Role of the interaction core in the excitation spectrum of 1D gases and liquids

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Outline



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- Target systems:
 - ID quantum systems in the continuum with different interaction cores: hard-rods, ID ⁴He, soft-rods

• How?

- Mainly Path Integral projector methods (T=0)
 ⇒ imaginary time densitydensity correlation functions
- Dynamic structure factor via "statistical" inversion of Laplace transform
- Results:
 - Mainly dynamic properties beyond Tomonaga Luttinger Liquid (TLL) theory



Collaborators

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Dimensions are relevant!





The effect of thermal and quantum fluctuations increase as we reduce the number of spatial dimensions (Mermin–Wagner theorem: no continuous symmetry breaking for $d \le 2$)



fluctuations destroy long range order, even at T = 0

1D is special

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- Well-defined low energy collective modes for many 1D Fermi & Bose systems, in fact, ...
- Interacting 1D Bose systems with (short-range) repulsive interactions the reduced dimensionality of the space naturally induces presence of collective modes
- 1D Fermi statistics imposes a nodal structure which mimicks contact hard core interaction ⇒ Bose-Fermi mapping

[Girardeau, J. Mat. Phys. (1960)] Same static and dynamic properties (except for momentum distribution)



⇒ Tomonaga Luttinger liquid (TLL) theory

[Tomonaga, Prog. Theor. Phys. (1950); Luttinger, J. Mat. Phys. (1963)] universal field-theoretical/hydrodynamic description of interacting 1D Fermions or Bosons characterized by low-energy phonon modes

1D universal behaviour



$$\hat{H}_{1D} = -\frac{\hbar^2}{2m} \int dx \,\hat{\Psi}^+(x) \,\partial^2 \hat{\Psi}(x) + \frac{1}{2} \int dx \int dx' \,\hat{\Psi}^+(x) \hat{\Psi}^+(x') V(|x-x'|) \hat{\Psi}(x') \hat{\Psi}(x)$$

• Rewrite field operators in term of new fields: density and phase fluctuations [Haldane, Phys. Rev. Lett. (1980)] $\hat{\Psi}(x) = \sqrt{\rho + \frac{1}{\pi} \partial \hat{\phi}(x)} e^{i\hat{\theta}(x)}$

⇒ effective harmonic Hamiltonian

• H_{TLL} is exactly solvable; dynamic structure factor:

$$S(q,\omega) = \frac{\hbar q}{\frac{\omega \to 0}{q \to 0}} \frac{\hbar q}{2mv_s} \delta(\omega - v_s q)$$

The low-energy ...

- ... excitations are collective density fluctuations
- ... physics is universal (independent of interaction details and statistics)
- ... physics (Galileian invariant systems) is completely specified by K_L

Density fluctuation spectrum



• Dynamic structure factor:

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

density fluctuation:
$$\rho_{\vec{q}}(t) = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{-i\vec{q}\cdot\vec{r}_{j}(t)}$$

Density fluctuation
wave-length:
$$\lambda = 2\pi/|\vec{q}|$$



Bragg spectroscopy



Dispersion relation



• Dynamic structure factor: One can read the dispersion relation of coherent modes







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 H_{TLL} fixes also the long range behaviour of spatial correlation functions in terms of K_L only [Haldane, Phys. Rev. Lett. (1981)]

- pair distribution function

$$g(|x - x'|) \approx \frac{1}{|x - x'| > \frac{L}{N}} \frac{1}{\left(2\pi\rho |x - x'|\right)^2} + \sum_{l=1}^{\infty} A_l \frac{\cos\left(2\pi\rho l |x - x'|\right)}{\left(2\pi\rho |x - x'|\right)^{2l^2 \kappa_L}}$$



The TLL parameter: K_L



$$\mathcal{K}_{L} = \frac{\hbar\pi}{m} \frac{\rho}{\mathbf{v}_{s}} \qquad \Rightarrow \mathcal{K}_{L} \text{ depends on the ratio } \rho/\mathbf{v}_{s}$$

Note also that: $K_L \propto \sqrt{\kappa} \Rightarrow$ is a dimensionless compressibility

- Hard-core interactions with finite range a: when $\rho \approx 1/a$ by increasing n one should expect that $\rho/v_s \rightarrow 0 \Rightarrow K_L \rightarrow 0$
- Interactions inducing a self-bound state \Rightarrow sound velocity $v_s \rightarrow 0$ at the spinodal density (liquid/gas phase separation) $\Rightarrow K_L \rightarrow +\infty$



What about higher energies?



