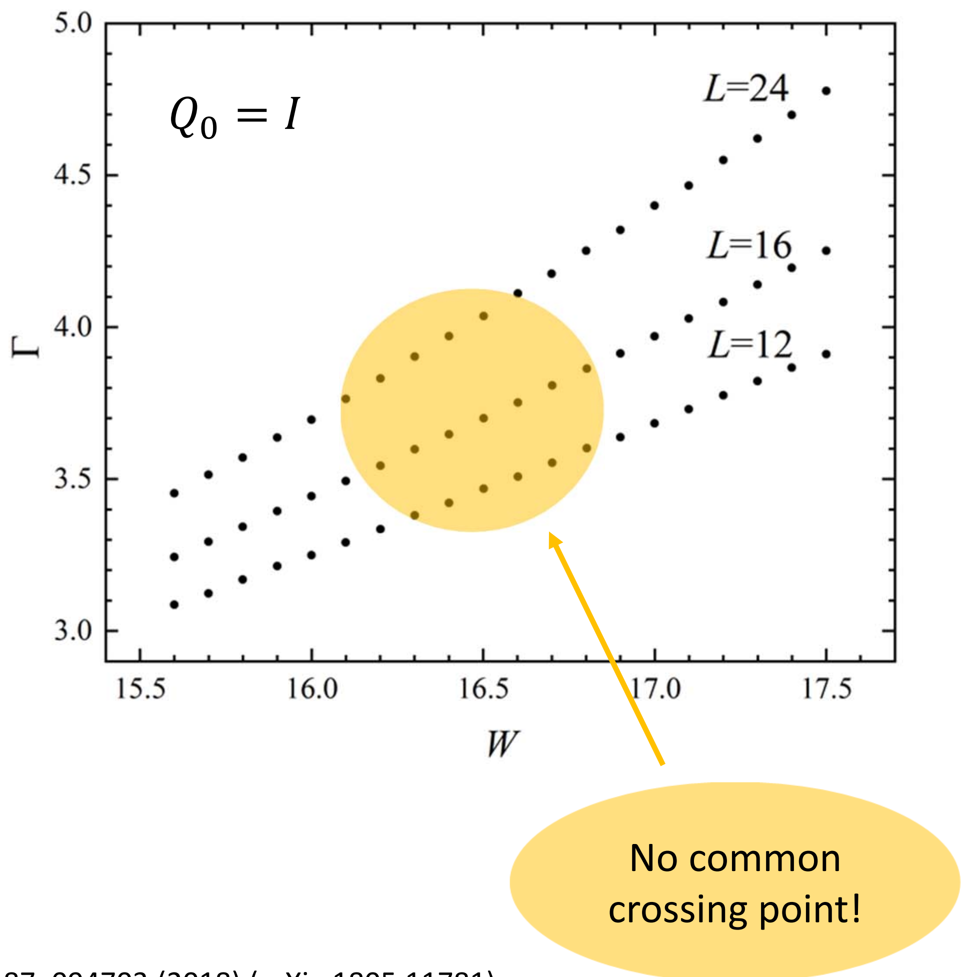
- Scaling law

$$\langle \tilde{\gamma}_N \rangle L_x = f\left(\frac{L_x}{\xi}, \frac{L}{\xi}, \frac{L}{\xi}\right)$$

- For cubes

$$\langle \tilde{\gamma}_N \rangle L = f\left(\frac{L}{\xi}, \frac{L}{\xi}, \frac{L}{\xi}\right)$$

$$\boxed{\Gamma = \langle \tilde{\gamma}_N \rangle L = f_{3\mathrm{D}}\left(\frac{L}{\xi}\right)}$$



