HEAT CONDUCTIVITY AS A TESTING GROUND FOR THE CHARACTERIZATION OF OUT-OF-EQUILIBRIUM STEADY STATES

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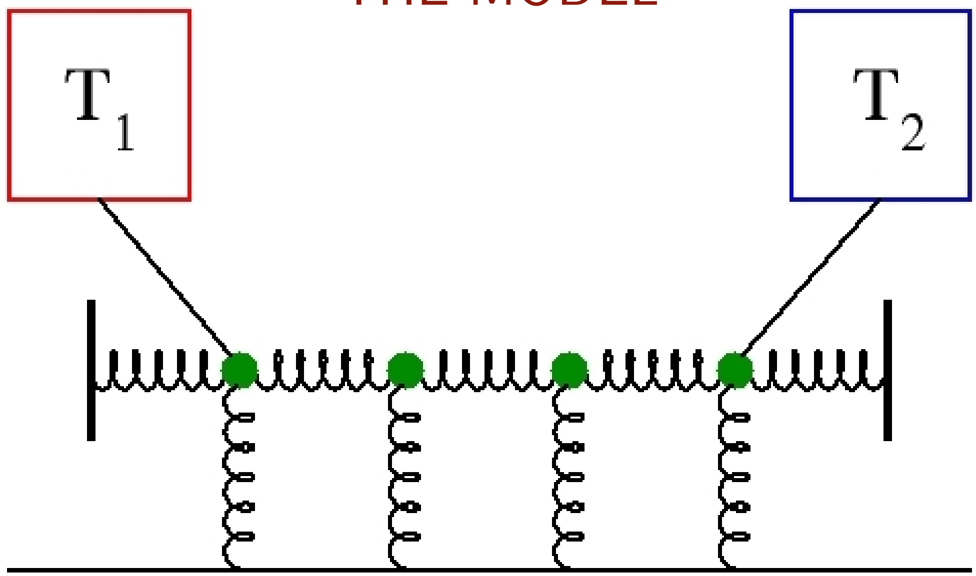
Wien – June 2008

OUTLINE

- MODELS AND DEFINITIONS
- ANOMALOUS VS. NORMAL TRANSPORT IN 1D SYSTEMS
- A SOLVABLE STOCHASTIC MODEL
- ANALYSIS OF THE STATIONARY REGIME
- "NORMAL" MODES

THE MODEL



$$H = \sum_{i=1}^{N} \left[\frac{p_i^2}{2m_i} + V(q_{i+1} - q_i) + U(q_i) \right] ,$$

m_i particle mass

$V(\cdot)$ potential energy of internal interactions

$U(\cdot)$ on-site potential

HEAT FLUX

$$j_i = \frac{1}{2}(q_{i+1} - q_i)(p_{i+1} + p_i) f(q_{i+1} - q_i) + p_i h_i$$

$j_i = \frac{a}{2}(p_i + p_{i+1}) f_{i+1}$ (in the limit of small fluctuations)

$a =$ lattice spacing

$f_{i+1} = f(q_{i+1} - q_i) =$ force due to the $i \longrightarrow (i+1)$ particle interaction

$j_i = \frac{1}{2} p_i^3$ (for an ideal gas)

THERMAL CONDUCTIVITY

$$\kappa(L) = \frac{\texttt{average\ \ heat\ \ flux}}{\texttt{thermal\ \ gradient}}$$

normal behaviour

$$\kappa(L)_{\lim L\to\infty} \qquad \texttt{finite}$$

sub/super conductive behaviour ($\alpha < 0, > 0$)

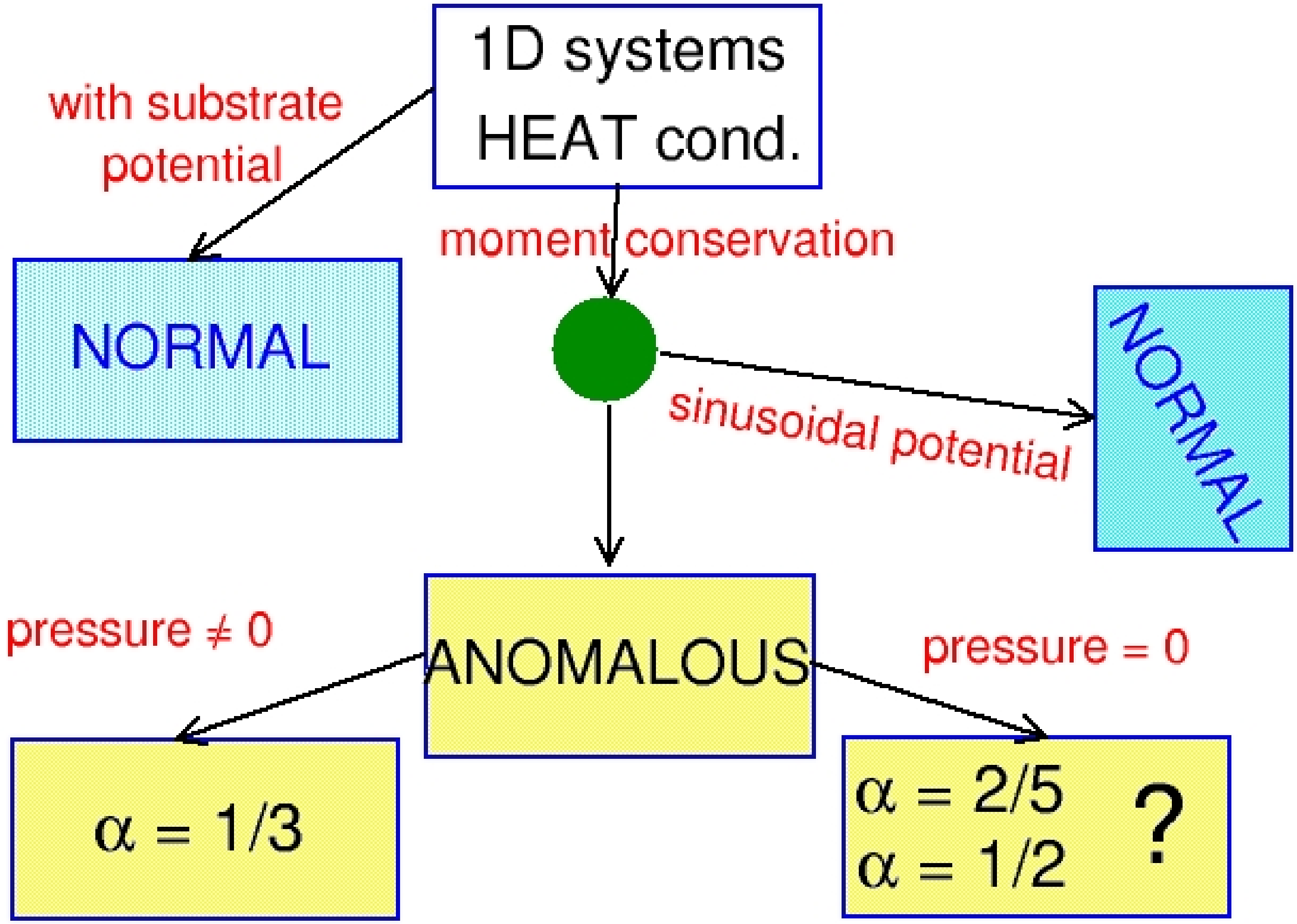
$$\kappa(L)_{\lim L\to\infty} \approx L^{\alpha}$$

