Quantum relaxation after a quench in systems with boundaries

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AGENDA

- Introduction
  - nonequilibrium quantum processes
    - quench dynamics
    - adiabatic relaxation
  - experimental examples
  - theoretical questions
  - challenging problems in this talk
    - effect of surfaces and finite sizes
    - evolution towards a quasi-thermal state
- Model and the numerical method
  - quantum Ising chain
  - free fermion description
  - calculation of time-dependent observables
    - local magnetization
    - correlation and autocorrelation function

- Relaxation of the local magnetization - Relaxation regimes
  - free relaxation regime
  - quasi-stationary regime
  - reconstruction regime
  - approximate periodicity
- Interpretation in semiclassical theory
  - quasi-particle interpretation
  - magnetization relaxation and reconstruction due to kinks
  - thermal vs. quantum quasi-particle occupation
- Relevant nonequilibrium scales
  - correlation length
  - relaxation time
- Conclusions

Quantum quench dynamics

- Phenomena
  sudden change of a parameter in the Hamiltonian
  - for $t < 0$
    - Hamiltonian $\mathscr{H}_0$
    - k-th eigenstate $|\Psi_k^{(0)}\rangle$
  - for $t > 0$
    - Hamiltonian $\mathscr{H}$
    - time-dependent state ($\hbar = 1$)

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

  - measured 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 through Feshbach resonance
  - weak couplings to dissipative degrees of freedem
  - coherent time evolution
    - Bose-Einstein condensates
    - spinor condensate
    - 1D Bose system noneq. relaxation

- Theoretical questions
  - nature of the stationary state
    - non-integrable models - thermalization?
    - integrable models - quasi-thermalization?
  - decay of correlations (space and time)
    - exponential (nonlocal operators)
    - power law (local operators)
- Questions studied in this talk
  - boundary and finite-size effects
  - evolution towards a quasi-thermal state

Model and numerical method

Quantum Ising chain

$$\mathcal{H} = -\frac{1}{2}\left[\sum_{l=1}^{L-1} \sigma_l^x \sigma_{l+1}^x - h \sum_{l=1}^{L} \sigma_l^z\right]$$

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

quantum quench at $t=0$

- for $t<0$: transverse field: h_0
- for $t \geq 0$: transverse field: h

equilibrium phase diagram:

- $h < h_c = 1$ ordered phase
- $h > h_c$ disordered phase
- $h = h_c$ quantum critical point

Free fermion representation

$$\mathscr{H} = \sum_{q=1}^{L} \varepsilon_q \left(\eta_q^\dagger \eta_q - \frac{1}{2} \right)$$

$\eta_q^\dagger, \eta_q$: fermion operators
ε_q: energy of modes:

$$\begin{aligned} \varepsilon_q \Psi_q(l) &= -h\Phi_q(l) - \Phi_q(l+1) , \\ \varepsilon_q \Phi_q(l) &= -\Psi_q(l-1) - h\Psi_q(l) \end{aligned}$$

spin operators:

$$\begin{aligned} \sigma_l^x &= A_1 B_1 A_2 B_2 \dots A_{l-1} B_{l-1} A_l , \\ \sigma_l^z &= -A_l B_l \end{aligned}$$

with Clifford (related to Majorana) operators

$$\begin{aligned} A_i &= \sum_{q=1}^{L} \Phi_q(i)(\eta_q^+ + \eta_q) , \\ B_i &= \sum_{q=1}^{L} \Psi_q(i)(\eta_q^+ - \eta_q) \end{aligned}$$

time evolution: $\eta_q^+(t) = e^{it\varepsilon_q}\eta_q^+$, $\eta_q(t) = e^{-it\varepsilon_q}\eta_q$
from this follows

$$A_l(t) = \sum_k \left[\langle A_l A_k \rangle_t A_k + \langle A_l B_k \rangle_t B_k \right],$$

$$B_l(t) = \sum_k \left[\langle B_l A_k \rangle_t A_k + \langle B_l B_k \rangle_t B_k \right],$$

with

$$\begin{aligned} \langle A_l A_k \rangle_t &= \sum_q \cos(\varepsilon_q t) \Phi_q(l) \Phi_q(k) , \\ \langle A_l B_k \rangle_t &= \langle B_k A_l \rangle_t = i \sum_q \sin(\varepsilon_q t) \Phi_q(l) \Psi_q(k) , \\ \langle B_l B_k \rangle_t &= \sum_q \cos(\varepsilon_q t) \Psi_q(l) \Psi_q(k) . \end{aligned}$$