K. Slevin and T. Ohtsuki, Journal of the Physical Society of Japan 87, 094703 (2018) (arXiv:1805.11781)

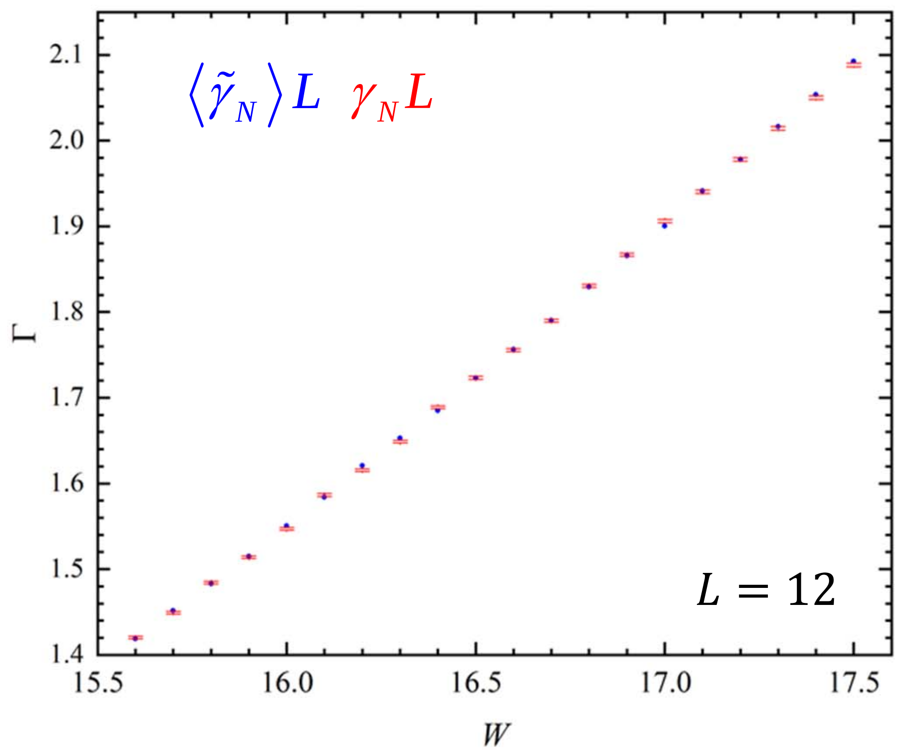
Stationary distribution

- Q_0 random matrix sampled from a distribution that is stationary under transfer matrix multiplication

$$Q'R = M_x Q$$

- For such a distribution

$$\langle \tilde{\gamma}_i \rangle = \frac{1}{l} \sum_{j=1}^{l} \left\langle \ln \left(R_j \right)_{i,i} \right\rangle$$
$$= \left\langle \ln \left(R_1 \right)_{i,i} \right\rangle$$
$$= \gamma_i$$
$$f_{Q1D} = f_{3D}$$



K. Slevin and T. Ohtsuki, Journal of the Physical Society of Japan 87, 094703 (2018) (arXiv:1805.11781)

Stationary distribution

- How to generate such matrices?
  - repeat several times

$$Q'R = M_q \cdots M_1 Q$$

discard R

  - use Kolmogorov-Smirnof test to check stationarity

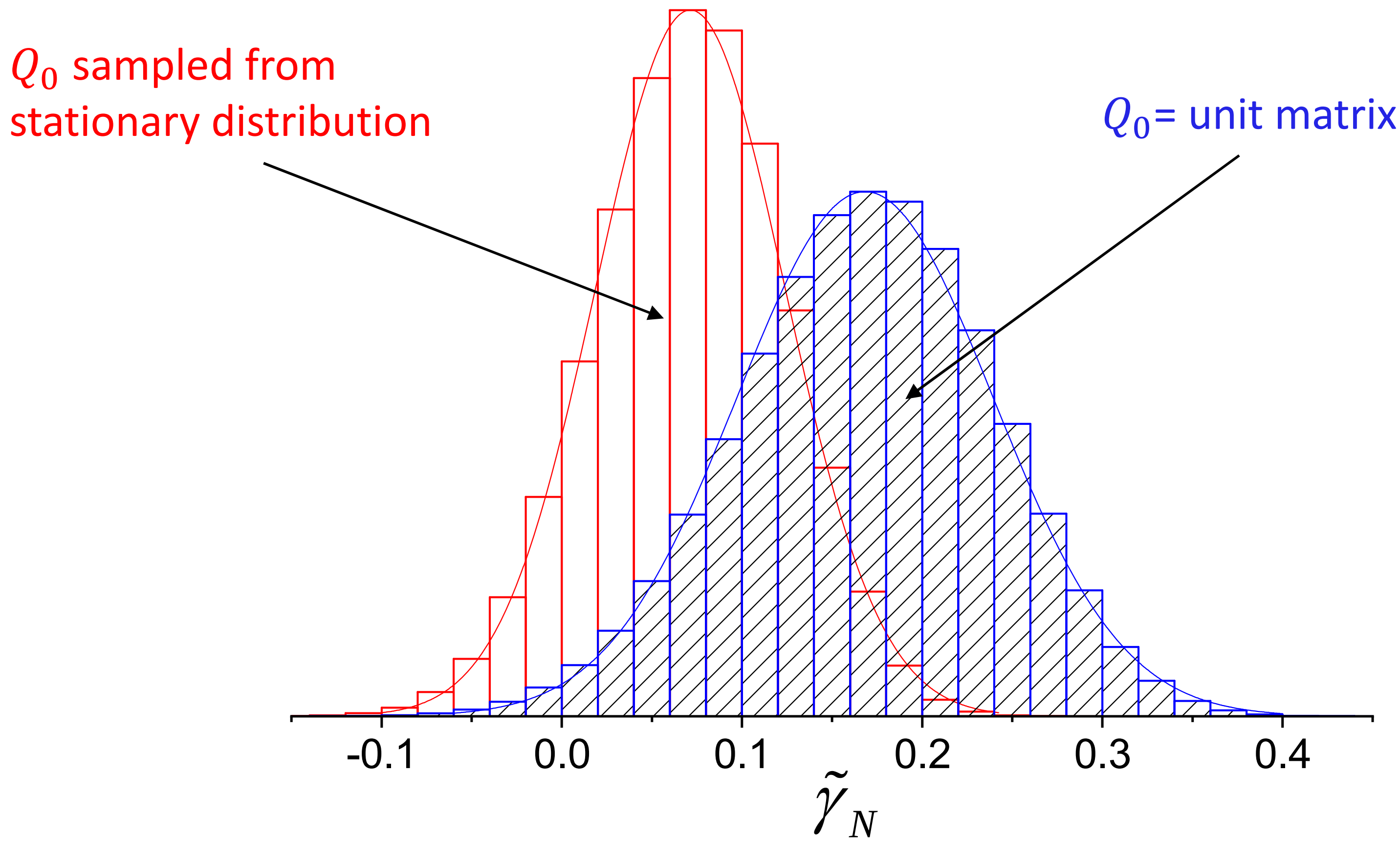
Table I. Example of the Kolmogorov-Smirnov test for cross section 48×48. The ensemble size is 589824. The table shows the p-value returned by the Kolmogorov-Smirnov test. The rows and columns are labeled by the number of randomizing multiplications.

