Semiclassical theory for quantum quenches in finite spin chains

Ferenc Iglói (Budapest)

in collaboration with

Heiko Rieger, Benjamin Blaß (Saarbrücken)

Phys. Rev. Lett. **106**, 035701 (2011), arXiv:1011.3664
Phys. Rev. B **84**, 165117 (2011), arXiv:1106.5248
arXiv:1205.3303

Firenze, 22nd May 2012

AGENDA

- Introduction
  - nonequilibrium quantum processes
    - experimental examples
    - theoretical questions
  - challenging problems in this talk
    - effect of surfaces and finite sizes
    - semiclassical theory
- Model and the numerical method
  - XY-chain in a transverse field
  - free fermion description
- Time-dependent observables
  - correlation function
  - local magnetization
  - entanglement entropy
- Interpretation in semiclassical theory
  - quasiparticle picture
  - entropy evolution
  - magnetization relaxation and reconstruction due to kinks
  - modified semiclassical theory
- Discussion
  - Generalized Gibbs ensemble

Quantum quench dynamics

- Phenomena
  sudden change of a parameter in the Hamiltonian
  - time: $\boxed{t<0} \to \boxed{t>0}$
  - Hamiltonian: $\mathscr{H}_0 \to \mathscr{H}$
  - k-th eigenstate: $|\Psi_k^{(0)}\rangle \to |\Psi_k(t)\rangle$

$$|\Psi_k(t)\rangle = \exp(-it\mathscr{H})\,|\Psi_k^{(0)}\rangle$$

- Studied quantities
  - observable $\hat{A}$
    $A(t) = \langle\Psi_k(t)|\hat{A}|\Psi_k(t)\rangle$
  - correlation function

$$C_{AB}(t_1,t_2) = \langle\Psi_k|\hat{A}(t_1)\hat{B}(t_2)|\Psi_k\rangle$$

$$\hat{A}(t) = \exp(-it\mathscr{H})\hat{A}\exp(it\mathscr{H})$$

- Experimental realizations
  - ultracold atomic gases in optical lattices
  - sudden change of parameters (c.f. through Feshbach resonance)
  - weak couplings to dissipative degrees of freedem
  - coherent time evolution
- Theoretical questions
  - nature of the stationary state
    - non-integrable models - thermalization?
    - integrable models - quasi-thermalization?
  - decay of correlations (space and time)
  - time-evolution of the entanglement entropy
- Questions studied in this talk
  - boundary and finite-size effects
  - semiclassical theory

Model and phase diagram

XY-chain in a transverse field

$$\mathscr{H} = -\frac{1}{2}\sum_l \left[\frac{1+\gamma}{2}\sigma_l^x\sigma_{l+1}^x + \frac{1-\gamma}{2}\sigma_l^y\sigma_{l+1}^y\right] - \frac{h}{2}\sum_l \sigma_l^z$$

$\sigma_l^{x,y,z}$: Pauli-matrices at site l

Free fermion representation

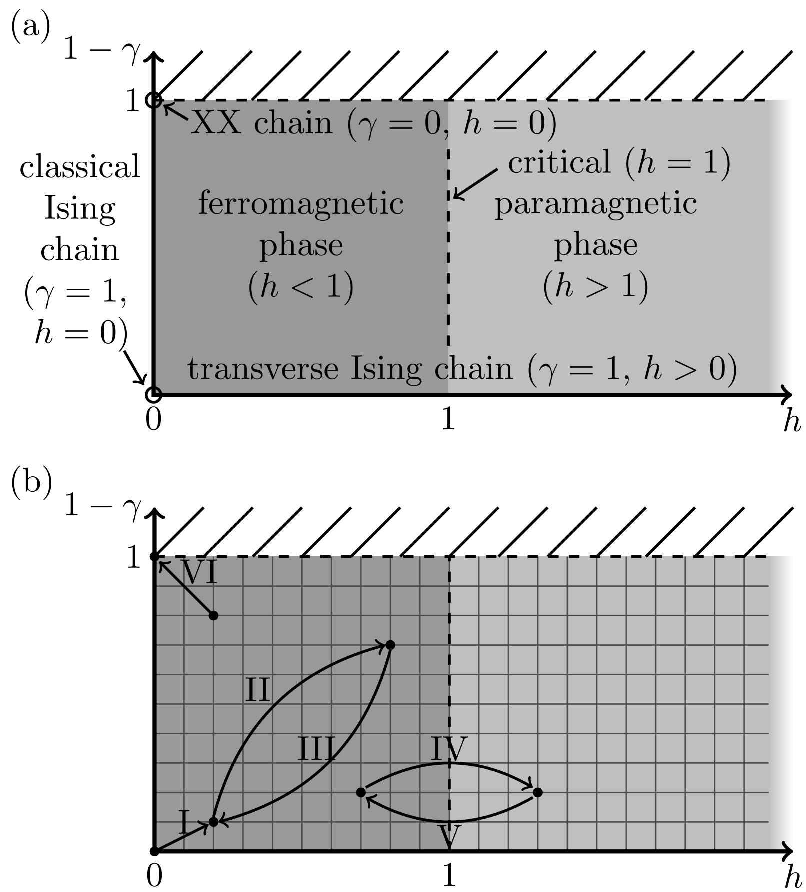
$$\mathscr{H} = \sum_p \varepsilon(p)\left(\eta_p^\dagger\eta_p - \frac{1}{2}\right)$$