The matrix-elements of time-dependent Clifford operators, such as $\langle \Psi_0^{(0)} | A_l(t) A_k(t) | \Psi_0^{(0)} \rangle$, involve the ground-state expectation values:

$$\langle \Psi_0^{(0)} | A_k A_l | \Psi_0^{(0)} \rangle = \delta_{k,l}, \;\; \langle \Psi_0^{(0)} | B_k B_l | \Psi_0^{(0)} \rangle = -\delta_{k,l}$$
$$\langle \Psi_0^{(0)} | A_k B_l | \Psi_0^{(0)} \rangle = -G_{kl}^{(0)}, \langle \Psi_0^{(0)} | B_k A_l | \Psi_0^{(0)} \rangle = G_{kl}^{(0)} .$$

with

$$G_{kl}^{(0)} = -\sum_q \Psi_q^{(0)}(k) \Phi_q^{(0)}(l)$$

.

Local magnetization

- **Definition:**

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

here $|\Psi_0^{(0)}\rangle_b$ is the ground state of the initial Hamiltonian in the presence of an external longitudinal field b.

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.

- **Calculation**

In the free-fermion representation:

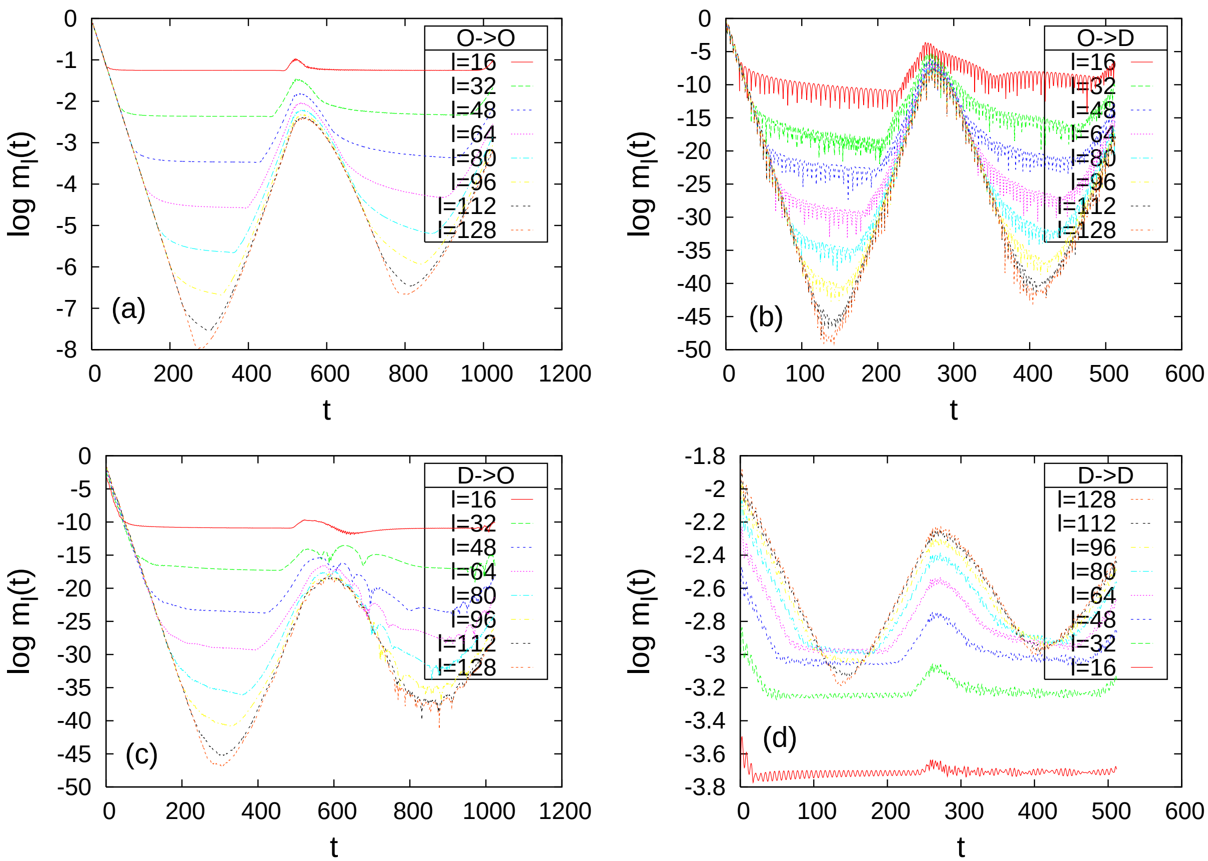
$$m_l(t) = \langle \Psi_0^{(0)} | A_1(t) B_1(t) \dots A_{l-1}(t) B_{l-1}(t) A_l(t) \eta_1^\dagger | \Psi_0^{(0)} \rangle$$

