Evidence of Quantum Critical Behavior of One-Dimensional Soft Bosons

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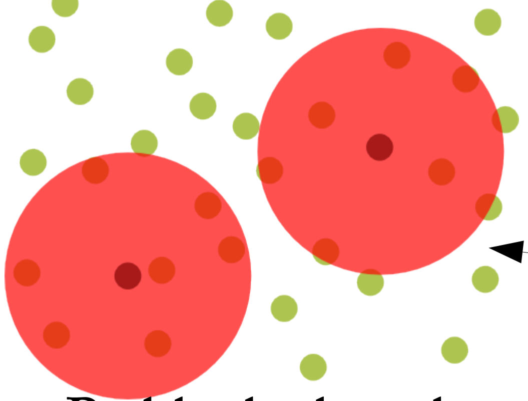
Motivation: soft core in dressed Rydberg gases

Ground state atoms

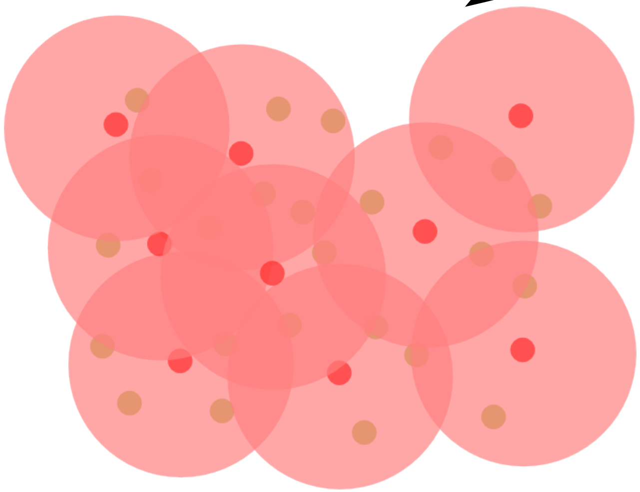


R_C blockade radius

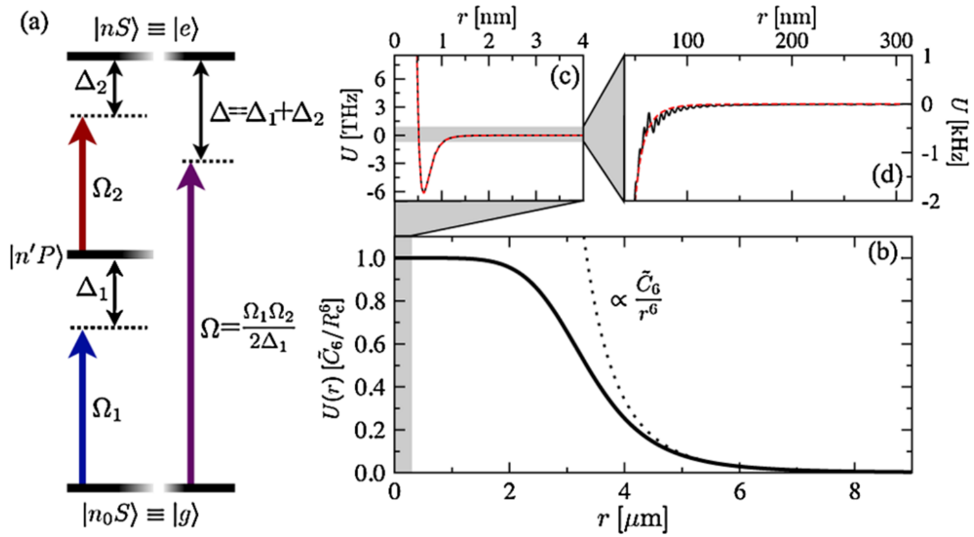
Rydberg state = Highly excited electronic state (n~200)
Couple ultracold atoms in ground-state to Rydberg state

A) Resonant light-atom coupling: hard-core freezed effective particles [Schauss et al., Nature (2012)]

B) Off-resonant: small quantum superposition of gs and Rydberg state, soft-core effective itinerant particles

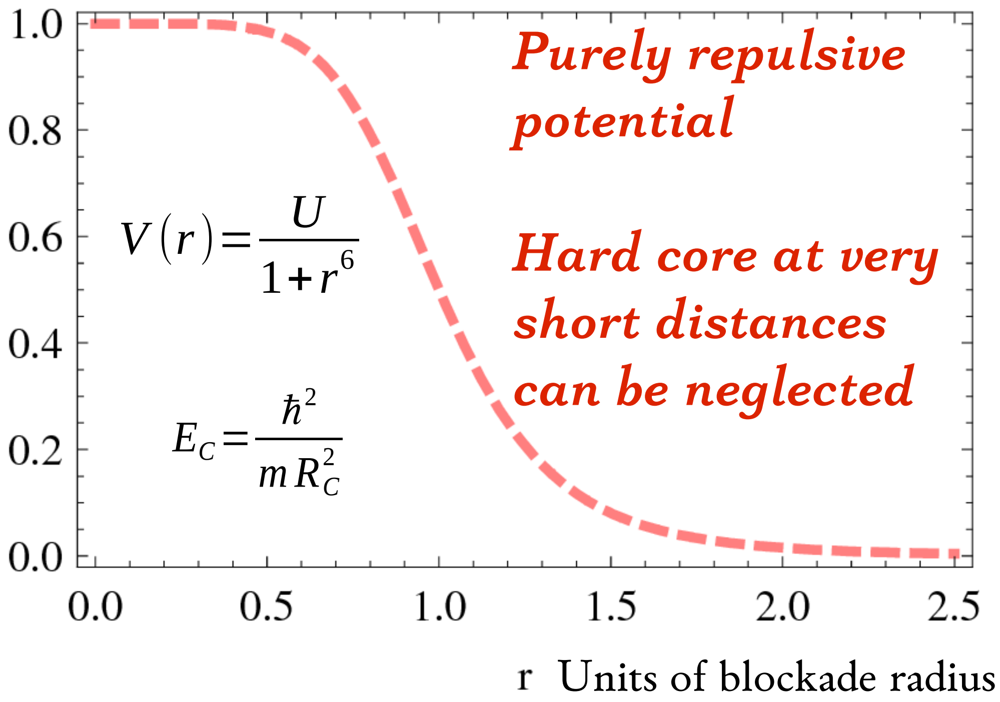


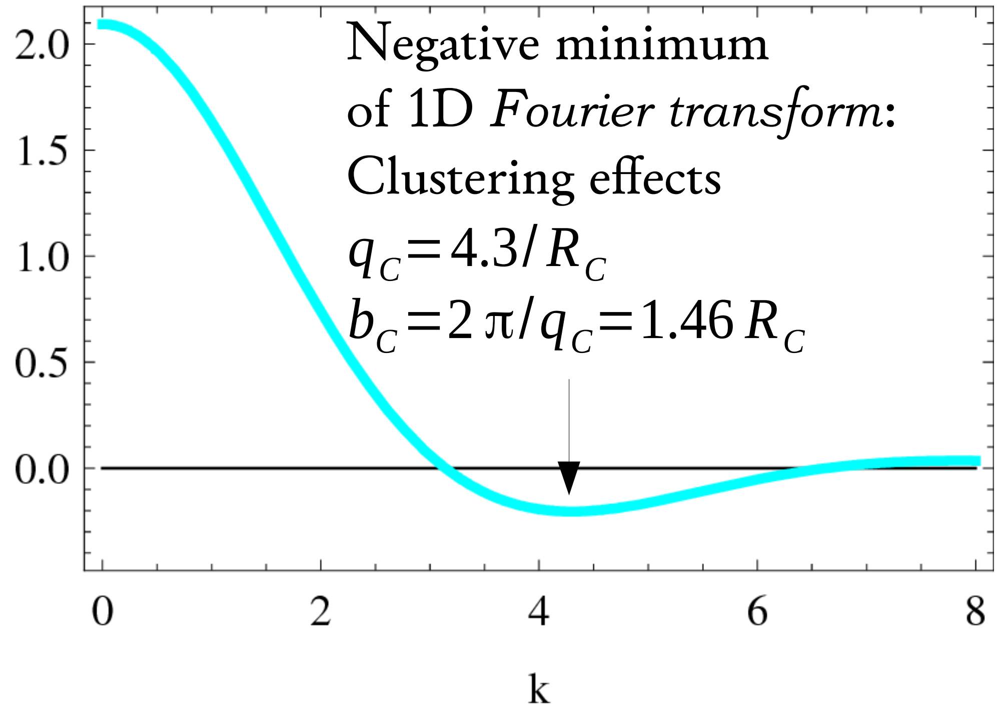
Henkel et al, PRL 104 (2010)



Quasi-1D: tight harmonic optical potential
Recent experiment Zeiher et al., arXiv:1705.08372
Finite lifetime ~ 1ms (lattice, still no overlap within soft-core)

Soft potentials and clustering





Classical soft systems: glassy behavior and polyamorphism [Mladek et al., PRL 96 (2006)]