THEORETICAL TOOLS

DYNAMICAL Renormalization Group

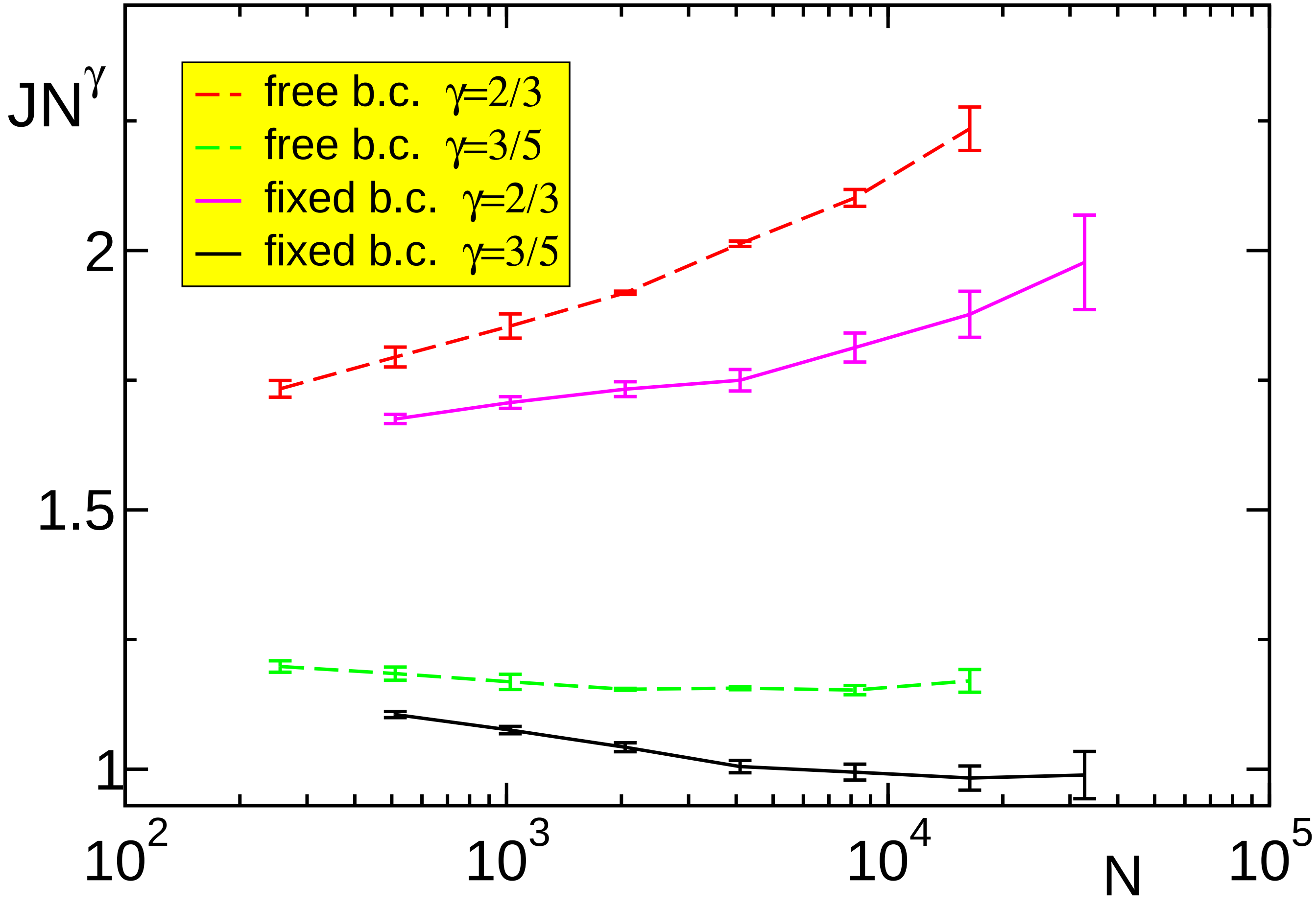
BOLTZMANN-PEIERLS EQUATION

SELF-CONSISTENT MODE COUPLING EQUATIONS

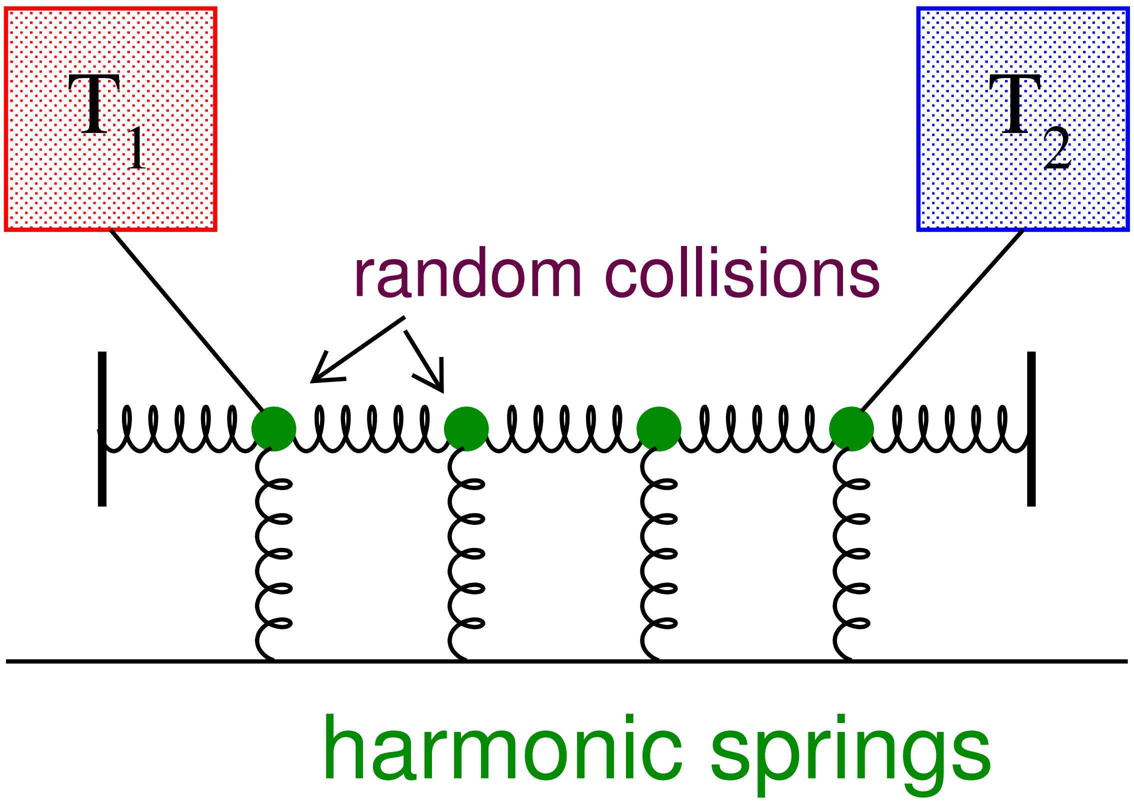

1D systems
HEAT cond.
with substrate potential
NORMAL
moment conservation
sinusoidal potential
NORMAL
ANOMALOUS
pressure ≠ 0
pressure = 0
α = 1/3
α = 2/5
α = 1/2
?