  - according to Wick-theorem it is expressed as sum of products of two-operator expectation values
  - it is given in the form of a Pfaffian, the elements are in a $2l \times 2l$ triangle
  - it is expressed as the square-root of the determinant of an antisymmetric matrix, with the elements of the Pfaffian above the diagonal

- **Behaviour in the initial state ($t < 0$)**

$$\begin{aligned} m_l(t<0) &= \left(1 - h_0^2\right)^{1/8}, \quad h_0 < h_c = 1, \\ m_l(t<0) &\sim L^{-1/8}, \quad h_0 = h_c = 1, \\ m_l(t<0) &\sim L^{-1/2}, \quad h_0 > h_c = 1. \end{aligned}$$

Relaxation of the magnetization profile



a) $h_0 = 0.0$ and $h = 0.5$ (**O** $\rightarrow$ **O**) b) $h_0 = 0.5$ and $h = 1.5$ (**O** $\rightarrow$ **D**)
c) $h_0 = 1.5$ and $h = 0.5$ (**D** $\rightarrow$ **O**)d) $h_0 = 1.5$ and $h = 2.0$ (**D** $\rightarrow$ **D**).

Interpretation in terms of quasi-particles

During the quench quasi-particles are created, which

- are emitted at every points of the chain
- travel with a constant speed, $v = v(h, h_0)$
- are reflected at the boundaries.

Properties of quasi-particles

- originating at nearby region $O(\xi)$ are quantum entangled
- others are incoherent
- incoherent particles arriving at a reference point, l, cause relaxation of the local observable (c.f. magnetization).
- the same particle arriving at a reference point, l, after reflection, induces quantum correlations in time, signalized by the reconstruction of the value of the local observable.

Relaxation regimes

- **Free relaxation regime** $t < t_l = l/v$
  - only incoherent quasi-particles pass the reference point
  - the magnetization has an exponential decay

$$\boxed{m_l(t) \equiv m(t) \approx A(t)\exp(-t/\tau)}$$

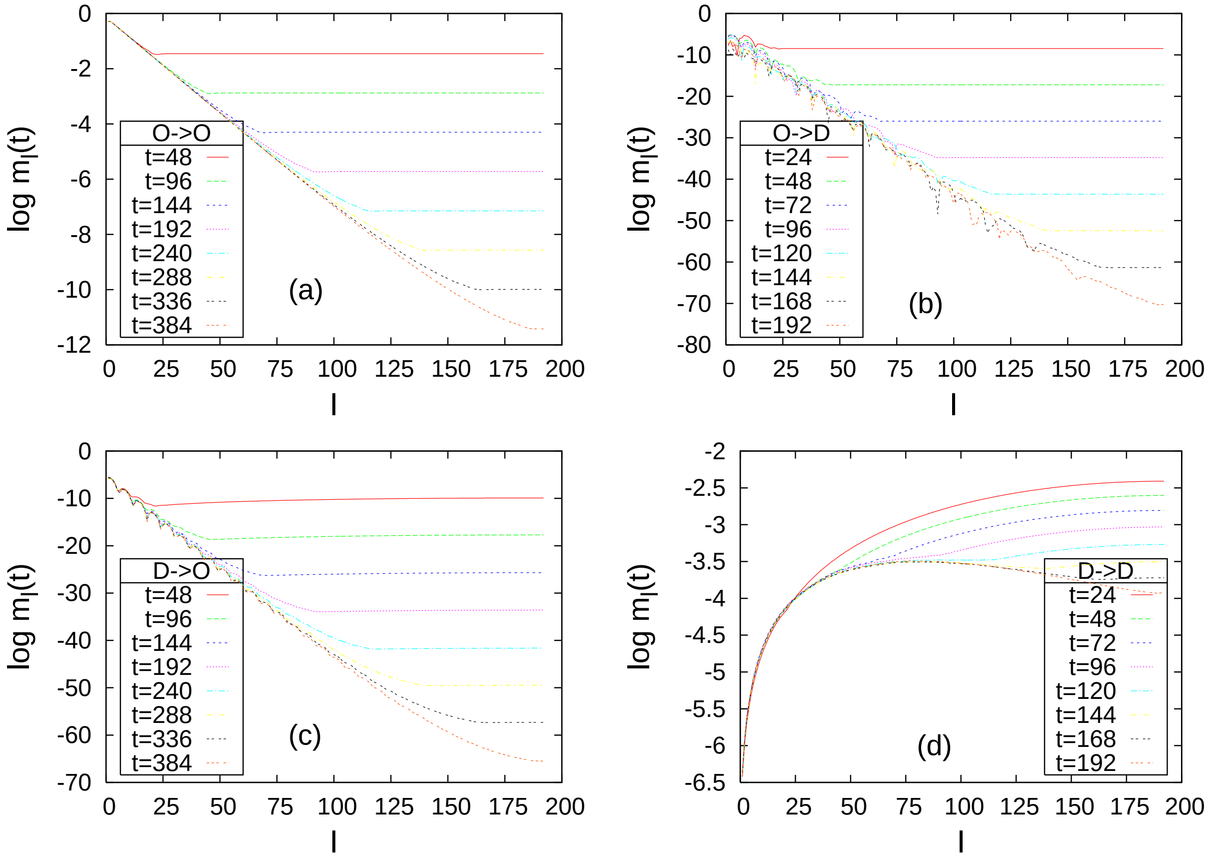
  - $A(t)$ oscillating prefactor
    - $h > h_c$ and $h_0 < h_c$: $A(t) \sim \cos(at+b)$ $A(t)$ changes sign
    - otherwise: $A(t) \sim [\cos(at+b)+c]$ $c > 1$, $A(t)$ always positive
  - $\boxed{\tau \text{ relaxation (phase-coherence) time}}$
  - quasi-thermalization for bulk sites

