

# Correlations and dynamics of 1d cold atoms

*integrability in and out of equilibrium*

*Workshop on Low-dimensional quantum gases out of equilibrium  
Minneapolis, 11 May 2012*

**Jean-Sébastien Caux**  
Universiteit van Amsterdam



Work done in collaboration with:

J. Mossel, M. Panfil, G. Brandino

R. Konik, A. Shashi, A. Imambekov, ...



# Plan of the talk

- Quick review: integrability for dynamics
- Interaction turnoff in Bose gas
- Numerical renormalization using integrability  
*1d Bose gas in a trap*
- *Interlude: generalized TBA and generalized Gibbs*  
*Time-dependent dynamics after release*
- Conclusions

Quick review:  
dynamics  
from  
integrability

# Bethe Ansatz (1931)



July 2, 1906 – March 6, 2005

Integrable Hamiltonian:

$$H = \int_0^L dx \mathcal{H}(x)$$

‘Reference state’: vacuum, FM state, ...

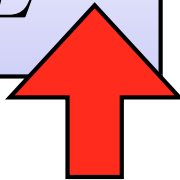
‘Particles’: atoms, down spins, ...

Exact many-body wavefunctions (in N-particle sector):

$$\Psi_N(\{x\}, \{\lambda\}) = \sum_P (-1)^{[P]} A_P(\{\lambda\}) e^{i x_j k(\lambda_{P_j})}$$

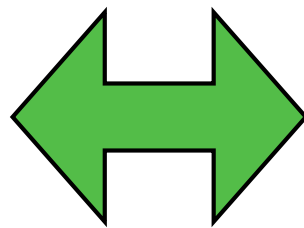
... parametrized by rapidities, made up of free waves ...  
... and obeying some form of Pauli principle

Imposing boundary conditions quantizes the allowable rapidities according to the **Bethe equations**

$$\theta_{kin}(\lambda_j) + \frac{1}{L} \sum_k \theta_{scat}(\lambda_j - \lambda_k) = \frac{2\pi}{L} I_j$$


Eigenstates: labeled by set of **quantum numbers**

Constructing all states in the Hilbert space



Obtaining all solutions to the Bethe equations

# The general idea, simply stated:

Start with your favourite quantum state  
(expressed in terms of Bethe states)

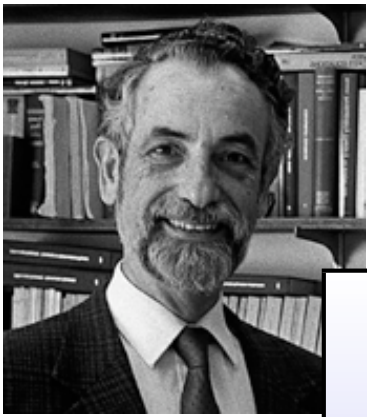
$$\mathcal{O} \rightarrow |\{\lambda\}\rangle$$

Apply some operator on it

Reexpress the result in the basis of Bethe states:

$$\mathcal{O}|\{\lambda\}\rangle = \sum_{\{\mu\}} F_{\{\mu\},\{\lambda\}}^{\mathcal{O}} |\{\mu\}\rangle$$

using 'matrix elements'  $F_{\{\mu\},\{\lambda\}}^{\mathcal{O}} = \langle\{\mu\}|\mathcal{O}|\{\lambda\}\rangle$



# The Lieb-Liniger model

$$\mathcal{H}_N = - \sum_{j=1}^N \frac{\partial^2}{\partial x_j^2} + 2c \sum_{1 \leq j < l \leq N} \delta(x_j - x_l)$$

Interaction: **repulsive** ( $c > 0$ ) or **attractive** ( $c < 0$ )

Second-quantized form:

$$H_0 = \int_0^L dx \left\{ \partial_x \Psi^\dagger(x) \partial_x \Psi(x) + c \Psi^\dagger(x) \Psi^\dagger(x) \Psi(x) \Psi(x) \right\}$$

Bethe equations

$$e^{i\lambda_j L} = \prod_{l \neq j} \frac{\lambda_j - \lambda_l + ic}{\lambda_j - \lambda_l - ic}, \quad j = 1, \dots, N$$

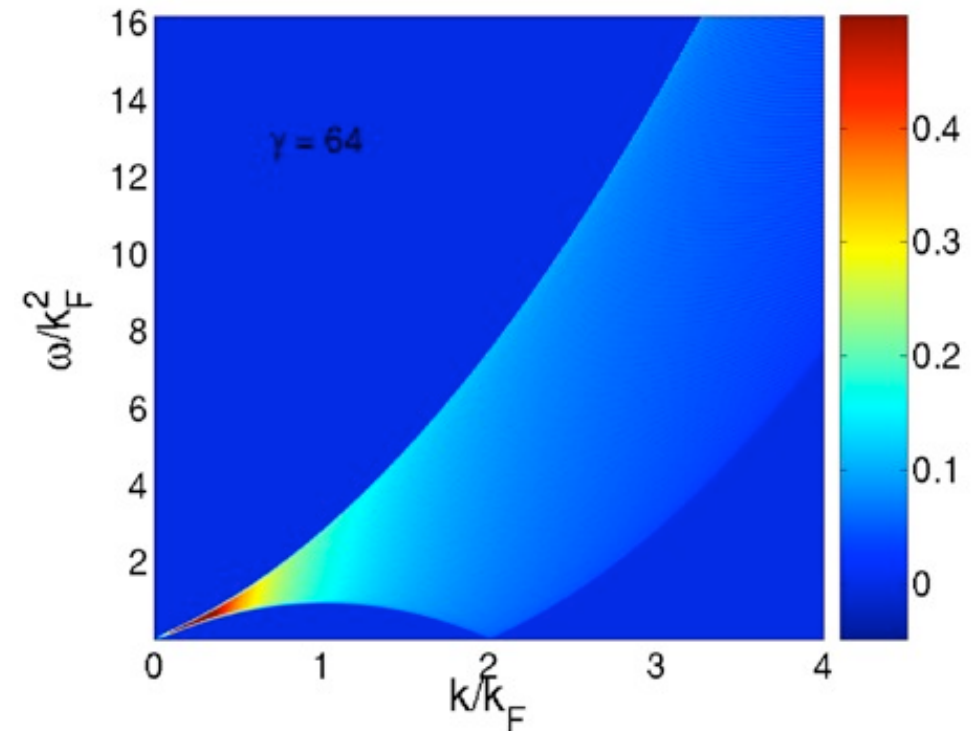
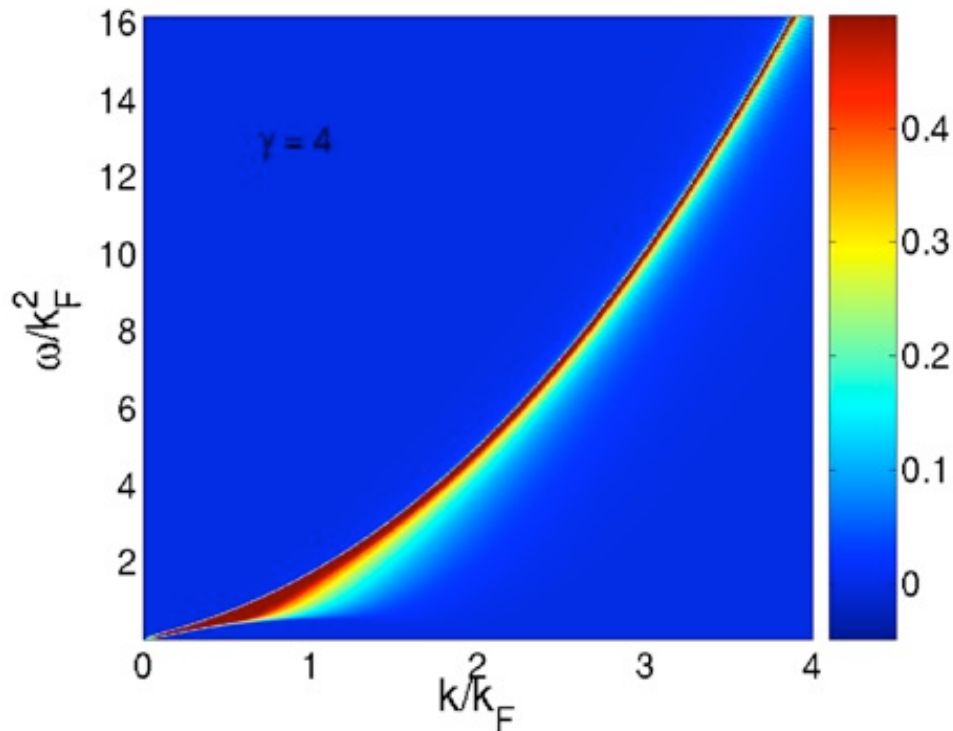


# Repulsive Lieb-Liniger gas

Density-density (dynamical SF)

