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Kinetic Approach to 1D Energy Transport

Herbert SPOHN

Technische Universitaet Muenchen TUM, Zentrum Mathematik M5, Garching Germany

Strada Costiera, 11 - 34151 - Trieste - Italy • Tel. +39 0402240111 • Fax. +39 040224163 • sci_info@ictp.it • www.ictp.it
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Kinetic Approach to 1D Energy Transport

Herbert Spohn

TU München

jointly with J. Lukkarinen, P. Mei (Univ. Helsinki)

M. Fürst, C. Mendl (TUM)

goal: kinetic theory as a universal tool to study 1D energy transport

Example 1: FPU type chain

in competition with

- molecular dynamics
- mode coupling theory ⇒ lectures Livi

⇒ van Beijeren 2012, link to KPZ

Example 2: Hubbard chain

draw back: small nonlinearity

I. FPU type chain

A: on-site potential, no momentum conservation

$$H = \sum_j \left\{ \frac{1}{2} p_j^2 + \frac{1}{2} \omega_0^2 q_j^2 - \delta \omega_0^2 q_j q_{j+1} + \frac{1}{4} \lambda q_j^4 \right\}$$

"coupling"

on-site non-linear

stability $\Rightarrow$ $0 < \delta \leq \frac{1}{2}$

- kinetic equation small λ
- dispersion relation $\omega(k)^2 = (1 - 2\delta \cos k)\,\omega_0^2$
- normal modes $a(k) = \frac{1}{\sqrt{2}} \left(\sqrt{\omega}\, \hat{q}(k) + i \frac{1}{\sqrt{\omega}} \hat{p}(k) \right)$

$|k| \leq \pi$, $\mathbb{T} = [-\pi, \pi]$

- average Wigner function   spatially homogeneous

$$\langle a(k)^* a(k') \rangle_t = W^\lambda(k,t)\,\delta(k-k')$$

variation on time scale λ^{-2} $(t \rightsquigarrow \lambda^{-2} t)$

momentum mod 2π

energy

$$\rightsquigarrow \frac{\partial}{\partial t} W_1 = \int_{\mathbb{T}^3} dk_2\, dk_3\, dk_4\, (\omega_1 \omega_2 \omega_3 \omega_4)^{-1}\, \delta(\underline{k})\, \delta(\underline{\omega})$$

$$\times \left[W_2 W_3 W_4 + W_1 W_3 W_4 - W_1 W_2 W_3 - W_1 W_2 W_4 \right]$$

$W_j = W(k_j)$, $\omega_j = \omega(k_j)$

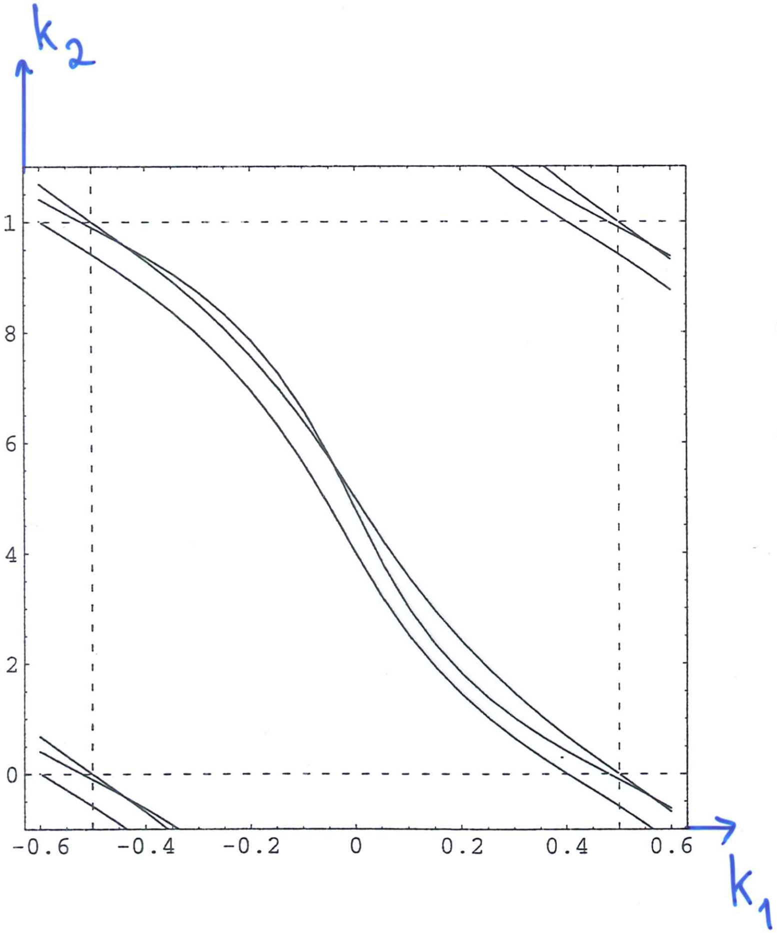
$\underline{\omega} = \omega_1 + \omega_2 - \omega_3 - \omega_4$