#multiplications	32	64	96
32	-	0.004	0.023
64	0.004	-	0.688
96	0.023	0.688	-

K. Slevin and T. Ohtsuki, Journal of the Physical Society of Japan 87, 094703 (2018) (arXiv:1805.11781)

Dependence on initial matrix!

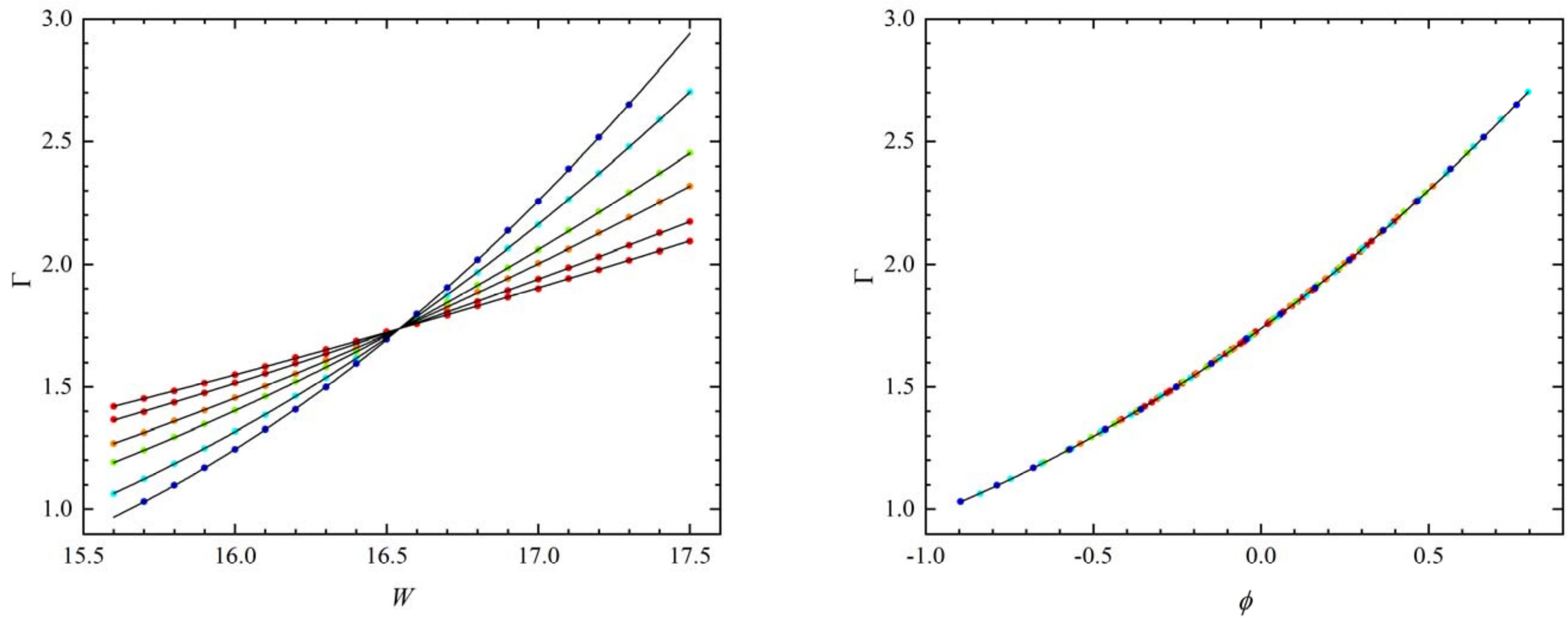
$$QR = MQ_0 = M_L \cdots M_1 Q_0$$



Finite size scaling

Energy $E = 0$ System size $L \times L \times L$ $L = 12, 16, 24, 32, 48, 64$
