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Workshop on Synergies between Field Theory and Exact Computational Methods in Strongly Correlated Quantum Matter

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Critical scaling in a trap

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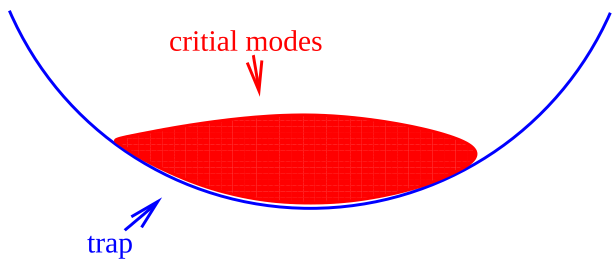
Physical systems are generally inhomogeneneous, homogeneous systems are often an ideal limit of experimental conditions.

General issue: How quantum and thermal critical behaviors develop in the presence of external space-dependent fields

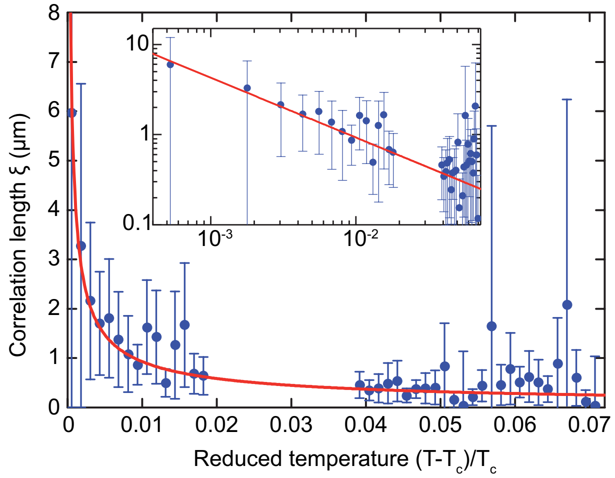
Ex.: interacting particles trapped within a limited region of space by an external potential, such as in experiments of



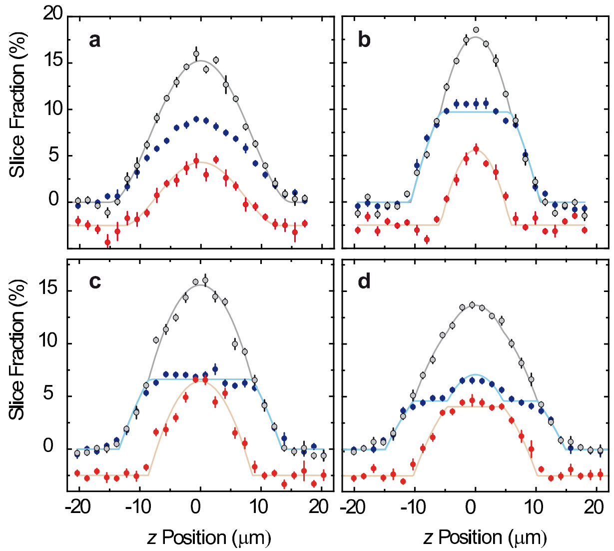
Bose-Einstein condensation in diluted atomic vapors and of cold atoms in optical lattices → interplay between quantum and statistical behaviors

Trap-size scaling provides a framework to describe the thermal and quantum critical behaviors of particle systems confined by an external field (M.Campostrini, EV, PRL 102,240601,2009; PRA 81,023606,2010)

Finite-T transition related to the **Bose-Einstein condensation in interacting gases**, experiments show an increasing correlation length compatible with a continuous transition (Donner, etal, Science 2007). Moreover, experimental evidences of the Kosterlitz-Thouless transition in 2D (e.g., Hung etal, Nature 2010)



Quantum Mott insulator to superfluid transitions and different Mott phases (where the density is independent of μ) have been observed in many experiments with ultracold atomic gases loaded in optical lattices (arrays of microscopic potentials induced by ac Stark effects of interfering laser beams)



A common feature is a **confining potential**, which can be varied to achieve different spatial geometries, allowing also to effectively reduce the spatial dims

A classical example:

The lattice gas model in a confining field $V(r) = (|\vec{r}|/l)^p$,

$$\mathcal{H}_{\rm Lgas} = -4J \sum_{\langle ij \rangle} \rho_i \rho_j - \mu \sum_i \rho_i + \sum_i 2V(r_i)\rho_i,$$

where $\rho_i = 0, 1$ whether the site is empty or occupied.

Far from the origin $\langle \rho_x \rangle \to 0$ (as $\langle \rho_x \rangle \sim e^{-2V(x)}$), thus particles are trapped.

It can be exactly mapped to a standard Ising model:

$$\mathcal{H} = -J \sum_{\langle ij \rangle} s_i s_j + h \sum_i s_i - \sum_i V(r_i) s_i, \qquad s_i = 1 - 2\rho_i, \qquad h = 2qJ + \mu/2$$

In the absence of the trap, liquid-gas transition and Ising critical behavior with a diverging length scale, at $T = T_c$ and $\mu = \mu_c = -4qJ$ ($h = h_c = 0$).

No diverging length scale in the presence of the confining potential

How is the critical behavior distorted by the trap, and recovered in the limit $l \to \infty$?

A quantum example:

Atomic gases loaded in optical lattices are generally described by the Bose-Hubbard (BH) model with a confining potential

$$H_{\rm BH} = -\frac{J}{2}\sum_{\langle ij\rangle}(b_i^\dagger b_j + b_j^\dagger b_i) + \sum_i [(\mu + V(r_i))n_i + U n_i(n_i - 1)],$$

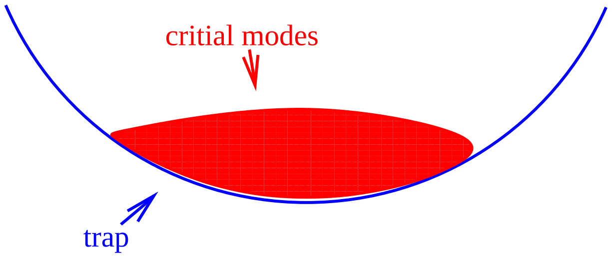
where $n_i = b_i^\dagger b_i$, $V(r) = v^p r^p$, and the trap length scale $l \equiv J^{1/p}/v$

The trapping potential strongly affects the critical behavior at the Mott transitions and within the superfluid phases: correlation functions are not expected to develop a diverging length scale.

A theoretical description of the critical correlations in trapped systems is important for experimental investigations.

In a trap, correlations do not develop a diverging length scale.

The critical behavior of the homogeneous system is observed around the middle of the trap only when $\xi \ll l_{\rm trap}$



If $\xi \gtrsim l_{\rm trap}$, it gets distorted by the trap, although it may still show universal effects controlled by the universality class of the transition of the unconfined system.

These universal effects are described by the trap-size scaling theory, resembling the finite-size scaling theory in critical phenomena, but characterized by a further nontrivial *trap critical exponent* θ, which describes how the critical length scale ξ depends on the trap size at criticality, i.e., $\xi \sim l_{\rm trap}^{\theta}$ (the above naive relations in magenta thus become respectively $\xi \ll l_{\rm trap}^{\theta}$ and $\xi \gtrsim l_{\rm trap}^{\theta}$)

Plan of the rest of the talk:

- Trap-size scaling at *thermal* transitions
  - Lattice gas models, static and dynamics
  - Finite-T transitions at the formation of BEC in interacting gases
- TSS at $T = 0$ quantum transitions in D-dim quantum systems (described by $(D + z)$-dim QFT's)
  - The XY chain in the presence of a space-dependent transverse field, as a laboratory model
  - The Bose-Hubbard (BH) model, describing cold bosonic atoms in optical lattices, at equilibrium and off-equilibrium

Critical behavior of homogeneous systems, scaling law

$$\mathcal{F}_{\rm sing}(u_1, u_2, \dots, u_k, \dots) = b^{-d} \mathcal{F}_{\rm sing}(b^{y_1} u_1, b^{y_2} u_2, \dots, b^{y_k} u_k, \dots)$$

u_k are nonlinear scaling fields (analytic functions of the model parameters)

In a standard continuous transition: **two relevant scaling fields** $u_t \sim t = T/T_c - 1$ (with $y_t = 1/\nu$) and $u_h \sim h$ (external field, with $y_h = (d - 2 + \eta)/2$), and irrelevant u_i ($i \geq 3$) with $y_i < 0$.

When $u_t, t \to 0$ and $u_h, h \to 0$

$$\mathcal{F}_{\rm sing} \approx \xi^{-d} \left[f(h\xi^{y_h}) + \xi^{-\omega} f_\omega(h\xi^{y_h}) + ... \right], \qquad \xi \sim t^{-\nu}$$

$O(\xi^{-\omega})$ arises from the leading irrelevant u_3, and $\omega = -y_3$.