Non-linear Luttinger (NLL) theory [Imambekov et al. Rev. Mod. Phys. (2012)]

- Assumes a low energy threshold for $S(q,\omega)$: $\omega_{th}(q)$
- $\omega_{th}(q)$ is a renormalization of $\omega(q)$: the curvature determines an effective mass m*
- \Rightarrow Exactly solvable Hamiltonian: S(q, ω) has a power-law behaviour near the edge with exponent $\mu(q)$



In general the physics is non-universal, numerical calculations or QMC are needed

Lieb Liniger model



• Integrable 1D model [Lieb, Liniger, Phys.Rev. (1963)]

• Hamiltonian: contact interaction
$$H = -\frac{\hbar^2}{2m} \left[\sum_{i=1}^N \partial_i^2 + c \sum_{i \neq j} \delta(x_i - x_j) \right]$$

dimensionless parameter $\gamma = c/\rho$ characterizes the interaction strength:

- $\gamma << 1$ weakly interacting regime
- $\gamma >> 1$ strong repulsion regime (Tonks-Girardeau)



Lieb Liniger model: $S(q,\omega)$



PHYSICAL REVIEW A 74, 031605(R) (2006)

Dynamical density-density correlations in the one-dimensional Bose gas

Jean-Sébastien Caux and Pasquale Calabrese Institute for Theoretical Physics, University of Amsterdam, 1018 XE Amsterdam, The Netherlands (Received 29 March 2006; published 29 September 2006)

• Calculation of $S(\vec{q}, \omega)$ at T=0 for the Lieb-Liniger model using a hybrid theoretical/numerical method based on the exact Bethe-ansatz solution:





Our "exact" QMC tool



We have used the "exact" T=0 K Path Integral Ground State (PIGS) projector method [Sarsa et al., J. Chem. Phys. (2000)]:

ground state \approx discrete imaginary time evolved trial quantum state, $\psi_{\rm T}$

Calculation of $\langle \psi_0 | \hat{O} | \psi_0 \rangle$ can be approximated, <u>with arbitrary precision</u> (for Bose systems) by $\frac{\langle \psi_\tau | \hat{O} | \psi_\tau \rangle}{\langle \psi_\tau | \psi_\tau \rangle}$

with
$$\psi_{\tau}(R) = \int dR_1 \cdots dR_{\rho} \left\langle R \left| e^{-\frac{\tau}{\rho} \hat{H}} \right| R_{\rho} \right\rangle \times \cdots \times \left\langle R_2 \left| e^{-\frac{\tau}{\rho} \hat{H}} \right| R_1 \right\rangle \psi_{\tau}(R_1)$$

 $R_i = \left\{ \vec{r}_1^i, \cdots, \vec{r}_N^i \right\}$ many-body coordinates

Notice: $\frac{\psi_{\tau}}{\sqrt{\langle \psi_{\tau} | \psi_{\tau} \rangle}} \xrightarrow[\tau \to \infty]{} \psi_{0}$ provided that $\langle \psi_{0} | \psi_{T} \rangle \neq 0$

ψ_T acts only at the
 beginning of the path
 ⇒ essentially
 unbiased like PIMC
 [Nava, Rossi, Reatto, Galli
 J. Chem. Phys. (2009)]

PIGS feature



The whole imaginary time evolution is sampled, via a Metropolis algorithm, at each MC step



Imaginary-time propagators

- For HR we employed the pair-product approximation to express the propagator relative to a small time step $\delta\tau$ as

$$G(R,R';\delta\tau) = \prod_{i=1}^{N} G_{0}(r_{i},r_{i}';\delta\tau) \prod_{i< j}^{N} G_{HR}(r_{i},r_{j};\delta\tau)$$

where G_0 is the free-particle propagator

$$G_{0}(r,r';\delta\tau) = \frac{e^{-(r-r')^{2}/4\lambda\delta\tau}}{\sqrt{2\pi\lambda\delta\tau}} \qquad \lambda = \frac{\hbar^{2}}{2m}$$

