Lieb-Liniger wavefunctions in a variational ansatz for interacting one-dimensional bosons

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Collaboration

Coworkers

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Outline

1. One-dimensional interacting bosons and Tomonaga-Luttinger liquid
2. The Lieb-Liniger model
3. Description of the ariational method
4. Cherny-Brand Ansatz for the static structure factor
5. Application to 1d dipolar gases

Interacting bosons in one-dimension

second quantized Hamiltonian

$$H = -\frac{1}{2m}\int dx \psi^\dagger(x)\frac{\partial^2\psi}{\partial x^2} + \frac{1}{2}\int dx dx' v(x-x')\psi^\dagger(x)\psi^\dagger(x')\psi(x)\psi(x')$$

Low energy description [Haldane, PRL **47**, 1840 (1981)]

$$H_b = \int \frac{dx}{2\pi}\left[uK(\pi\Pi)^2 + \frac{u}{K}(\partial_x\phi)^2\right]$$

$$uK = \frac{\pi n}{m} \quad \text{(Galilean invariance)}$$

$$\frac{u}{K} = \frac{1}{\pi L}\frac{d^2 E_{GS}(n)}{dn^2} \quad \text{(compressibility)}$$

Tomonaga-Luttinger liquid

Physical observables (Haldane, 1981)

$$\rho(x) = n - \frac{1}{\pi}\partial_x\phi + \sum_{m=1}^{+\infty} A_m \cos[2m(\phi(x) - \pi n x)]$$

$$\psi(x) = e^{i\theta(x)} \sum_{m=0}^{+\infty} B_m \cos[2m(\phi(x) - \pi n x)]$$

Ground state correlations (Haldane, 1981)

$$\langle e^{2in\phi(x)} e^{-2in\phi(x')}\rangle = \left(\frac{a}{|x-x'|}\right)^{2n^2K}$$

$$\langle e^{im\theta(x)} e^{-im\theta(x')}\rangle = \left(\frac{a}{|x-x'|}\right)^{\frac{m^2}{2K}}$$

Determination of the Tomonaga-Luttinger exponent

Numerics: two strategies

1. Deduce K from a correlation function
2. Deduce K from ground state energy

Analytics

- Bogolyubov approximation $K = \sqrt{\frac{n}{m\hat{v}(k=0)}}$ $(n \to +\infty)$
- Hard core bosons $K = 1$ $(n \to 0)$
- integrable models

The Lieb-Liniger model [Phys. Rev. 130, 1605 (1963)]

Hamiltonian ($v(x) = g\delta(x)$)

$$H = -\frac{1}{2m}\int dx \psi^\dagger(x)\frac{\partial^2\psi}{\partial x} + \frac{g}{2}\int dx (\psi^\dagger(x))^2\psi(x)^2$$

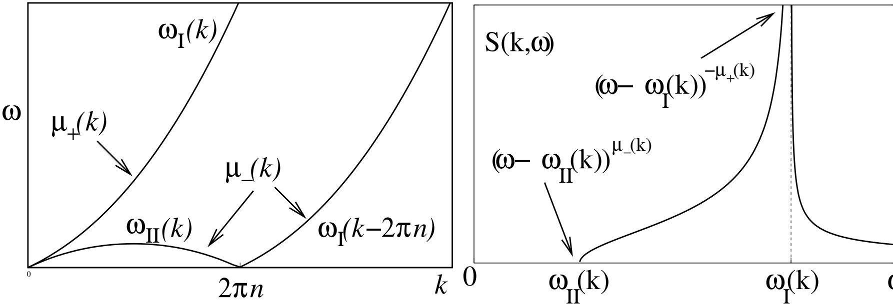
Exact ground state energy (Lieb Liniger Phys. Rev. 1963)

$$2\pi\rho(k) = 1 + \int_{-q_0}^{q_0}\frac{2mg}{(mg)^2 + (k-k')^2}\rho(k')dk'$$

$$\frac{E}{L} = \int_{-q_0}^{q_0} dk\rho(k)\frac{k^2}{2m} = \frac{n^3}{2m}\epsilon(\gamma)$$

$$n = \int_{-q_0}^{q_0} dk\rho(k) \quad \gamma = \frac{mg}{n}$$

Dynamical structure factor of the Lieb-Liniger model



J. S. Caux and P. Calabrese Phys. Rev A **74**, 031605 (2006)

Khodas *et al.* Phys. Rev. Lett. **99**, 110405 (2007)