(J-S C & P Calabrese, PRA 2006)

$$S(k, \omega) = \frac{2\pi}{L} \sum_{\alpha} |\langle 0 | \rho_k | \alpha \rangle|^2 \delta(\omega - E_{\alpha} + E_0)$$



Interaction  
turnoff  
in Lieb-Liniger

# Interaction quench in Lieb-Liniger

J. Mossel and JSC, arxiv:1201.1885

For all  $t < 0 : H = H_{c \neq 0}$

For all  $t > 0 : H = H_{c=0}$

Simplest time-dependent correlation:

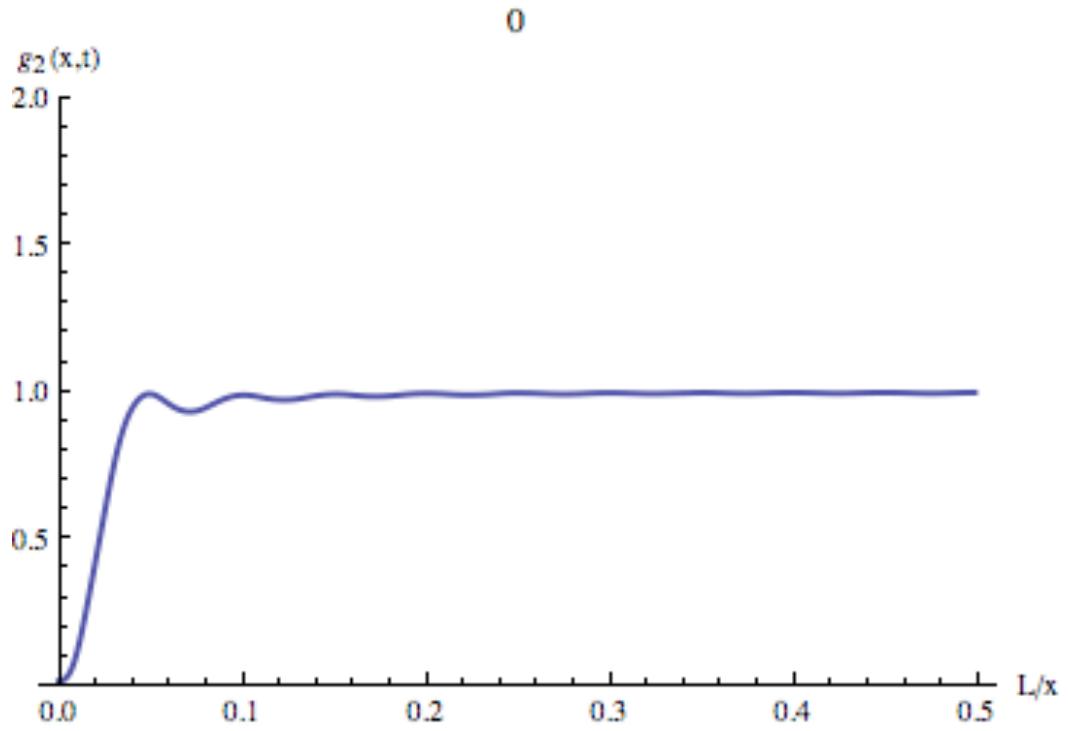
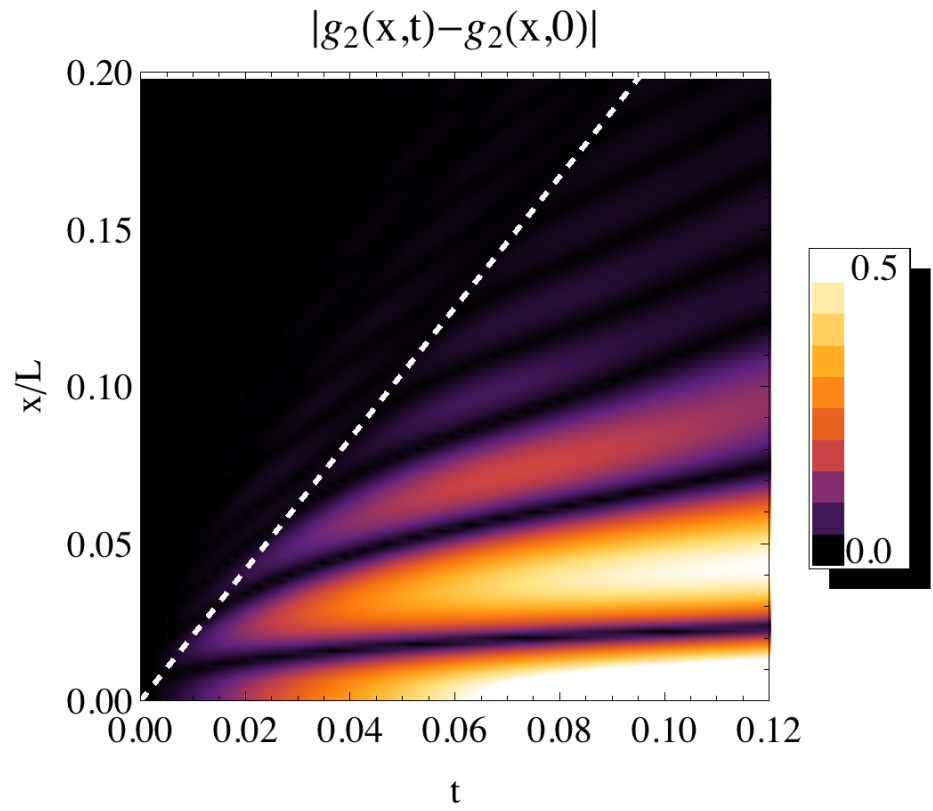
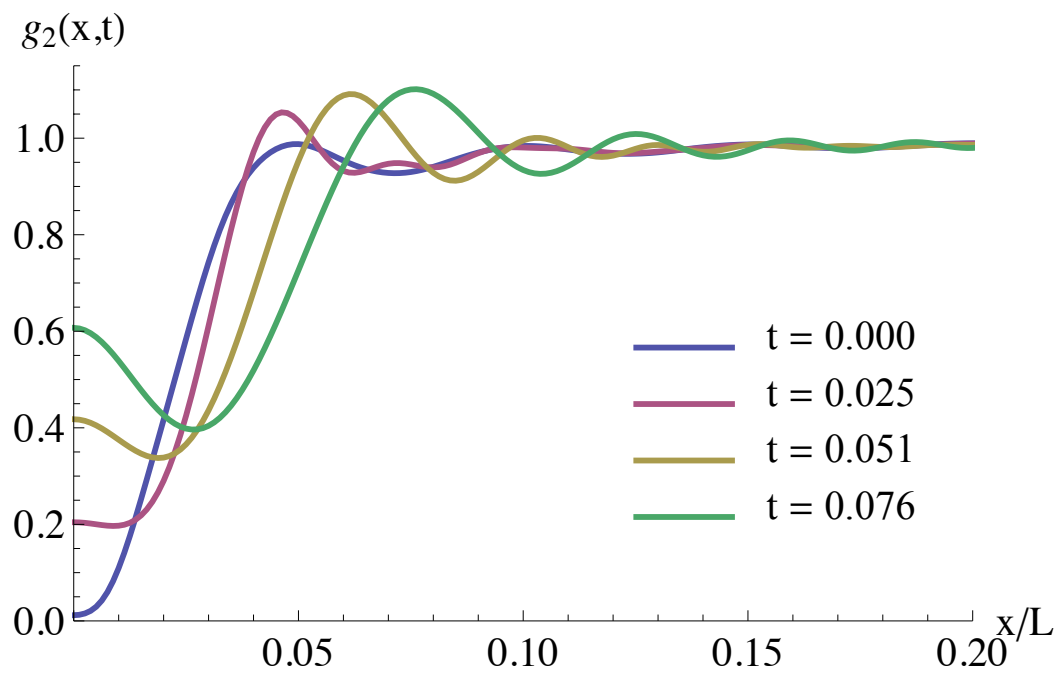
$$g_2(x; t) = \frac{\langle \phi(t) | \Psi^\dagger(x) \Psi^\dagger(0) \Psi(x) \Psi(0) | \phi(t) \rangle}{\langle \phi(t) | \Psi^\dagger(0) \Psi(0) | \phi(t) \rangle^2}$$

$$\begin{aligned} & \langle \phi(t) | \Psi^\dagger(x) \Psi^\dagger(0) \Psi(x) \Psi(0) | \phi(t) \rangle \\ &= \frac{1}{L^4} \sum_{k_1, k_2, k_3} e^{ik_{13}(x-2k_{23}t)} \langle \phi | \Psi_{k_1}^\dagger \Psi_{k_2}^\dagger \Psi_{k_3} \Psi_{k_1+k_{23}} | \phi \rangle \end{aligned}$$