AN ACCURATE NUMERICAL TEST

FPU-β : $T_+=1.1$; $T_-=0.9$



A STOCHATIC MODEL
ADAPTED FROM Basile Bernardin Olla



Kipnis, Marchioro, Presutti 1982
Bernardin, Olla 2005
Giardinà, Kurchan, Redig 2007

EQUATION FOR THE PROBABILITY DENSITY

$$\frac{\partial P}{\partial t}(x,t) \;=\; (\mathbb{L} + \mathbb{L}_{col})\, P(x,t) \qquad x \equiv (q,p)$$

$$\mathbb{L}P = \sum_{\mu,\nu} \left[a_{\mu\nu} \frac{\partial}{\partial x_\mu}(x_\nu P) + \frac{d_{\mu\nu}}{2} \frac{\partial^2 P}{\partial x_\mu \partial x_\nu} \right]$$

$$\mathbf{a} = \begin{pmatrix} \mathbf{0} & -\mathbf{I} \\ \omega^2 \mathbf{g} + k\mathbf{I} & \lambda \mathbf{r} \end{pmatrix}$$

$$\mathbf{d} = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & 2\lambda k_B T(\mathbf{r} + \eta \mathbf{s}) \end{pmatrix}$$

$$T = (T_+ + T_-)/2 \qquad \eta = (T_+ - T_-)/T$$

$$\mathbb{L}_{col} P = \gamma \sum_i [P(\ldots p_{i+1}, p_i \ldots) - P(\ldots p_i, p_{i+1} \ldots)]$$

Covariance matrix $c_{\mu\nu} = \langle x_\mu x_\nu \rangle \equiv \int dx\, P(x,t) x_\mu x_\nu$

$$\mathbf{c} = \begin{pmatrix} \mathbf{u} & \mathbf{z} \\ \mathbf{z}^\dagger & \mathbf{v} \end{pmatrix}$$

$$\dot{\mathbf{c}} \;=\; \mathbf{d} - \mathbf{ac} - \mathbf{ca}^\dagger + \dot{\mathbf{c}}_{col} \quad .$$

The contribution due to collisions reads

$$\dot{\mathbf{c}}_{col} = -\gamma \begin{pmatrix} \mathbf{0} & \mathbf{zg} \\ \mathbf{gz}^\dagger & \mathbf{w} \end{pmatrix}$$

where the auxiliary $N \times N$ matrix $\mathbf{w}$ is defined by

$$w_{ij} \equiv \begin{cases} v_{i+1j} + v_{i-1j} + v_{ij-1} + v_{ij+1} - 4v_{ij} & |i-j| > 1 \\ v_{i\pm1j} + v_{ij\mp1} - 2v_{ij} & i-j = \pm1 \\ v_{i-1j-1} + v_{i+1j+1} - 2v_{ij} & i = j \end{cases}$$

Stationary solution

$$\mathbf{z}^\dagger = -\mathbf{z}$$
$$\mathbf{v} = \omega^2 \mathbf{u}\mathbf{g} + k\mathbf{u} + \lambda \mathbf{z}\mathbf{r} + \gamma \mathbf{z}\mathbf{g}$$
$$\omega^2 \left(\mathbf{g}\mathbf{z} + \mathbf{z}^\dagger \mathbf{g}\right) + \lambda \left(\mathbf{r}\mathbf{v} + \mathbf{v}\mathbf{r}\right) + \gamma \mathbf{w} = 2\lambda k_B T (\mathbf{r} + \eta \mathbf{s})$$

Temperature profile: $T_i = \langle p_i^2 \rangle = v_{ii}$

Energy current: $J = J_i^d + J_i^c$

$$J_i^d \;=\; \omega^2 \langle q_{i-1} p_i \rangle \;=\; \omega^2 z_{i-1,i}$$

$$J_i^c \;=\; \frac{\gamma}{2}[\langle p_i^2 \rangle - \langle p_{i-1}^2 \rangle] \;=\; \frac{\gamma}{2}[v_{i,i} - v_{i-1,i-1}]$$

COORDINATE TRANSFORMATION

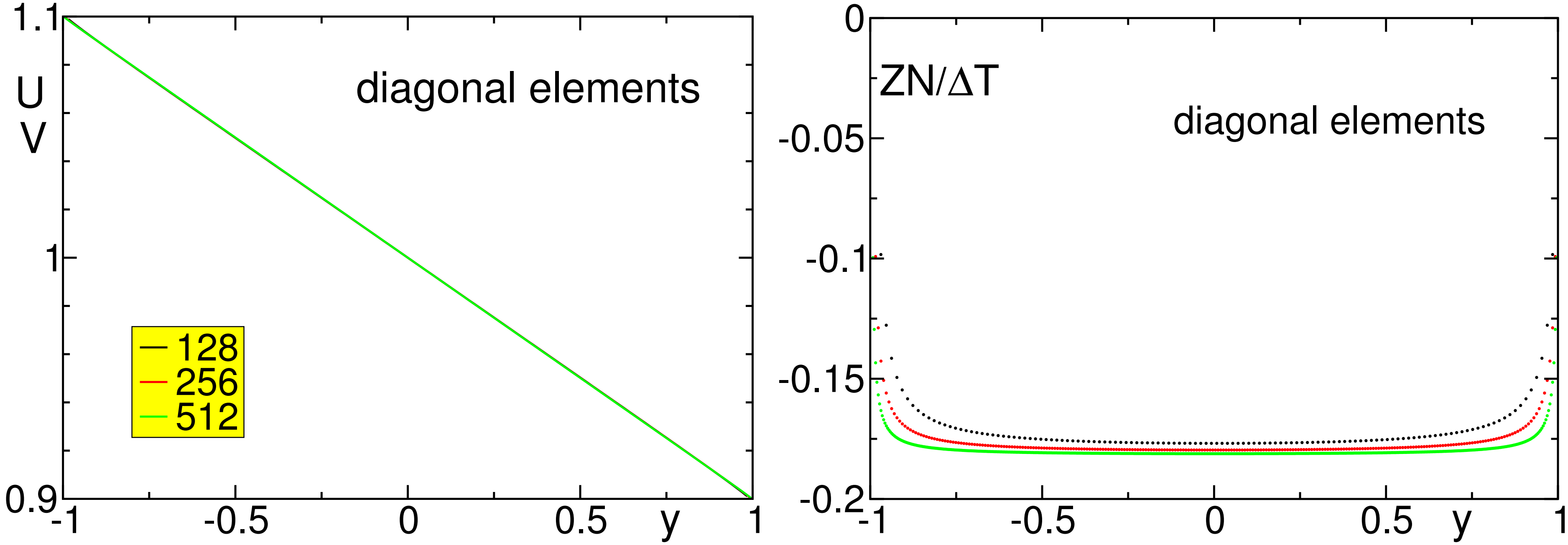
$$Q_i \; = \; a q_{i+1} - b q_i; \quad P_i = p_i$$

$$a = [\omega^2 + k/2 + (\omega^2 k + k^2/4)^{1/2}]^{1/2} \qquad b = \omega^2/a.$$