Shift function and auxiliary functions

Integral equation for the shift function

$$F_B(\nu|\lambda) - \frac{1}{2\pi}\int_{-q_0}^{q_0} \frac{2c}{(\nu-\mu)^2+c^2} F_B(\mu|\lambda) = \frac{1}{2} + \frac{1}{\pi}\arctan\left(\frac{\nu-\lambda}{c}\right),$$

$$\omega_p(\lambda) = \frac{1}{2m}\left[\lambda^2 - 2\int_{-q_0}^{q_0} \mu F_B(\mu|\lambda) d\mu\right]$$

$$k_p(\lambda) = \lambda + 2\int_{-q_0}^{q_0} \arctan\left(\frac{\lambda-\mu}{c}\right)\rho(\mu) d\mu$$

Lieb modes

Parametric representation

$$
\begin{aligned}
\omega_+(\lambda) &= \omega_p(q_0+\lambda) - \omega_p(q_0) \\
k_+(\lambda) &= k_p(q_0+\lambda) - k_p(q_0) \\
\omega_-(\lambda) &= \omega_p(q_0) - \omega_p(q_0-\lambda) \\
k_-(\lambda) &= k_p(q_0) - k_p(q_0-\lambda)
\end{aligned}
$$

- $\omega_+ > \omega_- \forall k$
- $\omega_I(k) = \omega_+(k_+^{-1}(k))$
- $\omega_{II}(k) = \omega_-(k_-^{-1}(k))$ for $k < 2\pi n$
- $\omega_-(k_-^{-1}(k)) = \omega_I(k - 2\pi n)$ for $k > 2\pi n$

Edge exponents

relation to the shift function

$$k_r(\lambda_r) = k$$

$$\delta_\pm(\lambda_r) = 2\pi F_B(\pm q_0, \lambda_r)$$

$$\mu_r(k) = 1 - \frac{1}{2}\left(\frac{1}{\sqrt{K}} + \frac{\delta_+(\lambda_r) - \delta_-(\lambda_r)}{2\pi}\right)^2$$

$$-\frac{1}{2}\left(\frac{\delta_+(\lambda_r) + \delta_-(\lambda_r)}{2\pi}\right)^2$$

Variational method

Variational principle

$$
\begin{aligned}
H &= H_0 + V \\
(H_0 + gU)|\psi_0(g)\rangle &= E_0(g)|\psi_0(g)\rangle \\
\langle\psi_0(g)|H|\psi_0(g)\rangle &\geq E_{GS}(H) \\
\Leftrightarrow E_0(g) - g\frac{dE_0}{dg} + \langle\psi_0(g)|V|\psi_0(g)\rangle &\geq E_{GS}(H)
\end{aligned}
$$

Ansatz

H_0 = Kinetic energy
V = Potential energy
$H_0 + gU$ = Lieb-Liniger Hamiltonian

Using the Lieb-Liniger Hamiltonian as variational Hamiltonian

Variational energy as a function of the structure factor

$$E_{var}(g) = E_0(g) - g\frac{\partial E_0(g)}{\partial g} + \frac{Nn}{2}\hat{v}(k=0)$$
$$+\frac{N}{2}\int_{-\infty}^{\infty}\frac{dk}{2\pi}\hat{v}(k)[S(k;g)-1].$$

The Cherny-Brand ansatz for the structure factor (I)