- **Quasi-stationary regime:** $t_l < t < T - t_l$, $T = L/v$,
  - two types of quasi-particles reach the reference point
    - type *1* passed l only once at a time $t' < t$
    - type *2* passed it twice at two times $t' < t'' < t$ with a reflection
  - these two types interfere, resulting in a slow relaxation
  - the quasi-stationary magnetization has an exponential dependence

$$\boxed{m_{l_1}(t_1)/m_{l_2}(t_2) \approx \exp[-(l_1 - l_2)/\xi]}$$

  - $\boxed{\xi \text{ correlation length}}$

Relaxation of the magnetization profile



a) $h_0 = 0.0$ and $h = 0.5$ (**O** $\to$ **O**) b) $h_0 = 0.5$ and $h = 1.5$ (**O** $\to$ **D**)
c) $h_0 = 1.5$ and $h = 0.5$ (**D** $\to$ **O**)d) $h_0 = 1.5$ and $h = 2.0$ (**D** $\to$ **D**).

Quasi-stationary limiting magnetization

- Definition

$$\overline{m}_l = \lim_{L\to\infty}\lim_{t\to\infty} m_l(L,t)$$

- Surface magnetization

$$\overline{m}_1 = \frac{(1-h^2)(1-h_0^2)^{1/2}}{1-hh_0}, \qquad h_0, h < 1,$$
$$\overline{m}_1 = 0, \qquad \text{otherwise.}$$

- nonequilibrium surface magnetization exponents:
  - $\beta_s = 1$: $h_0 < 1, h \to 1$
  - $\beta_s = 1/2$: $h_0 \to 1, h < 1$

- corrections to the quasi-stationary behaviour

	$h_0 < h_c$	$h_0 > h_c$
$h < h_0$	$t^{-1}\cos(at+b)$	$L^{-3/2}[\cos(at+b)+c]$, $c > 1$
$h > h_0$	$t^{-3/2}\cos(at+b)$	$t^{-1/2}[\cos(at+b)+cL^{-3/2}]$

- Bulk magnetization

$$\overline{m}_l > 0, \qquad h_0, h < 1,$$
$$\overline{m}_l = 0, \qquad \text{otherwise.}$$

- **Reconstruction regime:** $T - t_l < t < T$

- more and more type *2* quasi-particles reach the reference point

- incoherent spin flips in the past are progressively reversed

- for mono-disperse quasi-particles (velocity v) one would expect a T-periodicity: $m_l(t) = m_l(T-t)$

- observed behaviour:

$$\boxed{m_l(t) \equiv m(t) \approx B(t)\exp(t/\tau')}$$

- growth rate: $\tau'(h,h_0)$

- numerical observation:
  $\tau/\tau' = 0.883 \pm 0.002.$

- **Approximate periodicity:** $t > T$

- typical speed: $v(h,h_0) = \xi/\tau$

$$\begin{array}{ccl} \boxed{h<1} & , & v(h,h_0) \approx h a(h,h_0), \\ a(h,h_0) & \approx & 0.86 - 0.88, \\ \boxed{h>1} & , & v(h,h_0) \approx \text{const.} \end{array}$$