energy of modes: $\varepsilon(p) = \sqrt{\gamma^2\sin^2 p + (h-\cos p)^2}$

Bogoliubov angle: $\tan\Theta_p = -\gamma\sin p/(h-\cos p)$

Quantum quench:

$t<0$	$\rightarrow$	$t>0$
h_0, γ_0	$\rightarrow$	h, γ



equilibrium phase diagram and 6 quench protocols

Time-evolution of the entanglement entropy

Block of $i = 1, 2, \ldots, \ell$ spins

entanglement (von Neumann) entropy:

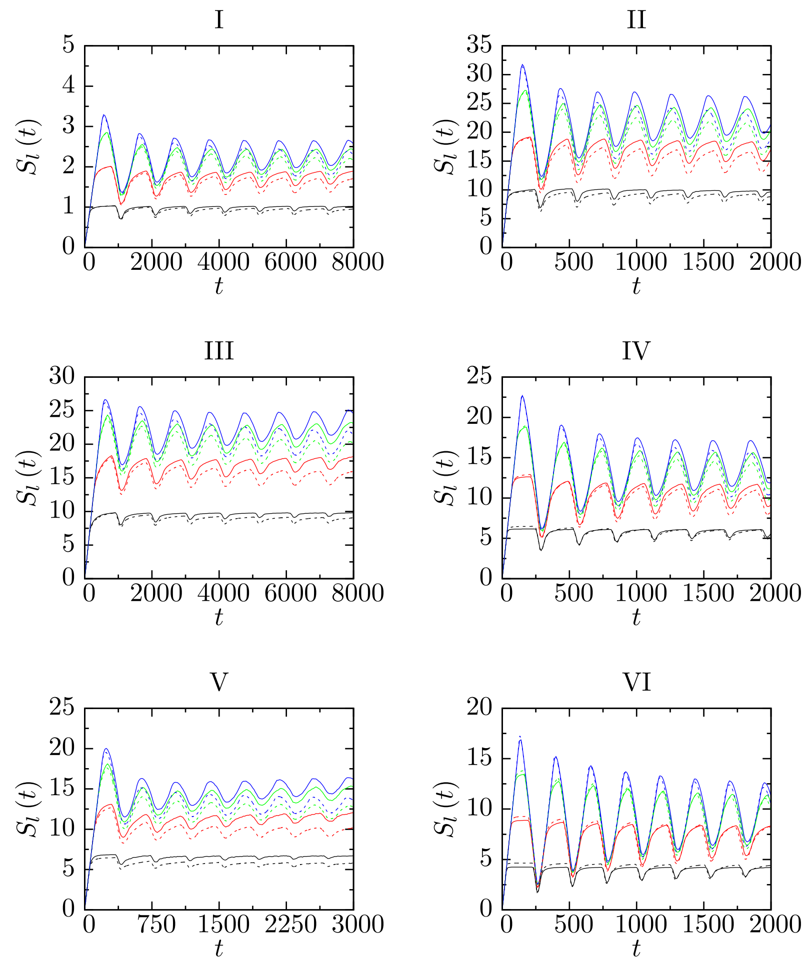
$$\mathscr{S}_\ell = \mathrm{Tr}_{i\leq\ell}[\rho_\ell \log \rho_\ell]$$

reduced density matrix:

$$\rho_\ell = \mathrm{Tr}_{i>\ell}|\Psi_0^{(0)}\rangle\langle\Psi_0^{(0)}|$$

$$\rho_\ell(t) = \exp(\imath\mathscr{H}t)\rho_\ell\exp(-\imath\mathscr{H}t)$$

in the free-fermion basis: $2\ell \times 2\ell$ eigenvalue problem



dynamical entropy for the 6 quench protocols
$(L = 256, l = 32 : -, 64 : -, 96 : -, 128 : -)$.