Finite-size scaling in a finite system

$$\mathcal{F}_{\rm sing}(u_1, u_2, \dots, L) = b^{-d} \mathcal{F}_{\rm sing}(b^{y_1} u_1, b^{y_2} u_2, \dots, L/b)$$

thus $\mathcal{F}_{\rm sing}(u_t, u_h) = L^{-d} \mathcal{F}_{\rm sing}(L^{y_t} u_t, L^{y_h} u_h)$

Trap-size scaling (TSS) in the presence of the confining potential

$$V(r) = v^p |\vec{r}|^p, \qquad l \equiv 1/v \quad \text{is the trap size}$$

Ex.: $\mathcal{H}_{\rm Lgas} = -4J \sum_{\langle ij \rangle} \rho_i \rho_j - \mu \sum_i \rho_i + \sum_i 2V(r_i) \rho_i$ with $\rho_i = 0, 1$

TSS Ansatz to allow for the confining potential:

$$\mathcal{F}(u_t, u_h, u_v, x) = b^{-d} \mathcal{F}(u_t b^{y_t}, u_h b^{y_h}, u_v b^{y_v}, x/b)$$

where $y_t = 1/\nu$, $y_h = (d + 2 - \eta)/2$, while y_v must be determined.

Then, fixing $u_v b^{y_v} = 1$, and defining the trap exponent $\theta \equiv 1/y_v$,

$$\text{TSS}: \qquad \mathcal{F} = l^{-\theta d} \mathcal{F}(u_t l^{\theta y_t}, u_h l^{\theta y_h}, x l^{-\theta})$$

resembling FSS: $\mathcal{F}_{\rm sing}(u_t, u_h) = L^{-d} \mathcal{F}_{\rm sing}(u_t L^{y_t}, u_h L^{y_h})$, with $L \to l^\theta$

Critical dynamics by adding the time dependence through the scaling variable $t l^{-z\theta}$ (Costagliola, EV, arXiv:1107.0815)

Finite-size effects by adding $L l^{-\theta}$ (de Queiroz, etal, PRE 81,051122,2010)

The correlation length ξ around the middle of the trap, or any generic length scale associated with the critical modes, behaves as

$$\xi = l^{\theta} \mathcal{X}(tl^{\theta/\nu}), \qquad \mathcal{X}(y) \sim y^{-\nu} \;\; \text{for} \;\; y \to 0$$

The trap induces a critical length scale $\xi \sim l^{\theta}$ at $t = 0$.

A generic quantity S is expected to asymptotically behave as

$$S = l^{-\theta y_s} f_s(tl^{\theta/\nu}, xl^{-\theta}) = l^{-\theta y_s} \bar{f}_s(\xi l^{-\theta}, xl^{-\theta})$$

The hard-wall limit, $p \to \infty$ of $V(r) = (|\vec{r}|/l)^p$, $\longrightarrow$ homogeneous system of size $L = 2l$ with open boundary conditions.

Standard finite size scaling for $p \to \infty$, thus $\lim_{p\to\infty} \theta = 1$ (in FSS the RG dimension of the size L is $y_L = -1$, since $\xi \sim L$ at T_c)

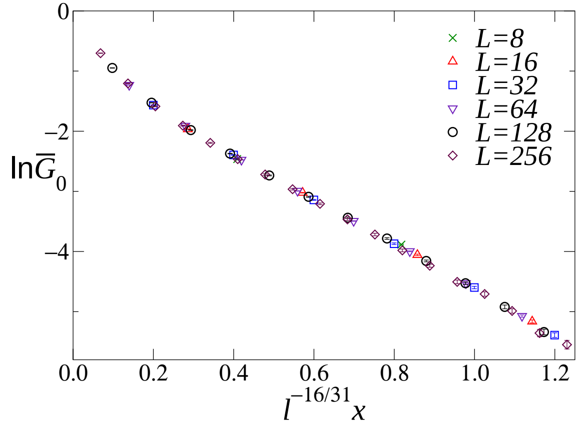
The trap exponent θ can be computed by analyzing the RG properties of the corresponding perturbation at the critical point.

In the lattice gas model, $\mathcal{H}_{\rm Lgas} = -4J\sum_{\langle ij\rangle} \rho_i\rho_j - \mu\sum_i \rho_i + \sum_i 2V(r_i)\rho_i$, the trapping potential is coupled to the order parameter, thus $P_V = \int d^dx\, V(x)\phi(x)$ to $H_{\phi^4} = \int d^dx \left[(\partial_\mu\phi)^2 + r\phi^2 + u\phi^4\right]$.

Using scaling relations ($y_V = p/\theta - p = d - y_\phi$, $y_\phi = (d-2+\eta)/2$) $\rightarrow$
$\theta = 2p/(d+2-\eta+2p)$, $p=2$: $\theta = 16/31,\ 0.4462,\ 2/5$ in 2,3 and 4D.

$$G_0(x) \equiv \langle\rho_0\rho_x\rangle - \langle\rho_0\rangle\langle\rho_x\rangle = l^{-2\theta y_\phi} f_g(tl^{\theta/\nu}, xl^{-\theta})$$

Results of MC simulations: $\overline{G}_0(x) \equiv l^{4/31}G_0(x)$ vs $xl^{-16/31}$ at T_c



Relaxational dynamics: time scale diverging as $\tau \sim l^{\theta z}$ where z is the dynamic exponent; confirmed by MC simulations with $z = 2.170(6)$.

Finite-T transitions in interacting Bose gases and BEC

The condensate wave function $\Psi(x)$ provides the $U(1)$ symm complex order parameter of the transition, thus expected to belong to

the XY universality class: $H_{XY} = \int d^d x \, (|\partial_\mu \Psi|^2 + r|\Psi|^2 + u|\Psi|^4)$

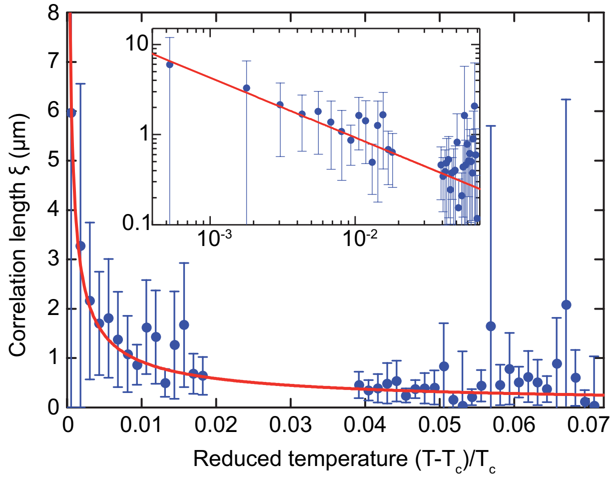
$\nu = 0.6717(1)$, $\eta = 0.0387(1)$ in 3D, shared with the superfluid transition in ^{4}He, superconductor transitions, transition in easy-plane magnets, etc...

No real BEC in 2D, but a finite-T Kosterlitz-Thouless transition with an exponential behavior of ξ, formally $\nu \to \infty$, to a quasi-long range order phase with one-body correlation functions decaying algebraically

In a harmonic trap, the confining potential $V(x) = v^2 x^2 \equiv (x/l)^2$ is coupled to the particle density, giving rise to $P_V = \int d^3x \, v^2 |x|^2 |\Psi(x)|^2$.

By scaling arguments: $\theta = 1/y_v = 2\nu/(1+2\nu)$, thus
$\theta = 0.57327(4)$ in 3D ($\nu = 0.6717(1)$) and $\theta = 1$ in 2D ($\nu = \infty$), for comparison, $\theta = 1/2$ for a Gaussian theory ($\nu = 1/2$)

Experimental results for a trapped Bose gas at BEC (Donner, etal, Science 2007) showed an increasing correlation length, leading to the estimate $\nu = 0.67(13)$ by fitting to $\xi \sim t^{-\nu}$ (to be compared with $\nu_{XY} = 0.6717(1)$).



Trap effects are negligible when $\xi \ll c l^{\theta}$, but relevant when $\xi \approx l^{\theta}$.

However, exp results are not sufficiently precise to show trap effects, (analogously to the experimental evidences of the KT transition in 2D)

Experiments may probe TSS, by varying the trapping potential and matching the trap-size dependence of the TSS Ansatz, analogously to experiments probing FSS behavior in ^{4}He at the superfluid transition.

One may exploit TSS, using it to infer the critical exponents from the data, analogously to FSS techniques to determine the critical parameters.

Quantum $T = 0$ transitions driven by quantum fluctuations: **quantum critical behavior** with a peculiar interplay between quantum and thermal fluctuations at low T.

Nonanaliticity of the ground-state energy, where the gap Δ vanishes

Continuous QPT $\longrightarrow$ diverging length scale ξ, and scaling properties.