G_{HR} is obtained from the exactly known solution of the two-body scattering problem, similarly to a standard approach for hard spheres in 3D [Cao, Berne, J. Chem. Phys. 97 (1992)]:

$$G_{_{H\!R}}(r,r';\delta\tau) = 1 - e^{-\frac{(r-a)(r'-a)}{2\lambda\delta\tau}}$$

ρα	K_L	$\delta \tau$ (1/E _F ($ ho$)
0.005	0.990	0.0025
0.077	0.852	0.0176
0.321	0.461	0.0509
0.471	0.280	0.0219
0.642	0.128	0.0142
0.700	0.090	0.0097
0.900	0.010	0.0012

For 1D ⁴He: fourth-order pair-Suzuki approximation [for example see: Nava et al., J. Chem. Phys. (2009)] and observe convergence of ground state estimates with a typical projection time τ =0.8 K⁻¹ using a time step $\delta\tau$ =1/160 K⁻¹.



Trial state: SWF & SPIGS



- HR: exact ψ_0 is known \Rightarrow the whole imaginary time propagation can be used to compute ground state properties like: $F(\vec{q}, \tau) = \langle \hat{\rho}_{\vec{a}}(\tau) \hat{\rho}_{-\vec{a}}(0) \rangle$
- When ψ_0 is not known we use a Shadow Wave function (SWF):

$$\psi_{SWF}(R) = \phi(R) \int dS \ K(R,S) \ \phi_{s}(S) \qquad S = \left\{ \vec{s}_{1}, \cdots, \vec{s}_{N} \right\}$$

which corresponds to a variationally optimized (first) projection step in imaginary-time.

PIGS+SWF ⇒ Shadow Path Integral Ground State (SPIGS)
 [Galli, Reatto, Mol. Phys. (2003)]:

shadow variables are integrated together with the other path-variables \Rightarrow add 2 more (many-body) variables at the tails of the path



Initial states



• Hard rods (exact!):

$$\psi_{0}^{HR}(x_{1}\cdots x_{N}) = \frac{1}{\sqrt{N!}} \det\left(\frac{e^{ik_{1}x_{j}}}{\sqrt{L'}}\right) \qquad L' = L - Na$$

$$k_{1} = \frac{2\pi}{L'}n_{1}$$

$$n_{1} = -\frac{N-1}{2} + (l-1)$$

$$l = 1, \cdots, N$$

• 1D ⁴He (SWF):
$$\psi_{SWF}(R) = \phi(R) \int dS \ K(R,S) \ \phi_s(S)$$

 $S = \{r_1, \dots, r_N\}$
 $S = \{s_1, \dots, s_N\}$

1D Reatto-Chester term [Phys. Rev. 155 (1967)] $\alpha = 1/\kappa_L$



Our analytic continuation method

F

- QMC: only imaginary time correlations functions
- Analytic continuation task: extract $S(q,\omega)$ from limited and noisy $F(q,\tau)$

$$(\vec{q}, l\delta\tau) = \left\langle \hat{\rho}_{\vec{q}}(l\delta\tau) \hat{\rho}_{-\vec{q}}(0) \right\rangle = \int_{0}^{\infty} d\omega \ e^{-\omega l\delta\tau} S(\vec{q}, \omega) \qquad l = 0, 1, 2, \cdots$$
In these conditions,
numerical inversion of
the Laplace transform:
ill-posed inverse problem

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PHYSICAL REVIEW B 82, 174510 (2010)

Ab initio low-energy dynamics of superfluid and solid ⁴He

E. Vitali, M. Rossi, L. Reatto, and D. E. Galli

GIFT ≡ Genetic Inversion via Falsification of Theories

Statistical inversion method: give up the idea to find *The Solution*, find (via a genetic algorithm) a wide class of spectral functions compatible with $F(q,\tau)$ and be confident only with properties shared by the large majority of them

GIFT: space of models



Chose a wide space of models compatible with a priori information $S(q, \omega) \ge 0$ $S(q, \omega) = 0 \text{ if } \omega \le \omega_{th}(q) (\ge 0)$ $(T=0) \quad \int_{0}^{+\infty} d\omega S(q, \omega) = S(q)$ $\int_{0}^{+\infty} d\omega \omega S(q, \omega) = \frac{q^{2}}{2m}$ \vdots

$$S(q,\omega) = \frac{S(q)}{M} \sum_{i=1}^{N_{\omega}} s_{q}^{(i)} \underbrace{\delta(\omega - \omega_{i})}_{i=1}$$