Disorder $W \in [15.6, 17.5]$ Ensemble size 589824 Precision 0.07% ~ 0.11%
<u>No irrelevant variable is needed</u>

$$\Gamma = F(\phi) \quad w = W - W_c \quad \phi = u(w) L^{\alpha} \quad \nu = \frac{1}{\alpha} > 0 \quad u(w) = \sum_{j=0}^{m} b_j w^j \quad F = \sum_{j=0}^{n} a_j \phi^j$$



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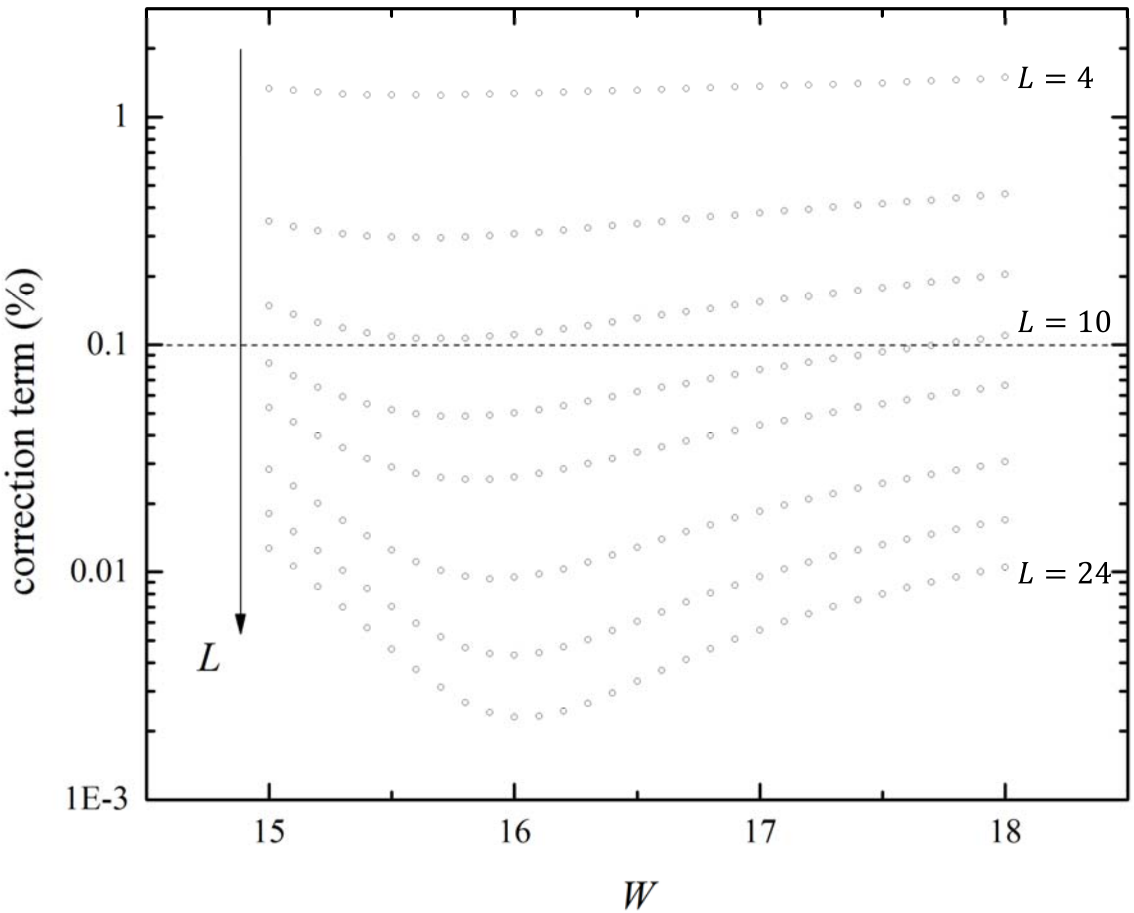
Corrections to scaling not needed