Expectation value: use triple resolution of identity

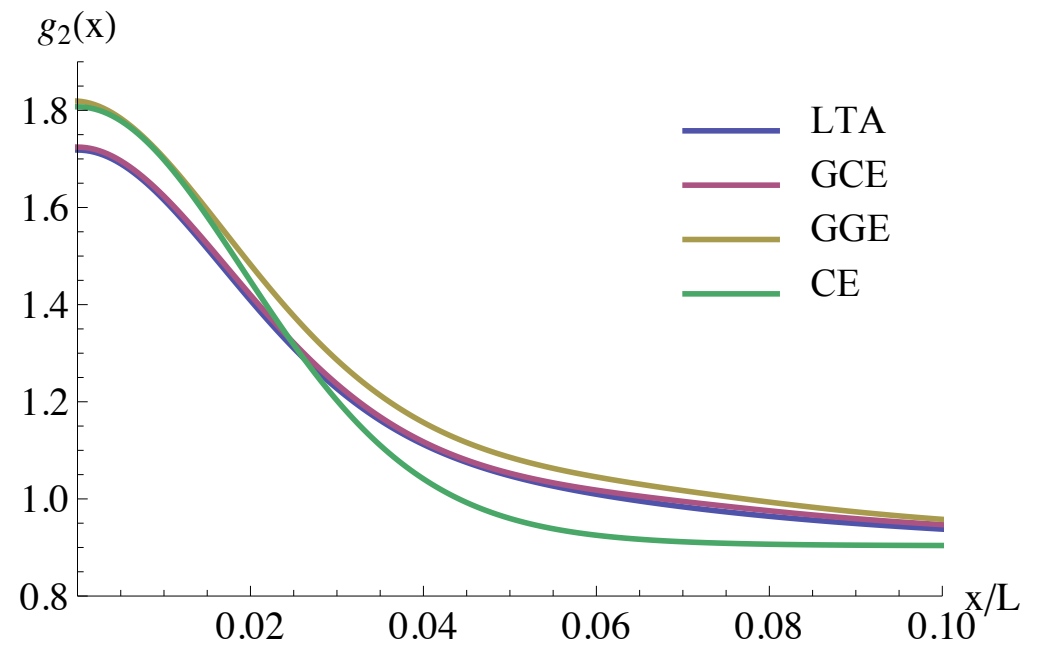
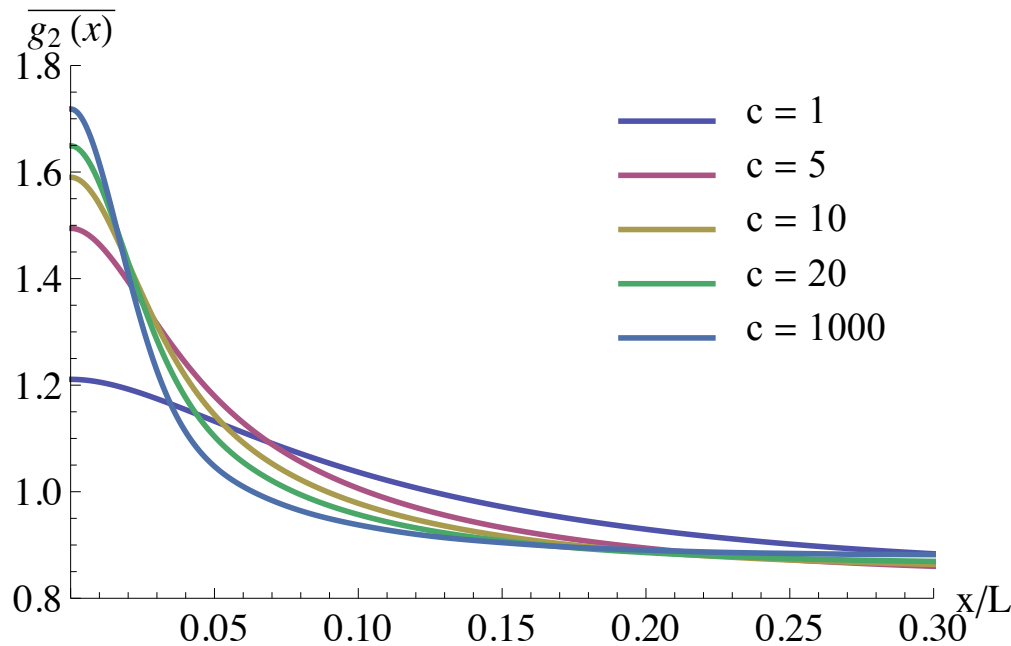
$$\sum_{n_1, n_2, n_3} \langle \phi | \Psi_{k_1}^\dagger | n_1 \rangle \langle n_1 | \Psi_{k_2}^\dagger | n_2 \rangle \langle n_2 | \Psi_{k_3} | n_3 \rangle \langle n_3 | \Psi_{k_1+k_2-k_3} | \phi \rangle$$

# Nonlocal density correlation as a function of time



# Long-time average of static density correlation

$$\overline{g_2(x; c)} = \lim_{T \rightarrow T_{LTA}} \frac{1}{T} \int_0^T g_2(x, t; c) dt$$



Compared to various ensembles ( $c = 1000$ )

GGE doesn't work here, but GenCanE does (finiteness?)

Numerical  
renormalization  
using  
integrability

# Renormalization from integrability

(nonrelativistic BA solvable models)

JSC & R. M. Konik | 203.0901

$$H = H_{int} + H_{pert}$$



Exactly solvable  
theory



Some perturbation

(with operator whose FF can  
be calculated)

Implementation of a 'fifth way' for RG  
(supplementing Wilson's original 'four ways')

# Numerical renormalization

- Summary of procedure:
- Choose a first set of  $N + dN$  states
  - Compute  $H$  and diagonalize it
  - Toss away highest-lying  $dN$  states
  - Include next  $dN$  states
  - Recompute  $H$  and diagonalize
  - ...

States basis: usually, free states or from exact diag

Here: **exact BA eigenstates**

Include states in order of expected importance

Usually: chosen only according to **energy**

Here: must use a more refined measure,  
exploiting knowledge of **matrix elements**



# Example: Lieb-Liniger in a trap

Hamiltonian:

$$H = -\frac{\hbar^2}{2m} \sum_{j=1}^N \frac{\partial^2}{\partial x_j^2} + 2c \sum_{i<j} \delta(x_i - x_j) + \sum_i V(x_i)$$

with simple harmonic trap  $V(x) = \frac{m}{2} \omega^2 x^2$

The perturbation can be written in terms of the density operator

$$H_{pert} = \int_0^L dx V(x) \rho(x)$$

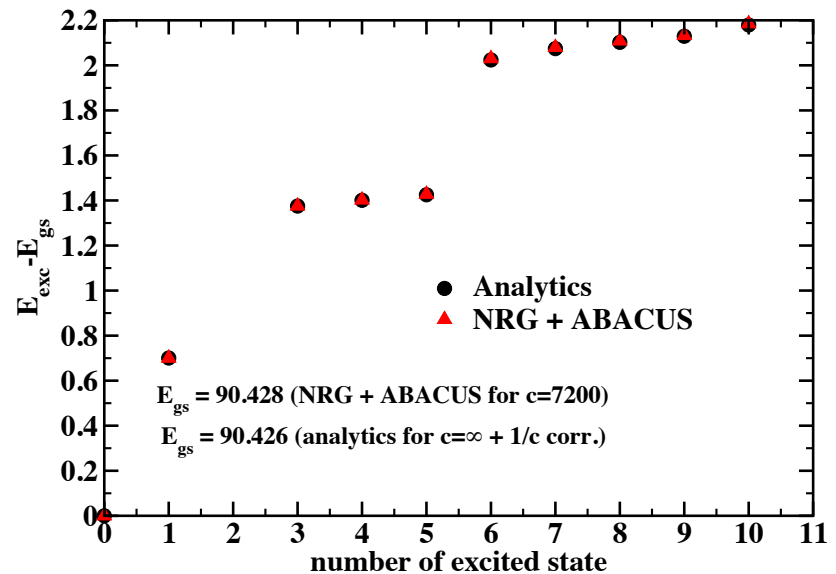
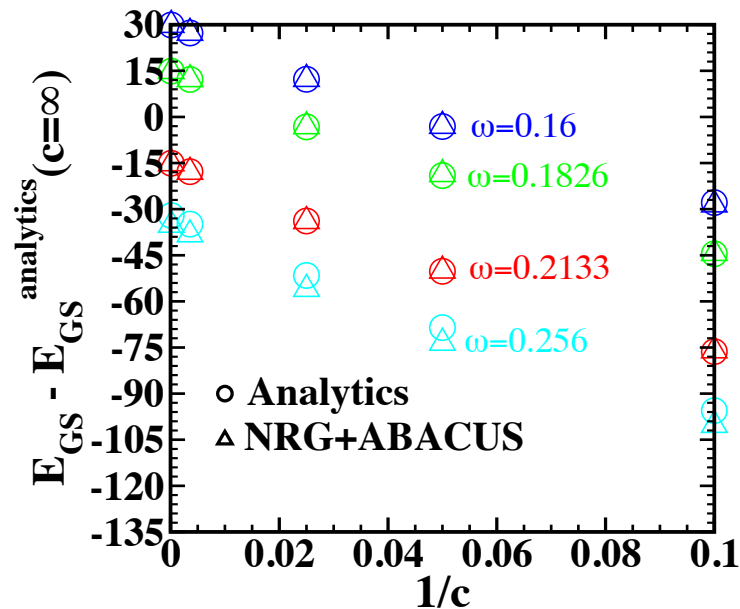
whose matrix element is available as a function of rapidities in bra and ket states