Semiclassical theory - entropy

- at $t=0$ QP pairs are created

$$\eta^{\dagger}_{\pm p}|\Psi_0^{(0)}\rangle$$

homogeneously in space, which are quantum entangled.

- for $t>0$ they move ballistically with constant velocity $\pm v_p$:
$$v_p = \frac{\partial \varepsilon(p)}{\partial p} = \frac{\sin p\left[h-\left(1-\gamma^2\right)\cos p\right]}{\varepsilon(p)}$$

- if at $t>0$ one of the QP pairs is in the block and its partner is in the environment: there is a contribution s_p to the entanglement entropy. Otherwise the contribution is 0.

- $\mathscr{S}_\ell =$ sum of the contributions of the pairs

- $s_p = -(1-f_p)\ln(1-f_p) - f_p \ln f_p$
entropy of free fermions

- $f_p = f_p(h_0,\gamma_0;h,\gamma)$: the occupation probability of mode p
$f_p = \left\langle \Psi_0^{(0)} \middle| \eta_p^{\dagger}\eta_p \middle| \Psi_0^{(0)} \right\rangle = \frac{1}{2}(1-\cos\Delta_p)$

- Δ_p: difference of the Bogoliubov angles:
$$\cos\Delta_p = \frac{(\cos p - h_0)(\cos p - h) + \gamma\gamma_0 \sin^2 p}{\varepsilon(p)\,\varepsilon^0(p)}$$

- In the $L\to\infty$, $\ell \gg 1$ limit:

$$\mathscr{S}_\ell(t) = t\frac{1}{2\pi}\int_0^{\pi} dp\, v_p s_p, \quad t < l/v_{max}$$

$$\mathscr{S}_\ell(t) = l\frac{1}{2\pi}\int_0^{\pi} dp\, s_p, \quad t \gg l/v_{max}$$

exact results (Fagotti & Calabrese)

- for finite L excellent agreement

Correlation function and local magnetization

General two-point function:

$$C^{xx}(l_1,t_1;l_2,t_2)=\left\langle \Psi_0^{(0)}\left|\sigma_{l_1}^x(t_1)\sigma_{l_2}^x(t_2)\right|\Psi_0^{(0)}\right\rangle$$

Equal-time correlation function:

$$C_t^{xx}(l_1,l_2)\equiv C^{xx}(l_1,t;l_2,t)$$

for large separation:

$$C_t^{xx}(l_1,l_2)=m_{l_1}(t)\,m_{l_2}(t)$$

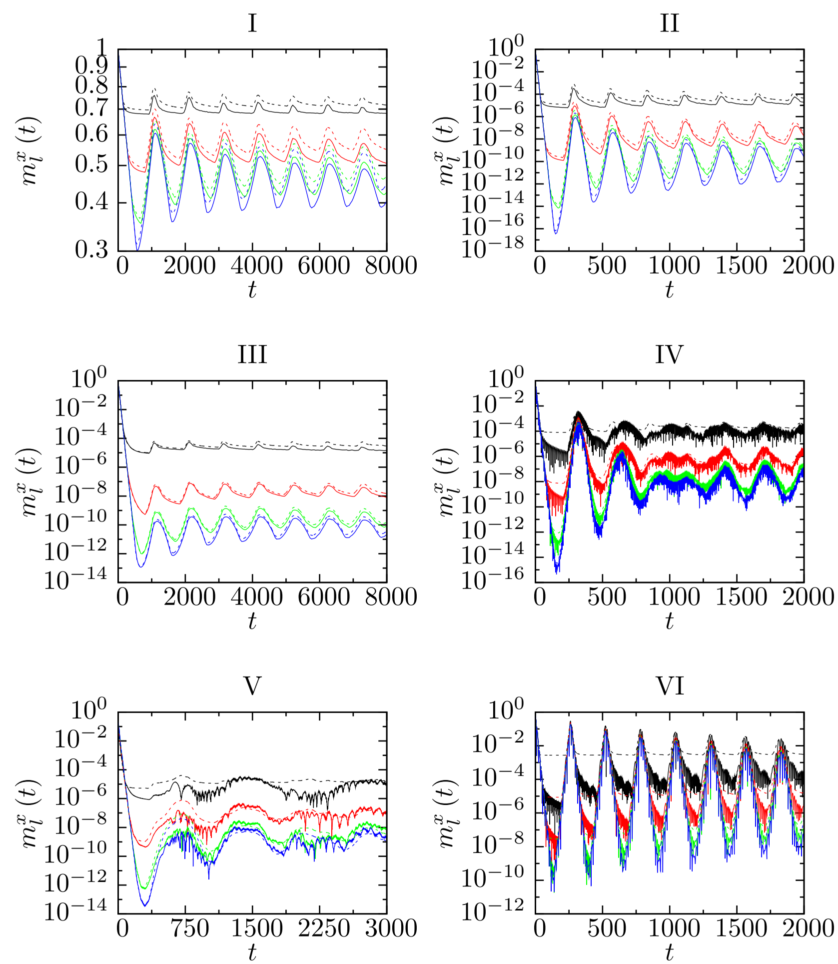
local magnetization:

$$m_l(t)=\lim_{b\to 0_+}\,{}_b\langle\Psi_0^{(0)}|\sigma_l^x(t)|\Psi_0^{(0)}\rangle_b$$

b: strength of a longitudinal field
According to Yang it can be written as the **off-diagonal matrix-element:**

$$m_l(t)=\langle\Psi_0^{(0)}|\sigma_l^x(t)|\Psi_1^{(0)}\rangle$$

here $|\Psi_1^{(0)}\rangle=\eta_1^\dagger|\Psi_0^{(0)}\rangle$ is the first excited state.



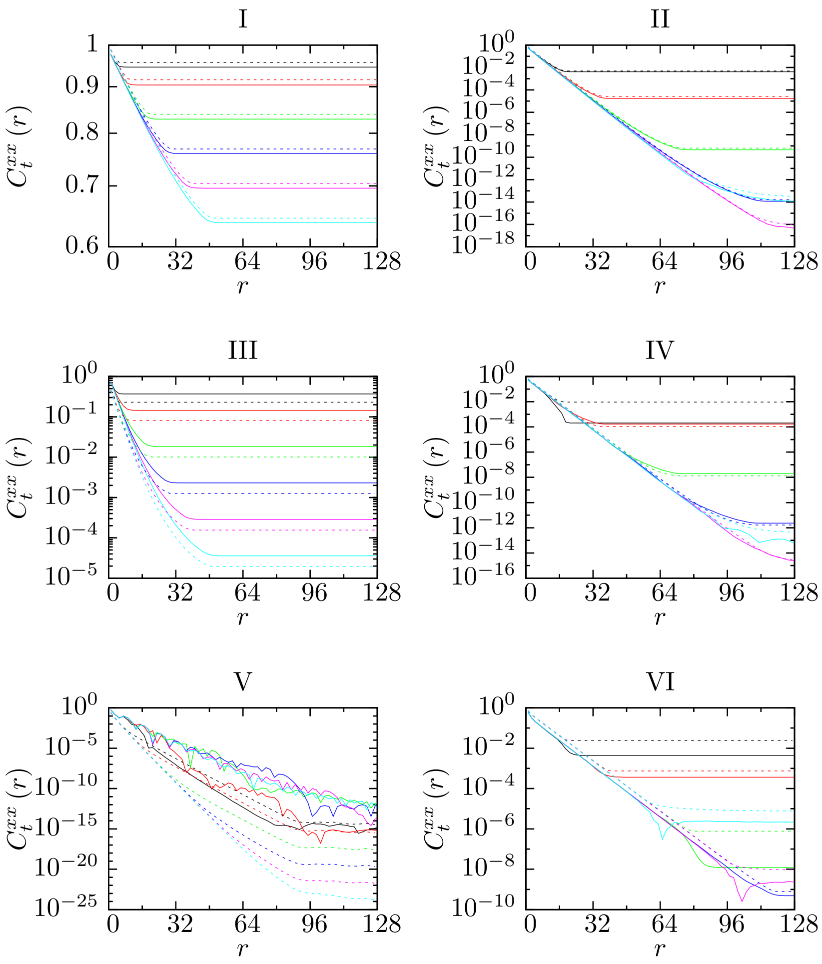
local magnetization for the 6 quenches
$(L=256, l=32:-, 64:-, 96:-, 128:-)$.