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FSS results

Stability of fit

95% confidence intervals

Goodness of fit probability

	ν	Γ_c	W_c	N_D	N_P	p
all data	1.572[1.566,1.577]	1.7372[1.7359,1.7384]	16.543[16.541,16.545]	117	7	0.5
restricted W	1.565[1.544,1.586]	1.737[1.736,1.739]	16.542[16.540,16.545]	48	6	0.6
restricted L	1.575[1.567,1.583]	1.740[1.738,1.742]	16.546[16.543,16.549]	77	7	0.8

Table II. The details of the finite size scaling fits to all the data, to data with the range of disorder W restricted to [16.2,16.9], and to data with larger system sizes $L = 24, 32, 48, 64$ only. The precisions are expressed as 95% confidence intervals. The values of the χ^2 statistic for the best fits are 112.1, 38.5, and 59.8 respectively.

$$\nu = 1.573 \pm .0055 \rightarrow \nu = 1.572 \pm .003$$

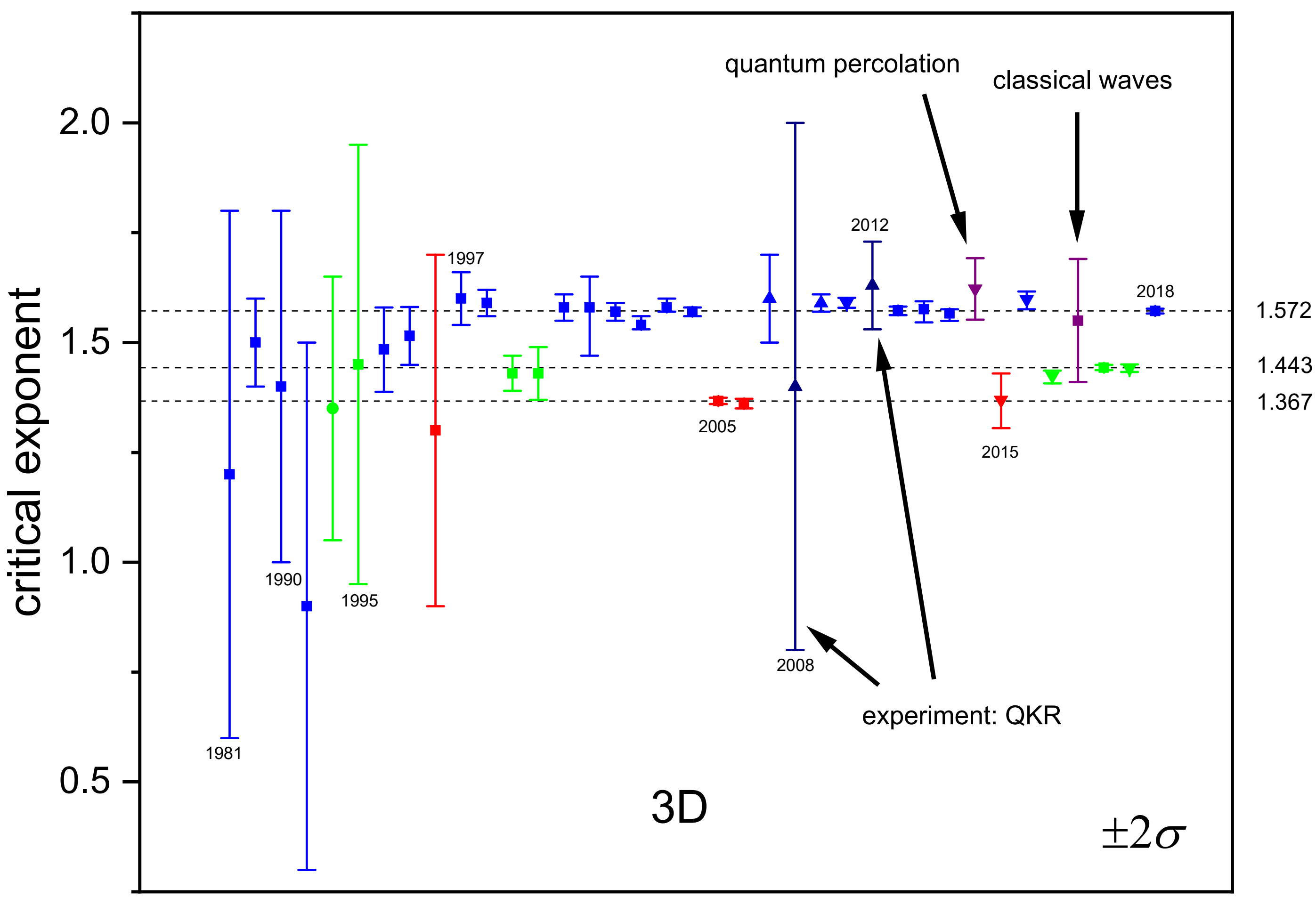
Monte Carlo simulation of synthetic datasets