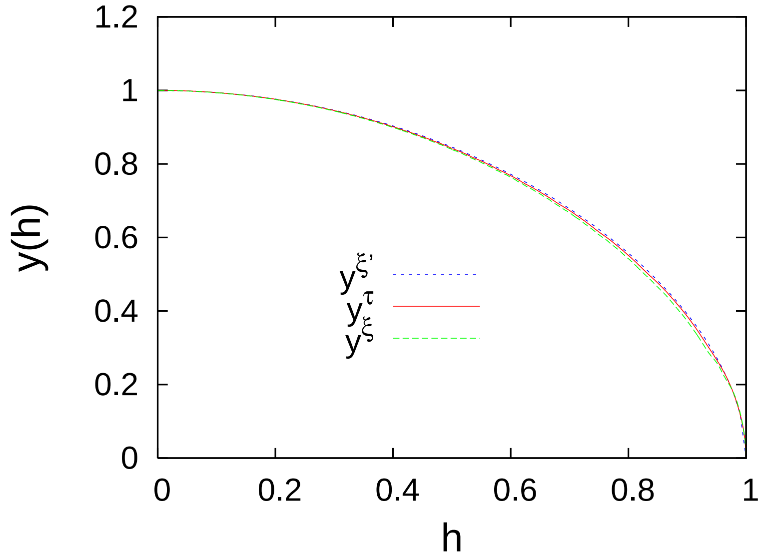
Relaxation time: $\tau(h, h_0)$

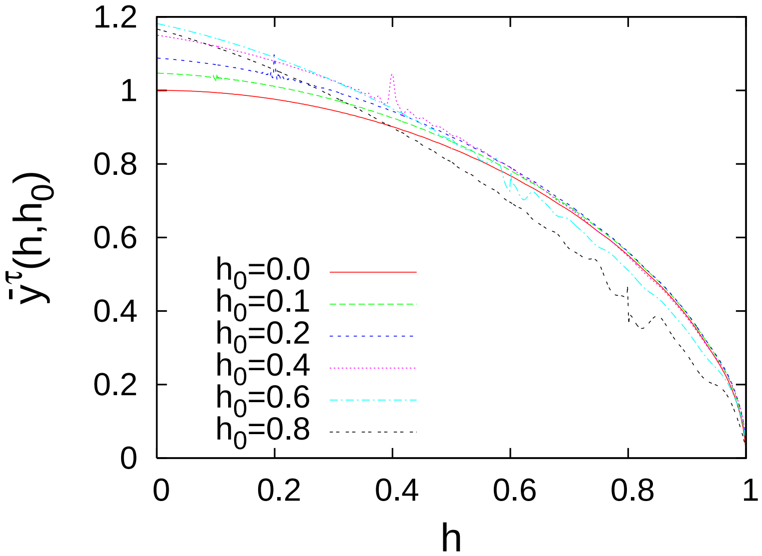
- divergent at the following points
  - stationary point: $h = h_0$
    $$\tau(h, h_0) \sim (h - h_0)^{-2}$$
  - for small h
    $$\tau(h, h_0) \sim h^{-1}$$
  - for $h_0 = 0$:
    $$\tau(h, h_0 = 0) \sim h^{-3}$$

- quench from a fully ordered state $h_0 = 0$
  - to the disordered phase $h \geq 1$
    $\tau(h \geq 1, h_0 = 0) = \pi/2$,
    independent of h.
  - to the ordered phase $h < 1$
    $\tau(h, h_0 = 0) = h^{-3}\tilde{\tau}(h, h_0 = 0)$
    * $h \to 0$ we obtain
      $\tilde{\tau}(h = 0, h_0 = 0) = 3\pi/2$
    * $h > 0$ we consider $\boxed{y^{\tau}(h) = \dfrac{\tilde{\tau}(h) - \tilde{\tau}(1)}{\tilde{\tau}(0) - \tilde{\tau}(1)}}$
    * compare with $\boxed{y^{\xi}(h) = \dfrac{\tilde{\xi}(h) - \tilde{\xi}(1)}{\tilde{\xi}(0) - \tilde{\xi}(1)}}$
      $\tilde{\xi}(h) = \xi(h) h^2$
      exact result:
      $\xi(h) = -1/\log((1 + \sqrt{1 - h^2})/2)$