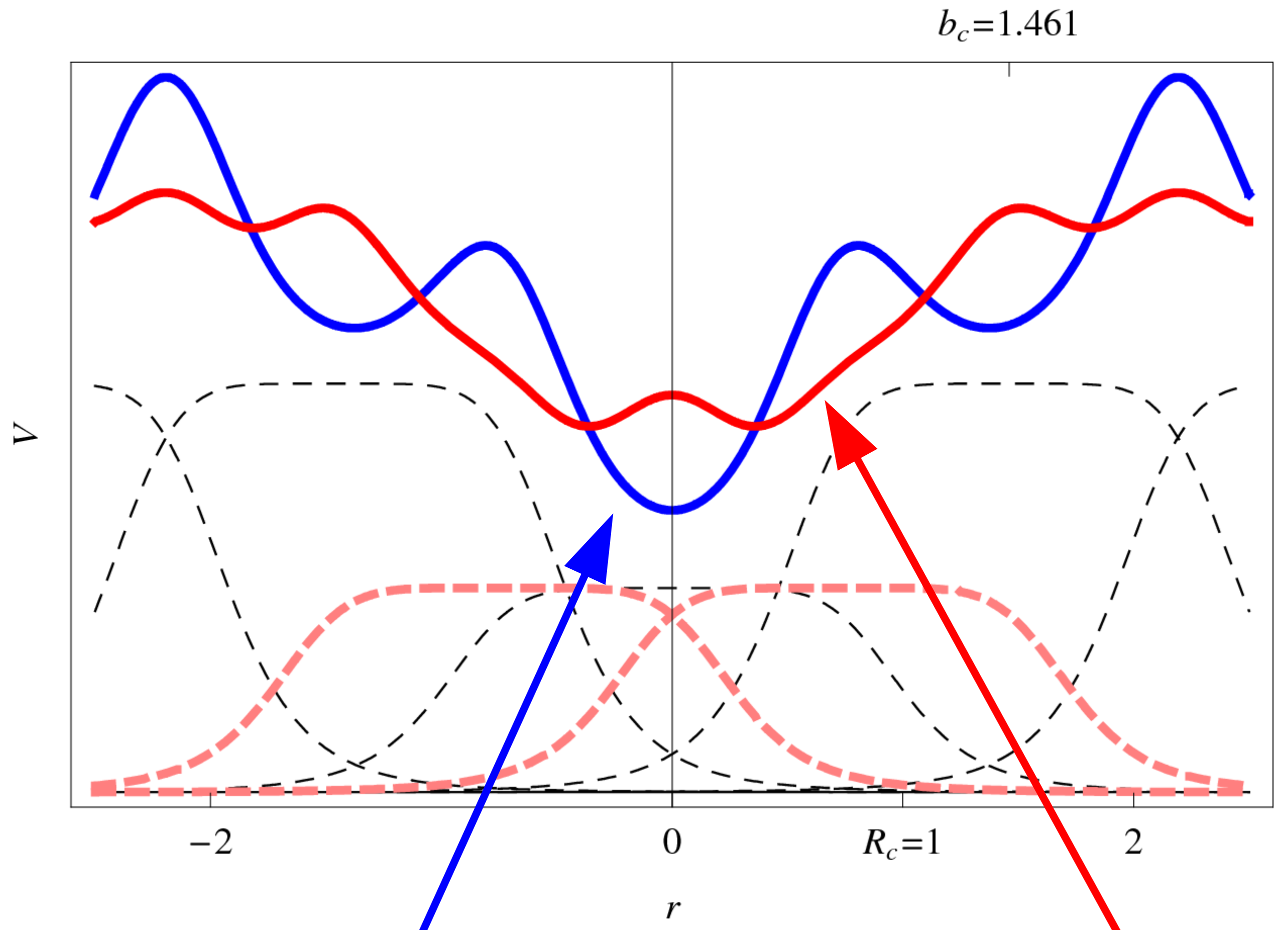
Quantum soft systems: 2D/3D *supersolids* *(crystals of clusters with coherence)*

[Henkel et al. PRL 104 (2010), Saccani et al. PRL 108 (2012), Macrì et al. PRA 87 (2013), Ancilotto et al. PRA 88 (2013), Cinti et al. Nat. Comm. 5 (2014) …]

1D Cluster Luttinger Liquids on a lattice [Mattioli et al., PRL 111 (2013)]

1D Classical cluster liquids [Prestipino et al, PRE 92 (2015)] 1D bulk quantum systems?

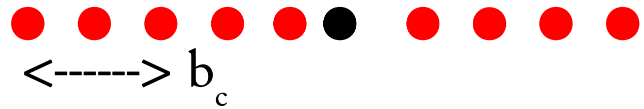
A simple mean-field picture in 1D



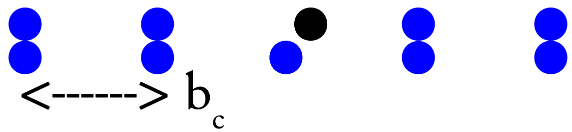
Fix high density $\rho = 2/b_C \approx 1.36$

Let particle ● to be free. What is the potential it experiences if:

1) All other particles are in a lattice of spacing b = b_c/2 ?



2) All other particles are in a lattice of spacing b=b_c (two particles per site) ?



Effective harmonic interaction: Stability

Effective double well: Instability

Kinetic energy (quantum effect at T=0) can induce a transition.

Density fluctuations are a good witness

Dynamical Structure Factor

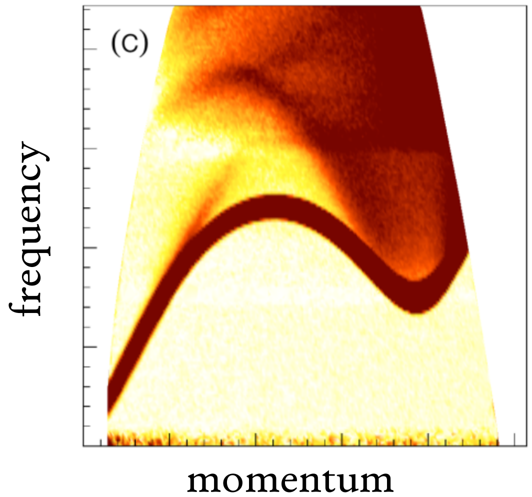
$$S(\vec{q},\omega)=\int_{-\infty}^{\infty}\frac{dt}{2\pi}e^{i\omega t}\langle\hat{\rho}_{\vec{q}}(t)\hat{\rho}_{-\vec{q}}(0)\rangle$$

$$\hat{\rho}_{\vec{q}}(t)=\frac{1}{\sqrt{N}}\sum_{j=1}^{N}e^{-i\vec{q}\vec{r}_j(t)}$$

Linear response to weak density perturbations
Spectral decomposition contains all many-body excited states, *weighted with coupling to density fluctuations*

→ *Spectrum of Density fluctuations*
(Sound or more localized quasi-particles)
One can read the dispersion relation of coherent modes

Beauvois et al.
PRB 94 (2016)



HOW TO MEASURE IT IN EXPERIMENTS?

QUANTUM LIQUIDS (Helium)

- Inelastic neutron scattering. Measure of partial differential cross section

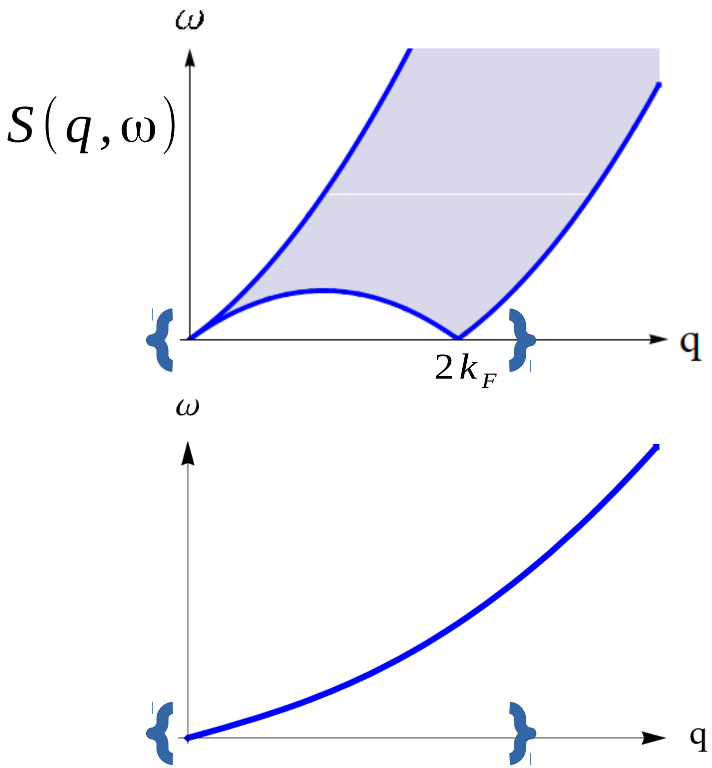
$$\frac{d^2\sigma}{d\Omega\, dE}\propto S(\vec{q},\omega)$$

ULTRACOLD GASES

- Bragg scattering. Photon absorption and stimulated emission into two lasers beams which fix q and ω.

1D: "Bosonization" of fermions (and bosons)

All low-energy modes are collective (Fermi liquid theory is not valid)
→ Luttinger liquids effective hydrodynamic theory [Haldane PRL 47 (1981)]
Small q and ω: phonons both for bosons and *fermions*



Luttinger parameter ~ compressibility
(Galilean invariant case)
K_L determines properties of correlation functions
Universality (independent of details of interaction and statistics!)

$$K_L = \sqrt{\frac{\hbar^2 \pi^2 \rho^3 \kappa_S}{m}} = \frac{v_F}{u} = \frac{\hbar \pi \rho}{m u}$$

Ideal Fermi Gas $K_L=1$

Ideal Fermions: *kinematically forbidden region for particle-hole excitations (flat spectrum)* Still, phonons at small q

$$\hbar \omega_{\pm} = \left| \frac{\hbar^2 q^2}{2m} \pm \frac{\hbar^2 k_F q}{m} \right|$$

In general: power-law decay above threshold (no true delta functions)

Properties of Luttinger liquids

Standard Luttinger liquids have density oscillations around lattice of spacing $1/\rho$

$$g(r) \underset{r\to\infty}{\simeq} 1 - \frac{2K_L}{(2\pi\rho r)^2} + \sum_{l=1} A_l \frac{\cos(2\pi l \rho r)}{r^{2K_L l^2}}$$

Low momenta

Umklapp momenta

→ If $K_L < 1/2$, the static structure factor shows quasi-Bragg peaks:

$$S(q=2\pi\rho) \propto N^{1-2K_L}$$

→ not a crystal (linear scaling) unless K_L=0 (namely, not a Luttinger liquid, but Mott insulator)

Coherence $$\langle \Psi^\dagger(r)\Psi(0)\rangle \underset{r\to\infty}{\simeq} \frac{1}{r^{2K_L}}$$

Algebraic decay (like 2D superfluids at finite T). Slow decay if K_L >> 1/2

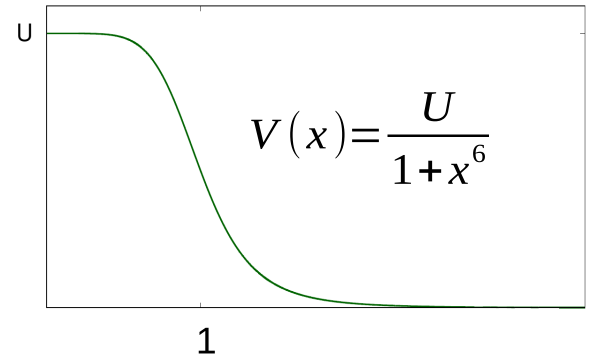
Drag force (dissipated power due to impurity with velocity v) $$F_v \underset{v\to 0}{\propto} v^{2K_L - 1}$$

Our model and methods

N bosons in pure 1D at zero temperature

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

We fully solve Schroedinger equation
in imaginary time



A) Path integral quantum Monte Carlo at T=0

Note: Hamiltonian description, we neglect dissipation
Close analogy to the Extended Bose-Hubbard model
Warning: strong interaction or high density would induce losses or quasi-1D zig-zag transition