Ex: **the Ising chain in a transverse field** $H_{\rm Is} = -J\sum_i \sigma^x_i \sigma^x_{i+1} - \mu\sigma^z_i$

$\mu \to \infty \longrightarrow$ ground state=$\prod_i |\uparrow_i\rangle$

$\mu = 0 \longrightarrow$ two degenerate ground states $\prod_i |\rightarrow_i\rangle$ and $\prod_i |\leftarrow_i\rangle$

These phases extend to finite μ, quantum transition at $\mu_c/J = 1$, between quantum paramagnetic and ordered phases

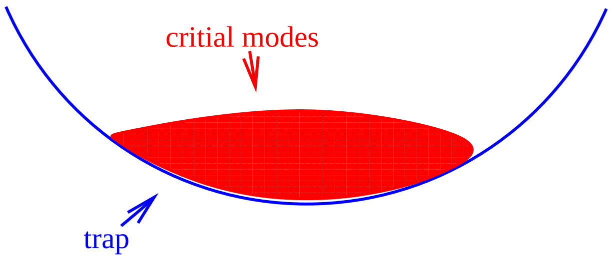
2D Ising quantum critical behavior with $\Delta \sim \xi^{-1} \sim |\mu - \mu_c|$

A QPT is generally characterized by a relevant parameter μ, with RG dimensions $y_\mu \equiv 1/\nu$, and dynamic exponent z:

$$\xi \sim |\bar{\mu}|^{-\nu}, \qquad \Delta \sim |\bar{\mu}|^{z\nu} \sim \xi^{-z}, \qquad \bar{\mu} = \mu - \mu_c$$

Scaling law of the free energy $F(\mu, T) = b^{-(d+z)} F(\bar{\mu} b^{1/\nu}, T b^z)$

A trapping potential significantly changes the phenomenology of QPT: correlations are not expected to develop a diverging length scale.



TSS to describe how critical correlations develop in large traps.

Scaling Ansatz in the presence of the trap $V(r) = v^p r^p \equiv (r/l)^p$:

$$F(\mu, T, v, x) = b^{-(d+z)} F(\bar{\mu} b^{y_\mu}, T b^z, v b^{y_v}, x/b)$$

$F = l^{-\theta(d+z)} \mathcal{F}(\bar{\mu} l^{\theta/\nu}, T l^{\theta z}, x l^{-\theta})$ where $\nu \equiv 1/y_\mu$ and $\theta \equiv 1/y_v$

For example, TSS of the gap and the length scale:

$$\Delta = l^{-\theta z} \mathcal{D}(\bar{\mu} l^{\theta/\nu}), \qquad \mathcal{D}(y) \sim y^{z\nu} \text{ for } y \to 0$$

$$\xi = l^{\theta} \mathcal{X}(\bar{\mu} l^{\theta/\nu}, T l^{\theta z}), \qquad \mathcal{X}(y,0) \sim y^{-\nu} \text{ for } y \to 0$$

implying a critical length scale scaling as $\xi \sim l^{\theta}$ at $\bar{\mu} = 0$.

The *trap exponent* θ depends on the universality class of the QPT, and the way the potential is coupled to the system.

θ can be computed using RG scaling arguments

The hard-wall limit $p \to \infty$ is equivalent to confining a homogeneous system in a box of size $L = 2l$ with open boundary conditions, thus $\theta \to 1$

TSS provides a general framework for quantum critical behaviors in confined systems.

The quantum XY chain in a transverse field is a standard theoretical laboratory for issues related to quantum transitions.

A space-dependent transverse field gives rise to an inhomogeneity analogous to a trapping potential in particle systems

$$H_{\rm XY} = -\sum_i \frac{1}{2}[(1+\gamma)\sigma_i^x\sigma_{i+1}^x + (1-\gamma)\sigma_i^y\sigma_{i+1}^y] - \mu\sigma_i^z - V(x_i)\sigma_i^z,$$

where $0 < \gamma \leq 1$, $V(x) = v^p|x|^p \equiv (|x|/l)^p$

Map into **spinless fermions** by a Jordan-Wigner transformation:
$\sigma_i^x = \Pi_{j<i}(1-2c_j^\dagger c_j)(c_i^\dagger + c_i)$, $\sigma_i^y = i\Pi_{j<i}(1-2c_j^\dagger c_j)(c_i^\dagger - c_i)$, $\sigma_i^z = 1 - 2c_i^\dagger c_i$

$$H = \sum [c_i^\dagger A_{ij} c_j + \frac{1}{2}(c_i^\dagger B_{ij} c_j^\dagger + \text{h.c.})], \qquad A_{ij} = 2\delta_{ij} - \delta_{i+1,j} - \delta_{i,j+1} + 2Q(x_i)\delta_{ij},$$

$$B_{ij} = -\gamma\left(\delta_{i+1,j} - \delta_{i,j+1}\right), \quad Q(x) = \bar{\mu} + V(x), \quad \bar{\mu} \equiv \mu - 1.$$

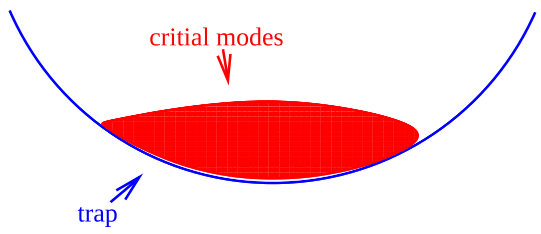
μ plays the role of *chemical potential* for the *c-particles*, and $V(x)$ acts as a *trap*

There are experimental realizations of Ising chains, such as the insulators $CsCoBr_3$, $CoNb_2O_6$, etc.., in a magnetic field.

In the absence of the trap, quantum transition at $\bar{\mu} \equiv \mu - 1 = 0$ in the 2D Ising universality class, separating a quantum paramagnetic phase for $\bar{\mu} > 0$ from a quantum ferromagnetic phase for $\bar{\mu} < 0$.

$$\xi \sim |\bar{\mu}|^{-\nu}, \quad \nu = 1/y_\mu = 1; \qquad\qquad \Delta \sim \xi^{-z}, \quad z = 1$$

In the presence of the confining potential $V(x) = v^p x^p$ ($l \equiv 1/v$ is the trap size), the critical behavior can be observed around the center of the trap in the large-l limit.



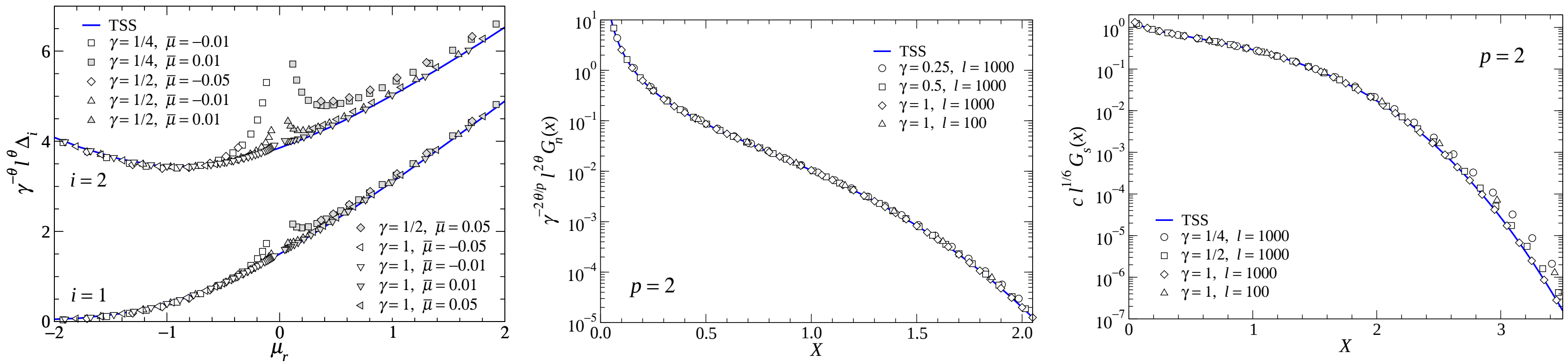
Analyzing the RG dim of the corresponding perturbation

$$P_V = \int d^d x \, dt \, V(x) \phi(x)^2 \quad \longrightarrow \quad \theta \equiv 1/y_v = p/(p+1)$$

Using the relations $y_V = p y_v - p$, $y_{\phi^2} = d + z - y_\mu$, $y_V + y_{\phi^2} = d + z$, $p y_v - p = y_\mu$, and the value $z = 1$ and $y_\mu = 1$

TSS can be analytically derived in the XY chain model, arriving at a continuum Schrödinger-like equation for the lowest states. The asymptotic trap-size dependence confirms the RG scaling arguments