- quench from partially ordered state $h_0 > 0$
  - define: $\tilde{\tau}(h, h_0) = h(h - h_0)^2 \tau(h, h_0)$
  - at $h = 1$: $\tilde{\tau}(h = 1, h_0) = \pi(1 - h_0)/2$.
  - for $h < 1$ we study:
    $\boxed{\overline{y}^{\tau}(h, h_0) = \Delta\tilde{\tau}(h, h_0)/\Delta\tilde{\tau}(0, 0)}$
    with $\Delta\tilde{\tau}(h, h_0) = \tilde{\tau}(h, h_0) - \tilde{\tau}(1, h_0)$

Ratios of the relaxation times





Semiclassical calculation

Quasiparticles (QP)

- wave packets: $\eta_p^{\dagger}|0\rangle$
- $\eta_p^{+}|0\rangle \rightarrow \sum_k a_k|k\rangle$
  superposition of kinks at position k
  $|k\rangle = |++\cdots+--\cdots-\rangle$
  $a_k \propto \sin(k\pi/L),\ k=1,\ldots,L.$
- energy of QP: $\varepsilon_p = \sqrt{1+h^2-2h\cos(p)}$
- $p = \pm\frac{\pi}{L}, \pm\frac{3\pi}{L}, \pm\frac{5\pi}{L}, \ldots,\ |k|<\pi$
- velocity of QP: $v_p = \frac{\partial\varepsilon_p}{\partial p} = \frac{h\sin(p)}{\varepsilon_p}$

- QP-s are created at arbitrary position, x_0,
- creation probability: $f_p(h_0,h)$.
  - if the system is thermalized at temperature T
    $f_p(h_0,h) = e^{-\varepsilon_p/T}$
  - in quantum relaxation
    $f_p(h_0,h) = \langle\Psi_0^{(0)}|\eta_p^{+}\eta_p|\Psi_0^{(0)}\rangle$
  - for small h and h_0 (periodic chain):
    $f_p(h_0,h) = \frac{1}{4}(h_0-h)^2\sin^2(p).$

Relaxation of the magnetization

- initial magnetization: $m_l(0)$ $(h_0 < h_c)$
- the magnetization for $t > 0$ is reduced due to spin flips
  - the local spin flips each time a kink passes the site l
  - the local spin has its initial state at t if even number of kinks has passed
- calculation of the magnetization
  - denote by $\boxed{q(t)}$ the probability that a given kink has passed odd times before t the site l
  - the probability that a given set of n kinks has passed (each odd times): $q^n(1-q)^{L-n}$
  - summing over all possibilities

$$
\begin{aligned}
\frac{m_l(t)}{m_l(0)} &= \sum_{n=0}^{L} (-1)^n q^n (1-q)^{L-n} \frac{L!}{n!(L-n)!} \\
&= (1-2q)^L \approx \exp(-2q(t)L)
\end{aligned}
$$

Calculation of $q(t)$

- definition of $q_p(t)$
  - refers to a pair of QPs with velocities v_p and $-v_p$
  - it is the probability, that the QP pair pass the site l together an odd number of times
  - the QP pairs emerge uniformly in space
  - definition of $q_p(x_0,t)$
    - $q_p(x_0,t) = 1$, if the p kink-pair of initial position x_0 pass the site l an odd number of times before t
    - $q_p(x_0,t) = 0$, otherwise
  - relation with $q_p(t)$:

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

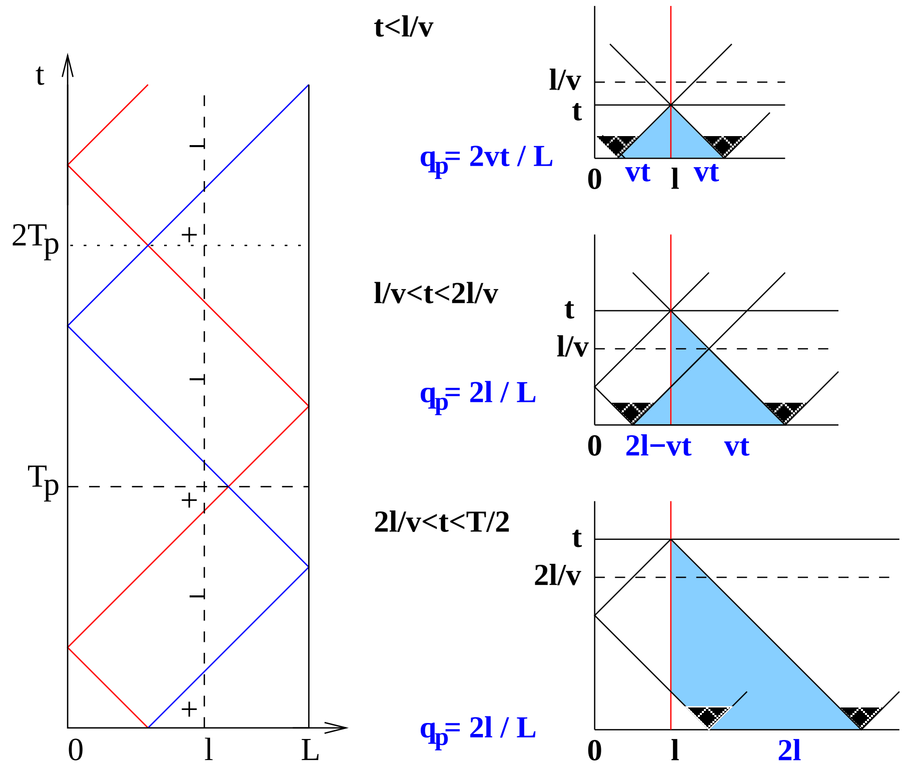
- relation with $q(t)$:

$$q(t) = \frac{1}{2\pi}\int_0^\pi dp f_p(h_0,h) q_p(t)$$

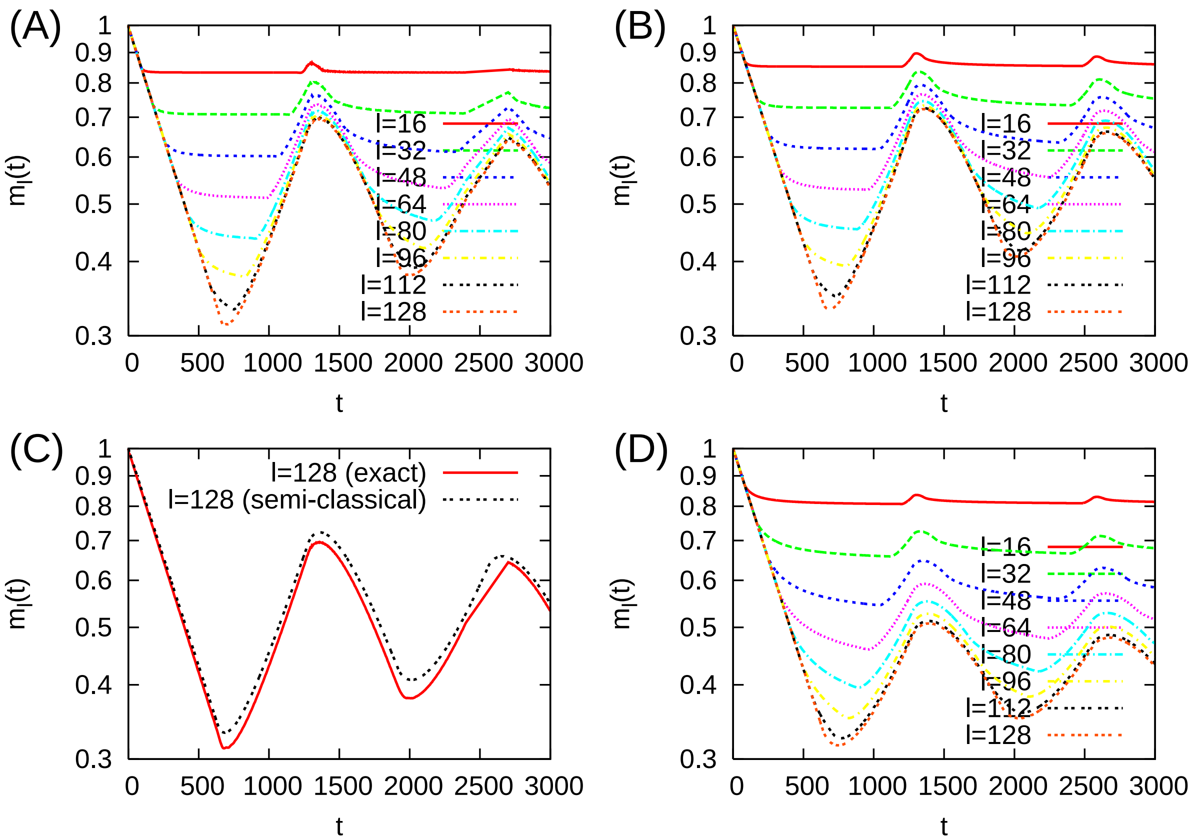
- value of $q_p(t)$:

$$Lq_p(t) = \begin{cases} 2v_p t & \text{for} & t \le t_1 \\ 2l & \text{for} & t_1 \le t \le t_2 \\ 2 - 2v_p t & \text{for} & t_2 \le t < T_p \end{cases} \tag{1}$$

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 $m_l(t)$. Full lines are quasi-particles or kinks moving with velocity v_p through the chain. The $\pm$ signs denote the sign of the spin at site l. **Right:** Sketch of the trajectories of kink pairs that flip the spin at position l exactly once for times $t < T_p/2$. Kink pairs with initial position x_0 outside the marked region either do not flip the spin at l (since they do not reach the position l within time t) or they flip it twice. q_p is the fraction of the marked intervals on the $t = 0$-axis.