K. Slevin and T. Ohtsuki, Journal of the Physical Society of Japan 87, 094703 (2018) (arXiv:1805.11781)

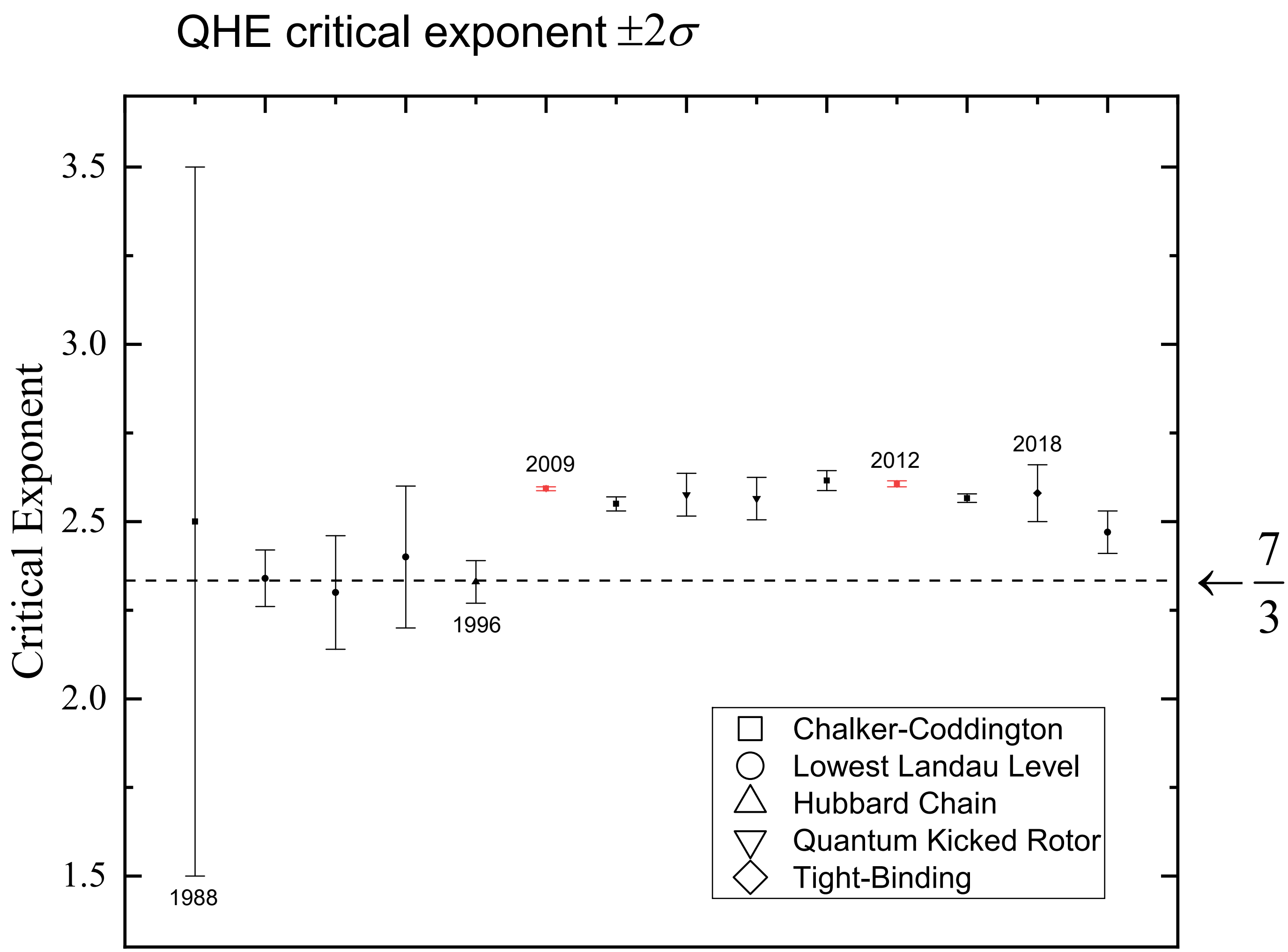
Computation

- System B of Supercomputer Center, ISSP, University of Tokyo
  - 288 MPI processes (144 nodes each with 2 CPUs).
  - Each process used 12 cores (OpenMP)
  - Parallel random number streams (MT2203 of Intel MKL)
- Computation time about 900 hours
  - mostly for L=64
- Computation time scales as L^7
  - $L = 24 \to L = 64$
  - ≈ 1000 times the total time of our 2014 calculation