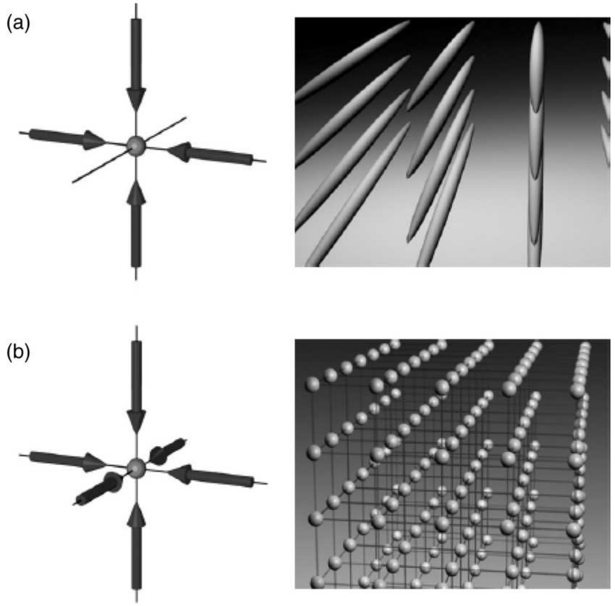
- any low-energy scale behaves as $\Delta \approx \gamma^{\theta} l^{-\theta} \mathcal{D}(\mu_r)$ where $\mu_r \equiv \gamma^{-\theta} l^{\theta} \bar{\mu}$
- particle-density correlator: $G_n(x) \equiv \langle n_0 n_x \rangle_c \approx \gamma^{2\theta/p} l^{-2\theta} \mathcal{G}_n(X)$
- two-point function: $G_s(x) \equiv \langle \sigma_0^x \sigma_x^x \rangle = a_s l^{-\theta\eta} \mathcal{G}_s(X)$
- its second moment correlation length: $\xi = a_\xi \gamma^{\theta/p} l^{\theta} [1 + O(l^{-\theta})]$



- Bipartite entanglement entropy: $\lim_{L\to\infty} S_{\rm vN}(L/2;L) \approx (c/6)\ln l^{\theta}$, instead of $S_{\rm vN}(L/2;L) \approx (c/6)\ln L$ for homogeneous systems

Ultracold atomic gases in optical lattices (arrays of microscopic potentials induced by ac Stark effects of interfering laser beams, which constrain the atoms at the sites of a lattice)

Experiments are set up with a harmonic trap, inducing an effective external potential $V(r) = v^2 r^2$



Boson systems described by **the Bose-Hubbard model** ($[b_i, b_j^\dagger] = \delta_{ij}$, $n_i \equiv b_i^\dagger b_i$) (D. Jaksch etal, 1998)

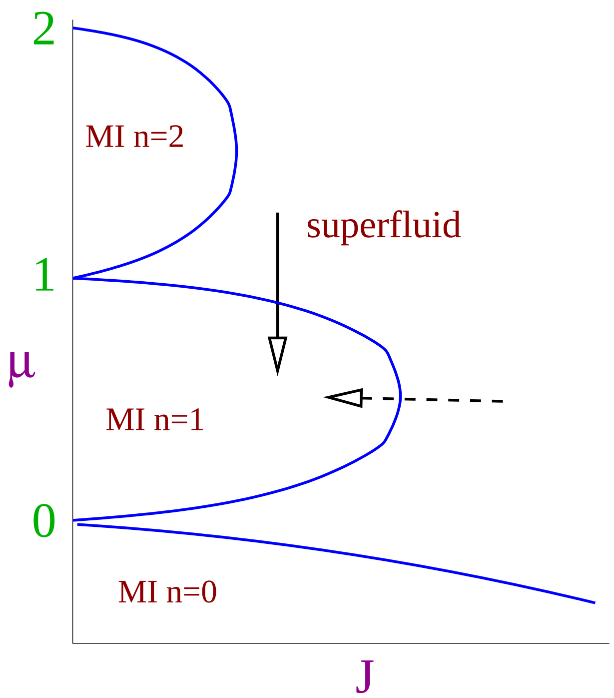
$$H_{\mathrm{BH}} = -\frac{J}{2} \sum_{\langle ij \rangle} (b_i^\dagger b_j + b_j^\dagger b_i) + \sum_i U n_i (n_i - 1) + \mu \sum_i n_i + \sum_i V(r_i) n_i$$

The BH model presents Mott insulators ($\partial\langle n_i\rangle/\partial\mu = 0$) and superfluid phases. At the transitions driven by μ (ex. along the full arrow), *nonrelativistic* bosonic field theory (Fisher etal, 1989)

$$Z = \int [D\phi] \exp(-\int_0^{1/T} dt\, d^d x\, \mathcal{L}_c),$$

$$\mathcal{L}_c = \phi^* \partial_t \phi + \frac{1}{2m} |\nabla\phi|^2 + r|\phi|^2 + u|\phi|^4,$$

where $r \sim \mu - \mu_c$.



The upper critical dimension is $d_c = 2 \rightarrow$ mean field for $d > 2$.

For $d = 2$ the FT is free (apart from logs), thus $z = 2, \quad y_\mu = 2$.

The 1D critical theory is equivalent to a free field theory of nonrelativistic spinless fermions, thus $z = 2, \quad y_\mu = 2$.

The special transitions at fixed integer density (along the dashed arrow) $\in$ the $d + 1$ XY universality class (*relativistic FT*), thus $z = 1, \quad y_\mu = 1/\nu_{\rm XY}$.

In the presence of a confining potential, experimental and theoretical results show the coexistence of Mott insulator and superfluid regions, but the critical behavior can only be observed in the large trap size limit.

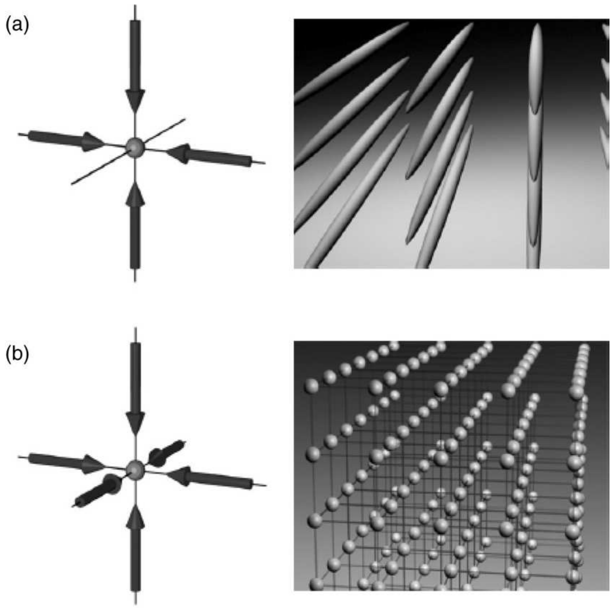
Within the TSS framework:

$$F(\mu, T, l, x) = l^{-\theta(d+z)} \mathcal{F}(\bar{\mu} l^{\theta/\nu}, T l^{\theta z}, x l^{-\theta}), \quad \langle O \rangle(\mu, l, x) \sim l^{-y_o \theta} \mathcal{O}(\bar{\mu} l^{\theta/\nu}, x l^{-\theta})$$

for several physically interesting observables, such as particle density and its correlators, one-particle density matrix, entanglement, etc...

The trap exponent θ can be determined by an analysis of the corresponding RG perturbation, $P_V = \int d^d x \, dt \, V(x) |\phi(x)|^2$, obtaining $\theta = p/(p + y_\mu)$. By replacing the corresponding value of y_μ, this relation yields the value of θ for each specific transition. $\theta = p/(p+2)$ at the μ-driven transitions.

The experimental capability of varying the confining potential allows to vary the effective spatial geometry, including quasi-1D geometries. Several exps on 1D systems, usually keeping the trap fixed.



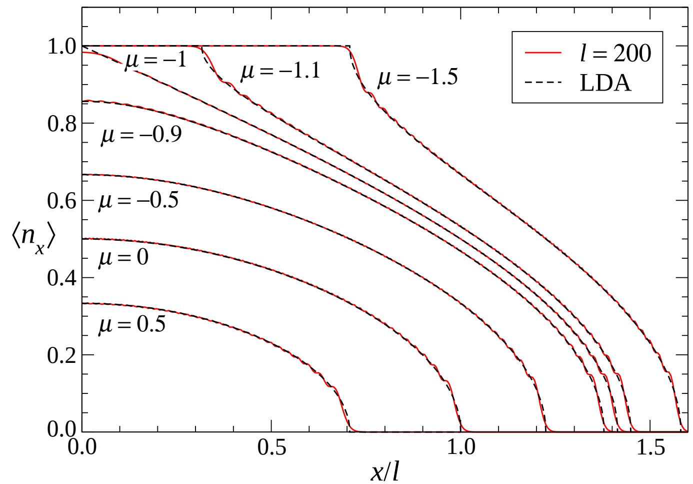
1D BH models allow accurate studies by analytical and numerical computations

The 1D hard-core Bose-Hubbard model. The hard-core $U \to \infty$ limit of $H_{\rm BH} = -\frac{J}{2}\sum_{\langle ij\rangle}(b_i^\dagger b_j + b_j^\dagger b_i) + \sum_i[(\mu + V(r_i))n_i + Un_i(n_i-1)]$ implies that the particle number is restricted to $n_i = 0, 1$. Exact mapping into a model of free spinless fermions $H_c = \sum_{ij} c_i^\dagger h_{ij} c_j$

