A Bose gas with impurities in one dimension

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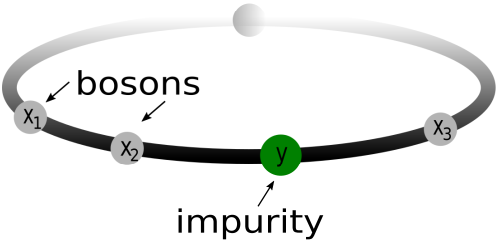
Outline

- System [A Bose gas with impurities in one dimension] and Goal
- Motivation
  1. Why to study systems with impurities
  2. Why to study our system
- Two techniques
  1. the similarity renormalization group
  2. the Gross-Pitaevski equation
- Outlook

System

System



$$H = -\frac{\hbar^2}{2m_B}\sum_i \frac{\partial^2}{\partial x_i^2} - \frac{\hbar^2}{2m_I}\frac{\partial^2}{\partial y^2} + g_{BB}\sum_{i>j}\delta(x_i - x_j) + c\sum_i \delta(x_i - y)$$

$c, g_{BB} > 0$

Goal: Understand the ground-state properties.

Motivation

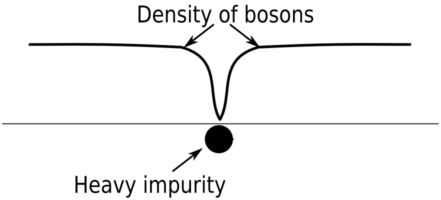
Why to study systems with impurities?

Properties of an environment change due to the presence of impurities.

Examples:

In Semiconductors: (Germanium + 0.001% Arsenic) has the electrical conductivity of Germanium times $\sim$ 10 000.

Transport properties of a Bose gas can be strongly affected by an impurity:

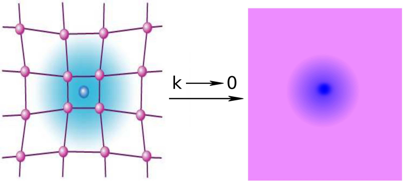


Why to study systems with impurities?

One-body dynamics change due to the presence of an environment.

Example:

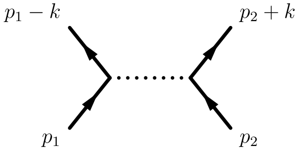
An electron in an ionic crystall forms a polaron



$$H_{real} \qquad \rightarrow \qquad H_{imp} = \epsilon - \frac{\hbar^2}{2m_{eff}}\frac{\partial^2}{\partial y^2}$$

Why to study systems with impurities?

To understand changes in few-body physics due to the presence of an environment, e.g., emergent potential between impurities



Formation of a bipolaron.

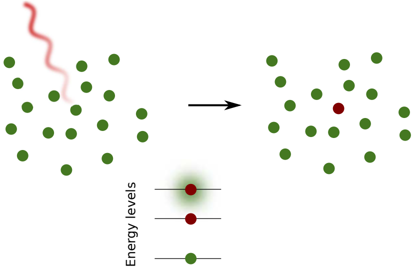
Examples of systems with impurities

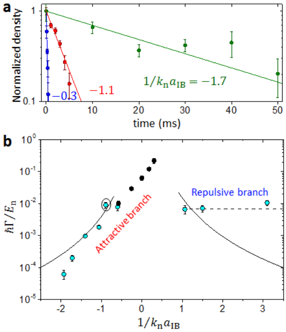
- e^- interacting with phonons,
- ^{3}He in ^{4}He,
- proton in a neutron star,
- ...

Simulations with cold atoms

The classic problems are often hard to solve, but one can create and study simpler systems using cold atoms (cf. talks of M. Köhl and M. Zwierlein)

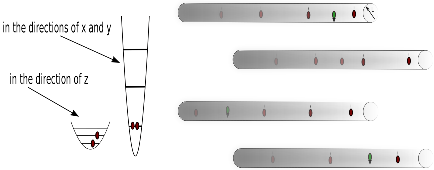
- to test theoretical models
- to understand the problem deeper



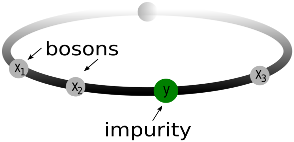


Right figure from : Ming-Guang Hu et al., PRL **117**, 055301 (2016)

In cold atom systems the geometry can be tuned,



The interaction potential can be modified using external fields.



One can create cold atomic systems that can be described by the Hamiltonian (neglecting decay)

$$H = -\frac{\hbar^2}{2m_B}\sum_i \frac{\partial^2}{\partial x_i^2} - \frac{\hbar^2}{2m_I}\frac{\partial^2}{\partial y^2} + g_{BB}\sum_{i>j}\delta(x_i - x_j) + c\sum_i \delta(x_i - y)$$

Below I will discuss how to calculate the ground state energy of this Hamiltonian non-perturbatively.

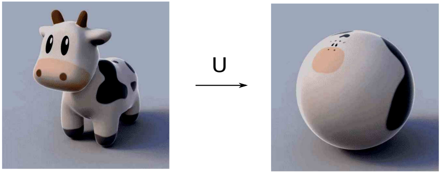
$$H \to H_{imp} = \epsilon(L) - \frac{\hbar^2}{2m_{eff}}\frac{\partial^2}{\partial y^2}$$

Approaches to the problem

Flow equations (Similarity Renorm. Group)

To diagonalize the problem

$$H_{diagonal} = UHU^{\dagger},$$

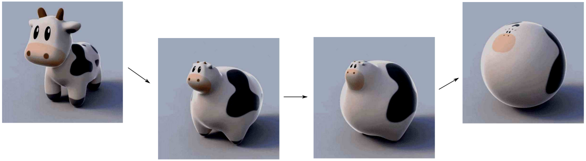


Flow equations (Similarity Renorm. Group)

The matrix U is usually not known, so instead we use the flow equations

$$\frac{\mathrm{d}\mathcal{H}(s)}{\mathrm{d}s} = \eta\mathcal{H} - \mathcal{H}\eta \equiv [\eta, \mathcal{H}(s)],$$

here $\mathcal{H}(0) = H$, and $\mathcal{H}(s \to \infty) \to H_{diagonal}$



S. Kehrein, *The Flow Equation Approach to Many-Particle Systems* (2006).
K. Tsukiyama, S. K. Bogner, and A. Schwenk, PRL **106**, 222502 (2011).