Equal-time correlation function

Correlations between symmetrically placed points:

$C_t^{xx}(r) = C^{xx}\left(\frac{L-r+1}{2}, t; \frac{L+r+1}{2}, t\right), r = 1, 3, \ldots, L-1$

.



equal-time correlation function for fixed time t for the 6 quench protocols ($-t = 10$, $-t = 20$, $-t = 40$, $-t = 60$, $-t = 80$, $-t = 100$).

Semiclassical theory - correlations

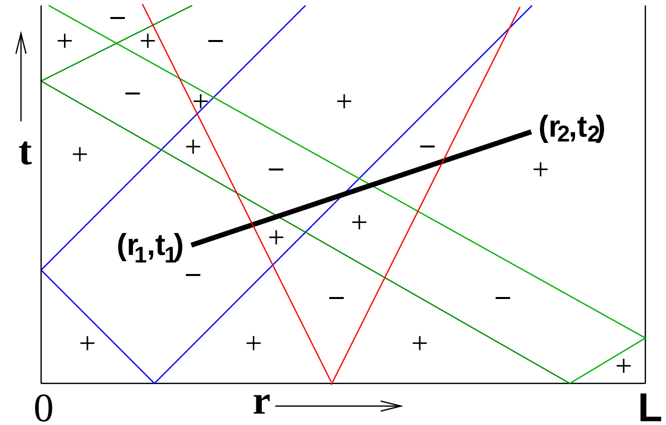
- The QPs in the spin basis are (for small h and $1-\gamma$)
  wave packets: $\eta_p^\dagger|\Psi_0^{(0)}\rangle \to \sum_k a_k|k\rangle$
  superposition of kinks at position k
  $|k\rangle = |++\cdots+--\cdots-\rangle$
  $a_k \propto \sin(k\pi/L),\ k=1,\ldots,L.$

- if the space-time trajectory of a kink passes the line: $(\mathbf{r_1},\mathbf{t_1};\mathbf{r_2},\mathbf{t_2})$ the correlation function changes sign

- the correlation function has its initial value if even number of kinks has passed the line

- calculation of the correlation function
  - denote by $\boxed{Q(r_1,t_1;r_2,t_2)}$ the probability that a given kink has passed odd times the line
  - the probability that a given set of n kinks has passed (each odd times): $Q^n(1-Q)^{L-n}$
  - summing over all possibilities

$$\frac{C(r_1,t_1;r_2,t_2)}{C_{\rm eq}(r_1,r_2)} = \sum_{n=0}^{L}(-1)^n Q^n(1-Q)^{L-n}\frac{L!}{n!(L-n)!}$$
$$= (1-2Q)^L \approx \exp[-2Q(r_1,t_1;r_2,t_2)L]$$



Typical semiclassical contribution to the correlation function $C(r_1,t_1;r_2,t_2)$.

Semiclassical theory - magnetization

$$m_l(t) = m_l^{\rm eq} \exp[-2q(t,l)L]$$

Here

$$q(t,l) = \frac{1}{2\pi}\int_0^\pi dp f_p q_p(t,l)$$

and

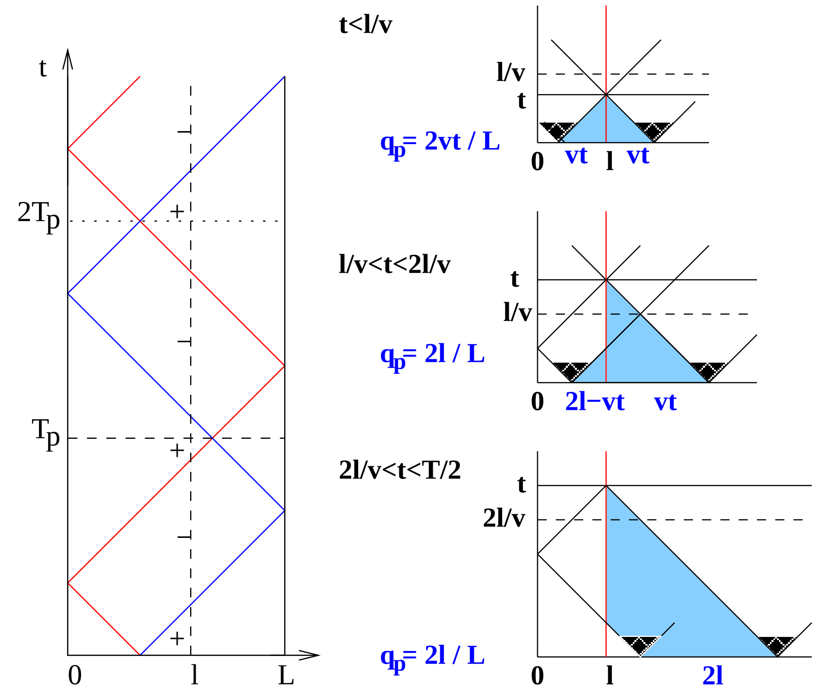
$$q_p(t,l) = \frac{1}{L}\int_0^L dx_0 q_p(x_0,t,l)$$