Delta function

$$\boldsymbol{s}_{q}^{(i)} \in \left\{0, 1, 2, \cdots, M\right\}$$

M = maximum number ofquanta of spectral weight

$$\omega_{i} = \omega_{th} + \Delta \omega (i - 1 / 2)$$
$$\frac{1}{M} \sum_{i=1}^{N_{\omega}} s_{q}^{(i)} = 1$$

Note that S(q) = F(q, 0) is part of QMC "observations"

 $\Delta \omega =$ width of the partition









Stochastic dynamics

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Hard Rods: exact properties



The hard-rods model is exactly solvable by Bethe-ansatz
[Nagamiya, Proc. Phys. Math. Soc. Japan (1940); Mazzanti et al., Phys. Rev. Lett. (2008)]

 PRL 116, 135302 (2016)
 PHYSICAL REVIEW LETTERS
 week ending 1 APRIL 2016

 One-Dimensional Liquid ⁴He: Dynamical Properties beyond Luttinger-Liquid Theory

 G. Bertaina,¹ M. Motta,² M. Rossi,^{3,4,5} E. Vitali,² and D. E. Galli¹

- Excited states are pseudo p-h excitations with renormalized mass $m^* = K_L m$
- Kowledge of excited states & $m^* \Rightarrow exact \omega_{th}$

 $\omega_{th}(q) = \omega_*(q - 2k_F j)$ $2k_F j \le q \le 2k_F(j+1) \quad j = 0, 1, 2, \cdots$

• Exact $\omega_{th} \Rightarrow$ exact exponent $\mu(q)$ of the nonlinear LL theory:

$$\mu(q) = -2\left(\frac{qa}{2\pi} - j\right)\left(\frac{qa}{2\pi} - j - 1\right)$$
$$2k_{F}j \leq q \leq 2k_{F}(j+1) \quad j = 0, 1, 2, \cdots$$

PHYSICAL REVIEW A 94, 043627 (2016) Dynamical structure factor of one-dimensional hard rods M. Motta,¹ E. Vitali,¹ M. Rossi,^{2,3} D. E. Galli,⁴ and G. Bertaina⁴ 1.0 0.5 0.0 -0.5 K₁ =0.99 ρα -1.0 ୍ରି -1.5 -2.0 -2.5 0.700 0.900 -3.0 1.000 K, =0.0 -3.5 -4.0 0.0 0.5 1.5 2.0 1.0 q (units of 2k_F)

Low density regime: spectral weight is broadly distributed inside the p-h band, reminiscent of the Tonks-Girardeau model of impenetrable point like bosons (Lieb Liniger $\gamma \rightarrow \infty$), to which HR model reduces in the $\rho a \rightarrow 0$ limit.

NLL & GIFT: For $q<2k_F \quad \mu(q)$ is slightly larger than zero \Rightarrow weak concentration of spectral weight close to ω_{th} . For $q>2k_F$, $\mu(q)<0$ and large \Rightarrow the support of $S(q,\omega)$ departs from ω_{th} .



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High-density regime: For $q/2k_F < 1.4$ the spectral weight concentrates in a narrow region of the $q-\omega$ plane that gradually departs from $\omega_{th}(q)$.

For $1.4 < q/2k_F < 1.8$, $S(q,\omega)$ broadens and flattens. Finally, for $1.8 < q/2k_F < 2$, the spectral weight again concentrates close to $\omega_{th}(q)$.

Agreement with an exact prediction: $S(q,\omega)$ constant on a finite range of ω for special wave vectors $q_j=2\pi j/a$ [Mazzanti et al., PRL (2008)]





1.10⁻³

9·10⁻⁴

8·10⁻⁴

7·10⁻⁴

6·10⁻⁴

5·10⁻⁴

4·10⁻⁴

3.10-4

2·10⁻⁴

1·10⁻⁴

0

18

 ρ a=0.9: we observe that above q/2k_F=10, S(q, ω) is no more peaked along ω _{th}(q);

stripe structure: repeated p-h band (every $2k_F$); stripes are bounded by the p-h band of the rescaled IFG obtained defining $\rho' = \rho/(1-\rho a)$:

$$\omega_{R}^{\pm} = \frac{\hbar}{2m} \Big| 2\pi \rho' q \pm q^{2} \Big|$$

S(q, ω) flat at special q_i=2 π j/a (red arrows)