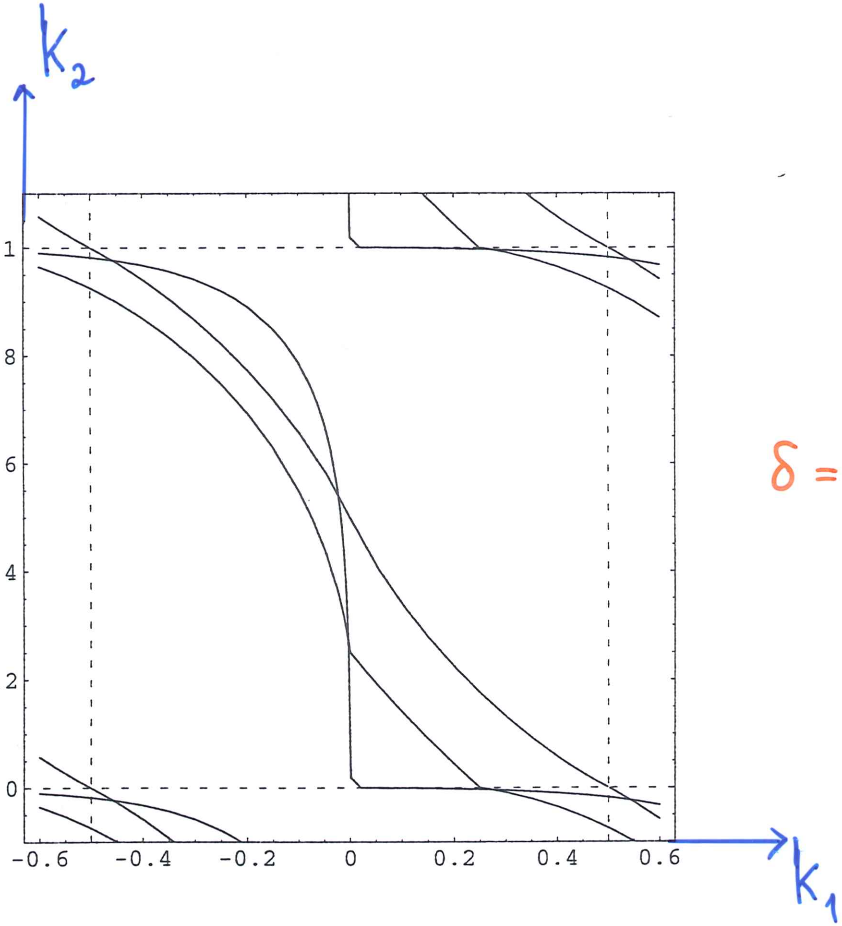
$\underline{k} = k_1 + k_2 - k_3 - k_4$

spatially inhomogeneous

$W(r,k,t)$ ADD $-\omega'(k)\frac{\partial}{\partial r}$

$\delta = 0.4$





$\delta = 0.5$

$$k_2 = k_2(k_1 ; k_3)$$

- stationary solutions: equilibrium $W_\beta(k) = \dfrac{1}{\beta\,\omega(k)}$

|| energy transport $\Leftrightarrow$ energy current correlation in equilibrium ||

$$J^{en}_{j,j+1} = -\frac{1}{2}\,\delta\,\omega_0^2\,(p_j\,q_{j+1} - p_{j+1}\,q_j)$$

$$C_\lambda(t) = \sum_j \langle J^{en}_{j,j+1}(t)\,J^{en}_{0,1}(0)\rangle_{eq}$$ total

- non-equilibrium

$$\langle J^{en}_{0,1}(t)\rangle = \delta \int_{\mathbb{T}} dk\,\underbrace{\sin 2k}_{\substack{\shortparallel \\ g\,=\,\omega'\omega}}\,W^\lambda(k,t)$$

small λ

as operators

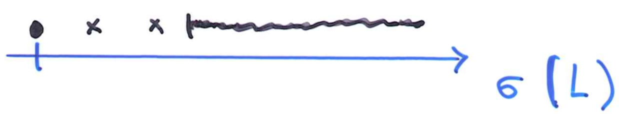
$$C^{\lambda}(\lambda^{-2}t) = \langle \omega g, e^{-\omega L \omega |t|} \omega g \rangle$$