Dynamical Structure factor [Cherny & Brand Phys. Rev. A 79 043607 (2009)]

$$S(k,\omega) \simeq C\frac{[\omega^\alpha - \omega_-^\alpha(k)]^{\mu_-}}{[\omega_+^\alpha(k) - \omega^\alpha]^{\mu_+}}\Theta(\omega - \omega_-(k))\Theta(\omega_+(k) - \omega)$$

$$\alpha = 1 + \frac{1}{\sqrt{K}}$$

$$\int_0^{+\infty} d\omega\omega S(k,\omega) = N\frac{k^2}{2m}$$

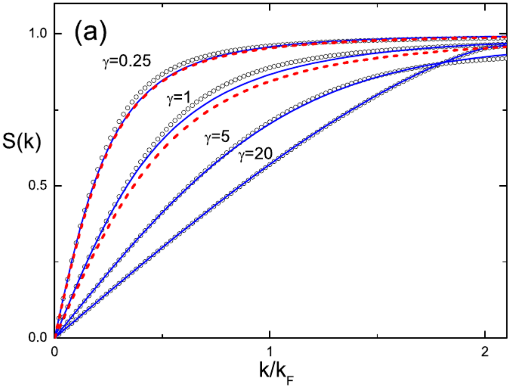
Cherny-Brand ansatz for the structure factor (II)

Static structure factor

$$S(k;g) \simeq \frac{k^2}{2m\omega_-} \times$$

$$\frac{{}_2F_1\left(1+\frac{\sqrt{K}}{1+\sqrt{K}}+\mu_-+\mu_+, 1+\mu_-; 2+\mu_--\mu_+, 1-\left(\frac{\omega_-}{\omega_+}\right)^2\right)}{{}_2F_1\left(1+\frac{2\sqrt{K}}{1+\sqrt{K}}+\mu_-+\mu_+, 1+\mu_-; 2+\mu_--\mu_+, 1-\left(\frac{\omega_-}{\omega_+}\right)^2\right)}$$

Comparison with the exact calculation of Caux and Calabrese



From Cherny and Brand Phys. Rev. A **79**, 043607 (2009)

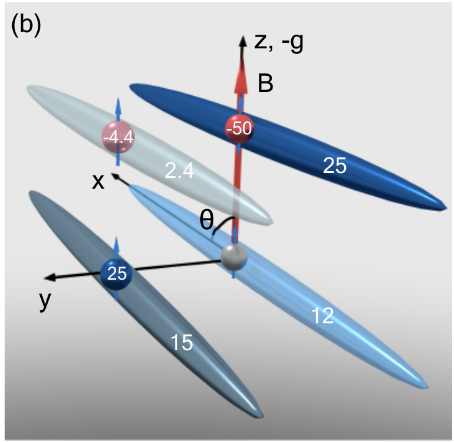
Algorithm

Description

1. For a given g, solve integrals equations for $\rho(k)$ and $F_B(\nu|\lambda)$ by Nystrom method.
2. Find $K, \omega_\pm(k), \mu_\pm(k)$ and deduce $S(k;g)$ from Cherny-Brand Ansatz.
3. Use $S(k;g)$ to obtain the variational energy by numerical integration.
4. Locate the minimum as a function of g with the Golden search algorithm.

Application to the dipolar gas

Realizations of dipolar gas



Magnetic atoms trapped in quasi-1d tubes and aligned by a magnetic field

- Chromium (^{52}Cr, $\mu_{Cr} = 6\mu_B$)
- Erbium (^{168}Er, $\mu_{Er} = 7\mu_B$)
- Dysprosium (^{162}Dy $\mu_{Dy} = 6\mu_B$)

From Tang *et al.* Phys. Rev. X **8**, 021030 (2018).

Potential in the dipolar gas with transverse trapping

Single Mode Approximation [Sinha& Santos Phys. Rev. Lett. **99**, 140406 (2007)]

$$V_{dd}(x-x') = V(\theta)\left[V^{1D}_{DDI}\left(\frac{x-x'}{l_\perp}\right) - \frac{8}{3}\delta\left(\frac{x-x'}{l_\perp}\right)\right],$$

$$V(\theta) = \frac{\mu_0\mu_D^2}{4\pi}\frac{1-3\cos^2\theta}{4l_\perp^3},$$

$$V^{1D}_{DDI}(u) = -2|u| + \sqrt{2\pi}\left[1+u^2\right]e^{\frac{u^2}{2}}\,\mathrm{erfc}\left(\frac{|u|}{\sqrt{2}}\right),$$