# Lieb-Liniger in a trap: static properties

Ground state in a trap obtained as linear combination of Bethe states

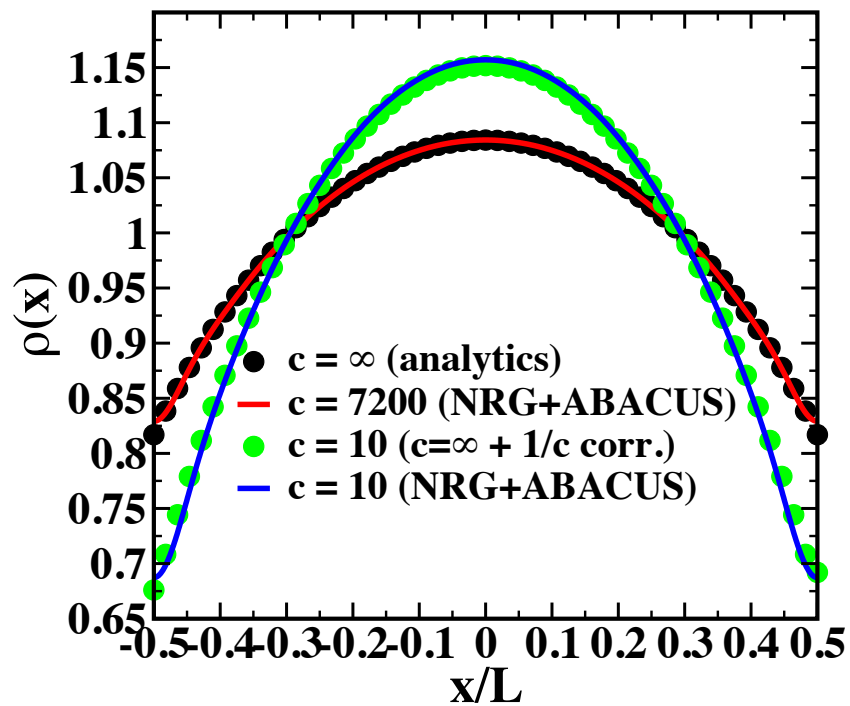
$$|\psi\rangle_{GS} = \sum_s c_s |s\rangle$$

Energies of ground and low-lying states can be tested at large  $c$  by comparing to analytical results



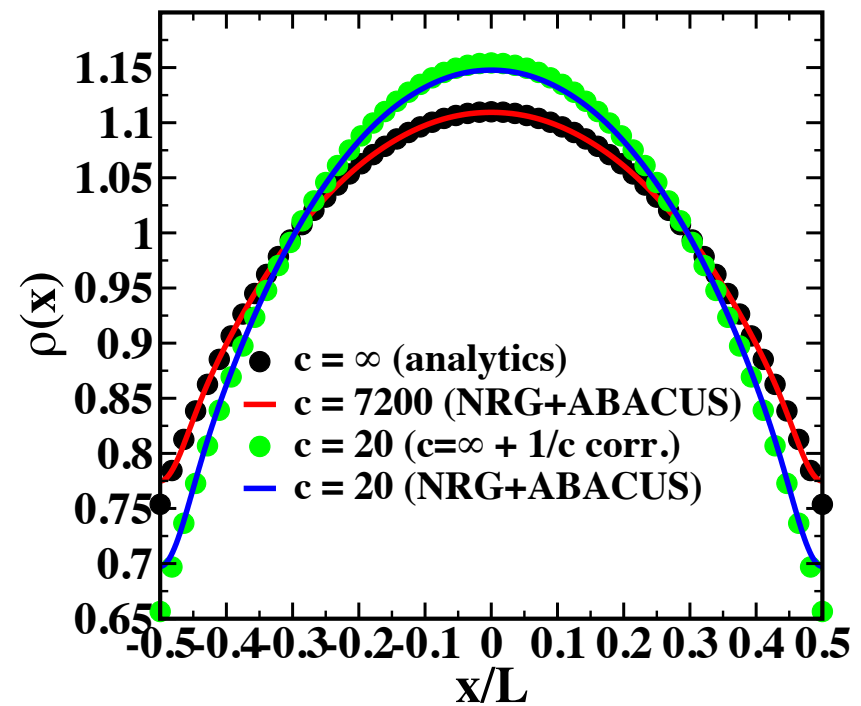
# Lieb-Liniger in a trap: static properties beyond energetics

Density profile in ground state of trapped gas



$$\omega = 0.16$$

$$N = 56$$



$$\omega = 0.183$$

# Time evolution after trap release

The time evolution is trivially given by

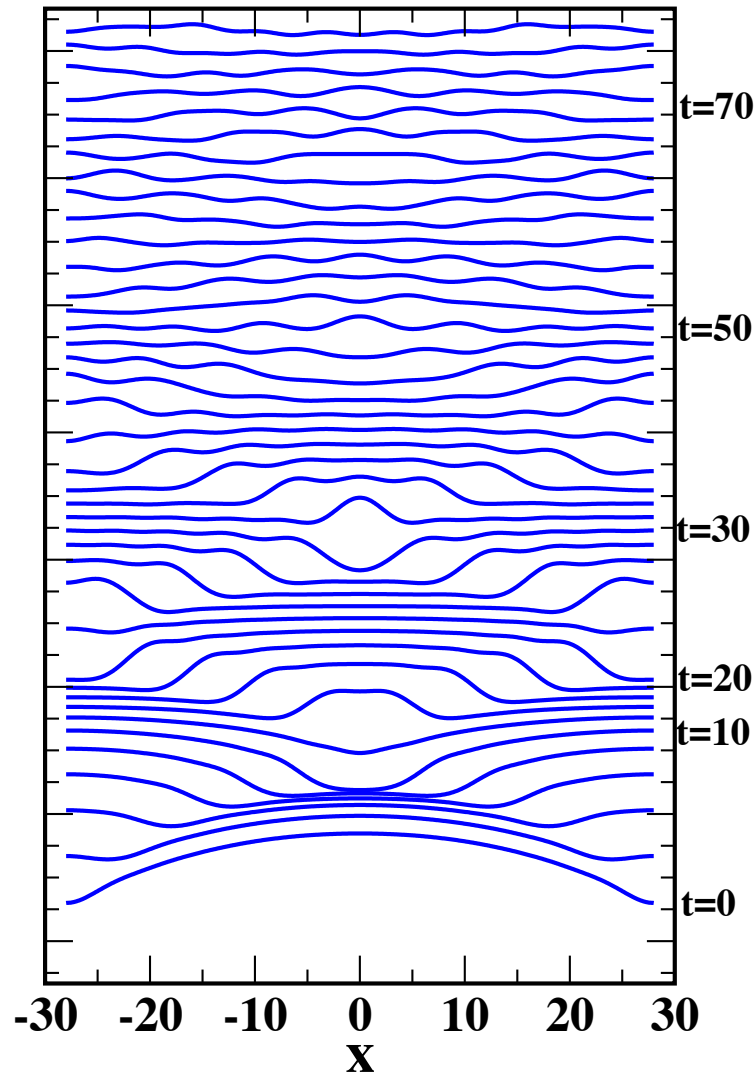
$$|\psi(t)\rangle_{GS} = \sum_s c_s e^{-iE_s t} |s\rangle$$

Advantage of using integrable basis:  
if post-quench evolution is via integrable H,  
**energies are known exactly**, and thus  
**arbitrary t is accessible** without loss of accuracy!