In the absence of the trap, **three phases**: $\langle n_i\rangle = 0$ (vacuum) for $\mu > 1$, $\langle n_i\rangle = 1$ for $\mu < -1$, and a gapless superfluid phase for $|\mu| < 1 \longrightarrow$ two Mott-insulator to superfluid transitions at $\mu = 1$ and $\mu = -1$

Thermodynamic limit of
$H_{\rm BH} = -\frac{J}{2}\sum_{\langle ij\rangle}(b_i^\dagger b_j + b_j^\dagger b_i) + \sum_i U n_i(n_i-1) + \sum_i [\mu + V(r_i)] n_i$, in the presence of the trapping potential ($V(0)=0$), at fixed μ, corresponding to $N, l \longrightarrow \infty$ keeping N/l^d fixed

$\langle n_x \rangle$ of the 1D HC BH model approaches its local density approximation in the large-l limit, i.e., the value of the particle density of the homogeneous system at $\mu_{\rm eff}(x) \equiv \mu + (x/l)^p$

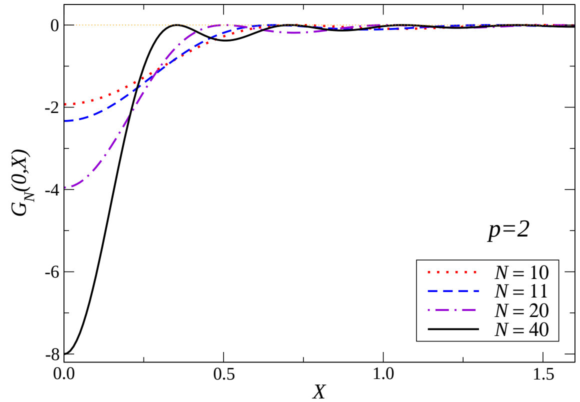


Corrections are suppressed by powers of l, and present a nontrivial scaling: $\langle n_x \rangle = \rho_{\rm lda}(x/l) + l^{-\theta}\mathcal{D}(x/l^\theta, Tl)$. This feature is likely shared by other particle systems, finite U or Hubbard models

Another interesting TSS regime is that at fixed particle number $N = \sum_i \langle n_i \rangle$, corresponding to the low-density regime $N/l \to 0$.

Results from various approaches:

• Analytical results: TSS in the dilute limit $\mu \to 1$, or TSS keeping N fixed (this regime shows universality within trapped boson gases with short ranged interactions, Lieb-Liniger model)



• Numerical results by exact diagonalization in the superfluid phase and at the $n = 1$ Mott transition at $T = 0$, showing a modulated TSS at $T = 0$, essentially due to level crossings of the lowest states at finite trap size,
$\Delta = l^{-2\theta} A_\Delta(\phi)[1 + O(l^{-\theta/2})]$, $\langle n_0 \rangle = 1 - l^{-\theta} D_0(\phi)[1 + O(l^{-\theta/2})]$

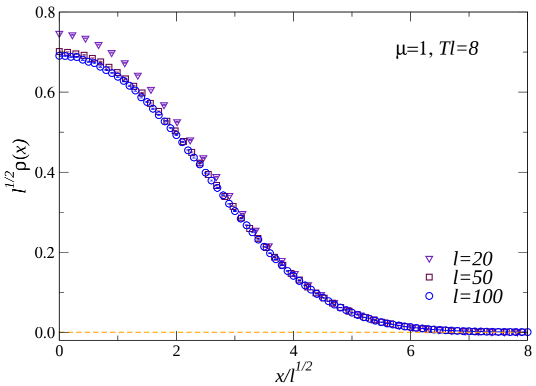
• Numerical results by DMRG to check universality when adding interaction terms in the Hamiltonian.

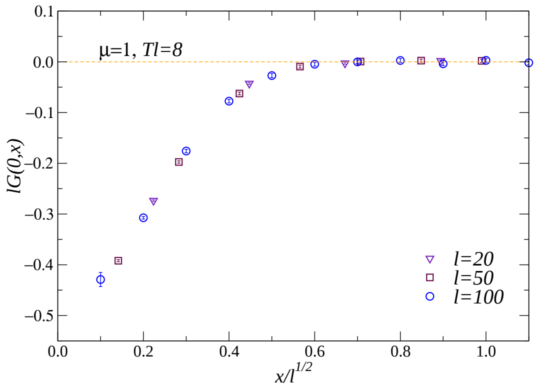
• Numerical results by quantum-MC at finite temperature, showing TSS, while the $T = 0$ modulation phenomenon disappears.

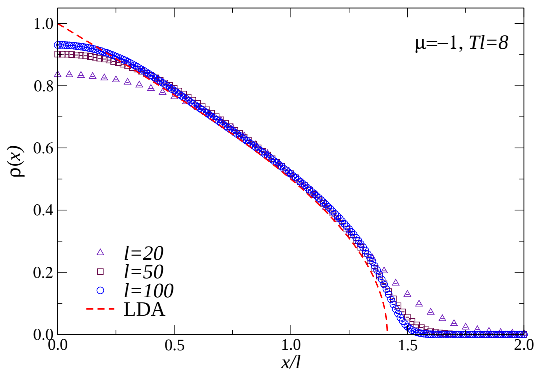
At the Mott transitions: $y_\mu = 2,\ z = 2,\ \theta = p/(p+2)$,

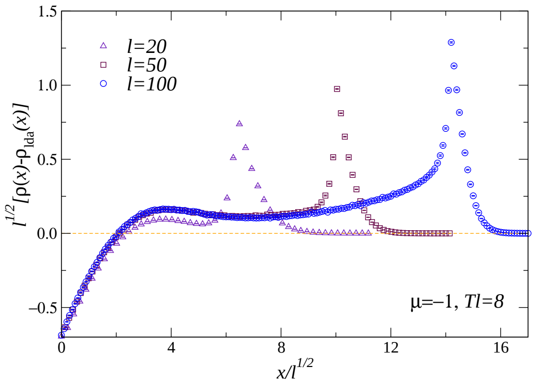
$\langle n_x \rangle = \rho_{\rm lda}(x/l) + l^{-\theta}\mathcal{D}(x/l^\theta, Tl)$ and $\langle n_x n_y \rangle_c = l^{-2\theta}\mathcal{G}(x/l^\theta, y/l^\theta, Tl)$

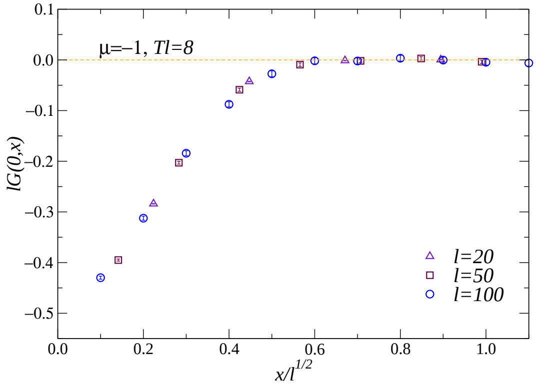
Numerical results by QMC at finite T showing TSS (modulations apparently cancel at finite T)











CONCLUSIONS: TSS provides a theoretical framework to describe thermal and quantum critical behaviors in confined particle systems.

- **At finite-T transitions**, the critical behavior of confined systems can be described by a universal TSS, resembling finite-size scaling theory.

$\mathcal{F} = l^{-\theta d}\mathcal{F}(u_t l^{\theta y_t}, u_h l^{\theta y_h}, x l^{-\theta})$, where the trap exponent θ describes how ξ scales with l: $\xi \sim l^\theta$ at T_c.

θ depends on the universality class, the power law $V(x) = (x/l)^p$, and the way it is coupled to the critical modes. θ can be computed by scaling arguments.

- Results for the static and dynamic critical behavior of
  - Lattice gas models
  - QLRO of 2D systems
  - finite-T transitions of interacting Bose gases with BEC

• **At QPT**, $\mathcal{F}(\mu, T, l, x) = l^{-\theta(d+z)}\mathcal{F}(\bar{\mu}l^{\theta/\nu}, Tl^{z\theta}, xl^{-\theta})$

• Analytic and numerical results by diagonalization, DMRG and QMC, for

• the quantum XY chain in a space-dependent transverse field

• the Bose-Hubbard model, in particular in 1D, which is relevant for the description of cold atomic gases confined in optical lattices.

• Further results for: • TSS of the unitary off-equilibrium quantum dynamics, e.g., in the presence of a time-dependent confining potential (M. Campostrini, EV, PRA 82 063636 2010)

• TSS of bipartite entanglement entropies in 1D BH models, which diverge logarithmically with increasing the trap size, and present notable scaling behaviors in the TSS limit (M. Campostrini, EV, J. Stat. Mech. P08020 2010)

FURTHER SLIDES ......

Interacting Bose gases in a trap

The confining potential $V(x) = v^2 x^2 \equiv (x/l)^2$ is coupled to the particle density, related to the energy operator $E = |\Psi(x)|^2$, it gives rise to the RG perturbation $P_V = \int d^3x\, v^2 |x|^2 |\Psi(x)|^2$.