$$\langle g, f \rangle = \int_{\mathbb{T}} dk \, g(k) f(k)$$

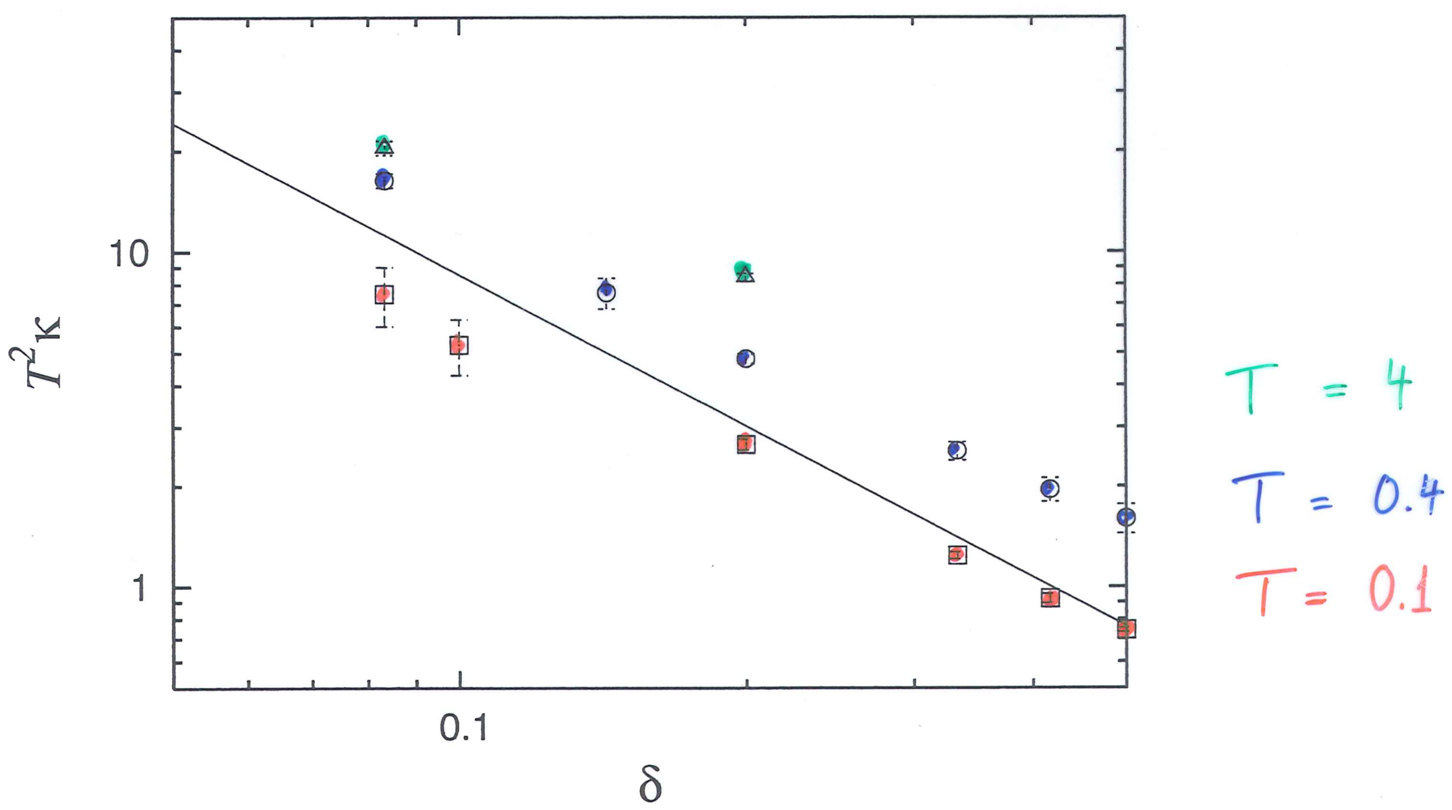
linearized collision operator

$$\langle f, L f \rangle = \int_{\mathbb{T}^4} d\underline{k} \, (\omega_1 \omega_2 \omega_3 \omega_4)^{-2} \delta(\underline{k}) \delta(\underline{\omega}) (f_1 + f_2 - f_3 - f_4)^2$$

$\omega L \omega$ has spectral gap



$\rightsquigarrow$ thermal conductivity $\int dt \, \langle \omega g, e^{-\omega L \omega |t|} \omega g \rangle > 0$, finite



10
1
0.1
$T^2\kappa$
δ
T = 4
T = 0.4
T = 0.1

B: β-chain momentum conservation

$$H = \sum_j \left\{ \frac{1}{2} p_j^2 + \frac{1}{2} (q_j - q_{j+1})^2 + \frac{1}{2}\lambda (q_j - q_{j+1})^4 \right\}$$

$$\omega(k) = \left| \sin\left(\frac{k}{2}\right) \right|$$

collision operator

$$\mathcal{C}(W)_1 = \int_{\mathbb{T}^3} dk_2 dk_3 dk_4 \, \omega_1 \omega_2 \omega_3 \omega_4 \; \delta(\underline{k}) \delta(\underline{\omega}) \left[W_1 W_3 W_4 + W_2 W_3 W_4 - W_1 W_2 W_3 - W_1 W_2 W_4 \right]$$

!

linearized

$$\langle f, L f \rangle = \int_{\mathbb{T}^4} d\underline{k} \; \delta(\underline{k}) \delta(\underline{\omega}) \left(f_1 + f_2 - f_3 - f_4 \right)^2$$

!