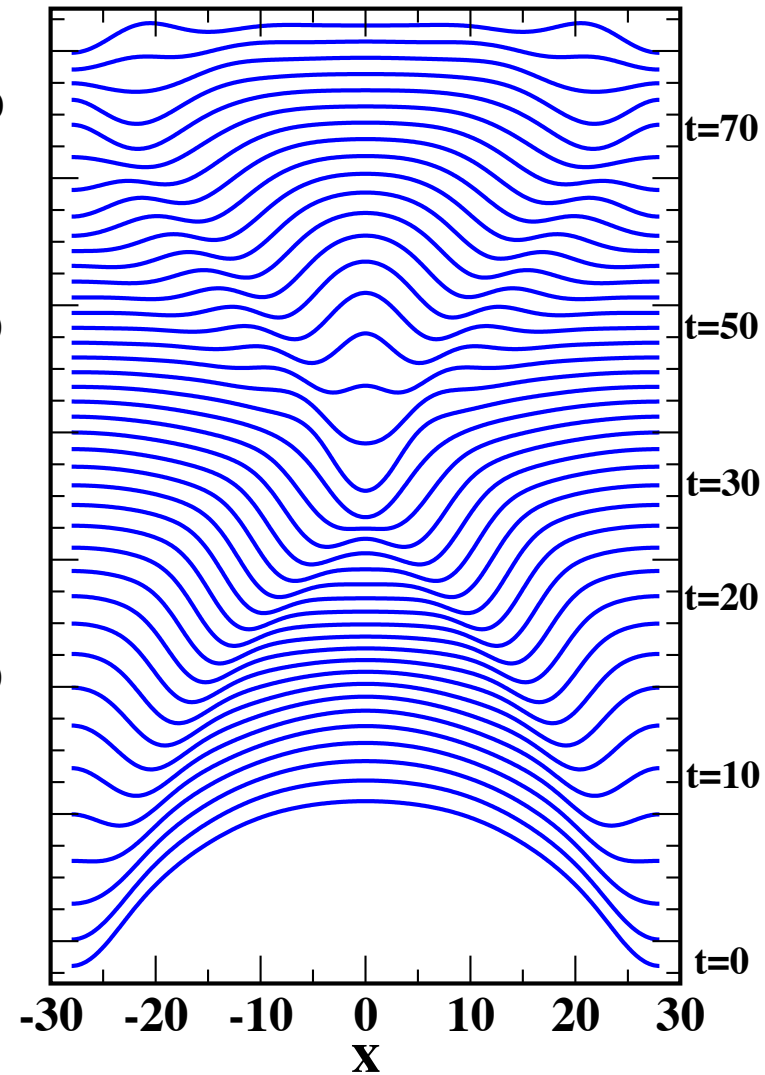
(note however that we always use  
**periodic boundary conditions**)

# Local density as function of time

$c=7200$



$c=1$

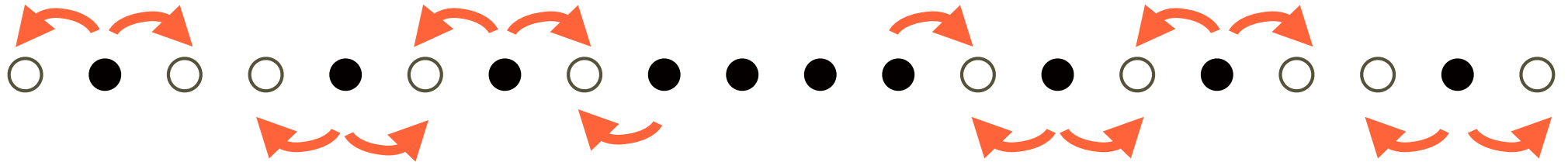


# Correlations long after release

(in other words: in the diagonal ensemble)

$$\langle \mathcal{O}^\dagger \mathcal{O} \rangle_{DE} \equiv \sum_s |c_s|^2 \langle s | \mathcal{O}^\dagger \mathcal{O} | s \rangle$$

Implementation of ‘ABACUS for arbitrary states’



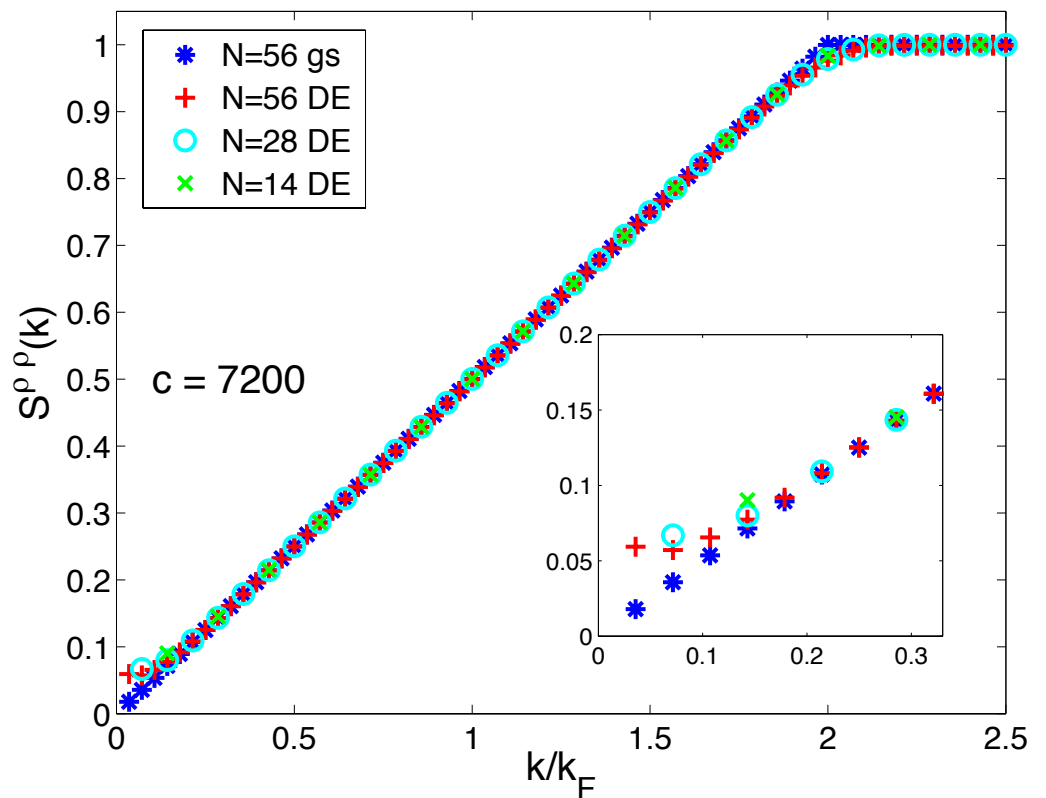
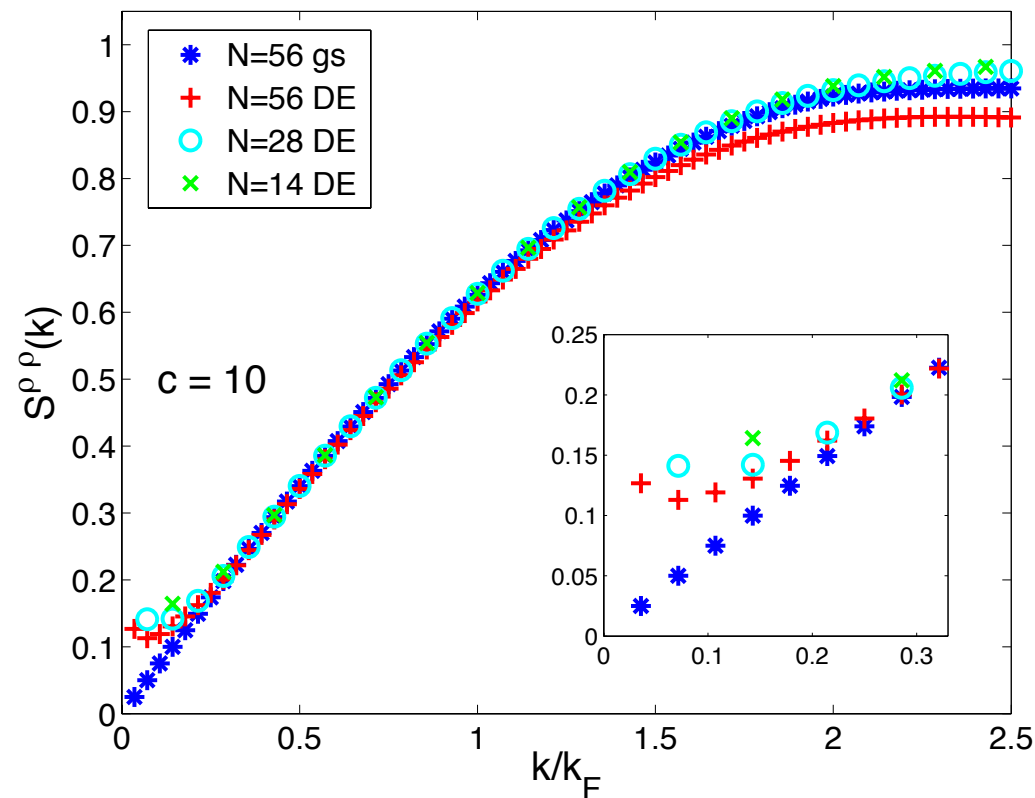
Matrix elements: are not suppressed as ‘rapidly’ as around the ground state. Large summation.