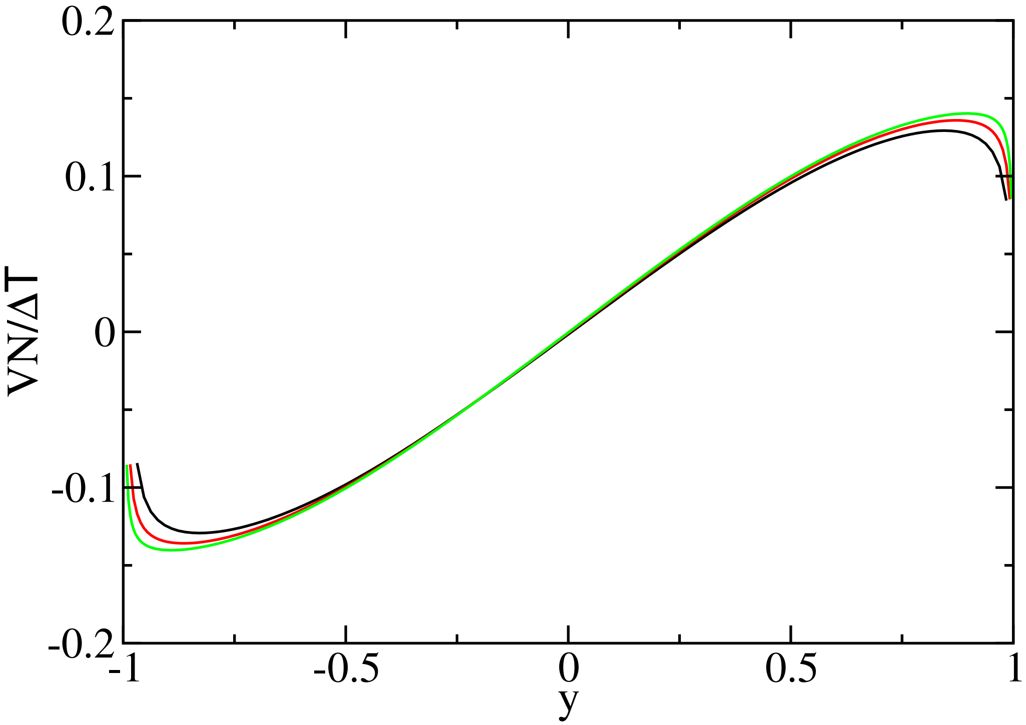
NEW COVARIANCE MATRIX

$$\mathbf{C} = \begin{pmatrix} \mathbf{U} & \mathbf{Z} \\ \mathbf{Z}^\dagger & \mathbf{V} \end{pmatrix}$$