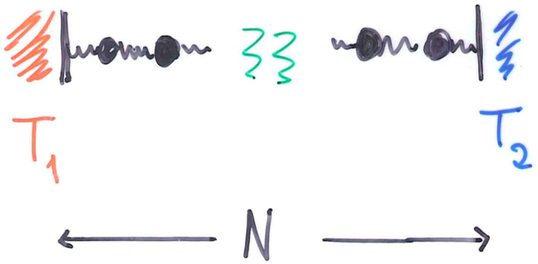
$$(\omega L \omega f)(k) = \int dk' \underbrace{R(k,k')}_{\text{explicit}} f(k') - \underbrace{V(k)}_{1/\text{relaxation time}} f(k)$$

R is "nice" integral operator,

$$V(k) \cong |k|^{5/3} \qquad k \to 0$$

NO spectral gap $\quad \langle \omega', e^{-\omega L \omega |t|} \omega' \rangle \cong t^{-3/5}$

super diffusive energy transport



steady state energy current $\quad N^{-3/5}$

mode coupling $\quad N^{-2/3}$

II. Hubbard chain

A: some theory

fermions on lattice $\mathbb{Z}$, weak on-site interaction

(similarly $\mathbb{Z}^D$, several bands,

example: graphene $D=2$, 2 bands, honeycomb)

Fermi field $\quad a_\sigma(x), \; a_\sigma^*(x), \; \sigma = \pm 1, \; x \in \mathbb{Z}$

$$\| \; H = \sum_{x,y} \underbrace{\alpha(x-y)}_{\text{hopping}} \, a(x)^* \cdot a(y) + \frac{1}{2} \lambda \sum_x \underbrace{(a(x)^* \cdot a(x))}_{\text{on-site}}{}^2 \; \|$$

$$a^* \cdot a = \sum_{\sigma = \pm 1} a_\sigma^* a_\sigma$$

dispersion $\quad \omega(k) = \hat{\alpha}(k)$

NO square

SU(2) invariant

$$\langle \hat{a}_\sigma(k)^* a_{\sigma'}(k') \rangle_t = \delta(k-k') W^\lambda_{\sigma\sigma'}(k,t)$$ spatially homogeneous

$W(k,t)$ is 2×2 matrix-valued $\quad 0 \leq W \leq 1$

$|\lambda| \ll 1$, kinetic time scale λ^{-2}.

$\rightsquigarrow$ $$\frac{d}{dt} W = \mathcal{C}(W) \qquad \mathcal{C} = \mathcal{C}_{col} + \mathcal{C}_{dis}$$

$$\mathcal{C}_{dis}(W) = -i[H_{eff}, W]$$

depends on $W(t)$

unitary, no entropy production

$$H_{eff,1} = \int_{\mathbb{T}^3} dk_2\, dk_3\, dk_4\ \delta(\underline{k})\ \mathcal{P}\left(\frac{1}{\underline{\omega}}\right) \left[W_3 W_4 - W_2 W_3 - W_3 W_2 - (\operatorname{tr} W_4) W_3 + (\operatorname{tr} W_2) W_3 + W_2 \right]$$

order !!

$\mathcal{P}$ principle value

$\mathcal{C}_{col}$

use $\mathcal{J}(W) = \operatorname{tr} W - W$ $\qquad \begin{pmatrix} a & b \\ c & d \end{pmatrix} \longmapsto \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$

$$\mathcal{C}_{col,1} = \int_{\mathbb{T}^3} dk_2\, dk_3\, dk_4\ \delta(\underline{k})\ \delta(\underline{\omega})$$

$$\times \left[\tilde{W}_1 W_3 \mathcal{J}(\tilde{W}_2 W_4) + \mathcal{J}(W_4 \tilde{W}_2) W_3 \tilde{W}_1 - W_1 \tilde{W}_3 \mathcal{J}(W_2 \tilde{W}_4) - \mathcal{J}(\tilde{W}_4 W_2) \tilde{W}_3 W_1 \right]$$

$\tilde{W} = 1 - W$

order !!