Relaxation of the local magnetization, $\log m_l(t)$, at different positions in a $L=256$ chain with free ends after a quench with parameters $h_0=0.0$, $h=0.2$ and $L=256$. **A** Exact (free fermion calculation). **B** Semi-classical prediction with the passing probability and the occupation probability. **C** Comparison between exact and QP calculation for $m_l(t)$ for $L=256$, $l=128$ for a quench from $h_0=0$ to $h=0.1$. **D** Semi-classical prediction using a thermal occupation number probability with an effective temperature, T_{eff}.

Calculation of τ and ξ

- free relaxation regime

$$\ln\left[\frac{m_l(t)}{m_l(0)}\right] = -t/\tau,$$
$$\frac{1}{\tau} = \frac{2}{\pi}\int_0^\pi \mathrm{d}p f_p|\mathcal{V}_p|$$

in the small h, h_0 limit:

$$\frac{1}{\tau} \approx \frac{h(h-h_0)^2}{2\pi}\int_0^\pi \mathrm{d}p\sin^3 p$$
$$= h(h-h_0)^2\frac{2}{3\pi}$$

"numerically exact" result

- quasi-stationary regime ($l_1, l_2 \ll L$)

$$\ln\left[\frac{m_{l_1}(t)}{m_{l_2}(t)}\right] = -\frac{l_1-l_2}{\xi},$$
$$\frac{1}{\xi} = \frac{2}{\pi}\int_0^\pi \mathrm{d}p f_p$$

in the small h, h_0 limit:

$$\frac{1}{\xi} \approx \frac{(h-h_0)^2}{2\pi}\int_0^\pi \mathrm{d}p\sin^2 p$$
$$= \frac{(h-h_0)^2}{4}$$

exact result for $h_0 = 0$

- reconstruction regime
for $l = L/2,\ t_m = L/v_{max}$,

$$\ln\left[\frac{m_{L/2}(t_m)}{m_{L/2}(t_m/2)}\right] = \frac{t_m/2}{\tau'},$$
$$\frac{1}{\tau'} = \frac{2}{\pi}\left\{\int_{\pi/6}^\pi \mathrm{d}p - \int_0^{\pi/6}\mathrm{d}p\right\} f_p|\mathcal{V}_p|$$

in the small h, h_0 limit:

$$\frac{1}{\tau'} = \frac{h(h-h_0)^2}{\pi}\frac{9\sqrt{3}-8}{12}$$
$$\frac{\tau}{\tau'} = \frac{9\sqrt{3}-8}{8} = 0.948$$

- Summation of the contributions (Calabrese et al)
effective occupation rate:

$$f_p \to \frac{1}{2}\ln(1-2f_p)$$

Generalized Gibbs ensemble (GGE)

- Nonintegrable systems
  - Thermalization
  - stationary state is a Gibbs state
  - one effective temperature: T_{eff}
- Integrable systems
  - Quasi-thermalization
  - stationary state is a GGE
  - effective temperature for each mode: $T_{\mathrm{eff}}(p)$
- Semi-classical theory

$$f_p(h_0,h) = \exp\left(-\frac{\varepsilon_h(p)}{T_{\mathrm{eff}}(p)}\right)$$

- Summation of the contributions

$$f_p(h_0,h) = \frac{1}{\exp\left(\frac{\varepsilon_h(p)}{T_{\mathrm{eff}}(p)}\right)+1}$$

classical kinks $\rightarrow$ free fermions
Boltzmann distr. $\rightarrow$ Fermi distr.

Conclusion

- effect of a free boundary on the quantum relaxation of the boundary magnetization
  - power-law relaxation
  - non-thermal behavior
  - finite limiting value
- relaxation in finite systems
  - different relaxation regimes
    - free relaxation
    - quasi-stationary regime
    - reconstruction regime
  - approximate periodicity in time
- explanation in terms of quasi-particles
  - emerging at quench at each sites
  - travel with a speed, v_p
  - reflected at the boundaries
  - by passing the reference point flip the spin
  - characteristic time and length-scales
- possible relevance of the results for another
  - integrable
  - nonintegrable

  systems