 $\begin{array}{c}
\omega_{\pm}^{R} & - - - - \\
\omega_{\pm}^{*} & - - - \\
\omega_{\mu} & - - - - \\
\omega_{\mu} & - - - - \\
\omega_{\mu} & - - - - \\
0 & \rho a = 0.900 \\
K_{L} = 0.010 \\
\end{array}$

8

q (units of 2k_F)

6

10

12

14

16

HR spectrum can be described by the synergy of two IFGs:

- one with the same ρ , but renormalized mass m^{*}=K_Lm
- the other with the same m, but renormalized density $\rho' = \rho / \sqrt{K_L}$

1000

Only in the unphysical $\rho a \rightarrow 1$ limit, S(q, ω) would attain perfect periodicity

1D ⁴He: K_L from S(q) & E(n)



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1D ⁴He: low density regime





- Agreement with LL theory for every ρ : S(q, ω) always peaked around phonon dispersion $\omega = v_s q$ when $q \rightarrow 0$ and $\omega \rightarrow 0$
- Similar to Lieb-Liniger at large K_L (Bogoliubov-like) here due to critical behaviour not to weak coupling
- At large momentum (q \gtrsim k_F) and energy: broadening of spectral weight, filling of the 1D IFG particle-hole band
- By further increasing ρ, the spectral weight starts to concentrate again, emerging as a phonon and then bending downwards to approach ω⁻(q): mixture of Bose & Fermi dynamical properties!

1D ⁴He: high density regime





• For $K_{L} \approx 1$ S(2 k_{F},ω) flat for $\omega \leq E_{F}/\hbar$ but, in contrast with IFG, HR & Lieb-Liniger models, S(q, ω) is not flat for $\omega > E_{F}/\hbar \Rightarrow$ strong non-universality.

- For $K_{L} < 1$, $S(q,\omega)$ is mostly distributed in a region with boundaries $\omega_{*}^{\pm}(q)$, which are modified like HRs: we notice that $\omega_{*}^{-}(q)=\omega_{-}(q)/K_{L}$ which again suggests that $m^{*}=K_{L}m$
- For $K_L \approx 0.13$ using a=2.139 Å (scattering length of repulsive part of V_{He-He}) in the HR analytical expression for $\mu(q)$, we found agreement with NLL and the presence of a special wave vector where $S(q, \omega)$ flattens



1D ⁴He: drag force



• Energy loss per unit time due to an heavy impurity (Fermi's golden rule):

$$\frac{d\varepsilon}{dt} = -F_{v} v \approx -\left(\int_{0}^{\infty} dq \left|\tilde{V}_{q}\right|^{2} \rho \hbar q S(q, qv)\right) v$$
$$\left(\hbar \omega_{q} = \hbar q v - \frac{\hbar^{2} q^{2}}{2m} \approx \hbar q v\right)$$



J Low Temp Phys (2017) 187:419–426 DOI 10.1007/s10909-016-1704-8

Linear Response of One-Dimensional Liquid ⁴He to External Perturbations

M. Motta¹ · G. Bertaina² · E. Vitali¹ · D. E. Galli² · M. Rossi^{3,4}

Used contact potential with the same scattering length of the repulsive part of the ⁴He interaction

This is a perturbative estimate relevant for "soft" impurities. For hard-core impurities (like ³He pinned to ⁴He dislocations) superfluid response is suppressed.

Soft rods

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Conclusions (for hard-core interactions)

• We have computed T=O $S(q,\omega)$ of 1D quantum systems by means of state-of-the-art Path Integral projector and analytic continuation techniques.

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- The low-energy properties of $S(q,\omega)$: agreement with the TLL and nonlinear LL theory and with new analytical relations derived for the HR model
- Quantitative estimation of $S(q,\omega)$ also in the high-energy regime, beyond the predictions of LL theories.
- Non-universality/similarities in HRs and 1D ⁴He. In particular, at high densities both systems show a flat $S(q,\omega)$ at special wave vectors $q_j=2\pi j/a$, in agreement with a previous theoretical prediction for HR.
- Peculiar structure of the HR spectrum in the high-density and highmomentum regime, which can be described in terms of the p-h boundaries of two renormalized IFGs