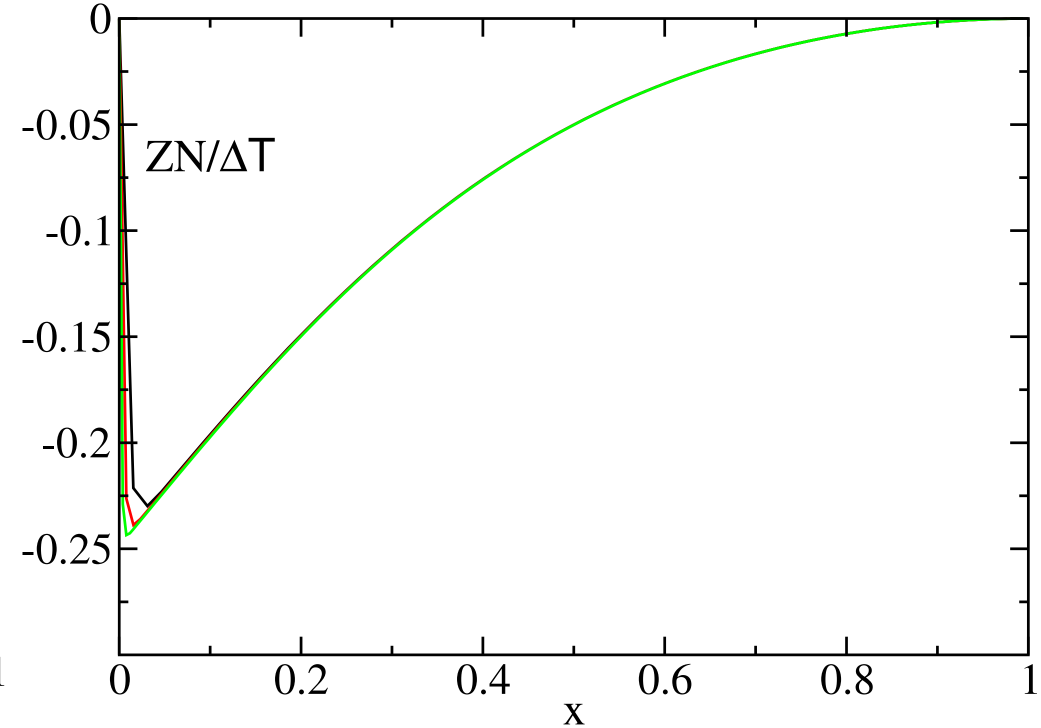
WITH ON-SITE POTENTIAL



$$y = (i + j - N)/N \qquad x = (i - j)/N$$



$i - j = 1$



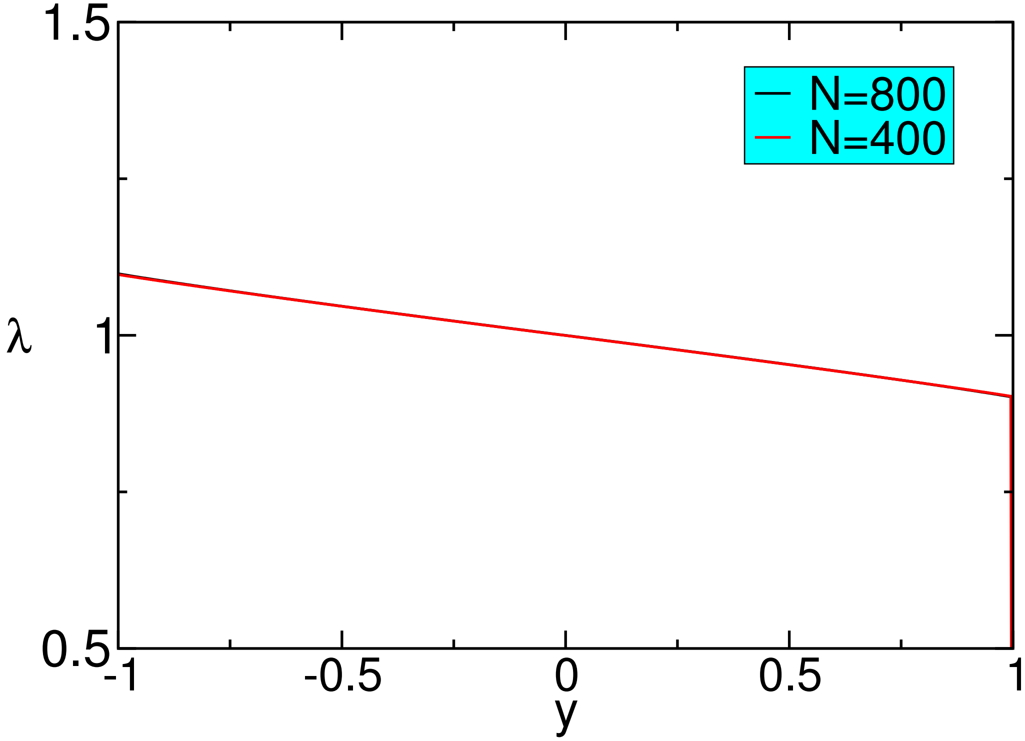
$y = 0$

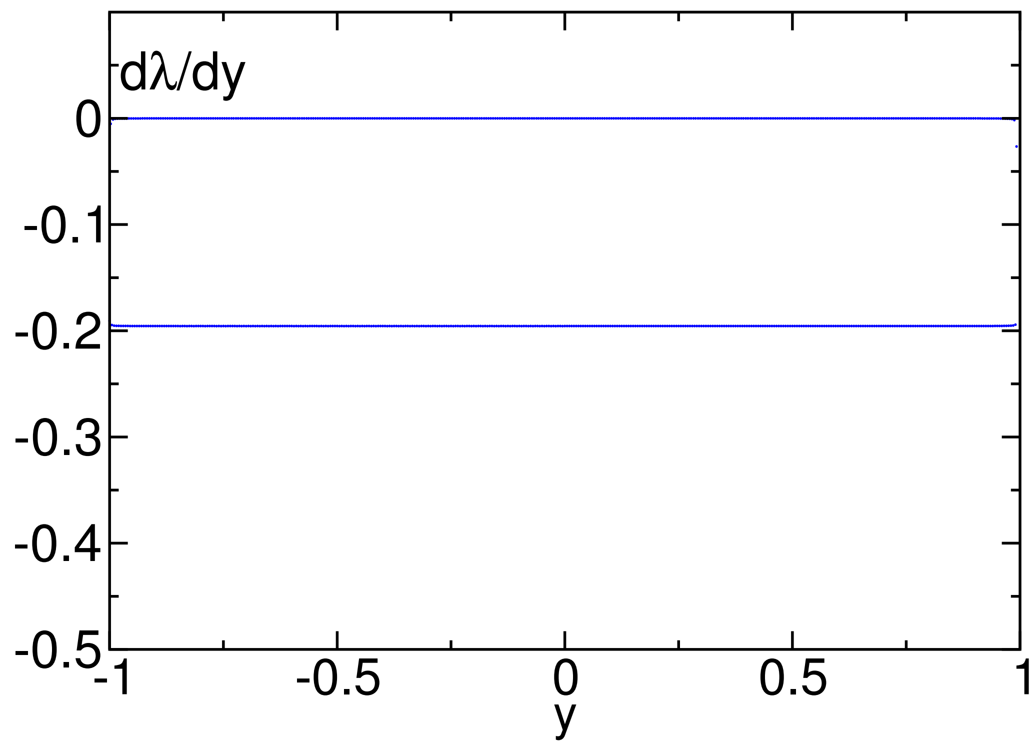
antidiagonal

PRINCIPAL COMPONENT ANALYSIS

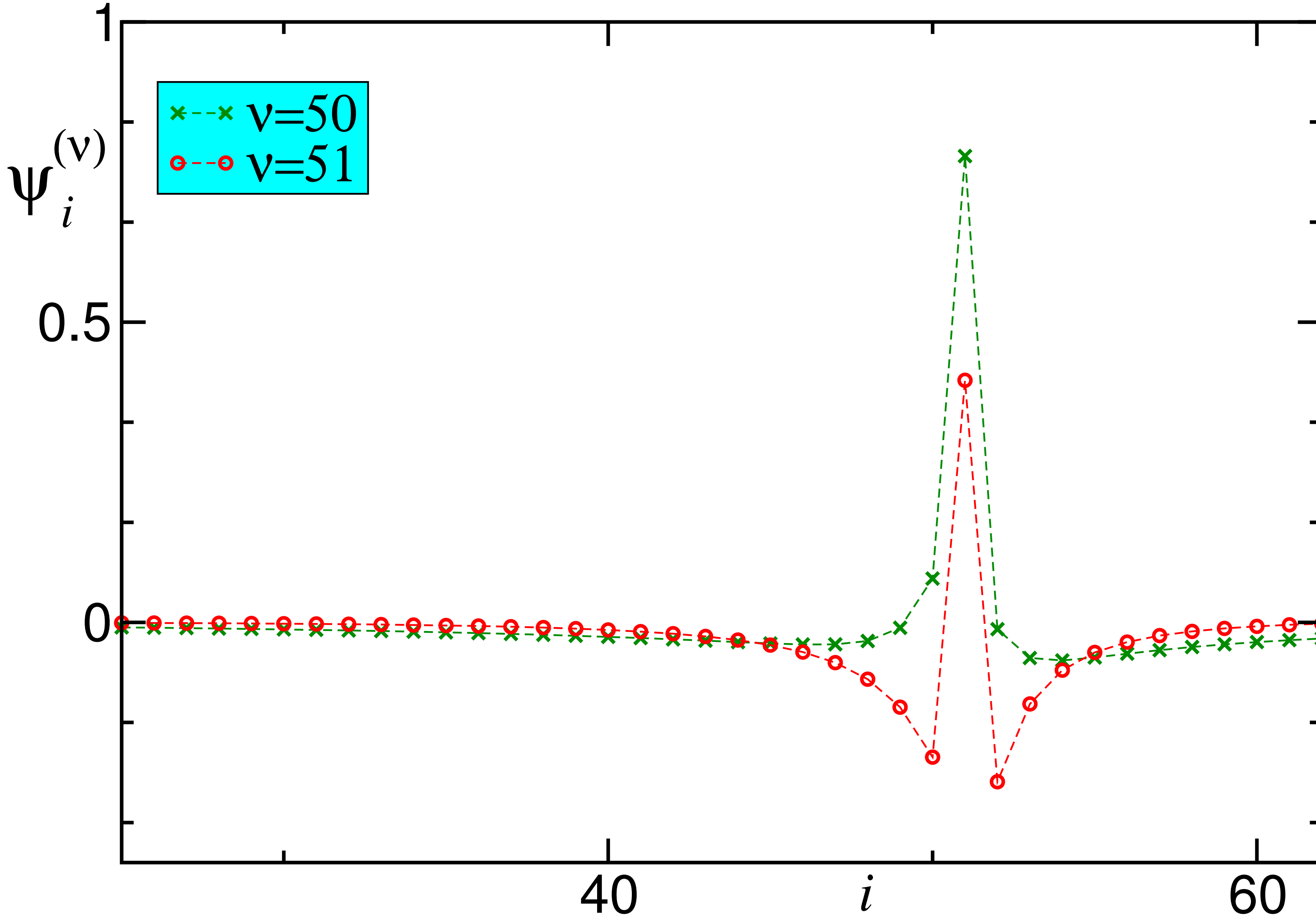
$$\mathbf{C}\psi^{(\nu)} \;=\; \lambda_\nu \psi^{(\nu)}, \qquad \nu = 1, \ldots, 2N$$