$\Rightarrow$ in condensed matter it is always assumed

$$W_{\sigma\sigma'}(k,t) = \delta_{\sigma\sigma'} W_\sigma(k,t)$$

$\rightsquigarrow$ $\mathcal{C}_{dis} \equiv 0$

$\rightsquigarrow$ two component classical Boltzmann

$$\frac{d}{dt} W_+ = \mathcal{C}_+(W_+, W_-)$$

$$\frac{d}{dt} W_- = \mathcal{C}_-(W_+, W_-)$$

properties of Hubbard-Boltzmann

- $\mathcal{C}(W)^* = \mathcal{C}(W^*)$

- Fermi constraint propagates $\quad 0 \leq W(k,t) \leq 1$

based on the inequality

matrices: A, B, C hermitean, ≥ 0

$$\| ABC + CBA - \mathrm{tr}(AB)\,C - \mathrm{tr}(CB)\,A \leq 0 \|$$

- conservation laws, approach to equilibrium

SU(2) $\quad \frac{d}{dt} \int dk\, W(k,t) = 0$

energy $\quad \frac{d}{dt} \int dk\, \omega(k)\, \mathrm{tr}\, W(k,t) = 0$

SU(2) fixes basis energy

2 eigenvalues $\rightsquigarrow$ μ_+ , μ_- , β

in the intial basis $\Rightarrow$ off-diagonal $\to 0$

$t \to \infty$

$\Rightarrow$ diagonal $\to \dfrac{1}{1 + e^{\beta(\omega(k) - \mu_\pm)}}$

- H-theorem

entropy $S(W) = - \int dk \{ W \log W + \tilde{W} \log \tilde{W} \}$

entropy production $\sigma = \frac{d}{dt} S$

$\sigma \geq 0$

- stationary solutions $\quad \mathcal{C}(W) = 0$

$\mathcal{C}(W) = 0 \iff \sigma(W) = 0 \quad \Rightarrow$ collision invariants

$D \geq 2$, generic ω,

$\sigma(W) = 0$, then there exists k-independent basis ψ_+, ψ_- such that

$$W = \sum_{\alpha = \pm} \left(1 + e^{\beta(\omega(k) - \mu_\alpha)}\right)^{-1} |\psi_\alpha\rangle\langle\psi_\alpha|$$

B: some simulations

// $\mathcal{C}$ has to be mollified //

- nearest neighbor hopping — integrable quantum model —

stationary solutions are

$$W_{st}(k) = \sum_{\alpha=\pm} \left(1 + e^{f(k) - c_\alpha}\right)^{-1} |\psi_\alpha\rangle\langle\psi_\alpha|$$