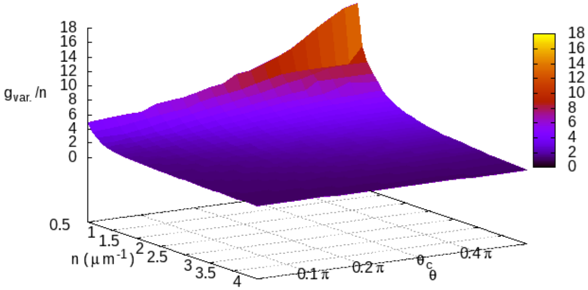
Full Hamiltonian

Van der Waals (contact) and dipolar

$$H_{Q1D} = -\frac{\hbar^2}{2m}\sum_i \frac{\partial^2}{\partial x_i^2} + \sum_{i<j} V_{dd}(x_i - x_j)$$
$$+ g_{VdW} \sum_{i<j} \delta(x_i - x_j)$$

We will fix θ,$l_\perp$,g_{VdW} and vary n

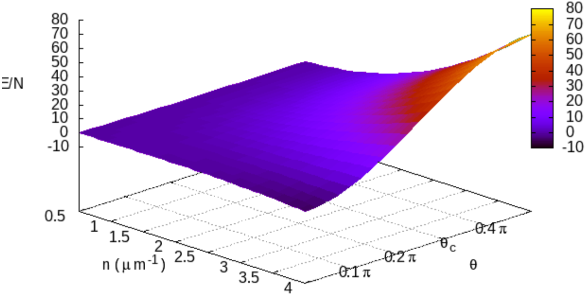
Calculated variational parameter



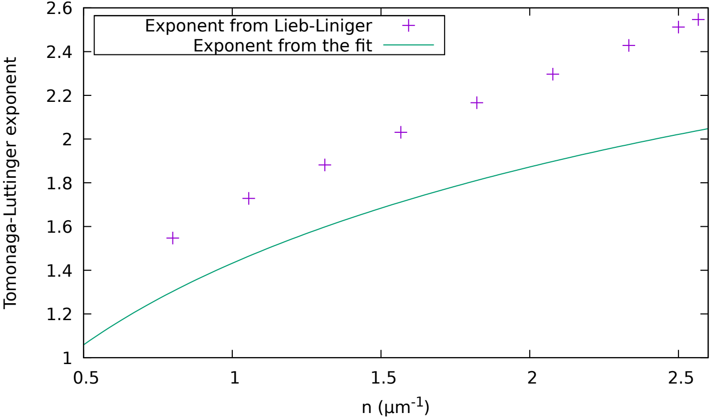
Interactions are more repulsive at low density

Dipolar interactions lead to strong angular dependence

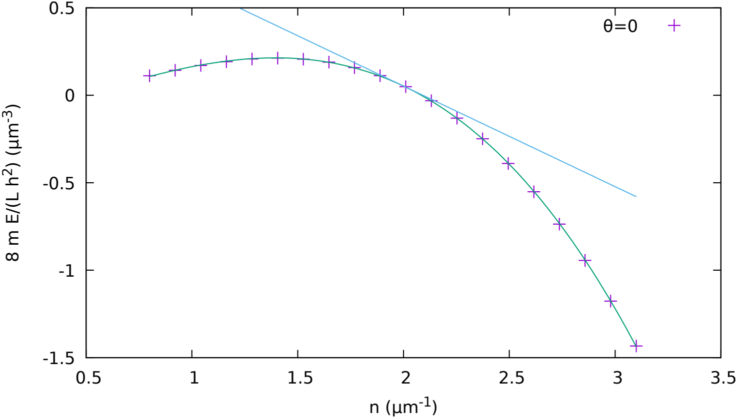
Calculated energy per particle



Tomonaga-Luttinger exponent for $\theta = \frac{\pi}{2}$



Instability for $\theta = 0$



Conclusion

Summary

- Variational calculation of ground state energy of interacting bosons
- Fast technique (12min on desktop PC)
- allows numerical computation of Tomonaga-Luttinger exponent
- suggest instability for attractive dipolar interaction

Perspectives

- More accurate calculation using the form factor approach
- Application to other models (shoulder potential)
- Application to the super-Tonks state