# Correlations long after release

(in other words: in the diagonal ensemble)

$$\langle \mathcal{O}^\dagger \mathcal{O} \rangle_{DE} \equiv \sum_s |c_s|^2 \langle s | \mathcal{O}^\dagger \mathcal{O} | s \rangle$$

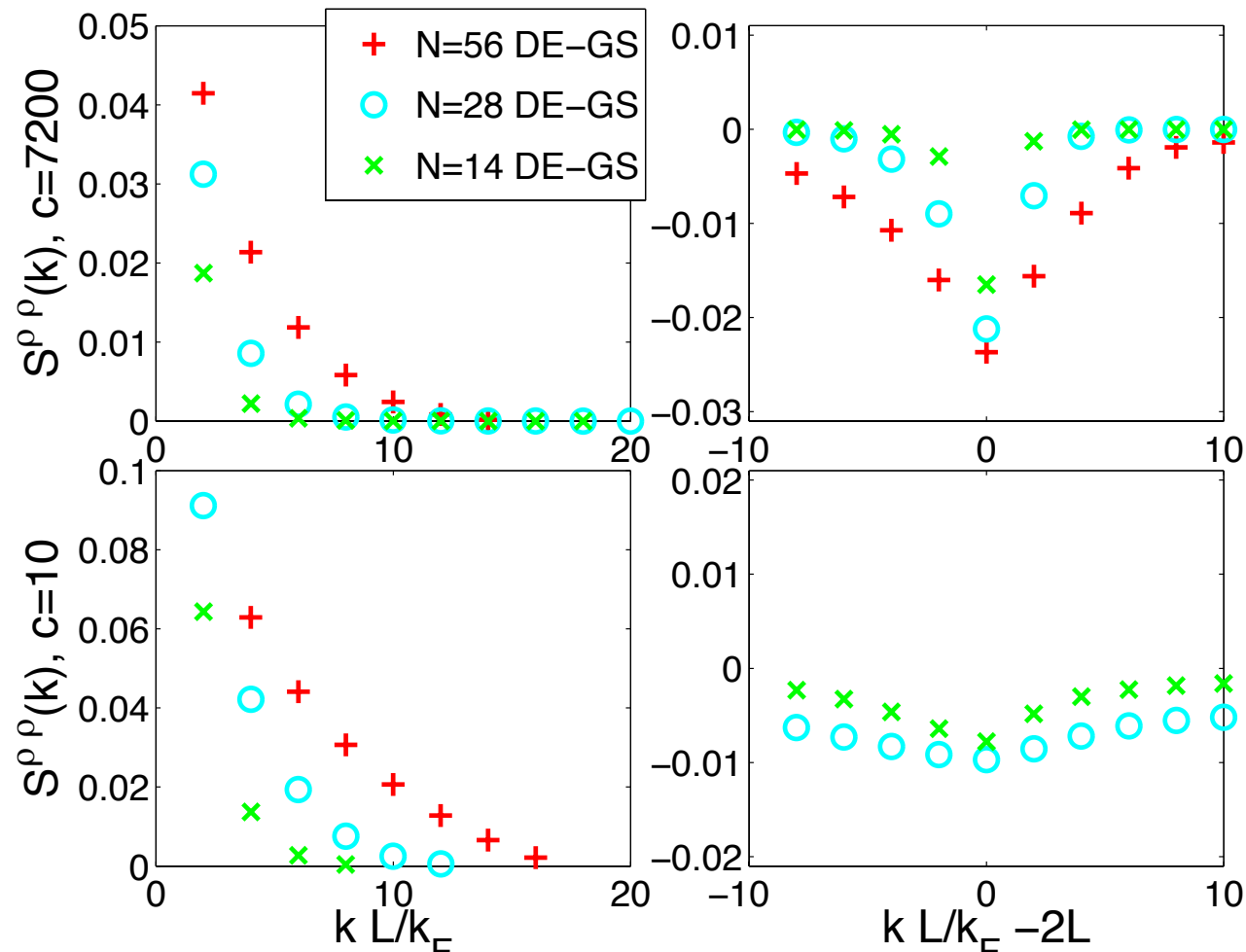
## I) Static structure factor



# Correlations long after release

(in other words: in the diagonal ensemble)

$$\langle \mathcal{O}^\dagger \mathcal{O} \rangle_{DE} \equiv \sum_s |c_s|^2 \langle s | \mathcal{O}^\dagger \mathcal{O} | s \rangle$$



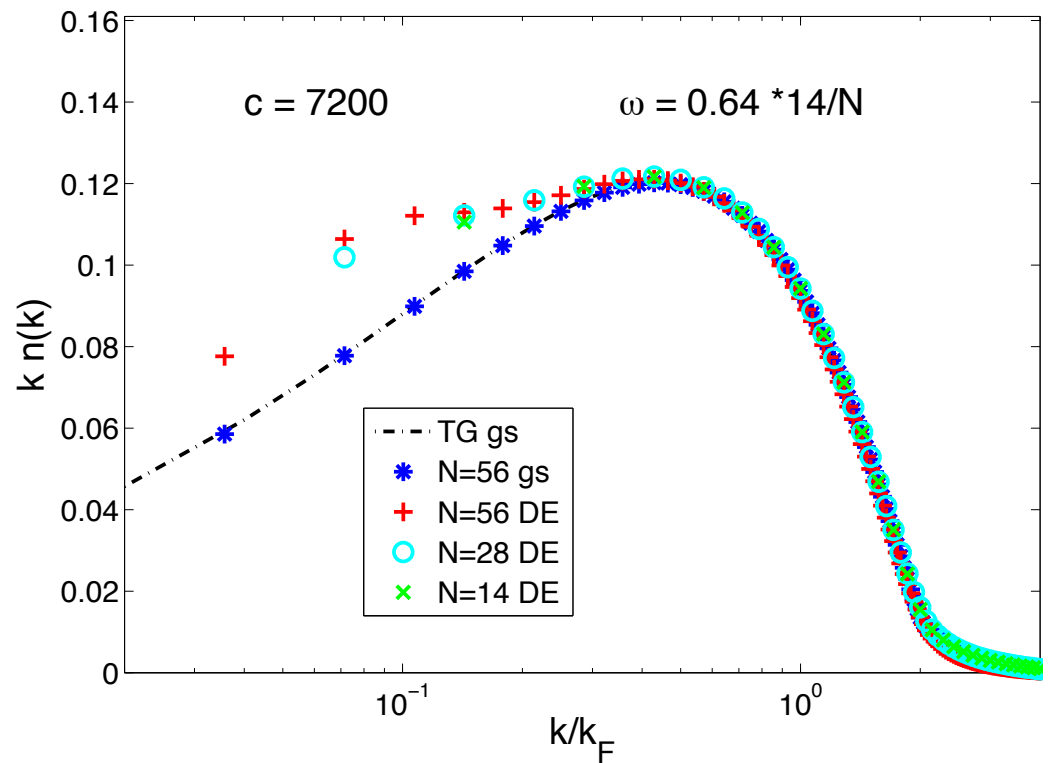
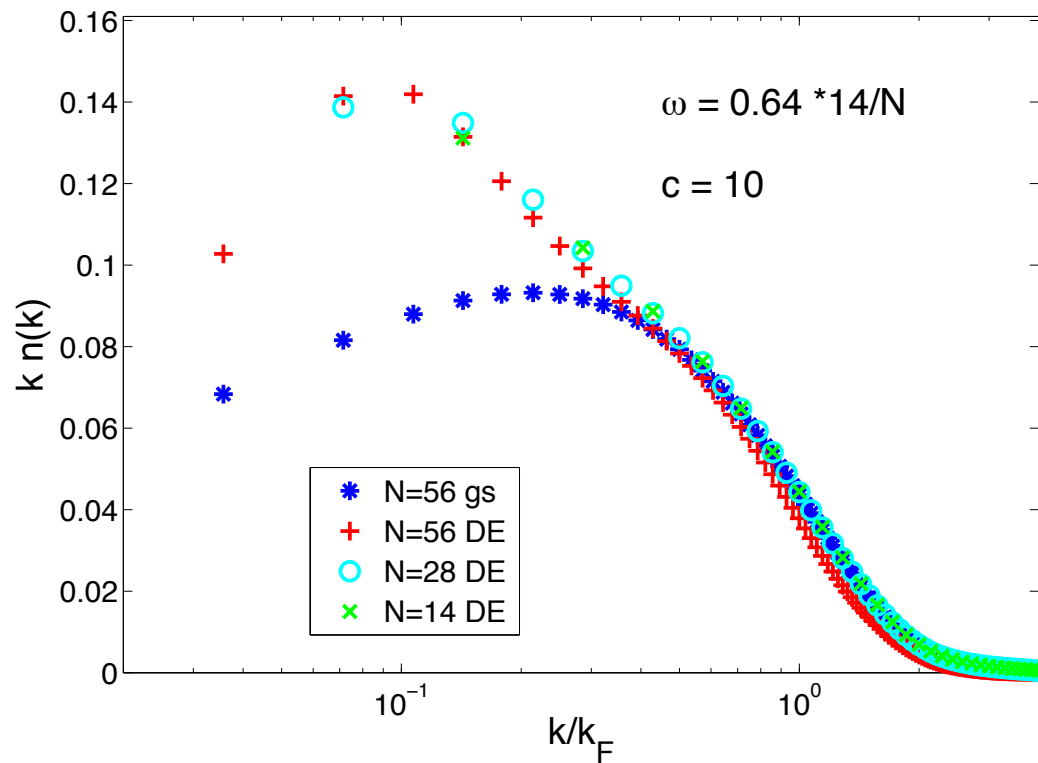