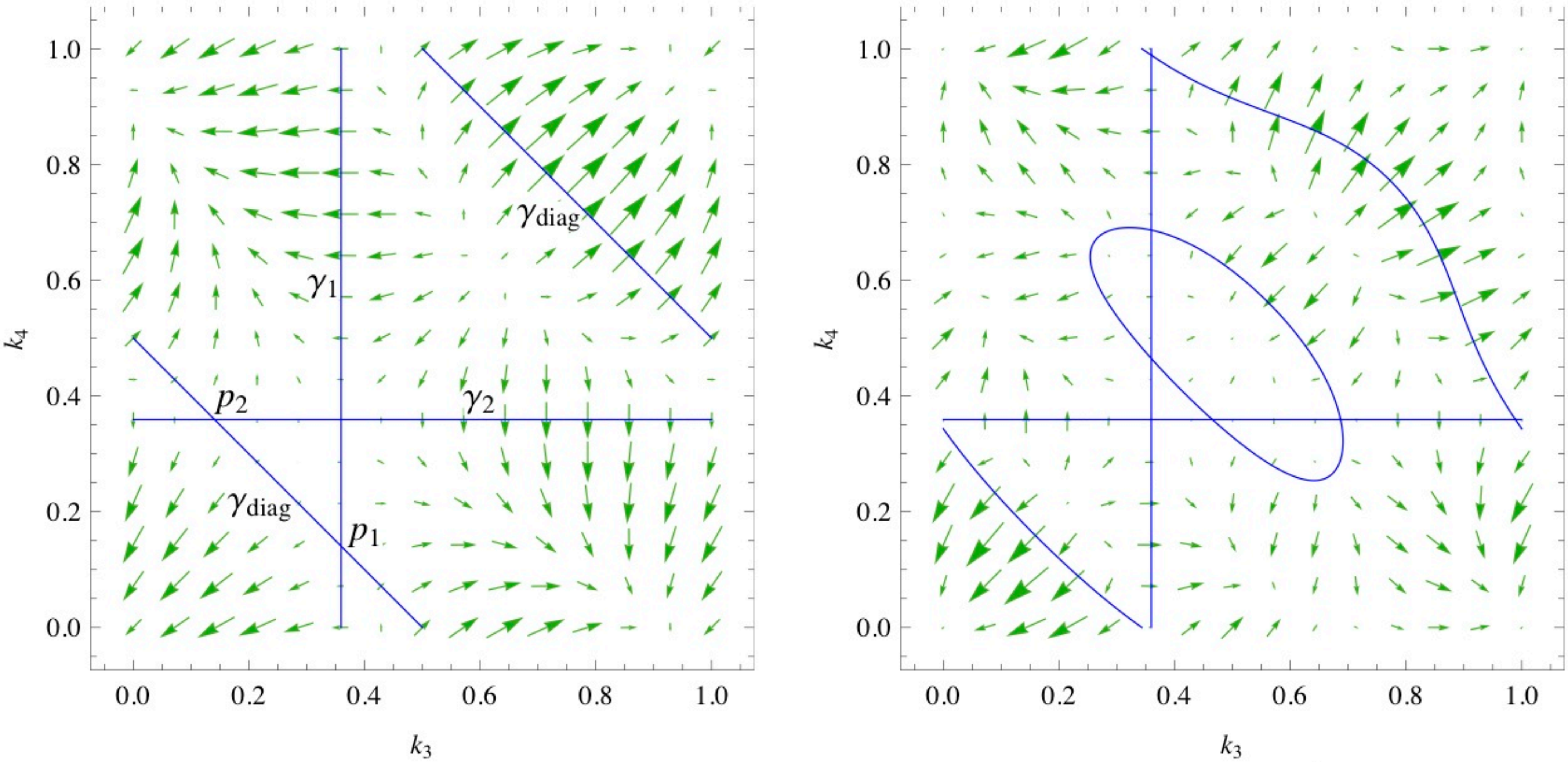
and $f(k) = -f(\pi - k)$

- next nearest neighbor hopping — non-integrable —

thermal

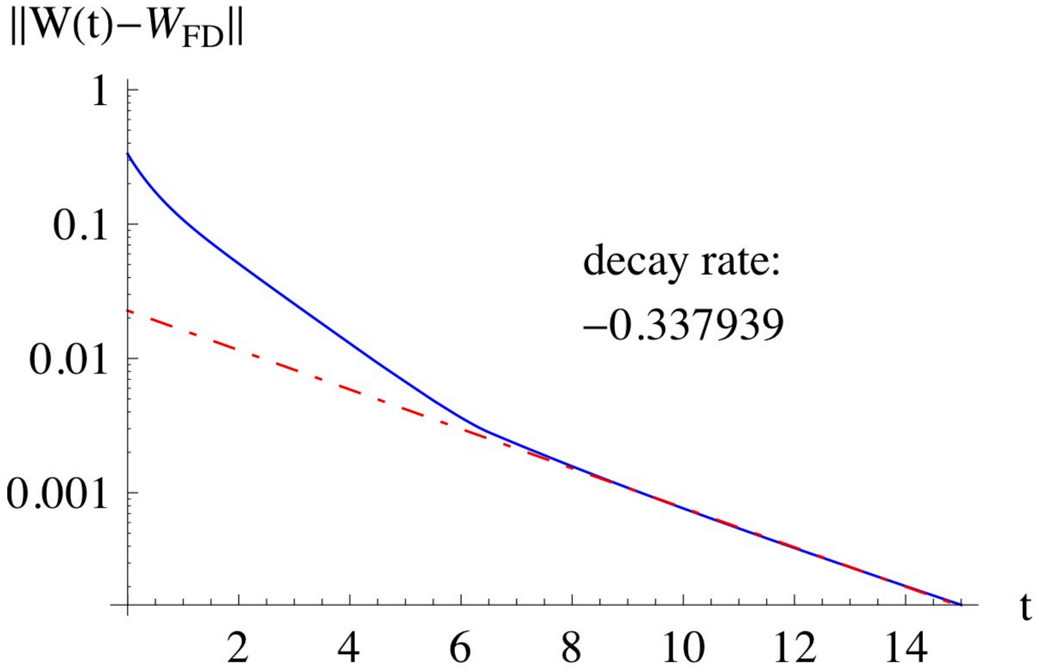
- n.n.