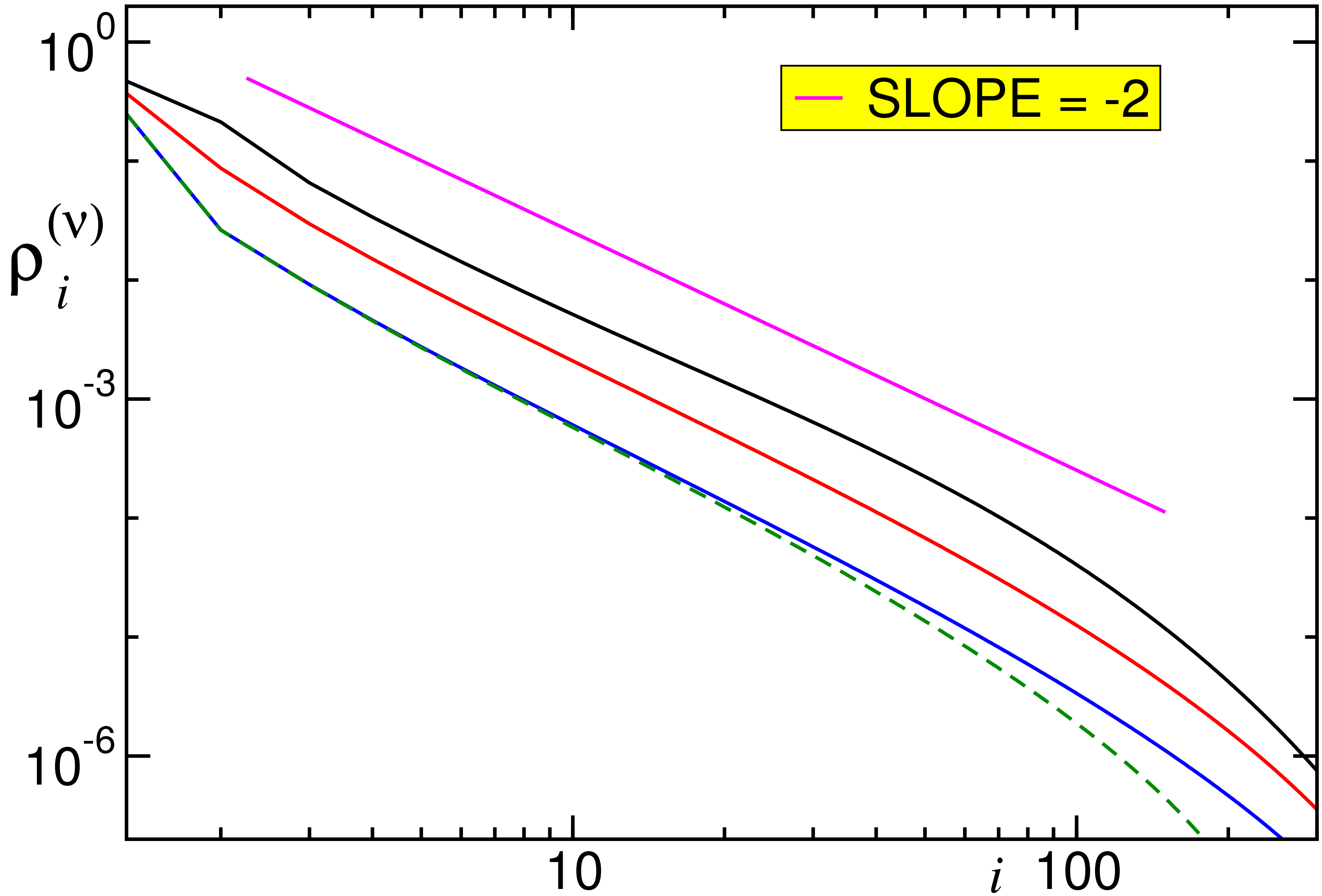
EIGENVALUES



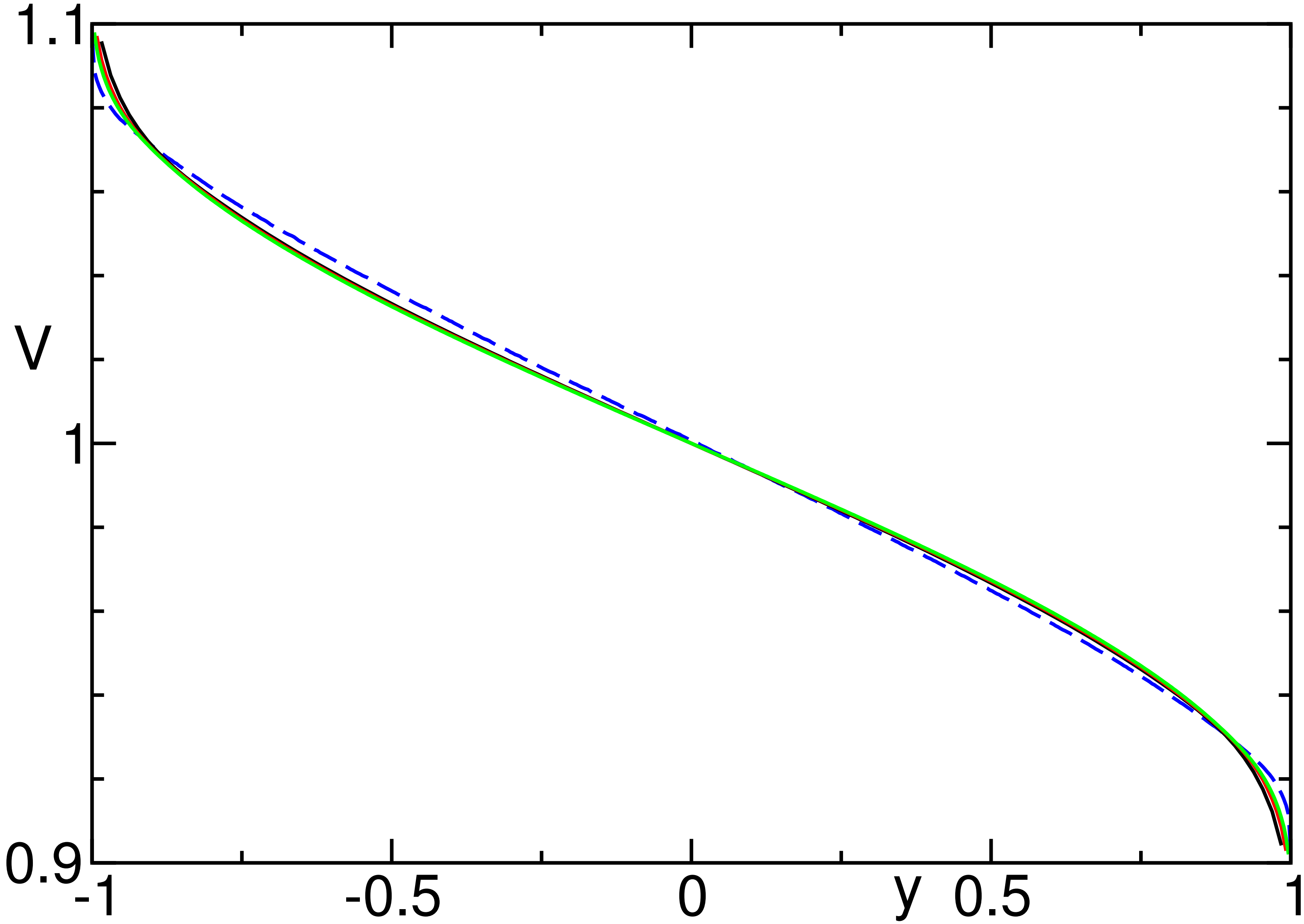


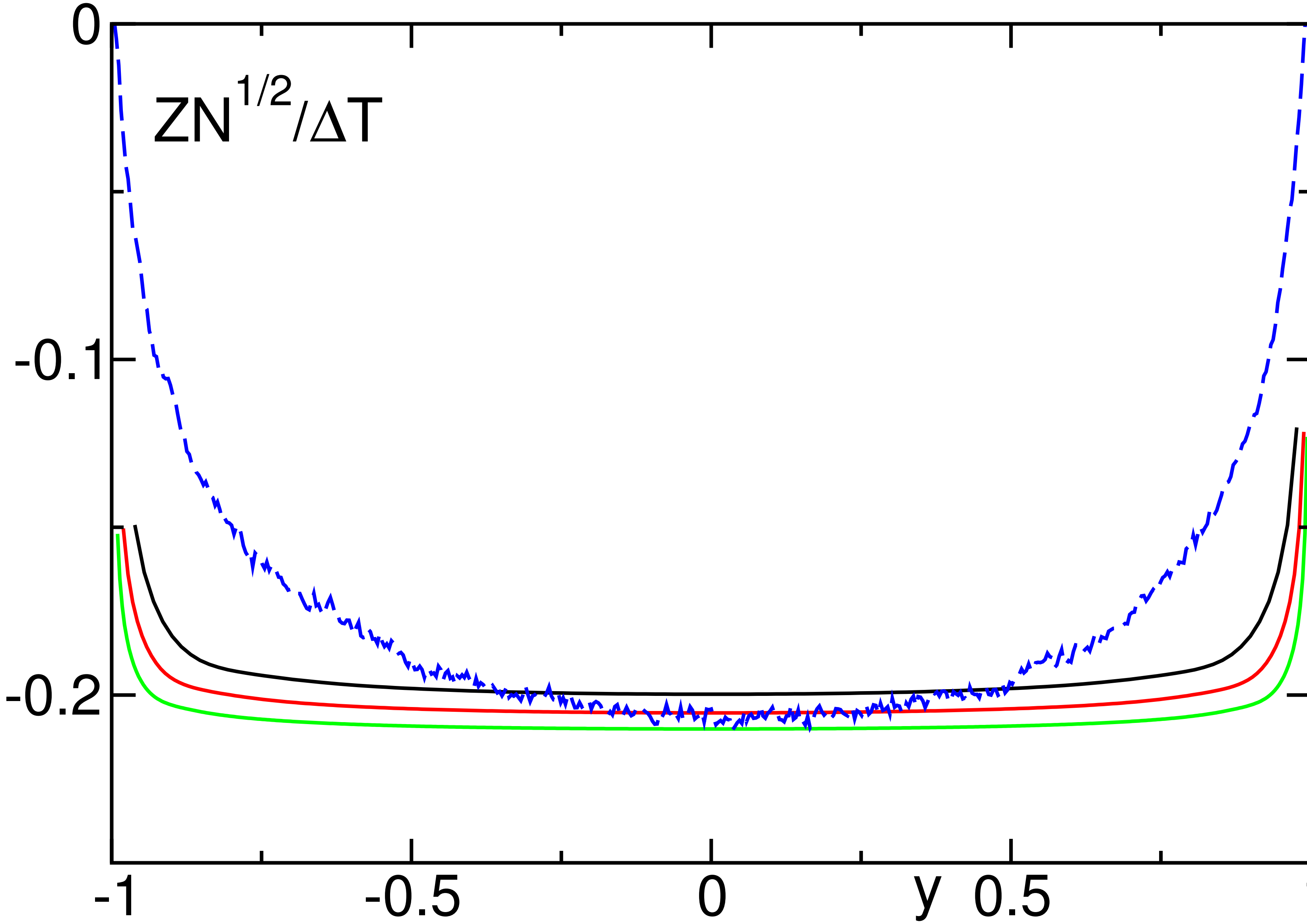
EIGENVECTORS



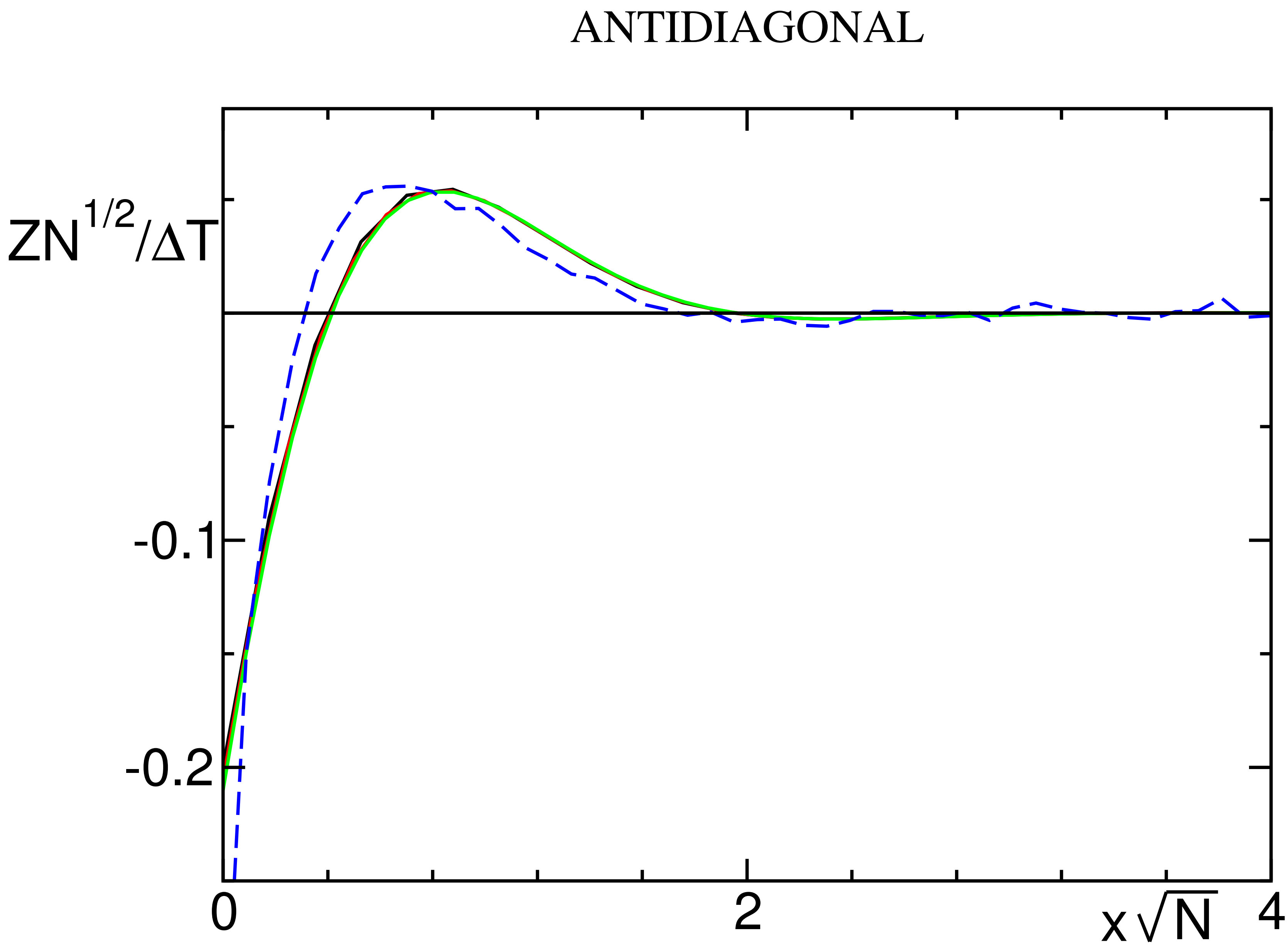

SLOPE = -2
10^{0}
10^{-3}
10^{-6}
$\rho_i^{(\nu)}$
10
100
i

WITH TRANSLATIONAL INVARIANCE





0