# Correlations long after release

(in other words: in the diagonal ensemble)

$$\langle \mathcal{O}^\dagger \mathcal{O} \rangle_{DE} \equiv \sum_s |c_s|^2 \langle s | \mathcal{O}^\dagger \mathcal{O} | s \rangle$$

## 2) Momentum distribution function



# Interlude: Generalized TBA

# Generalized TBA and generalized Gibbs

J. Mossel and JSC, arxiv:1203.1305

Integrable Hamiltonian  $H_0$  and its conserved charges  $\hat{Q}_n$

$$\left[ H_0, \hat{Q}_n \right] = 0, \quad \left[ \hat{Q}_n, \hat{Q}_m \right] = 0, \quad \forall n, m$$

Generic Hamiltonian:  $H(\{\beta\}) = \sum_n \beta_n \hat{Q}_n$

shares wavefunctions with  $H_0, \forall \{\beta_n\} \in \mathbb{R}$

Density matrix:  
generalized Gibbs  
ensemble (GGE)

$$\hat{\rho}_{GGE} = e^{-\sum_n \beta_n \hat{Q}_n}$$

Conjecture: after a quantum quench, GGE describes state at asymptotically large time

Rigol, Dunjko, Yurovsky, Olshanii, PRL 2007

Jaynes, Phys. Rev. 1957

Generalized inverse temperatures are set by initial conditions

$$\langle \hat{Q}_m \rangle = \text{Tr} \left\{ \hat{Q}_m e^{-\sum_n \beta_n \hat{Q}_n} \right\} / \mathcal{Z}_{GGE} \quad m = 0, 1, 2, \dots$$

$$\text{where } \mathcal{Z}_{GGE} = \text{Tr} e^{-\sum_n \beta_n \hat{Q}_n}$$

In reality, two major difficulties:

Conserved charges are generically nontrivial

Self-consistency problem difficult to solve

In practice: only implemented for free theories

# Generalized TBA for Lieb-Liniger

Eigenvalues of conserved charges trivial on Bethe states

$$\hat{Q}_n |\{\lambda\}\rangle = Q_n |\{\lambda\}\rangle, \quad Q_n = \sum_j \lambda_j^n$$

(although charges themselves are nontrivial *Davies & Korepin*)

The generalized Hamiltonian is trivially diagonalized by the Bethe states

$$H(\{\beta\}) |\{\lambda\}\rangle = E(\{\beta\}) |\{\lambda\}\rangle,$$

$$E(\{\beta\}|\{\lambda\}) = \sum_{n=0}^{\infty} \sum_{j=1}^N \beta_n \lambda_j^n \equiv \sum_{j=1}^N \varepsilon_0(\lambda_j)$$

$$\varepsilon_0(\lambda) \equiv \sum_{n=0}^{\infty} \beta_n \lambda^n \quad \text{‘Driving’ term for generalized TBA}$$

## Thermodynamic limit: root density distributions

$$\rho(\lambda) + \rho_h(\lambda) = \frac{1}{2\pi} + a_2 * \rho(\lambda), \quad a_2(\lambda) \equiv \frac{1}{\pi} \frac{c}{\lambda^2 + c^2}$$

Eigenvalue of conserved charges simply given by

$$Q_n = L \int_{-\infty}^{\infty} d\lambda \lambda^n \rho(\lambda)$$

Knowing the *root density distribution*  
is thus equivalent to  
knowing the *eigenvalues of all conserved charges*

# Solving the generalized TBA

Simply repeat logic of Yang & Yang

$$\mathcal{Z} = \int \mathcal{D}[\rho] e^{-G[\rho, \rho_h[\rho]]} \quad G[\rho, \rho_h] = \sum_{n=0} \beta_n Q_n - S[\rho, \rho_h]$$
$$S = L \int_{-\infty}^{\infty} d\lambda [(\rho + \rho_h) \ln(\rho + \rho_h) - \rho \ln \rho - \rho_h \ln \rho_h]$$

Usual saddle-point reasoning gives

$$\varepsilon(\lambda) + a_2 * \ln(1 + e^{-\varepsilon(\lambda)}) = \varepsilon_0(\lambda) \quad \varepsilon(\lambda) = \ln \frac{\rho_h(\lambda)}{\rho(\lambda)},$$

Solution exists and is unique, density obtained from

$$\rho(\lambda) = \vartheta(\lambda) \left( \frac{1}{2\pi} + a_2 * \rho(\lambda) \right) \quad \vartheta(\lambda) = \frac{\rho(\lambda)}{\rho(\lambda) + \rho_h(\lambda)} = \frac{1}{1 + e^{\varepsilon(\lambda)}}$$

Thus: two different ways of proceeding in practice:

1) given (by some 'beta-oracle') a set  $\{\beta_n\}$   
solve for  $\varepsilon(\lambda)$  from which  $\rho(\lambda)$  can be obtained

2) given (by some 'rho-oracle') a  $\rho(\lambda)$   
solve for  $\varepsilon(\lambda)$  from which  $\{\beta_n\}$  can be obtained

$$\beta_n = \left. \frac{\partial^n}{\partial \lambda^n} \left( \varepsilon(\lambda) + a_2 * \ln[1 + e^{-\varepsilon(\lambda)}] \right) \right|_{\lambda=0}$$



# Constructing the GGE explicitly

JSC & R. M. Konik | 203.0901

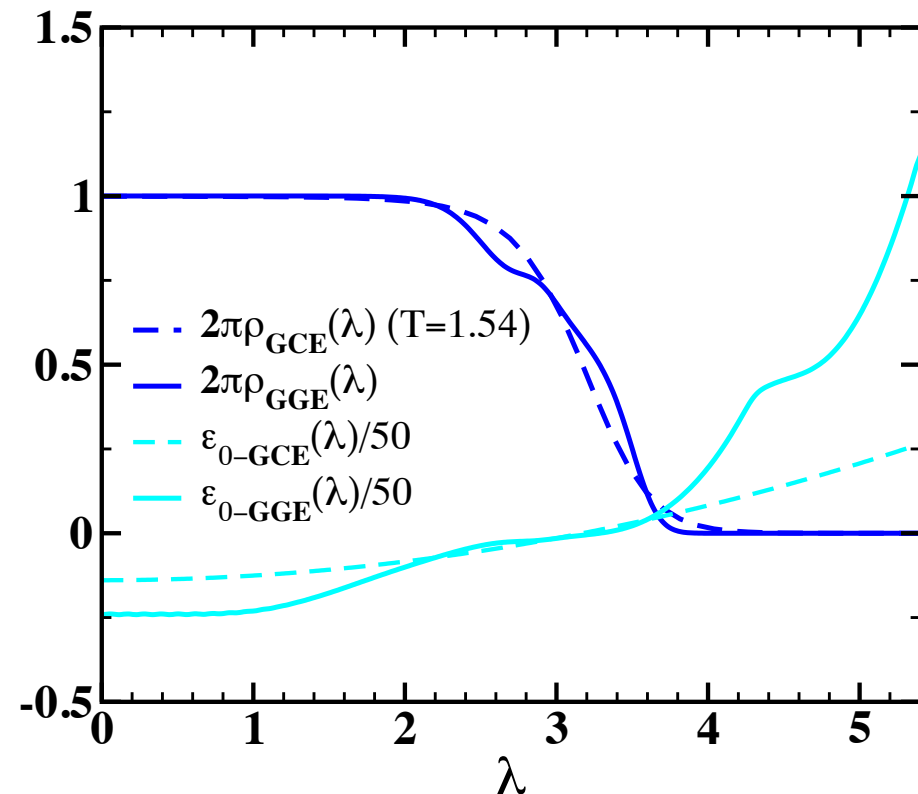
Lieb-Liniger in a trap, long after release