B) Statistical analytic continuation of imaginary-time correlations
Warning: ill-posed problem, needs regularization or stochastic approach

$$F(q,\tau) \rightarrow S(q,\omega)$$

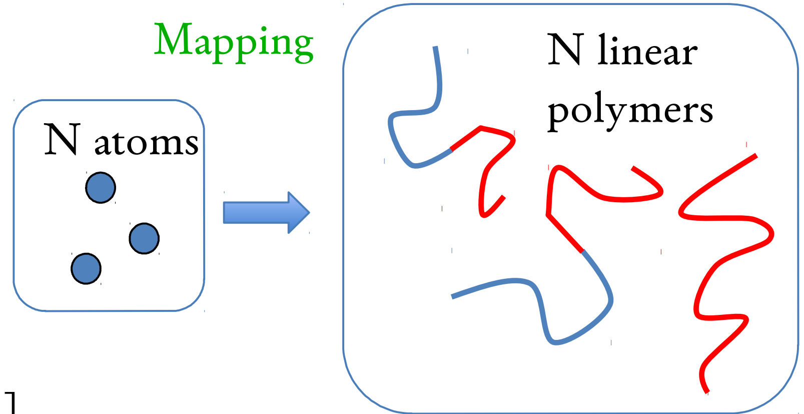
A) Path Integral Ground State method

"Exact" Path Integral Ground State (PIGS) quantum Monte Carlo method
[Sarsa et al., J. Chem. Phys. (2000)]

Imaginary-time projection of initial trial wavefunction

$$\Psi_\tau = e^{-\tau H}\Psi_T$$

For smooth potentials: Pair-Suzuki-Chin propagator
[Rossi et al., J. Chem. Phys. 131, (2009)]



We calculate energy

Pair distribution function $g(r)=\langle \hat{\rho}(r)\hat{\rho}(0)\rangle$

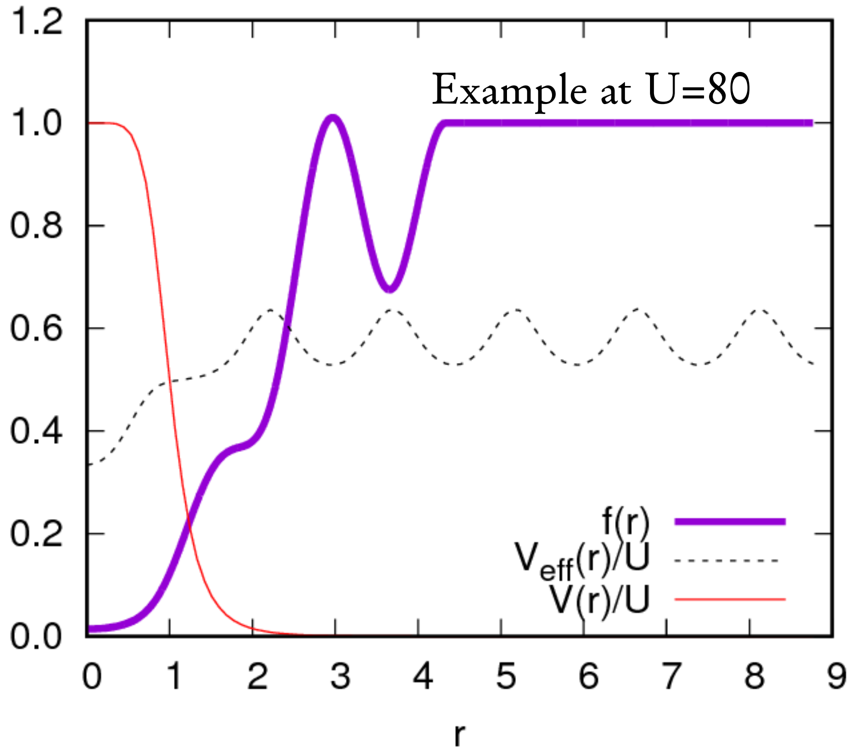
Static structure factor $S(q)=1+\rho\int dr\, e^{-iqr}[g(r)-1]$

Central chain in the paths equilibrates to ground state: exact imaginary-time correlation functions are available

Intermediate scattering function *in imaginary time* $F(\vec{q},\tau)=\langle \hat{\rho}_{\vec{q}}(\tau)\hat{\rho}_{-\vec{q}}(0)\rangle$

A) Details about trial wavefunction

Trial initial wavefunction of 2-body Jastrow type $\Psi_T = \prod_{i<j} f(r_{ij})$



f(r) is solution of 2-body problem with effective interaction

$$V_{eff}(r) = c_1 V(r) + c_2 \sum_l V(r - l\,b)$$

and $f(c_3)=1$

(times a long range phonon contribution à la Reatto-Chester, Phys. Rev. 155 1967)

Parameters are optimized within Variational Monte Carlo with simulated annealing, minimizing energy *plus* the difference of g(r) with preliminary PIGS simulations

$$\lambda = \lambda_E(\beta, \boldsymbol{\xi}) \cdot \lambda_g(\beta, \boldsymbol{\xi}) = \exp\left\{-\beta\left[E(\boldsymbol{\xi}) + \zeta\,\chi(\boldsymbol{\xi})\right]\right\}$$

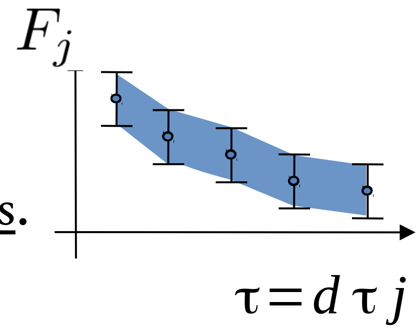
B) Numerical analytic continuation

No single exact solution of numerical inverse Laplace transform:
we use a stochastic method
Genetic Inversion via Falsification of Theories (GIFT)

$$F(\vec{q},\tau)=\langle\hat{\rho}_{\vec{q}}(\tau)\hat{\rho}_{-\vec{q}}(0)\rangle=\int_0^{\infty} d\omega\, e^{-\omega\tau} S(\vec{q},\omega)$$

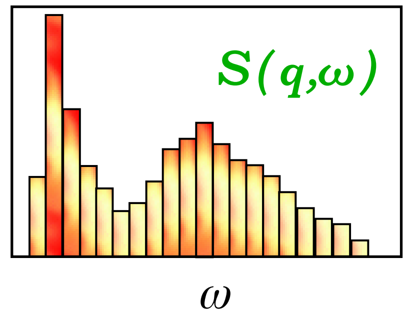
[Vitali et al, PRB 82 (2010), Bertaina et al, PRL 116 (2016),

Bertaina et al, Adv. Phys. X 2 (2017)]



No explicit entropic prior (unlike MaxEnt)
Genetic dynamics: survival of the fittest in a population of spectral functions.

Average over many solutions with X^2 ~ 1 (like Sandvik's ASM)
Initial sampling of imaginary-time data to "explore" error-bars
Sum rules or other exact information can be enforced
Good capability to resolve low energy sharp or broad features



Other stochastic methods:
[Sandvik, PRB 57 (1998), Mishchenko et al. PRB 62 (2000),
Reichman and Rabani JCP 131 (2009),
Fuchs et al., PRE 81 (2010), Goulko et al. PRB 95 (2017)]

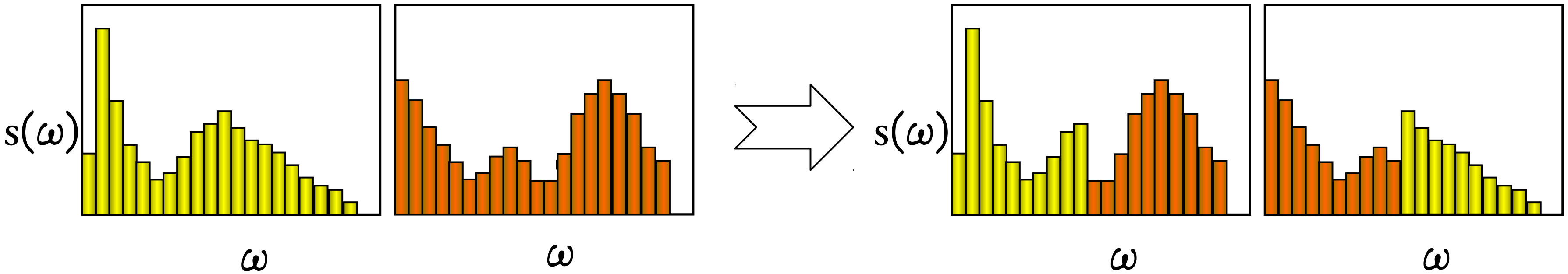
B) Details about GIFT

Initial Population: large random collection of models s(ω) = sum of delta functions

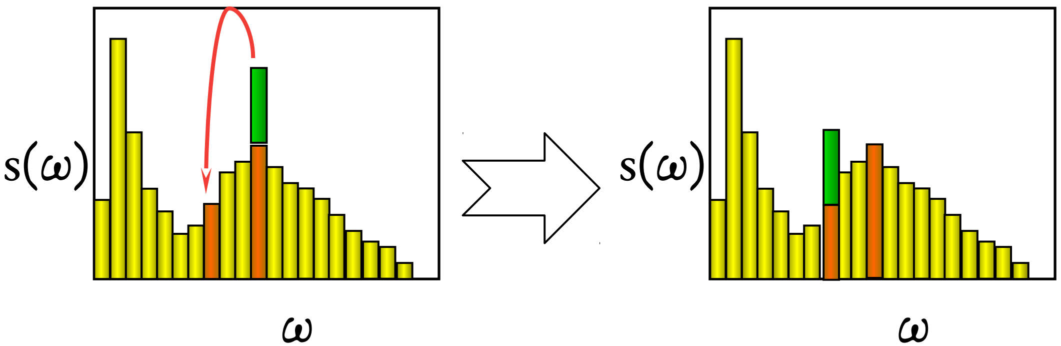
Generation: replace the population (with elitism: the best s(ω) is cloned) with a new one using genetic processes:

Selection: couples of individuals are selected for reproduction depending on their fitness

Crossover: an amount of spectral weight is exchanged between the two selected s(ω), at the same ω