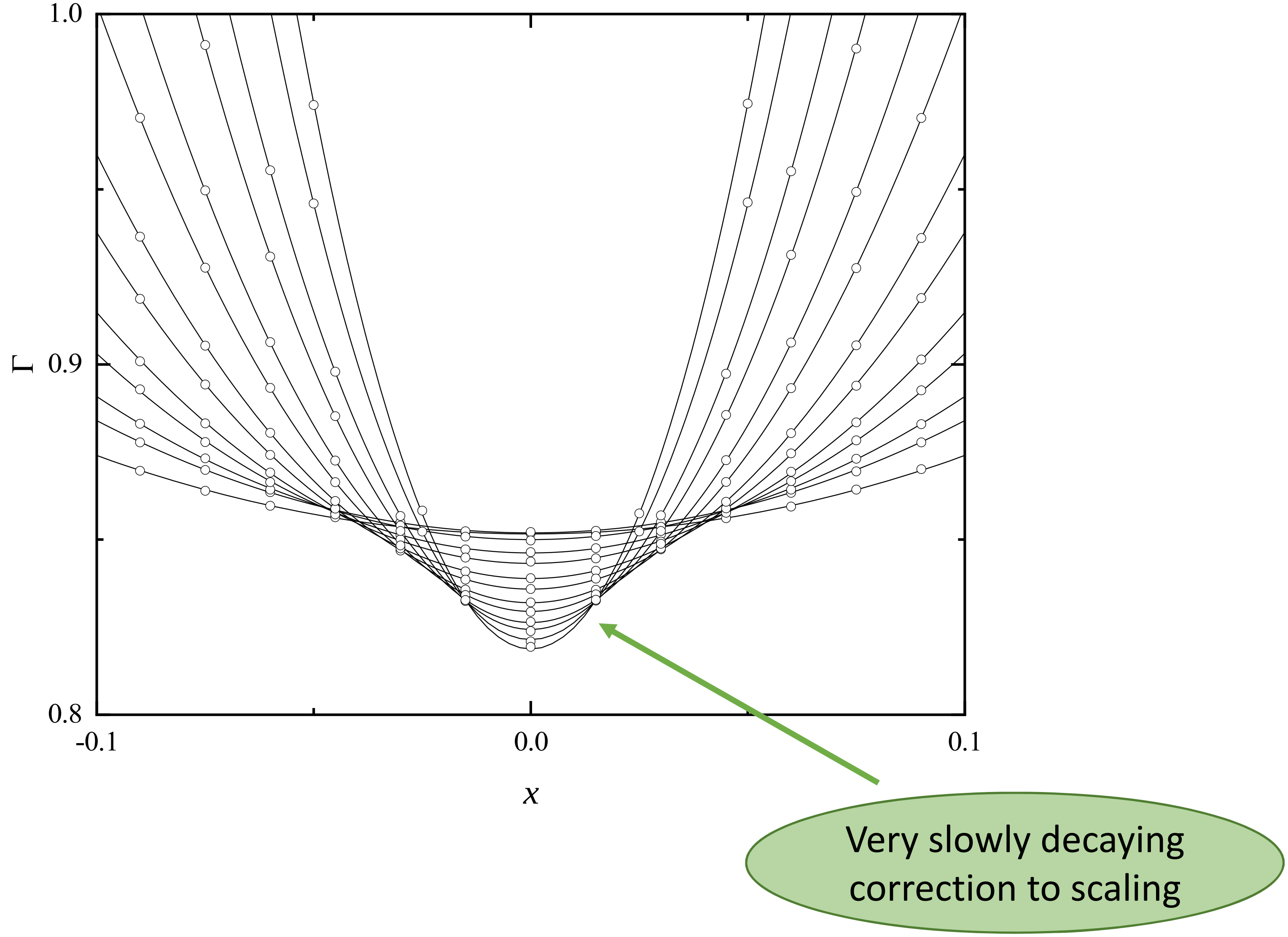
Anderson Transition in 3D



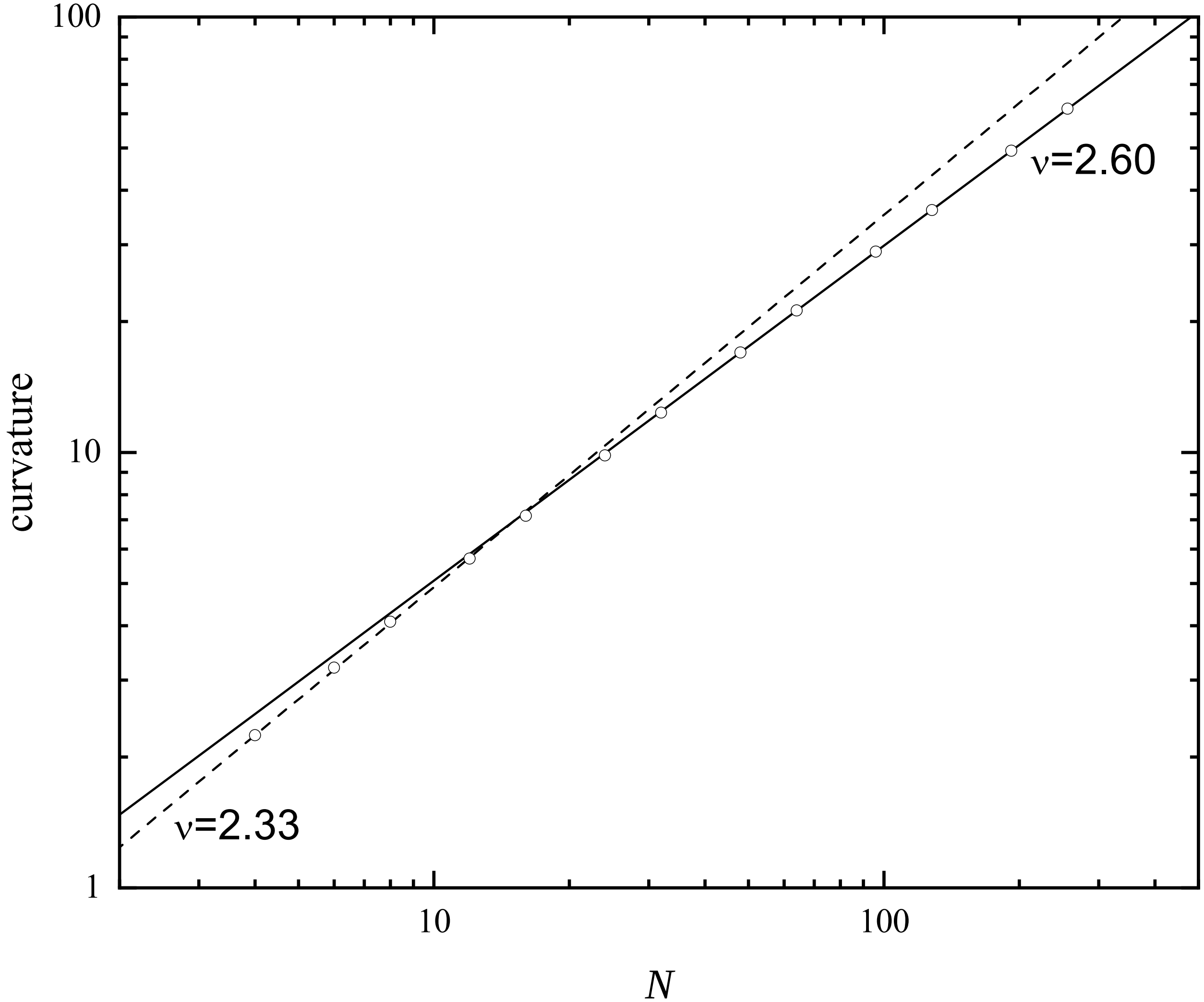
Quantum Hall Effect



QHE Finite Size Scaling



QHE Curvature vs N



Summary

- Parallel version of the transfer matrix method
  - full use of MPI
  - sample initial matrix from stationary distribution
  - system size increased from $L = 24 \to L = 64$
  - $\nu = 1.573 \pm .0055 \to \nu = 1.572 \pm .003$
- We used cubes
  - not optimal: precision of data depends on total number of transfer matrix multiplications
  - short systems better suited to generation of correlated random potentials (QHE, cold atoms,…)

- Acknowledgement
  - This work was supported by JSPS KAKENHI Grants No. 15H03700, 17K18763 and 26400393.
  - Thanks to the Supercomputer Center, ISSP, University of Tokyo for the use of System B.