Using $y_V = p y_v - p$, $y_E = d - 1/\nu$, and $y_V + y_E = d$,

$$\theta = \frac{1}{y_v} = \frac{2\nu}{1 + 2\nu}$$

thus $\theta = 0.57327(4)$ in 3D $(\nu = 0.6717(1))$ and $\theta = 1$ in 2D $(\nu = \infty)$, for comparison, $\theta = 1/2$ for a Gaussian theory $(\nu = 1/2)$

Trap effects are negligible when $\xi \ll c l^\theta$, but relevant when $\xi \approx l^\theta$.

Trap-size dependence casted in a **trap-size scaling** framework

Quasi-long range order in 2D trapped systems

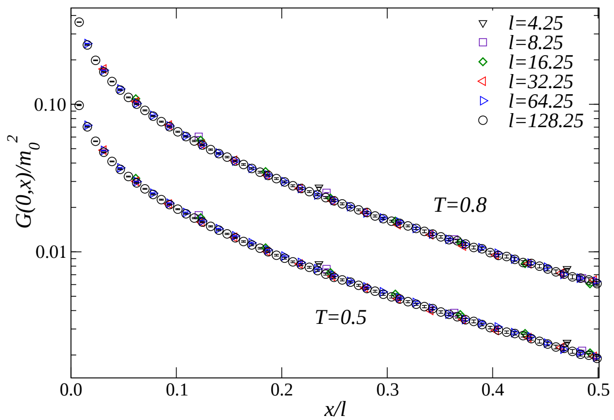
No real BEC in 2D, but a low-T QLRO, where the one-body correlation decays as $|x-y|^{-\eta(T)}$ with $\eta(T) = T/(2\pi) + O(T^2)$ up to $\eta(T_{\rm KT}) = 1/4$

How does the presence of the trap change the QLRO features?

In the spin-wave limit: $H_{\rm sw} = \int d^2x \, \frac{1}{2}(\nabla\varphi)^2 \longrightarrow \int d^2x \, \frac{1}{2}(1+v^p r^p)(\nabla\varphi)^2$

TSS with $\theta = 1$ in the whole QLRO phase, from $T=0$ to $T=T_{\rm KT}$:
$G(x,y) \equiv \langle \bar\psi(x)\psi(y)\rangle_c = l^{-\theta\eta(T)}\mathcal{G}(xl^{-\theta}, yl^{-\theta})$

From simulations of the 2D XY models:
$H_U = -J\sum_{\langle ij\rangle} {\rm Re}\, \bar\psi_i U_{ij}\psi_j,$
$U_{ij} = 1 + V(r_{ij}), \quad V(r) = v^p r^p$
(F. Crecchi, EV, PRA 83,035602,2011)



TSS can be proved in the XY chain model:

The Hamiltonian can be solved by exact numerical diagonalization, even in the presence of the trapping potential:

- New fermi variables $\eta_k = g_{ki} c_i^\dagger + h_{ki} c_i$ so that $H = \sum_k \omega_k \eta_k^\dagger \eta_k$, $(\omega_k \geq 0)$
- Introduce $\phi_{ki} = g_{ki} + h_{ki}$ and $\psi_{ki} = g_{ki} - h_{ki}$ satisfying the equations $(A + B)\phi_k = \omega_k \psi_k$ and $(A - B)\psi_k = \omega_k \phi_k$
- Solution by solving $(A - B)(A + B)\phi_k = \omega_k^2 \phi_k$,
- The continuum limit, by rewriting the discrete differences in terms of derivatives, has a nontrivial TSS limit: by rescaling

$$x = \gamma^{1/(1+p)} l^{p/(1+p)} X, \quad \bar{\mu} = \gamma^{p/(1+p)} l^{-p/(1+p)} \mu_r, \quad \omega_k = 2\gamma^{p/(1+p)} l^{-p/(1+p)} \Omega_k,$$

- Keeping only the leading terms in the large-l limit, Schrödinger-like eq

$$(\mu_r + X^p - \partial_X)(\mu_r + X^p + \partial_X)\phi_k(X) = \Omega_k^2 \phi_k(X)$$

Thus, $\theta = p/(p+1)$ **in agreement with RG**. Next-to-leading terms in the large-trap limit give rise to $O(l^{-\theta})$ scaling corrections.

Entanglement in a 1D quantum lattice system

Let us consider a pure state $|\Psi\rangle$, so that its density matrix is $\rho = |\Psi\rangle\langle\Psi|$. Let us divide the system into two parts A and B. $\rho_A = \mathrm{Tr}_B \rho$ is the reduced density matrix of the subsystem A. Entanglement entropies:

$$S_{\text{von Neumann}} = -\ln \mathrm{Tr}[\rho_A \ln \rho_A], \qquad S_{\text{Renyi}} = \frac{1}{1-\alpha} \ln \mathrm{Tr}\rho_A^\alpha$$

Quantum critical behaviors described by 2D conformal field theories show logarithmically divergent entanglement entropies.

Dividing the chain in two parts of length l_A and $L - l_A$, CFT predicts

$$S_\alpha(l_A; L) \approx C_\alpha \left[\ln L + \ln \sin(\pi l_A / L) + e_\alpha\right], \qquad C_\alpha = c\frac{1+\alpha^{-1}}{12}$$

where c is the central charge

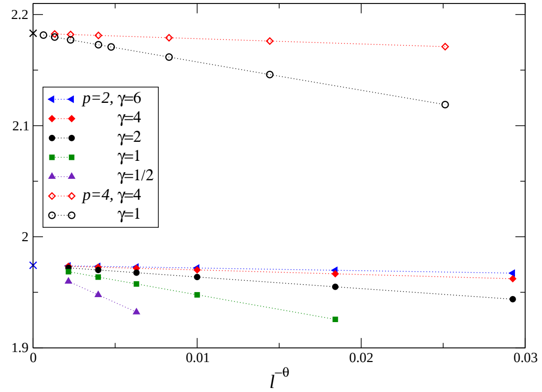
The trap destroys conformal invariance. What is the scaling behavior of the entanglement entropies in the TSS limit?

Bipartite entanglement in a trap at the critical point

In the presence of the trap of size l, the dependence on L disappears when $L \to \infty$. Thus, for sufficiently large $L \gg l$,

$$S_{\rm vN}(L/2;L) \approx \frac{c}{6}\left(\ln \xi_e + e_1\right),$$

$$\xi_e = a_e \gamma^{\theta/p} l^{\theta}[1 + O(l^{-\theta})]$$



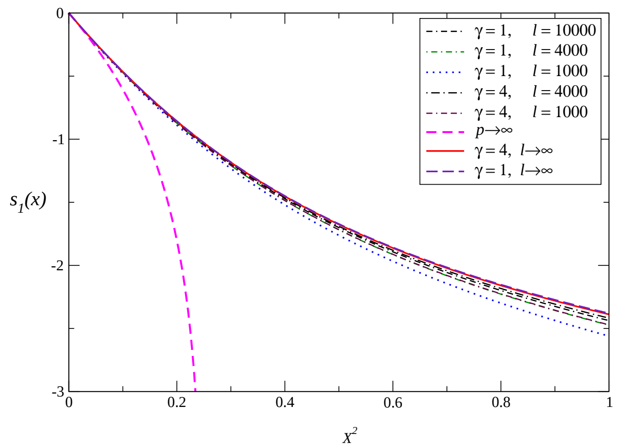
which defines an entanglement length ξ_e, scaling with $\theta = p/(1+p)$ (M. Campostrini, EV, J. Stat. Mech. P08020, 2010)

The spatial dependence:

$$S_{\rm vN}(L/2 - x; L) \approx$$

$$C_\alpha \left[\ln \xi_e + e_1 + f(X) + O(\xi_e^{-1/\alpha})\right],$$

$$X \equiv x/\xi_e, \qquad\qquad f(X) \longrightarrow$$



Two interesting regimes of TSS:

• TSS at fixed particle number $N = \sum_i \langle n_i \rangle$ in the low-density regime, in particular, the asymptotic large-$l_{\rm trap}$ dependence of

$$H_{\rm BH} = -\frac{J}{2} \sum_{\langle ij \rangle} (b_i^\dagger b_j + b_j^\dagger b_i) + U \sum_i n_i(n_i - 1) + \sum_i (r_i/l)^p n_i$$

keeping N fixed (recall that $[\hat{N}, H_{\rm BH}] = 0$), and increasing $l_{\rm trap}$

(M.Campostrini, EV, PRA 82 063636 2010)

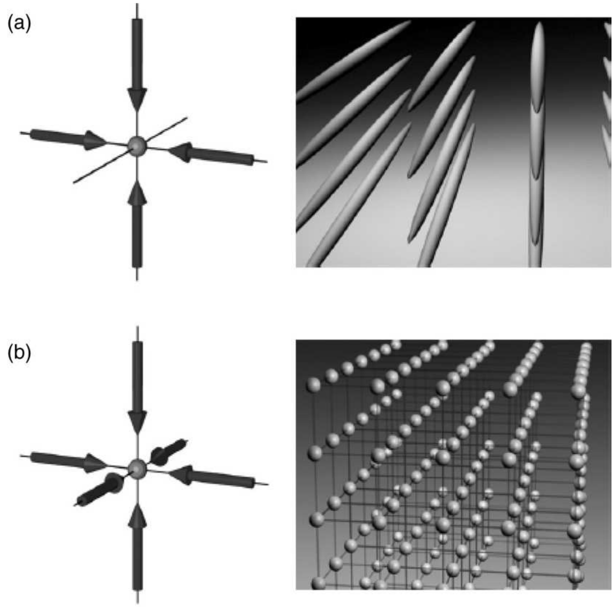
• TSS in the thermodynamic limit, achieved by adding a chemical potential, i.e., $\mu \sum_i n_i$, which corresponds to the limit

$$N, l \to \infty \quad \text{keeping} \quad N/l^d = f(\mu) \quad \text{fixed}$$

TSS at the Mott phase transitions and within the superfluid regions

(M.Campostrini, EV, PRA 81 063614 2010)

The experimental capability of varying the confining potential allows to vary the effective spatial geometry, including quasi-1D geometries. Several exps on 1D systems, usually keeping the trap size fixed.