Mutation: shift spectral weight between two intervals

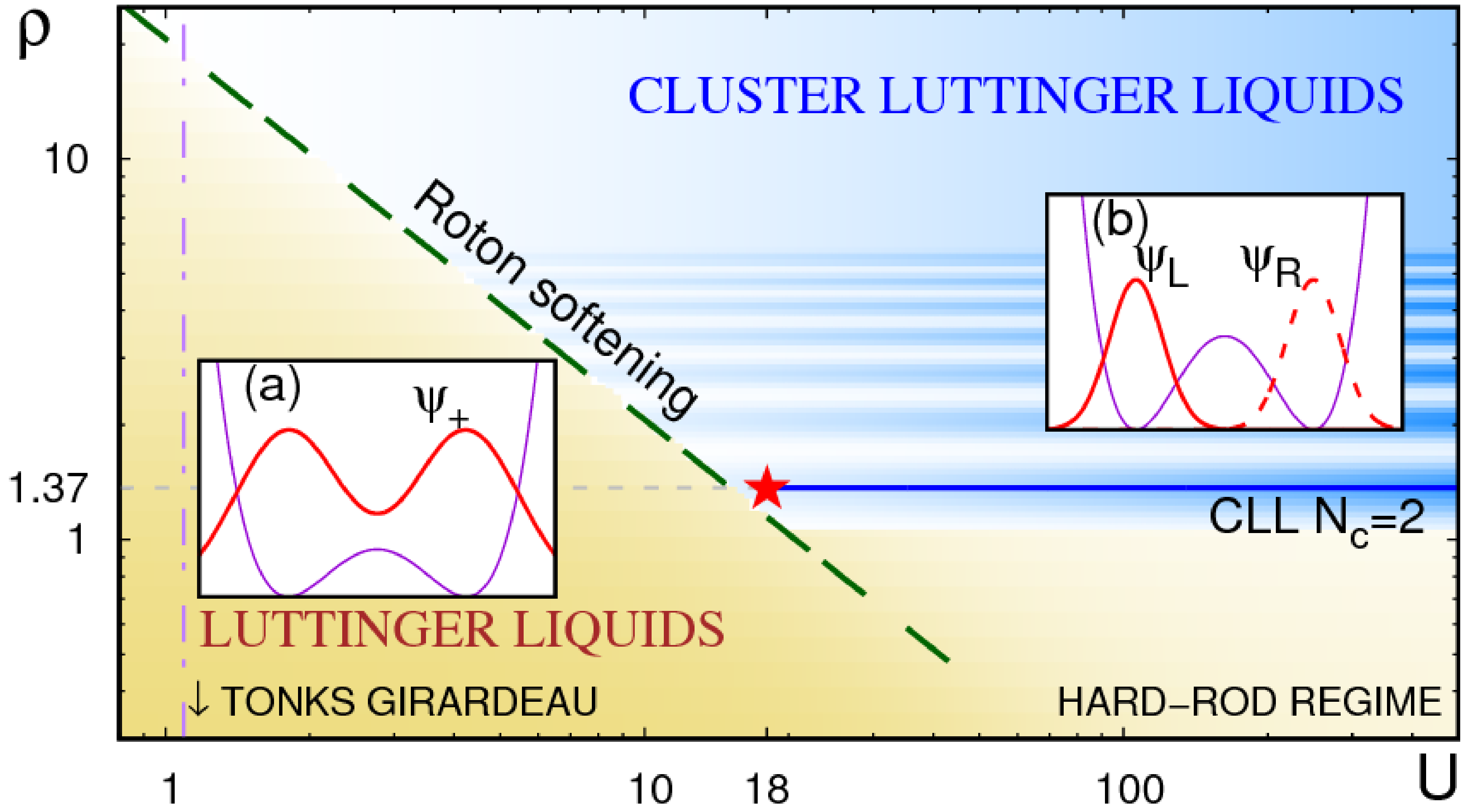


Simulated annealing : moves are accepted with a weight Exp[-X^2/T], with T decreasing (this is only a way to avoid destructive moves, no detailed balance)

Phase Diagram (T=0)

Density

The classical T=0 state would be a cluster crystal



Strength

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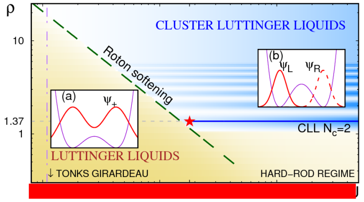
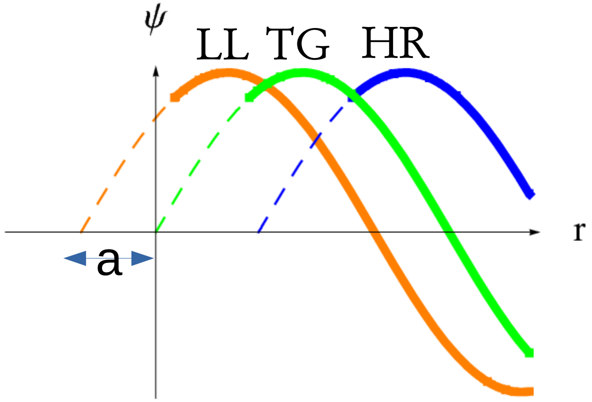


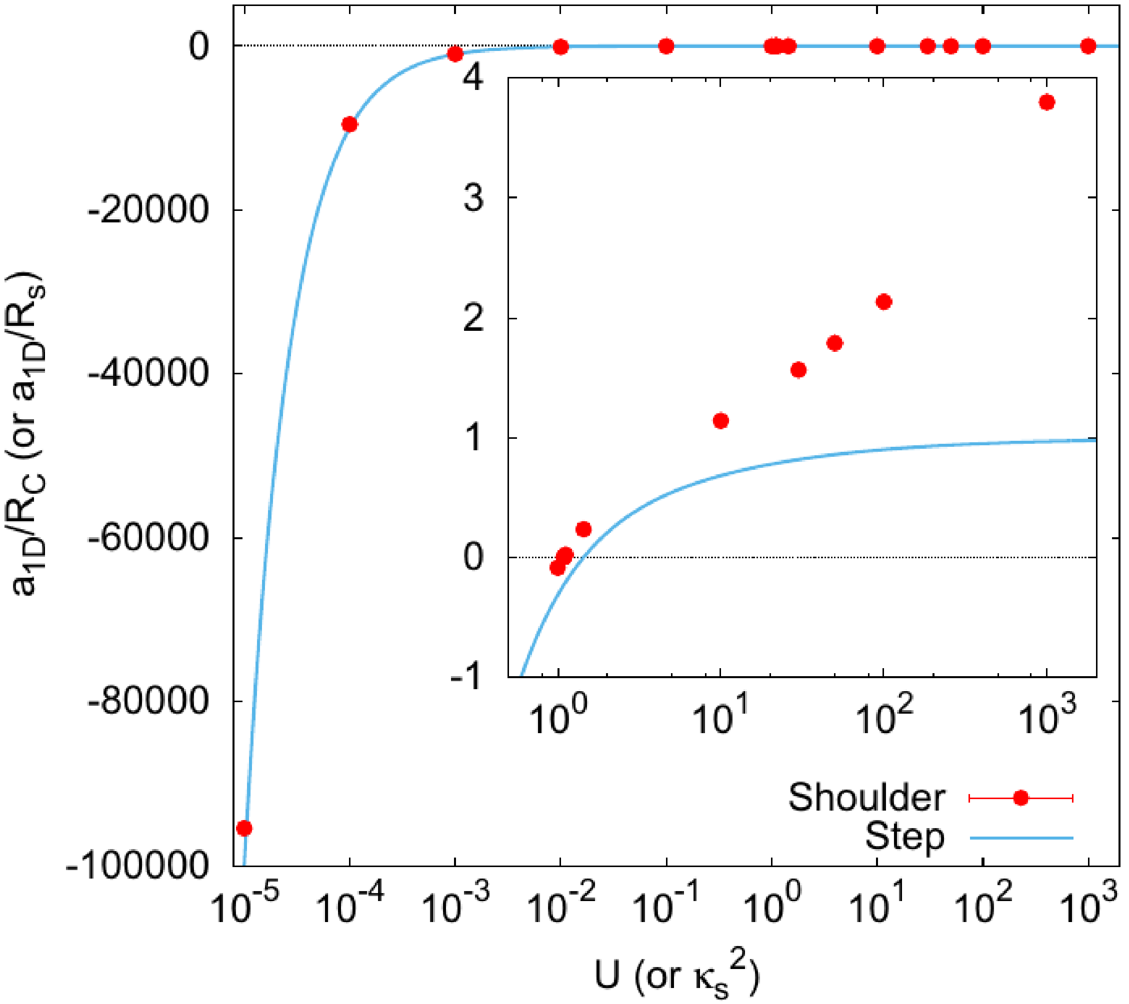
Dilute regime (ρ<0.01)

At low density the scattering length only is relevant

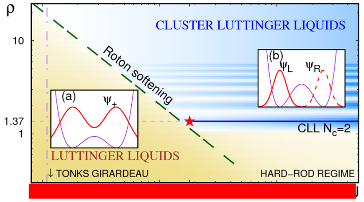


We recover the Lieb Liniger, Tonks Girardeau and Hard-Rod models

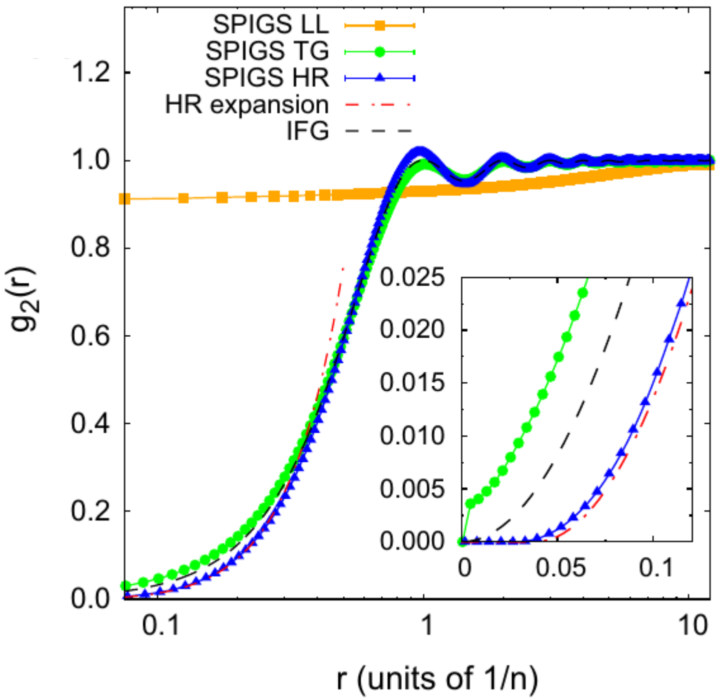
Standard Luttinger liquid theory is valid