GGE root density distribution is simply

$$\rho_{GGE}(\lambda) = \sum_s |c_s|^2 \rho_s(\lambda)$$

which is obtained from NRG+ABACUS

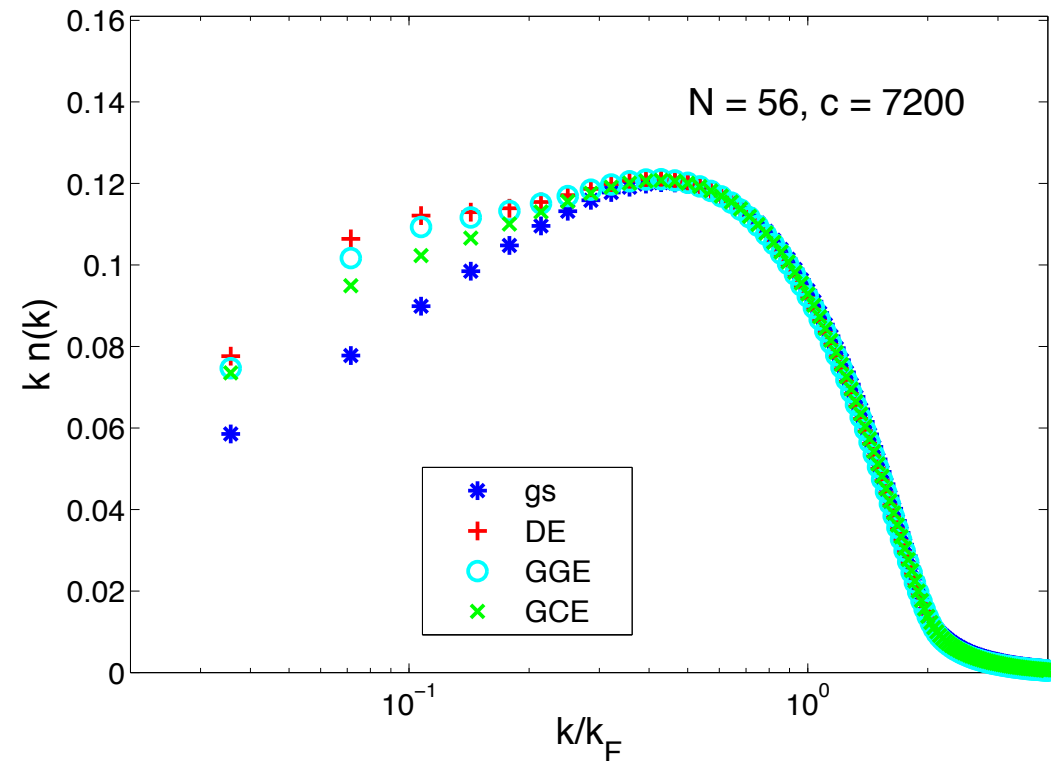
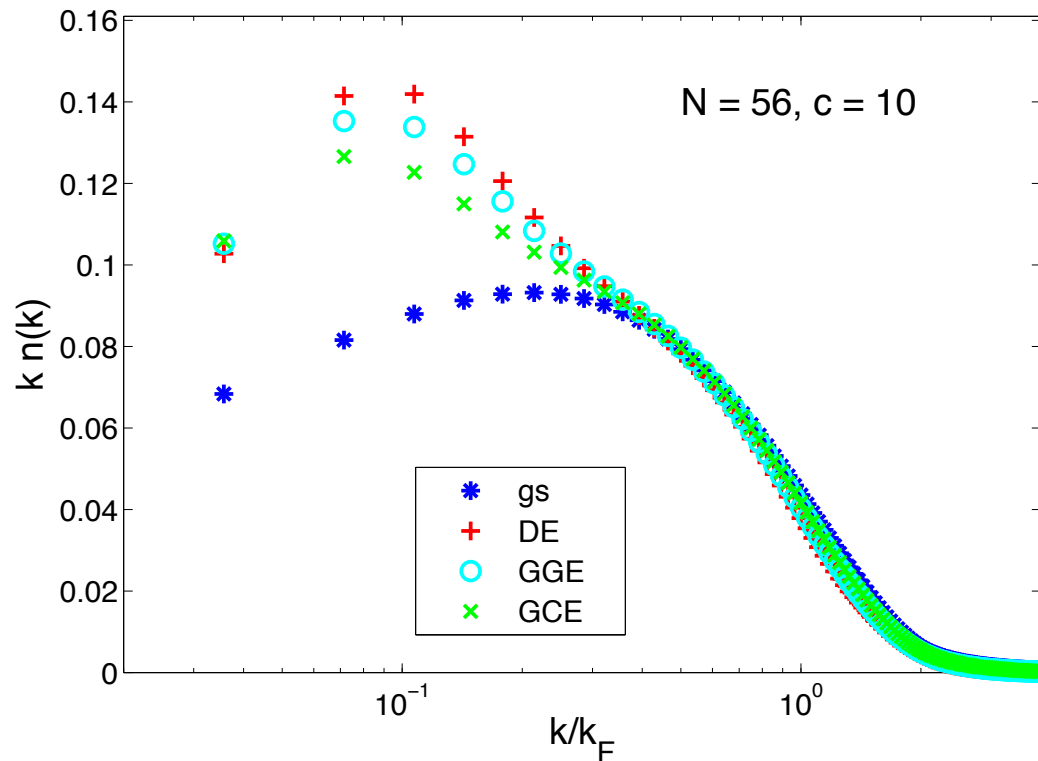
This root density is non-thermal



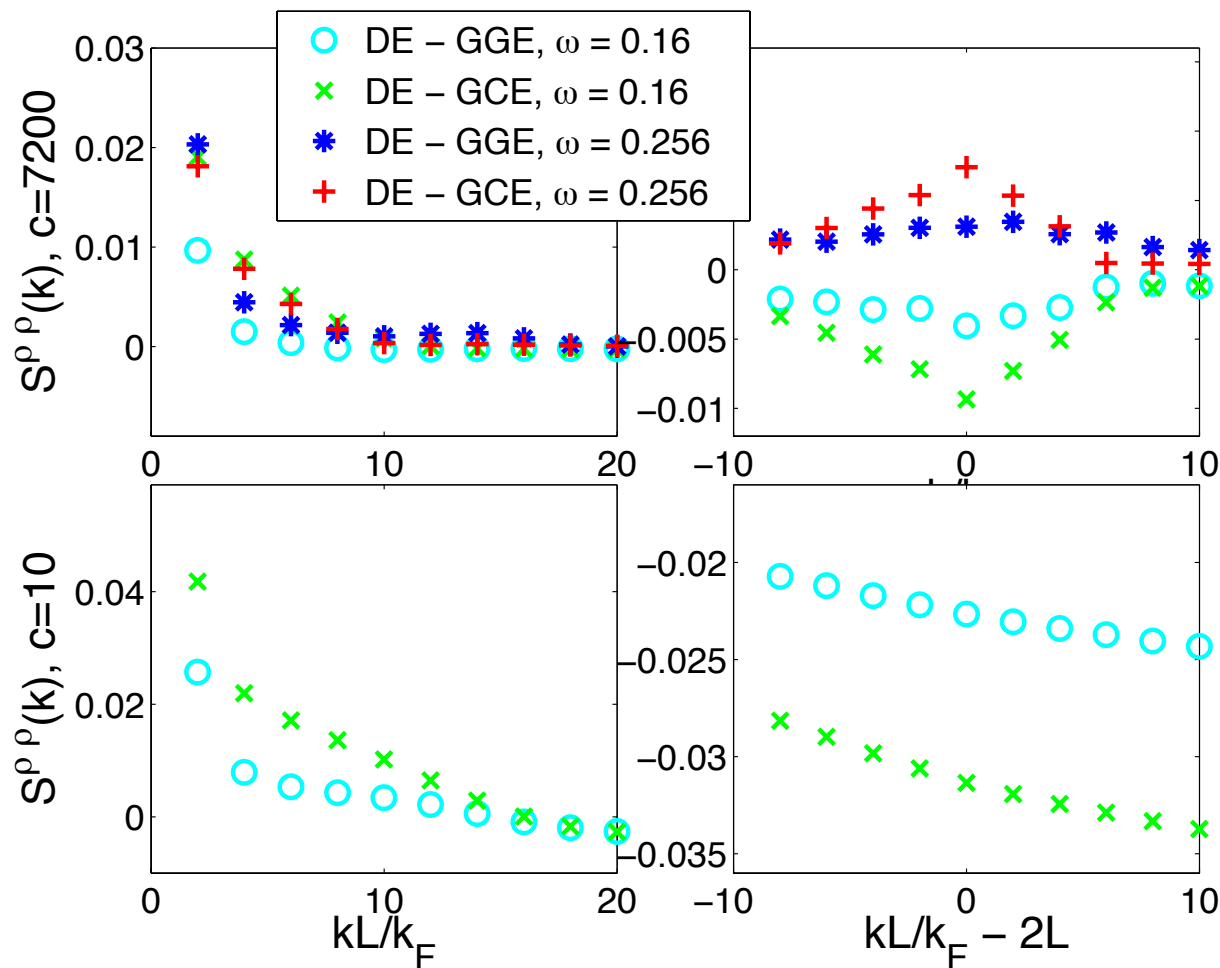
We are now in position to compare  
three different ensembles:

- 1) diagonal
- 2) grand canonical
- 3) generalized Gibbs

## Momentum distribution function



# Static structure factor



- both GCE and GGE disagree with DE
- disagreement grows with trap strength
- disagreement grows as interactions decrease
- GGE considerably better match to DE than GCE

# Conclusions

- Interaction turnoff in Lieb-Liniger
  - *simple explicitly solvable case*
  - *in this finite system, GenCan better than GenGibbs*
- NRG + ABACUS
  - *now able to tackle 'deformed' integrable models*
  - *method gives access to time evolution after quench*
- Not discussed here (for private discussions):
  - *correlation prefactors*
  - *thermal correlations*
  - *correlations on Moses states*