-0.1
-0.2
$ZN^{1/2}/\Delta T$
-1
-0.5
0
y
0.5
1


ANTIDIAGONAL
ZN^1/2/ΔT
-0.1
-0.2
0
2
x √N
4

THE CONTINUUM LIMIT
work in progress

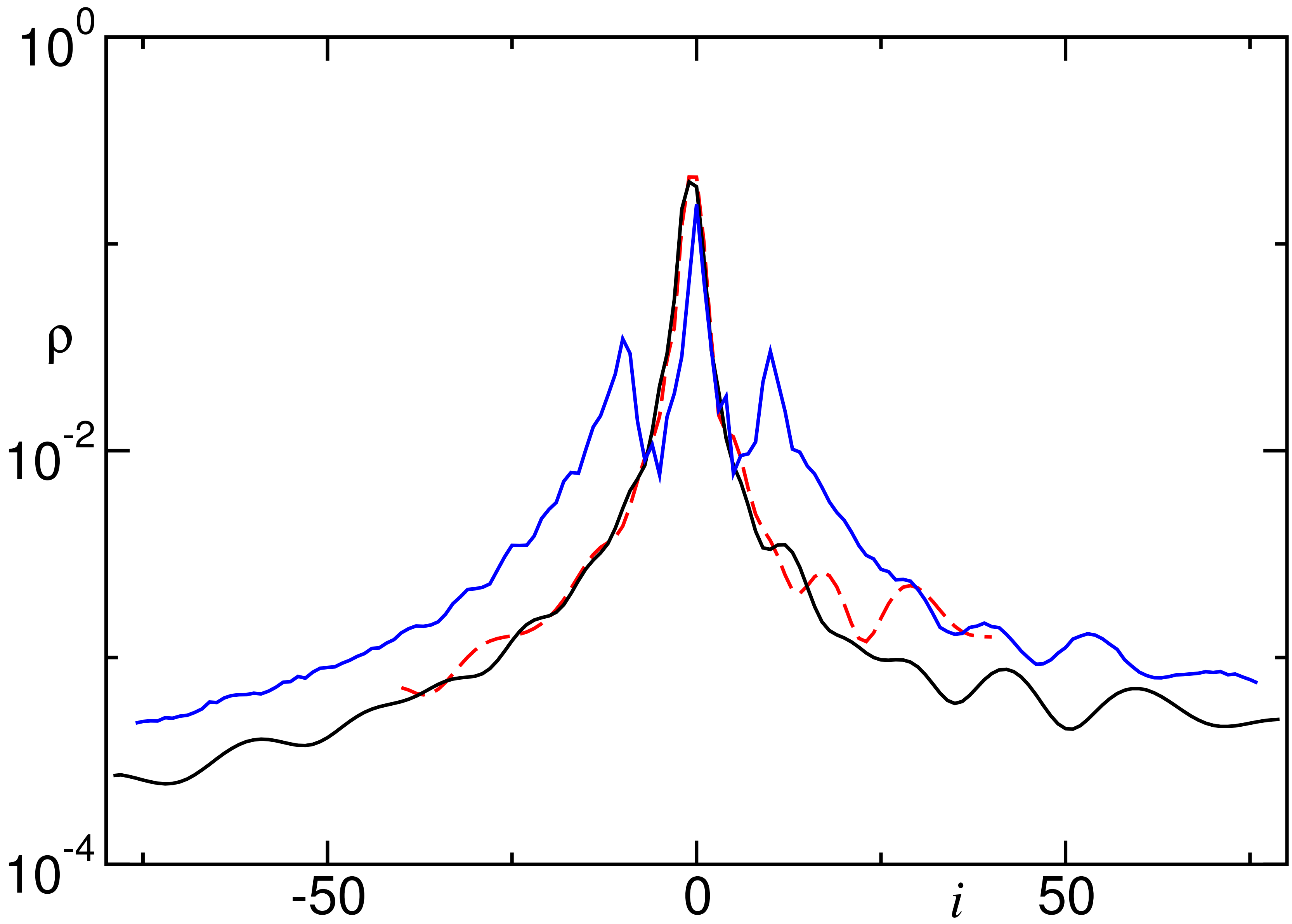
$$x = (i-j)\varepsilon \qquad y = \frac{(i+j)\varepsilon^2 - 1}{|1-(i-j)\varepsilon^2|}$$

where ε is a smallness parameter,