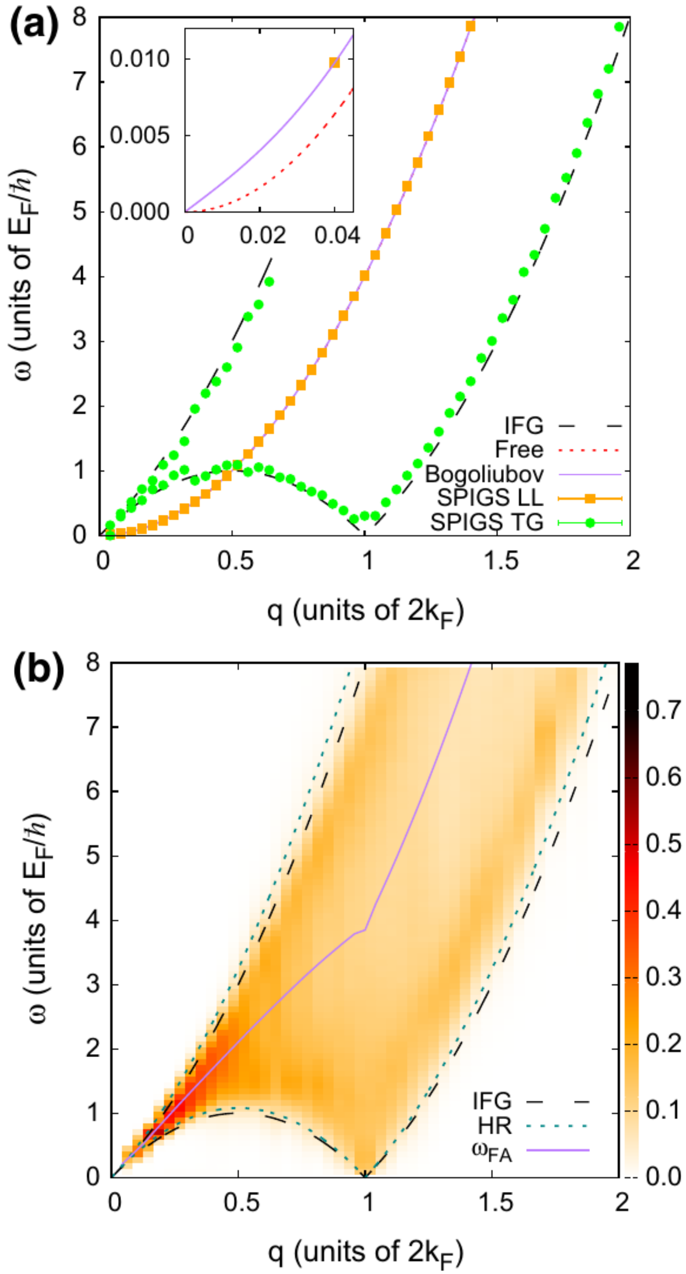
[M. Teruzzi, D.E. Galli, and G. Bertaina, J. Low Temp. Phys. 187, 719 (2017)]



Dilute regime (ρ<0.01)



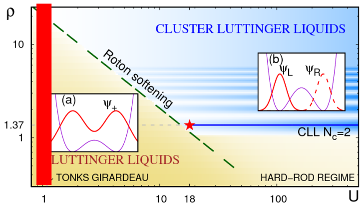
$S(q,\omega)$
in LL and TG regimes



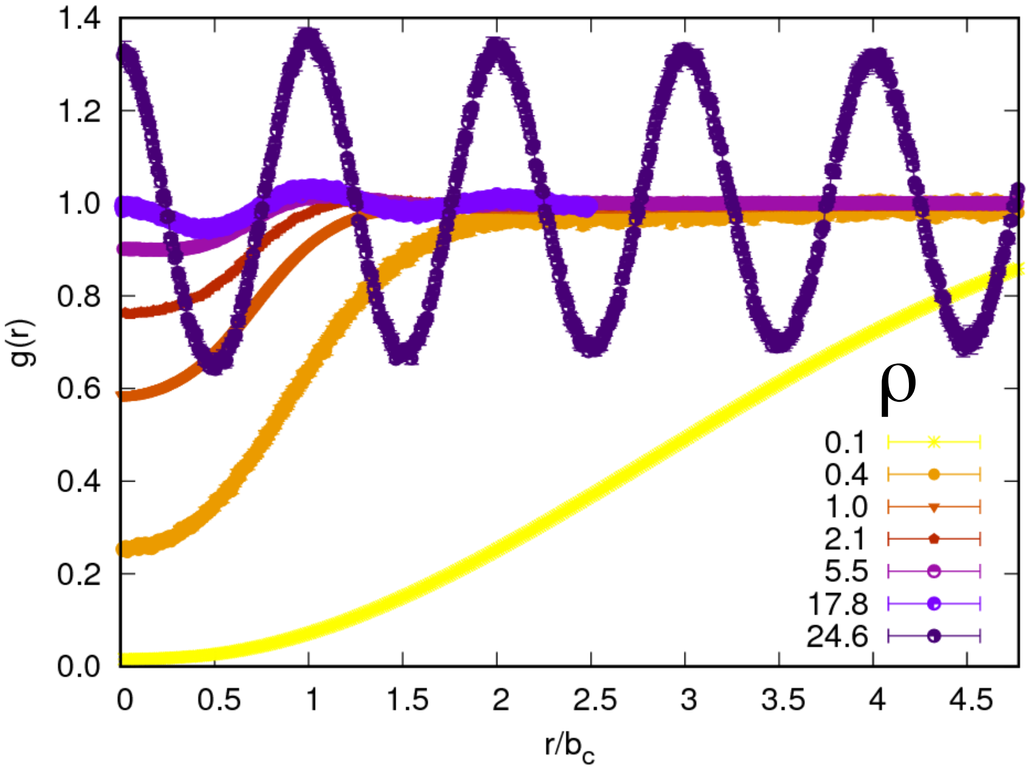
Pair distribution function from weak interaction $U=10^{-5}$, to intermediate U=1.09, to strong $U=10^{3}$

$S(q,\omega)$ in HR regime has renormalized threshold that agrees with [Motta et al., PRA 94 (2016)]

$$2k_F = 2\pi\rho$$
$$E_F = \hbar^2(\pi\rho)^2/2m$$



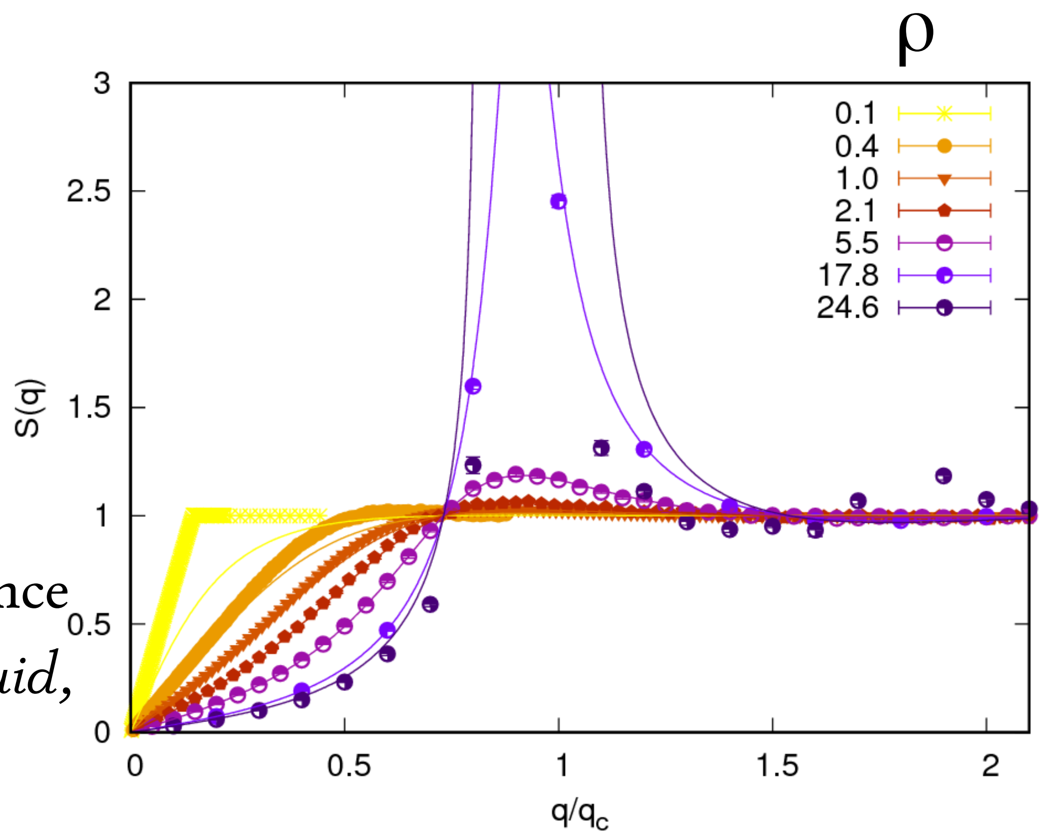
Homogeneous liquid (U~1.09)



← Pair distribution function: at high density maxima in zero and $b_C = 2\pi/q_C \sim 1.46\ R_c$

Independent of density!

(usually: peak at ~ 1/density)



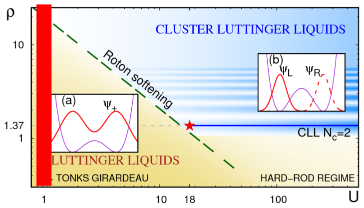
Static structure factor →

Bogoliubov treatment (lines) is good at intermediate densities.

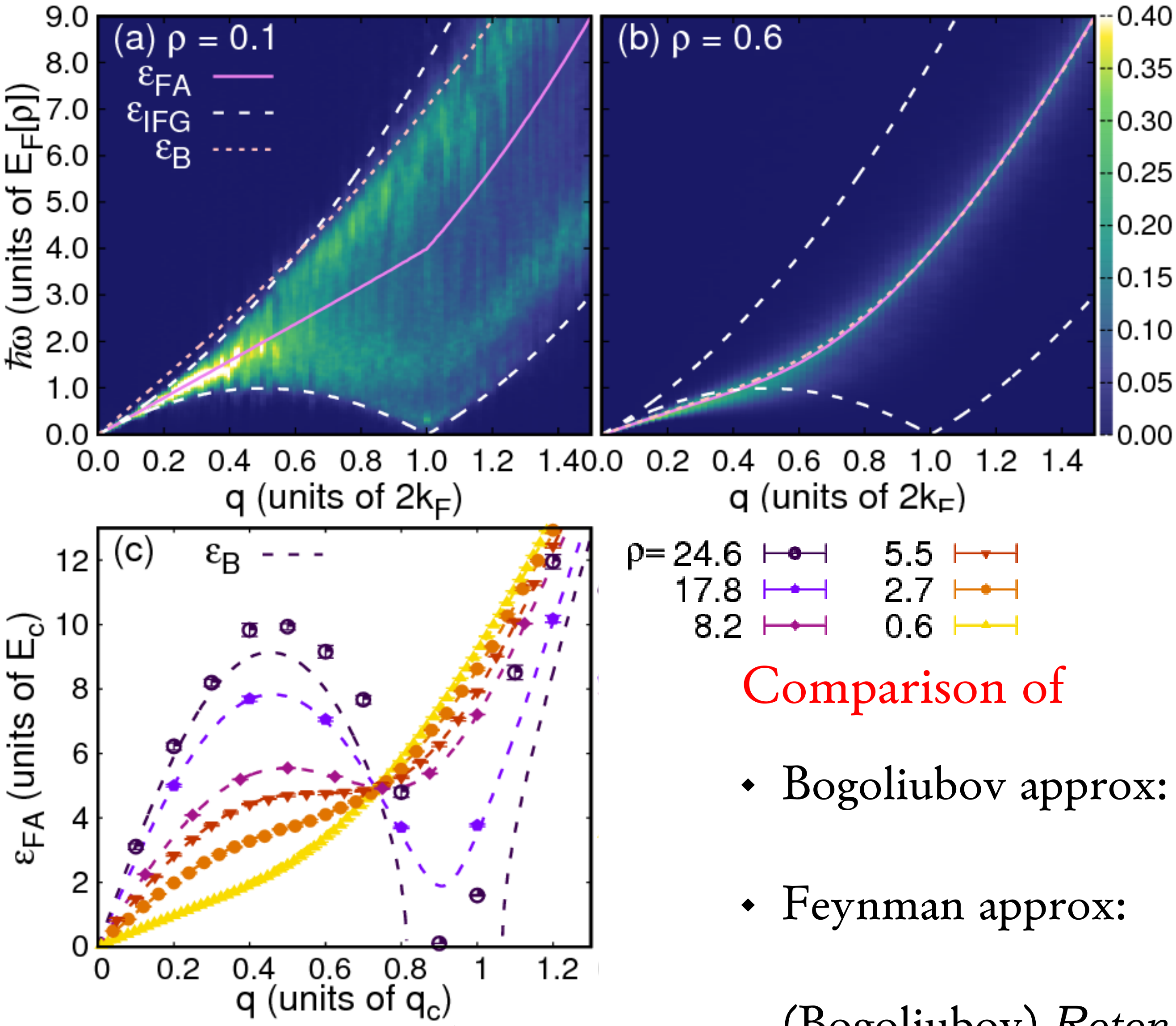
The maximum of S(k) goes to q_C → Divergence