1D BH models allow accurate studies by analytical and numerical computations

Critical trap-size dependence within the TSS framework:

$$F(\mu, T, l, x) = l^{-\theta(d+z)} \mathcal{F}(\bar{\mu} l^{\theta/\nu}, T l^{\theta z}, x l^{-\theta}),$$

$$\langle O \rangle(\mu, l, x) \sim l^{-y_o \theta} \mathcal{O}(\bar{\mu} l^{\theta/\nu}, x l^{-\theta}) \quad \text{at fixed } \mu,$$

$$\langle O \rangle(N, l, x) \sim l^{-y_o \theta} \mathcal{O}_N(x l^{-\theta}) \quad \text{at fixed } N,$$

for several physically interesting observables, such as particle density and its correlators, one-particle density matrix, entanglement, etc...

The 1D hard-core Bose-Hubbard model. The hard-core $U \to \infty$ limit of $H_{\rm BH} = -\frac{J}{2}\sum_{\langle ij\rangle}(b_i^\dagger b_j + b_j^\dagger b_i) + \sum_i[(\mu + V(r_i))n_i + U n_i(n_i-1)]$ implies that the particle number is restricted to $n_i = 0, 1$.

Exact mapping into the XX chain model in the presence of a space-dependent field, by $\sigma_i^x = b_i^\dagger + b_i$, $\sigma_i^y = i(b_i^\dagger - b_i)$, $\sigma_i^z = 1 - 2b_i^\dagger b_i$,

$$H_{\rm XX} = -J\sum_i \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y\right) - \mu\sum_i S_i^z - \sum_i V(x_i) S_i^z$$

One can then map it into a model of free spinless fermions by a Jordan-Wigner transformation, $H_c = \sum_{ij} c_i^\dagger h_{ij} c_j$

$$h_{ij} = \delta_{ij} - \frac{1}{2}\delta_{i,j-1} - \frac{1}{2}\delta_{i,j+1} + [\bar\mu + V(x_i)]\delta_{ij}, \qquad \bar\mu \equiv \mu - 1$$

In the absence of the trap, **three phases**: two Mott insulator phases, for $\mu > 1$ with $\langle n_i\rangle = 0$ (actually vacuum) and for $\mu < -1$ with $\langle n_i\rangle = 1$, and a gapless superfluid phase for $|\mu| < 1$. $\longrightarrow$ two Mott insulator to superfluid transitions at $\mu = 1$ and $\mu = -1$, related by the particle-hole symmetry

TSS of a N-particle system within the low-density regime $N/l \ll 1$

thus, approaching the low-density-to-vacuum transition, which may effectively be considered as a $n = 0$ Mott transition.

The power-law behavior is controlled by the continuum *nonrelativistic* complex Φ^4 theory, i.e., the theory describing the quantum critical behavior at Mott transitions driven by the chemical potential

Thus $\theta = p/(2+p)$ and $z = 2$, and $\langle O\rangle(N,l,x) \sim l^{-y_o\theta}\mathcal{O}_N(xl^{-\theta})$.

In particular, the gap behaves as $\Delta_N \approx A_N l^{-z\theta}$, the particle density as $\rho(x) \equiv \langle n_x\rangle = l^{-\theta}\mathcal{D}_N(x/l^\theta)$, etc...

The universal TSS can be analytically derived in the hard-core limit (exploiting the exact mapping to a quadratic spinless fermion model)

Universal with respect to the on-site repulsion coupling $U > 0$, also shared with continuum gas models such as the 1D Lieb-Liniger model
$\mathcal{H}_{\rm LL} = \sum_{i=1}^N \left[\frac{p_i^2}{2m} + V(x_i)\right] + g\sum_{i\neq j}\delta(x_i - x_j)$

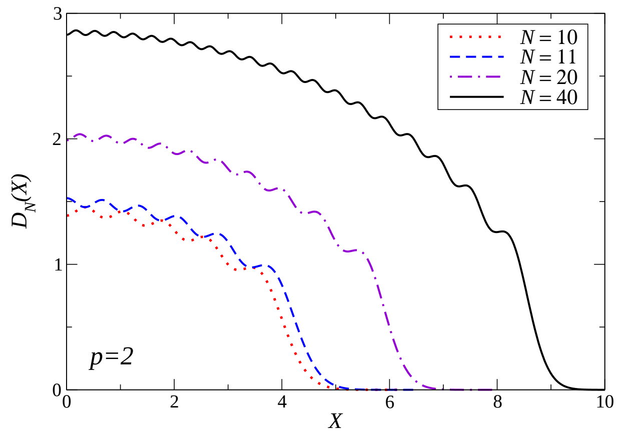
$$\langle n_x \rangle = l^{-\theta} \mathcal{D}_N(X) \left[1 + O(l^{-2\theta}) \right]$$

$$\mathcal{D}_N(X) = \sum_{k=0}^{N-1} \varphi_k^2(X)$$

where $\theta = p/(p+2)$, $X = x/l^{\theta}$,

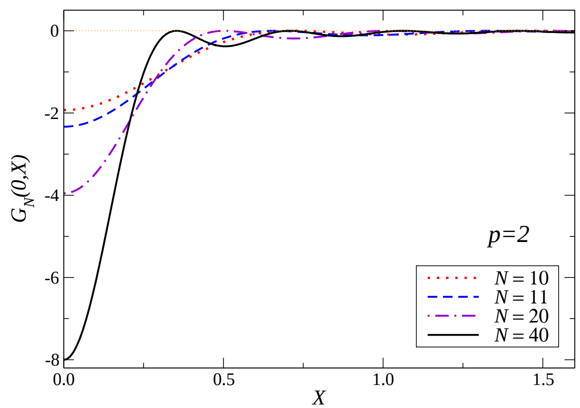
and $\varphi_k(X) = c_k H_k(X) \exp(-X^2/2)$

(solutions of $\left(-\frac{1}{2}\frac{d^2}{dX^2} + \frac{1}{2}X^2\right)\varphi_k(X) = e_k \varphi_k(X)$ with $e_k = k + 1/2$)



$$\langle n_x n_y \rangle_c \approx l^{-2\theta} \mathcal{G}_N(X, Y)$$

$$\mathcal{G}_N(X, Y) = -[\sum_{k=0}^{N-1} \varphi_k(X) \varphi_k(Y)]^2$$



Large-N: $\mathcal{D}_N(X) \approx N^{1/2} R_D(N^{-1/2} X)$ and $\mathcal{G}_N(X, Y) \approx N R_G(N^{1/2} X, N^{1/2} Y)$

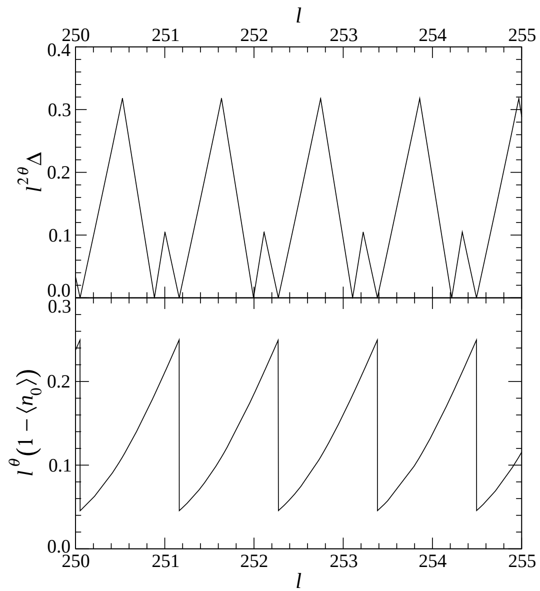
Modulated TSS keeping μ fixed, thus N/l constant, essentially due to level crossings of the lowest states at finite trap size, the particle number is conserved even in the presence of the trapping potential, thus the eigenvectors do not depend on μ, even though the eigenvalues do.