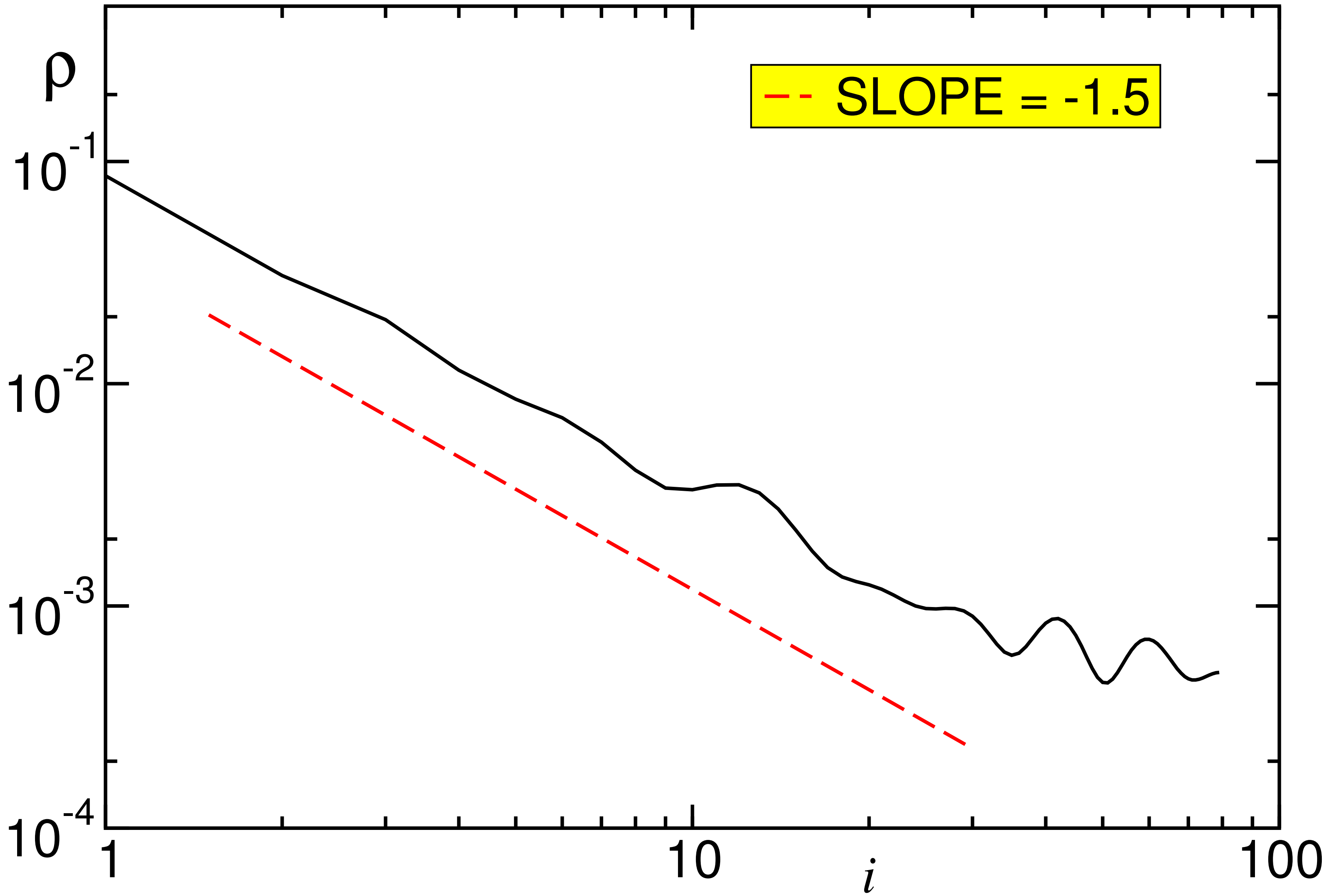
$$\varepsilon \; = \; \frac{1}{\sqrt{N}}$$

The leading component of the matrix Z satisfies the equation

$$4\omega^2 Z^{(0)}_{yy} = \gamma^2 Z^{(0)}_{xxxx}$$



10^0
10^{-2}
10^{-4}
ρ
-50
0
50
i


ρ
SLOPE = -1.5
10^{-1}
10^{-2}
10^{-3}
10^{-4}
1
10
100
i