$q_p(x_0,l,t) = 1$, if the p kink-pair of initial position x_0 pass the site l an odd number of times before t

$q_p(x_0,l,t) = 0$, otherwise

$$Lq_p(t) = \begin{cases} 2v_p t & \text{for} \quad t \le t_1 \\ 2l & \text{for} \quad t_1 \le t \le t_2 \\ 2 - 2v_p t & \text{for} \quad t_2 \le t < T_p \end{cases}$$

with $t_1 = l/v_p$, $T_p = L/v_p$ and $t_2 = T_p - t_1$.



Left: Typical semi-classical contribution to the time dependence of the local magnetization $m_l(t)$. **Right:** Sketch of the trajectories of kink pairs that flip the spin at position l exactly once for times $t < T_p/2$. q_p is the fraction of the marked intervals on the $t = 0$-axis.

Half-infinite system: $L \to \infty$

- Local magnetization

$$m_l(t) = m_l(0)\exp\left(-t\frac{2}{\pi}\int_0^\pi dp\, v_p f_p \theta(l - v_p t) - l\frac{2}{\pi}\int_0^\pi dp\, f_p \theta(v_p t - l)\right)$$

relaxation time:

$$\tau_{\text{mag}}^{-1} = \frac{2}{\pi}\int_0^\pi dp\, v_p f_p$$

correlation length:

$$\xi_{\text{mag}}^{-1} = \frac{2}{\pi}\int_0^\pi dp\, f_p$$

- Correlation function

$$C_t^{xx}(r) = C_0^{xx}(r)\exp\left(-t\frac{4}{\pi}\int_0^\pi dp\, v_p f_p \theta(r - 2v_p t) - l\frac{2}{\pi}\int_0^\pi dp\, f_p \theta(2v_p t - r)\right)$$

– The characteristic time and length scales are:

$$\tau_{\text{corr}} = \tau_{\text{mag}}/2, \qquad \xi_{\text{corr}} = \xi_{\text{mag}}.$$

– Excellent agreement for quenches deep in the ferromagnetic phase.

– For quenches close to the critical point use the modified occupation probability:

$$\boxed{f_p \to \tilde{f}_p = -\tfrac{1}{2}\ln|\cos\Delta_p|}$$

– exact in the themodynamic limit (Calabrese, Essler, Fagotti 2012).

– Excellent agreement for finite systems, too.

Generalized Gibbs ensemble (GGE)

Question of thermalization

Compare the equilibrium correlation length at $T > 0$ temperature, ξ_T, with the nonequilibrium correlation length after the quench

- semiclassical theory (Sachdev & Young)

$$\xi_T^{-1} = \frac{2}{\pi}\int_0^\pi dp \exp\left(-\frac{\varepsilon(p)}{T}\right)$$

to be compared with:

$$\xi^{-1} = \frac{2}{\pi}\int_0^\pi dp\, f_p$$

from this follows

$$\boxed{f_p = \exp\left(-\frac{\varepsilon(p)}{T_{\text{eff}}(p)}\right)}$$

- exact result (Barouch & McCoy)

$$\xi_T^{-1} = -\frac{1}{\pi}\int_0^\pi dp \ln\left|\tanh\frac{\varepsilon(p)}{2T}\right|$$

to be compared with:

$$\xi^{-1} = \frac{2}{\pi}\int_0^\pi dp\, \tilde{f}_p$$

from this follows

$$\boxed{f_p = \frac{1}{\exp\left(\frac{\varepsilon(p)}{T_{\text{eff}}(p)}\right)+1}}$$

Conclusion

- mode-dependent effective temperature: $T_{\text{eff}}(p)$
- Generalized Gibbs ensemble

SC theory	$\rightarrow$	**exact results**
classical kinks	$\rightarrow$	**free fermions**
Boltzmann distr.	$\rightarrow$	**Fermi distr.**