At the $n = 1$ Mott transition $\longrightarrow$ periodic asymptotic behavior [figs for the energy gap $l^{2\theta}\Delta$ and the particle density $l^{\theta}(1 - \langle n_0 \rangle)$]

$$\Delta = l^{-2\theta} A_{\Delta}(\phi)[1 + O(l^{-\theta/2})]$$

$$1 - \langle n_0 \rangle = l^{-\theta} D_0(\phi)[1 + O(l^{-\theta/2})]$$

where $\theta = p/(p+2)$ as expected, and ϕ is a phase-like variable measuring the distance from the closest smaller level crossing



Universality with respect to the on-site coupling U, checked by DMRG

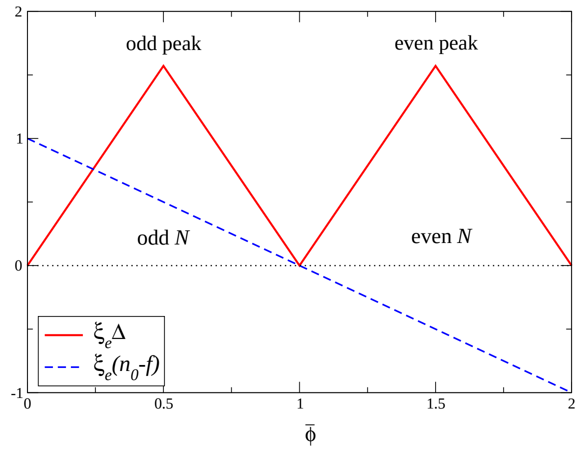
Modulated multi-TSS in the superfluid region

Beside the asymptotic modulation, multiscaling phenomenon $\rightarrow$ different length scales diverging with distinct power laws in the TSS.

$\xi_s \sim l$ for observables related to smooth modes, such as the gap and the half-lattice entanglement entropy

$\xi_F \sim l^{p/(p+1)}$ for modes at the Fermi scale $k_F = \pi f$, such as the density-density correlation.

$$\Delta \sim t(\varphi) l^{-1},$$
$$\langle n_0 \rangle - f \sim (1-\varphi) l^{-1}$$
$$\varphi \equiv 2(l - l_0^{(2k)})/(l_0^{(2k+2)} - l_0^{(2k)})$$



$$\langle n_0 n_x \rangle_c \approx l^{-2p/(p+1)} \mathrm{Re}[h(Y,\varphi) e^{2ik_F x} + g(Y,\varphi)], \quad Y = x/l^{p/(p+1)}$$

TSS at low density $N/l \ll 1$: varying l keeping N fixed

N particles: $H_{\rm BH} = -\frac{J}{2}\sum_{\langle ij\rangle}(b_i^\dagger b_j + b_j^\dagger b_i) + \sum_i [V(r_i) n_i + U n_i(n_i-1)]$

One can map its hard-core limit into spinless fermions by a Jordan-Wigner transformation, $H_c = \sum_{ij} c_i^\dagger h_{ij} c_j$, which can be diagonalized by $\eta_k = \sum_i \phi_{ki} c_i$ and $h_{ij}\phi_{kj} = \omega_k \phi_{ki}$, obtaining $H_c = \sum_k \omega_k \eta_k^\dagger \eta_k$

The ground state is given by N η-fermions at the lowest N one-particle levels, $E_0 = \sum_{k=0}^{N-1} \omega_k$.

TSS limit by taking the continuum limit, rescaling $x = l^{p/(2+p)} X$, $\omega_k = l^{-2p/(2+p)} e_k$, and setting $\varphi_k(X) \sim \phi_k(l^{p/(2+p)} X)$,

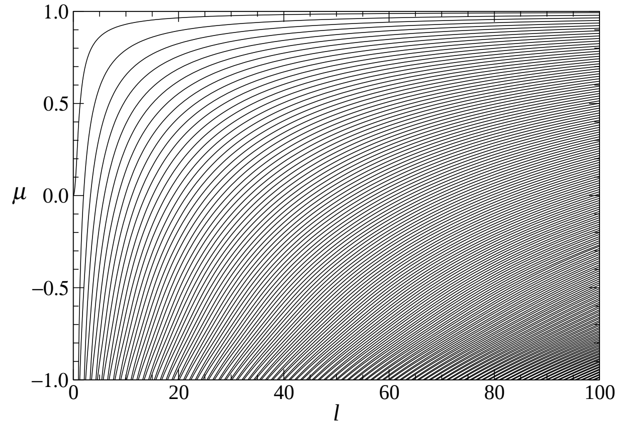
$$\left(-\frac{1}{2}\frac{d^2}{dX^2} + X^p\right)\varphi_k(X) = e_k \varphi_k(X),$$

For $p = 2$, $\quad e_k = 2^{1/2}(k + 1/2)$, and $\varphi_k(X) \propto (k!)^{-1/2} H_k(2^{1/4}X)\, e^{-X^2/\sqrt{2}}$.

From the rescaling of x, $\theta = p/(2+p)$, in agreement with RG.

Keeping the chemical potential fixed: subtle effects in the parameter region where the homogeneous model has a nonzero

Level crossings of the lowest states at finite trap size: the particle number is conserved even in the presence of the trapping potential, thus the eigenvectors do not depend on μ, even though the eigenvalues do.



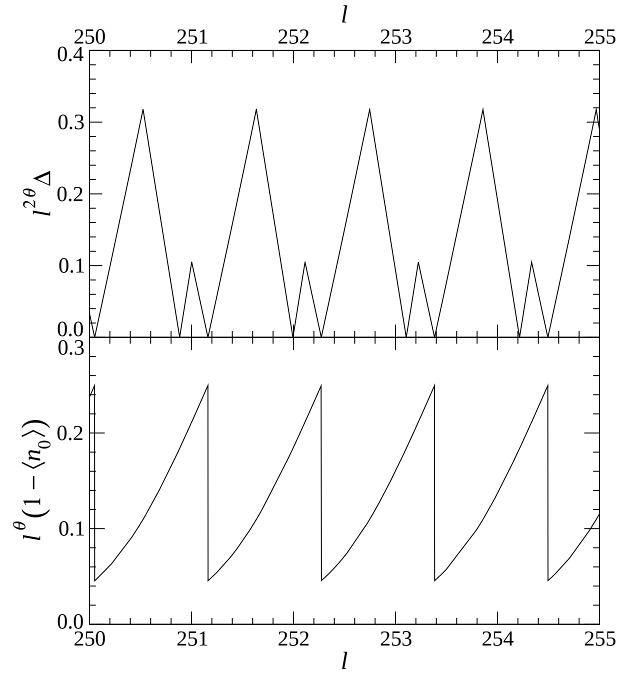
In the presence of the trap the particle number $N \equiv \langle \hat{N} \rangle$ is finite and increases as $N \sim l$ with increasing the trap size l.

As $l \to \infty$, there is an infinite number of level crossings where N jumps by 1 and the gap vanishes.

The length scale diverges only the in the large trap-size limit. The main effect of the infinite level crossings in the limit $l \to \infty$ is that the asymptotic power law behaviors gets modulated by periodic functions of the trap size l, giving rise to a modulated TSS.

Modulated TSS at **the $n = 1$ Mott insulator to superfluid transition**

The rescaled energy gap $l^{2\theta}\Delta$ (above) and the rescaled particle density in the middle of the trap $l^{\theta}(1-\langle n_0\rangle)$ (below) vs. l for $\mu = -1$ and $p = 2$, whose trap exponent is $\theta = 1/2$. This suggests a periodic asymptotic behavior with a period given by the interval between two even (or odd) zeroes,



$$P_l^{(k)} \equiv l_0^{(2k+2)} - l_0^{(2k)} = P_l^* + o(1/l)$$

For example: $P_l^* = 1.11072$ for $p = 2$ and $P_l^* = 1.10244$ for $p = 4$

The gap and the density at the origin behaves as

$$\Delta = l^{-2\theta} A_\Delta(\phi)[1 + O(l^{-\theta/2})], \qquad 1 - \langle n_0 \rangle = l^{-\theta} D_0(\phi)[1 + O(l^{-\theta/2})]$$

where $0 \leq \phi < 1$ is a phase-like variable $\phi \equiv (l - l_0^{(2k)})/(l_0^{(2k+2)} - l_0^{(2k)})$, $l_0^{(2k)} \leq l < l_0^{(2k+2)}$

$l^{2\theta}\Delta$ (above) and $l^{\theta}(1 - \langle n_0 \rangle)$ (below) vs. ϕ, for $p = 2$ $(\theta = 1/2)$. The extrapolation to $l \to \infty$ is obtained by assuming $O(l^{-\theta/2})$ leading corrections.

Check of universality within XXZ model (by DMRG).

Analogous results for other values of $p > 2$