Departure from homogeneous Luttinger liquid, Which has maximum in $2k_F = 2\pi\rho$

Article in preparation



Dynamical Structure Factor (U~1.09)



Roton at ~ q_c

Dilute regime: Almost flat spectrum

System still behaves as Tonks-Girardeau ~ Ideal Fermi Gas

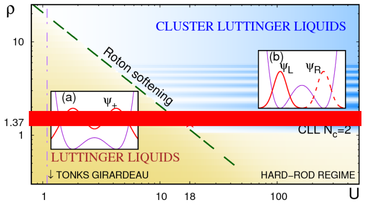
Higher density: spectrum starts to peak

Comparison of

- Bogoliubov approx: $$\varepsilon_B(q)=\sqrt{\frac{q^2}{2}\left(\frac{q^2}{2}+2\rho\tilde{V}(q)\right)}$$
- Feynman approx: $$\varepsilon_{FA}(q)=\frac{q^2}{2S(q)}$$

(Bogoliubov) *Roton softening* at $\rho U=20.6$

- Universal point at q_0 : $\tilde{V}(q_0)=0$

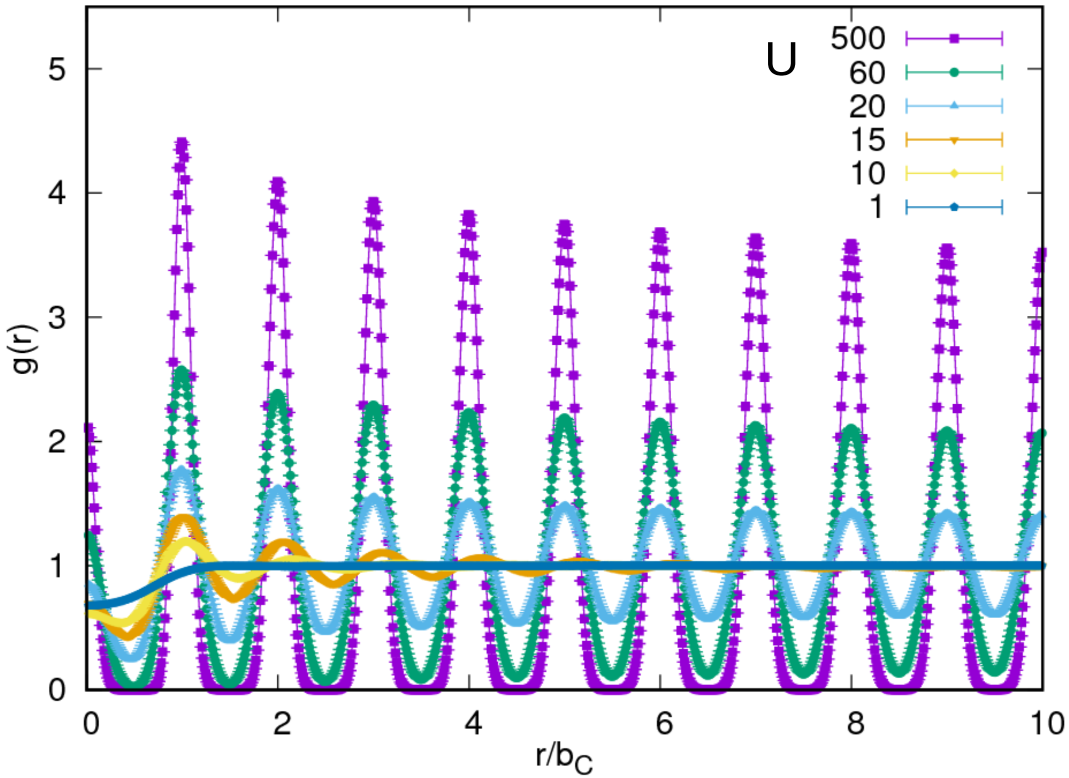


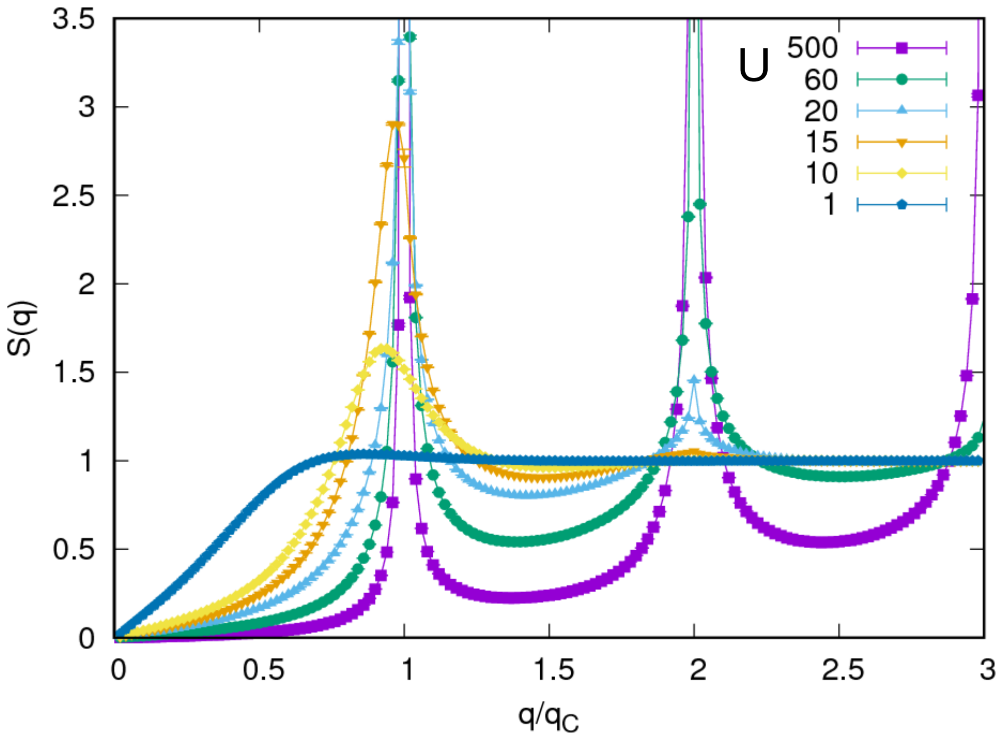
Commensurate cluster phase(s)

Focus on N_C=2 particles per cluster

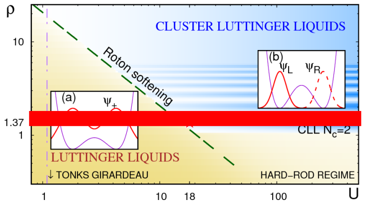
$$\rho = N_c / b_c \approx 1.36$$

Notice that clusters show algebraic long-range order (1D: not a solid)
→ Cluster Luttinger Liquid





Here Bogoliubov theory predicts roton softening at U ~ 15
We observe a divergence of $S(q_c)$ at U~18
(notice that at this density $q_c=k_F$
→ dimerization)



Cluster Luttinger liquids and K_L

Standard Luttinger liquids: density oscillations around auxiliary lattice of spacing $1/\rho$

$$g(r) \simeq 1 - \frac{2K_L}{(2\pi\rho r)^2} + \sum_{l=1} A_l \frac{\cos(2\pi l \rho r)}{r^{2K_L l^2}}$$

Cluster Luttinger liquids [Mattioli et al., PRL 111 (2013)] oscillate around auxiliary lattice depending on Fourier transform of the potential

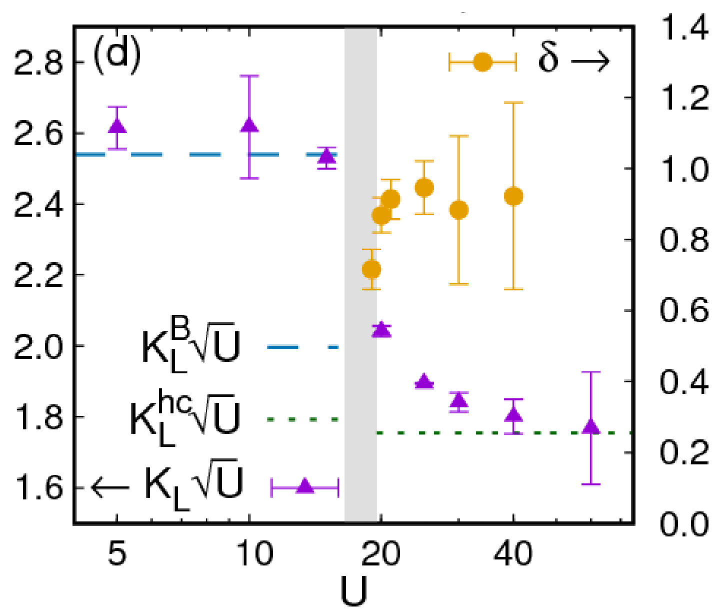
- We focus on commensurate Cluster Luttinger liquids (lattice spacing b_c) and obtain:

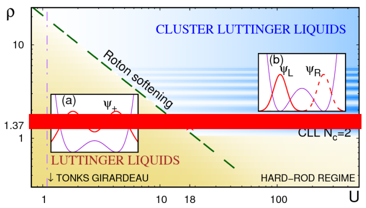
$$g(r) \simeq 1 - \frac{2K_L}{(2\pi\rho r)^2} + \sum_{l=1} A_l \frac{\cos(2\pi l \rho r / N_c)}{r^{2K_L l^2/N_c^2}}$$

- $K_L' = K_L / N_C^2$, while in standard LL: $K_L' = K_L$
- Estimate number of excess particles

$$\delta = \sqrt{K_L / K_L'} - 1$$

- Sudden increase after U~18
- Also K_L changes behavior (but dominant $U^{-1/2}$ trend)





Spectra in cluster regime (N_c=2)

Double harmonic chain spectrum (see also [Nehaus,Likos J. Phys.: Condens. Matter(2011)]) well describes acoustic mode

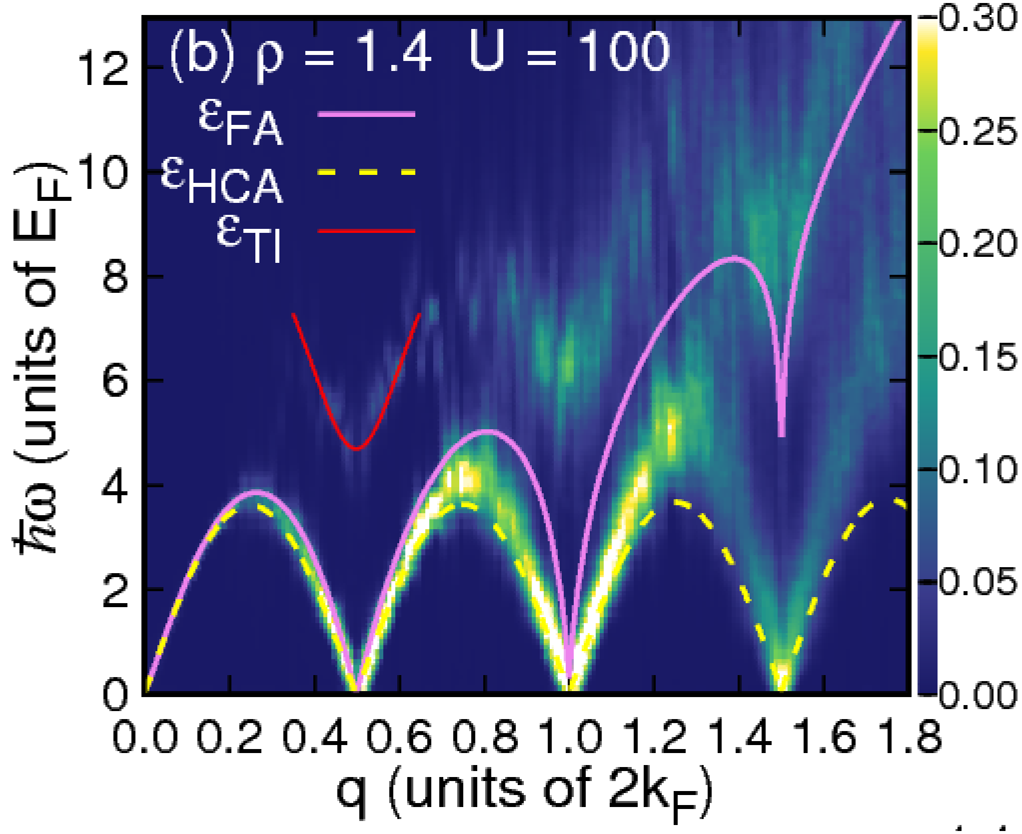
(notice 1D harmonic chain is not a crystal)

$$H_{cl} = \sum_{n\sigma} \frac{p_{n\sigma}^2}{2m} + \frac{\gamma}{2} \sum_{n,\sigma,\mu} (x_{n\sigma} - x_{n+1\mu})^2$$

$$\varepsilon_{HCA}(q) = 2\sqrt{N_c}\,\varepsilon_h \sin(q b_c/2)$$

$$\varepsilon_{HCO}(q) = \sqrt{2 N_c}\,\varepsilon_h \qquad (\textit{dispersionless})$$

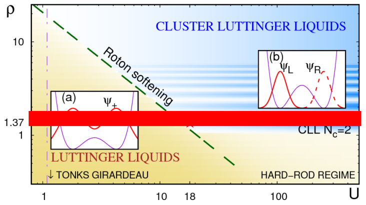
$$\varepsilon_h(b) = \sqrt{-(4\pi^2/b^3)\sum_j^\infty j^2 \tilde{V}(2\pi j/b)}$$



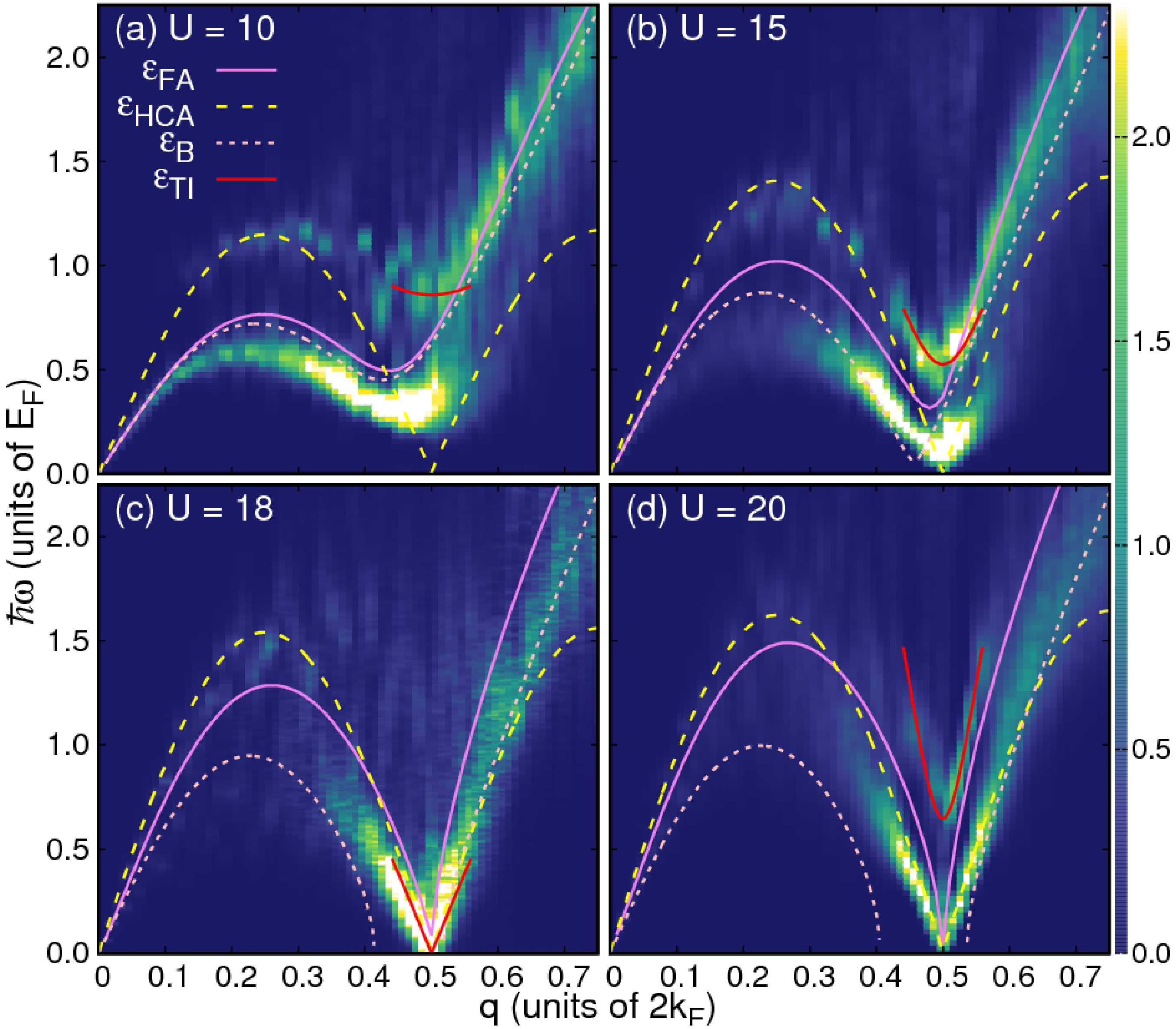
Higher frequencies:
multiphonons or *optical mode*
with anharmonic contributions [see also Saccani et al PRL 2012]

We have a liquid phase at small U, but also a liquid (cluster) phase at large U
Interesting behavior of the two modes at the transition...

Article in preparation



Spectra in transition region ($N_c=2$)



1) Secondary mode present also in liquid regime! Seems to avoid crossing Bogoliubov mode.

2) Gap of secondary mode at q_c goes to zero at transition U~18, but is finite in both phases.

3) At the transition the secondary mode and the Luttinger-HC mode are linear at q_c with the same velocity (within uncertainty)

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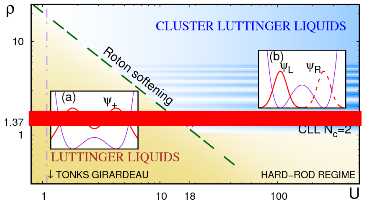
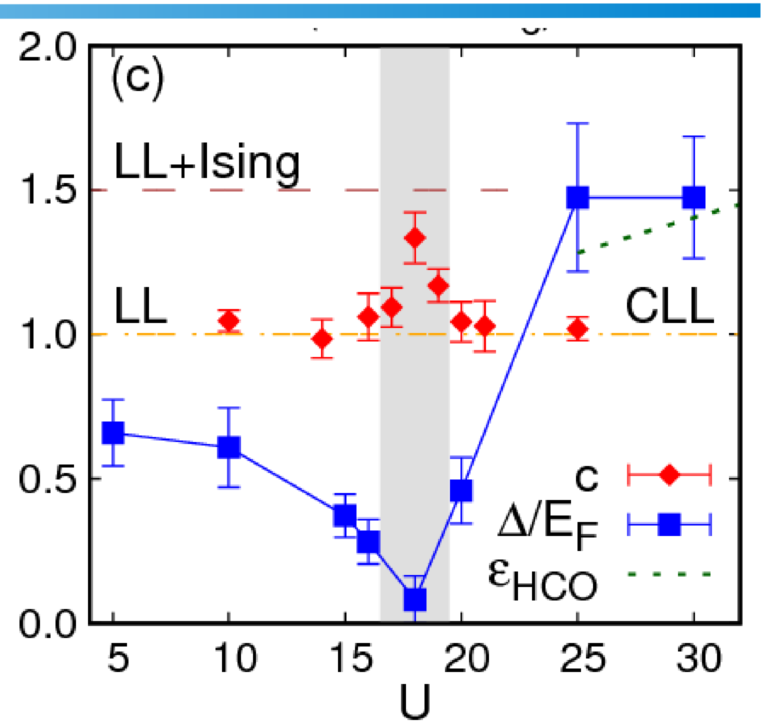