exponential convergence to steady state

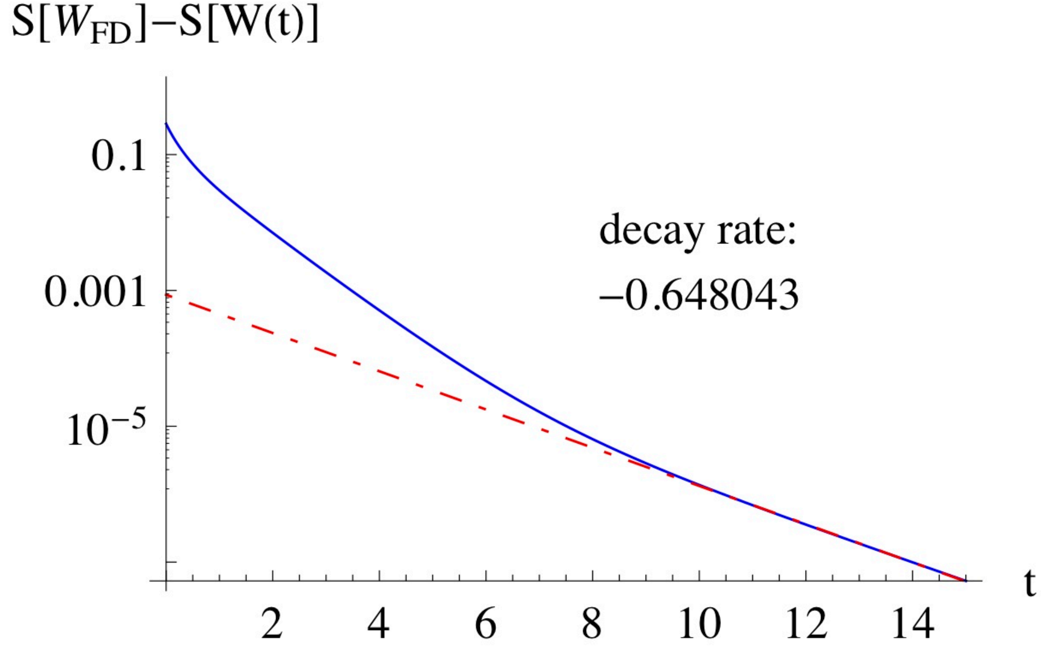


(a) $\omega(k) = 1 - \cos(2\pi k)$

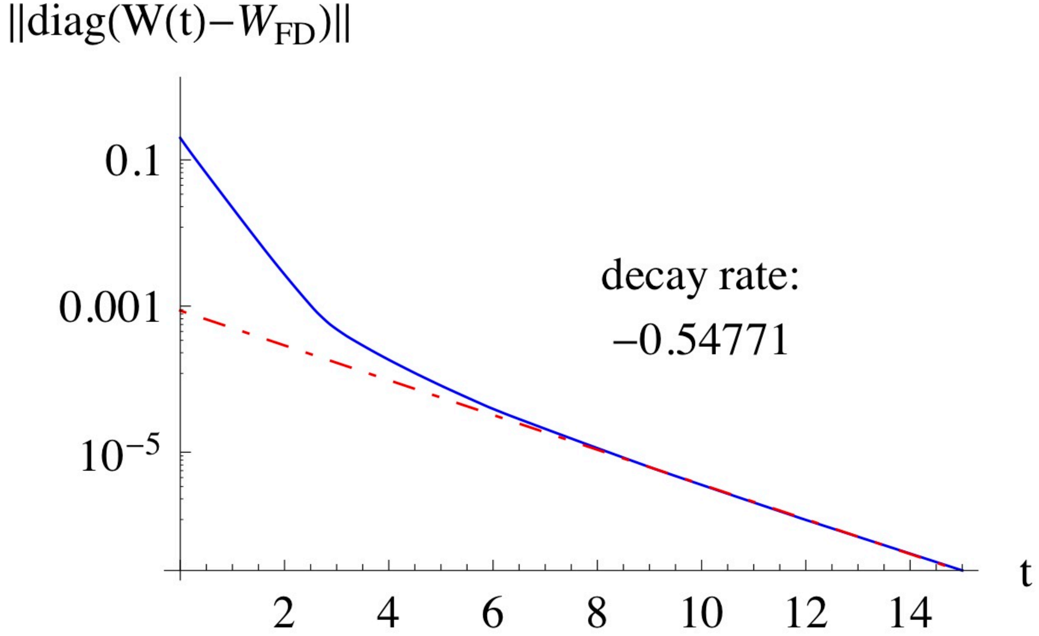
(b) $\omega_{\text{nnn}}(k) = 1 - \cos(2\pi k) - \frac{1}{2}\cos(4\pi k)$