Evidence of quantum criticality

We extract the gap of the secondary excitation at q_c
(uncertainty comes from slow convergence
close to transition and from analytic continuation)



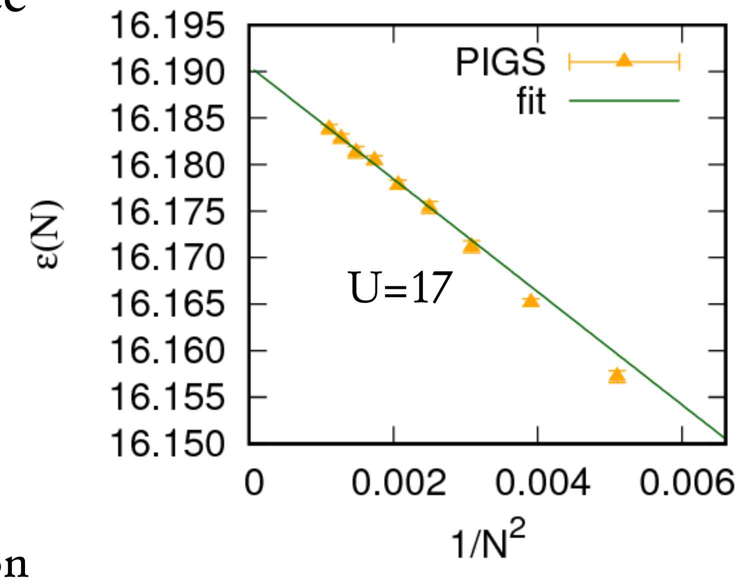
- Gap is linear close to transition

- Two gapless modes with same velocity at U~18
 Conformal Field Theory can tell us something

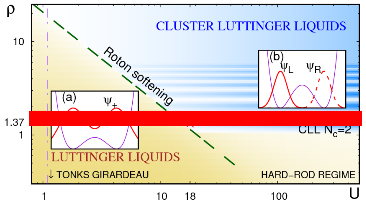
- Dalmonte et al, PRB 92 (2015) Transition on a lattice
 Central charge $c \sim 3/2 = 1 + 1/2$
 (Free boson class + free fermion class)
 From entanglement entropy
- We extract it from size effects in energy

$$\varepsilon(N) = \varepsilon_\infty - cE_F/(6\,K_L\,N^2)$$

 (most difficult point U=18: presence of small energy
 excitation)



Article in preparation



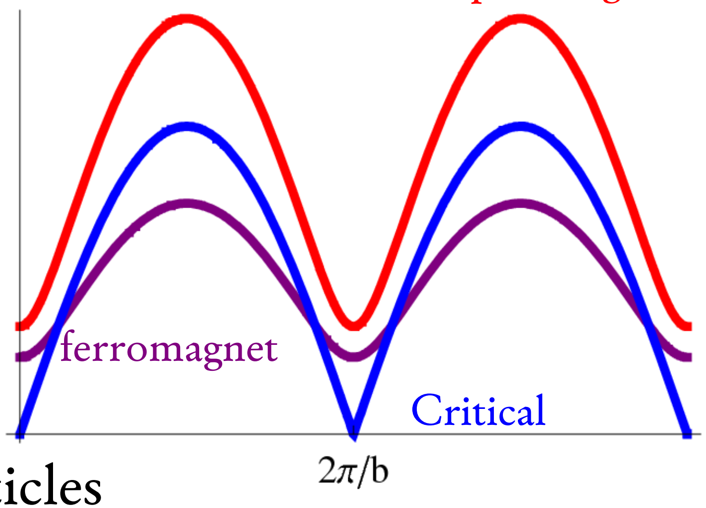
Quantum Ising model (N_c=2)

Emergent transverse Ising model describing the secondary excitation
(dual to 2D classical Ising, by mapping imaginary time to space dimension)

$$H_{TI} = -J\sum_i \sigma_i^z \sigma_{i+1}^z - h\sum_i \sigma_i^x$$

Alignment ↔ Quantum Delocalization

Let us call the eigenstates of σ^z : |L> and |R> (*hint: cluster left, cluster right*)
If h = 0: classical ferromagnet (T=0): all |L> or all |R>
Transverse field gives lowest energy to symmetrized state |+>=(|L> + |R>)/$\sqrt{2}$
→ delocalization: tunneling in a double well

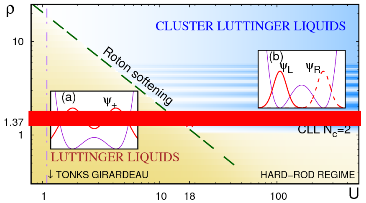


Exact spectrum is known, via a Jordan-Wigner transformation and Bogoliubov diagonalization

Δ=|J-h| $\qquad \varepsilon_{TI}(q) = \sqrt{\Delta^2 + 4Jh(\sin qa/2)^2}$

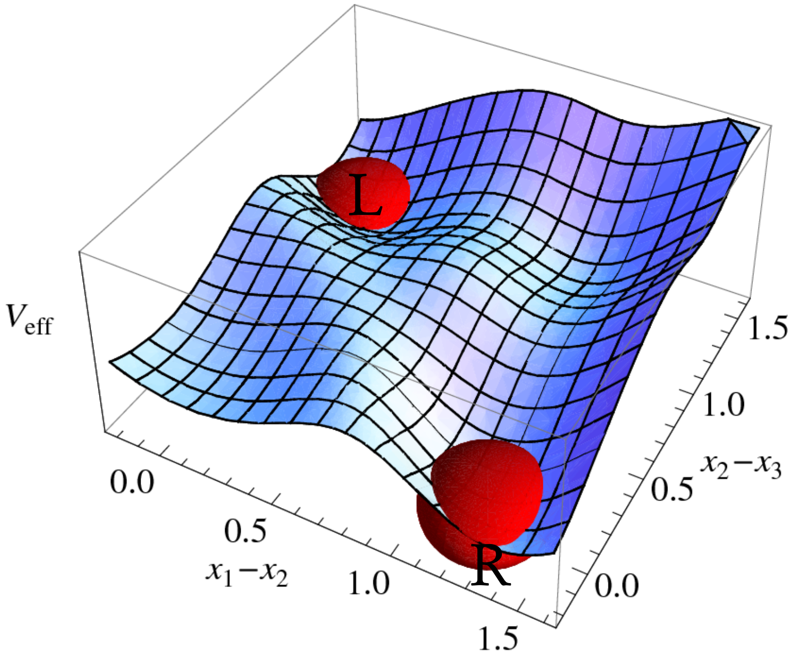
- Lattice spacing is b_c in our spectra: spins ↔ pairs of particles
- Difficult to microscopically determine

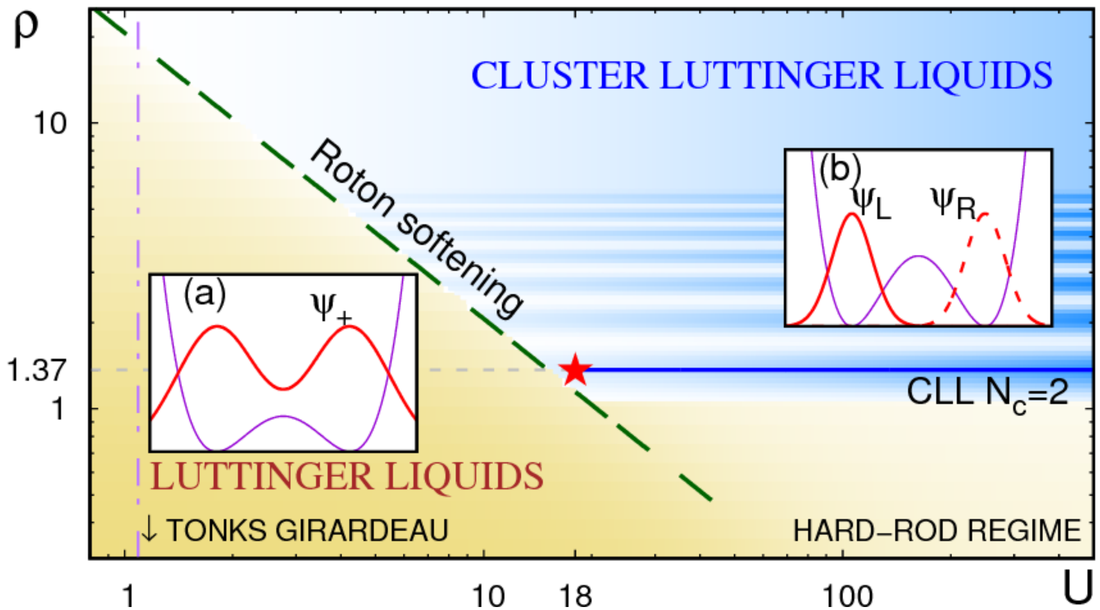
J~$\sqrt{U}$ optical modes, h~$\sqrt{U}\, e^{-\alpha\sqrt{(U)}}$ double-well tunneling (role of anharmonicity)

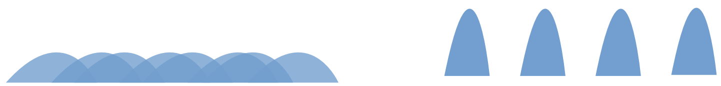


Quantum Ising model (N_c=2)

Effective double well potential in space of 3 particle distances, keeping center-of-mass and all other particles fixed







QUANTUM
PHASE TRANSITION

Liquid ... Cluster liquid

Paramagnet ... Ferromagnet

+ + + + ... ↓ ↓ ↓ ↓

Note: both are Luttinger liquids; close to transition Ising adds up

A non local order parameter is probably needed (no lattice is present)

Concluding Messages

- PIGS+GIFT methods useful to infer novel spectra, and theoretical interpretation with known models is complementary
- Clustering in a simple system of soft bosons, from rotons to harmonic chain spectrum
- Evidence of quantum critical behavior: peaks in $S(q_c)$; change in behavior of K_L; sudden increase of discrepancy δ ; secondary mode becoming gapless; central charge increasing
- Interpretation in terms of quantum Ising transition. Relevance for recent studies on $c = 3/2$ CFT

Interesting questions

- Higher N_C: what transitions?
- Consider non-commensurate density in the cluster phases
- Inhomogeneous systems to study boundary effects
- Microscopic study of Ising sector and definition of appropriate correlators
- Further investigation of what happens to optical modes across superfluid/supersolid transition in higher dimensions
- Use of quantum information measures to study the transition