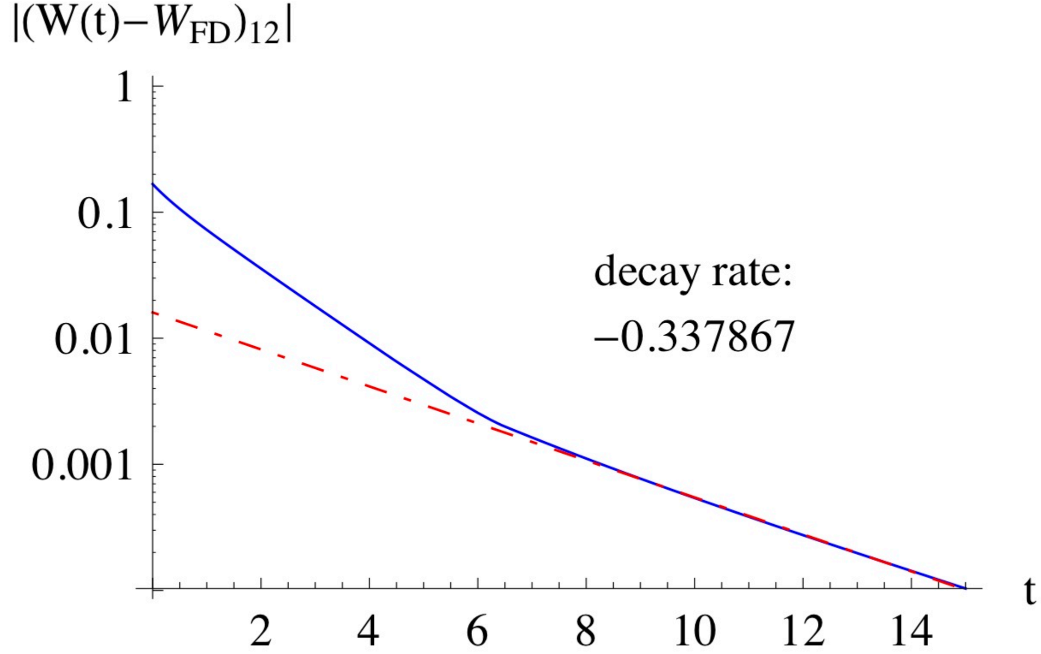
(a) convergence in Hilbert-Schmidt norm



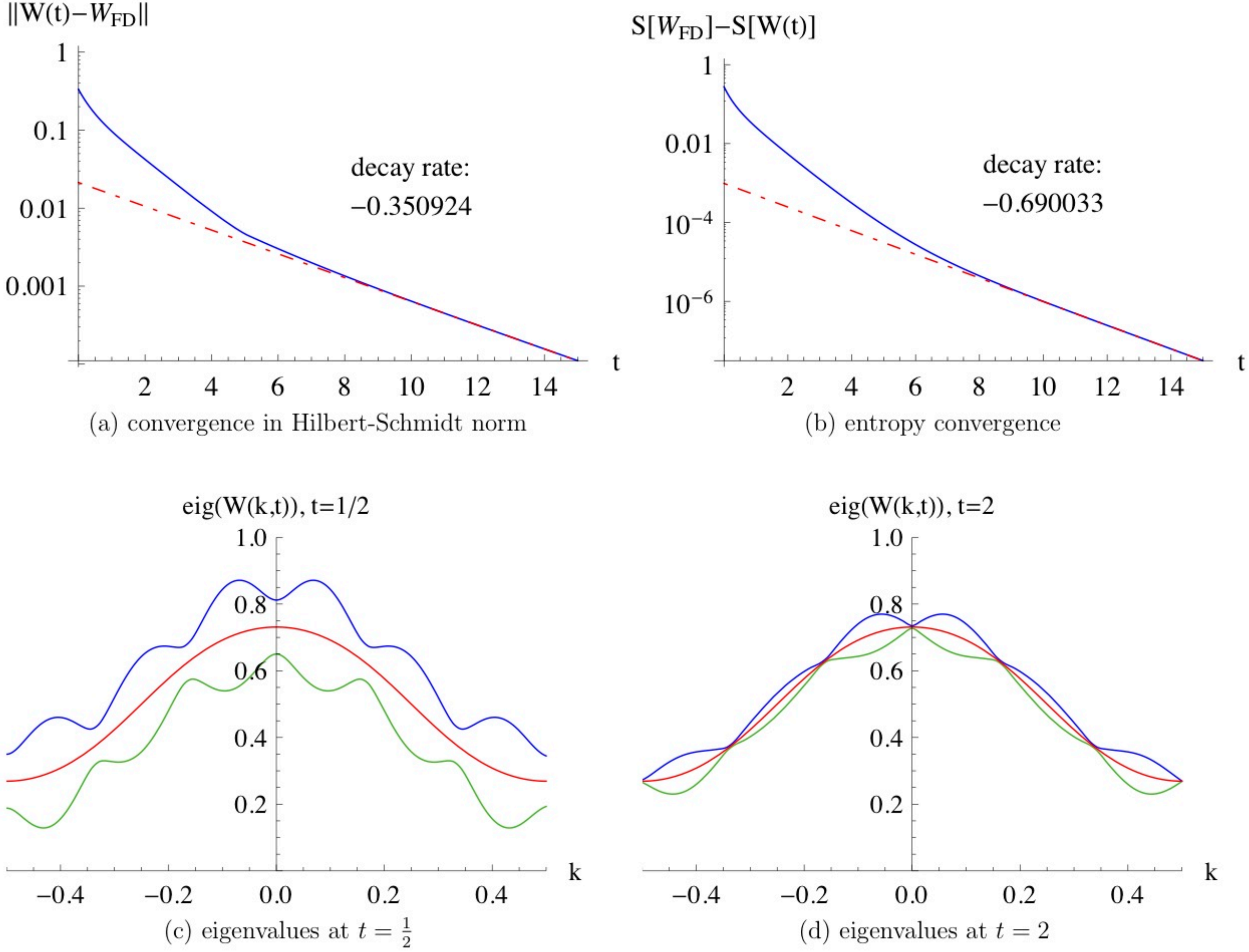
(b) entropy convergence



(c) convergence of the diagonal entries



(d) convergence of the off-diagonal entries



(a) convergence in Hilbert-Schmidt norm

(b) entropy convergence

(c) eigenvalues at $t = \frac{1}{2}$

(d) eigenvalues at $t = 2$

Conclusions

⇒ kinetic theory is a useful tool SEE wave turbulence

⇒ more work is needed

- linearization, energy transport
- quantum gases in optical lattices: expansion into vacuum

  ⇑ 2D Fermi-Hubbard

  via nonlinear diffusion
- graphene