Generators

The generator η defines the fixed points of the evolution. When $\eta = 0$ the dynamics stop.

For example, if we want to eliminate the coupling B_{ijkl} from the bosonic Hamiltonian (without the impurity)

$$H = \sum_{ij} A_{ij} a_i^\dagger a_j + \sum_{ijkl} B_{ijkl} a_i^\dagger a_j^\dagger a_k a_l$$

we can use

$$\eta(s) = B_{ijkl}(s) a_i^\dagger a_j^\dagger a_k a_l - H.C.$$

$$\frac{\mathrm{d}\mathcal{H}}{\mathrm{d}s}|_{s=0} = [\eta(0), H]$$

$$\downarrow$$

$$\mathcal{H}(\Delta s) = H + \Delta s \left(\sum_{ij} D_{ij} a_i^\dagger a_j + \sum_{ijkl} E_{ijkl} a_i^\dagger a_j^\dagger a_k a_l + \sum_{ijklmn} F_{ijklmn} a_i^\dagger a_j^\dagger a_k^\dagger a_l a_m a_n \right) + O(\Delta s^2)$$

Truncation

$$\mathcal{H}(s) = \sum_{ij} A_{ij}(s) a_i^\dagger a_j + \sum_{ijkl} B_{ijkl}(s) a_i^\dagger a_j^\dagger a_k a_l + \sum_{\mathrm{N}=3}^{\infty} \text{N-body interactions}$$

Truncation procedure:

$$\mathcal{H}(\Delta s) = H + \Delta s \left(\sum_{ij} D_{ij} a_i^\dagger a_j + \sum_{ijkl} E_{ijkl} a_i^\dagger a_j^\dagger a_k a_l + \sum_{ijklmn} F_{ijklmn} a_i^\dagger a_j^\dagger a_k^\dagger a_l a_m a_n \right) + O(\Delta s^2)$$

$$\sum_{ijklmn} F_{ijklmn} a_i^\dagger a_j^\dagger a_k^\dagger a_l a_m a_n = a_0^\dagger a_0 \sum L_{ijmn} a_i^\dagger a_j^\dagger a_m a_n + W$$

$$\mathcal{H}_{tr}(\Delta s) \simeq H + \Delta s \left(\sum_{ij} D_{ij} a_i^\dagger a_j + \sum_{ijkl} E_{ijkl} a_i^\dagger a_j^\dagger a_k a_l + N \sum_{ijkl} L_{ijmn} a_i^\dagger a_j^\dagger a_m a_n \right) + O(\Delta s^2)$$

Truncation

After Truncation:

$$\mathcal{H}_{tr}(s) = \sum_{ij} A_{ij}(s) a_i^\dagger a_j + \sum_{ijkl} B_{ijkl}(s) a_i^\dagger a_j^\dagger a_k a_l,$$
$$\eta(s) = \sum_{ij} \eta_{ij}(s) a_i^\dagger a_j + \sum_{ijkl} \eta_{ijkl}(s) a_i^\dagger a_j^\dagger a_k a_l$$

We are after only the ground state: block-diagonalization of the matrix.

A reference state includes preliminary information about the system.

We work with bosons – reference state is simply $\Psi(x_1, ..., x_N) = \prod \phi(x_i)$

AGV and H.-W. Hammer, New J. Phys. **19**, 113051 (2017)

Estimation of corrections

The error is due to truncation

$$\sum_{ijklmn} F_{ijklmn} a_i^\dagger a_j^\dagger a_k^\dagger a_l a_m a_n = a_0^\dagger a_0 \sum L_{ijkl} a_i^\dagger a_j^\dagger a_m a_n + W$$
$$\simeq N \sum L_{ijmn} a_i^\dagger a_j^\dagger a_m a_n$$

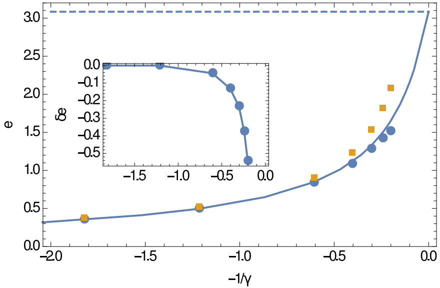
Use matrix perturbation theory to estimate corrections

$$\mathcal{H}(s) = \mathcal{H}_{tr}(s) + \int_0^s \tilde{W}(x)\mathrm{d}x + \int_0^s [\eta(x), \mathcal{H}(x) - \mathcal{H}_{tr}(x)]\mathrm{d}x$$

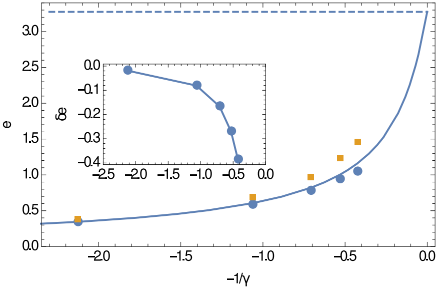
Without impurity (Lieb-Liniger gas)

$$H = -\frac{1}{2}\sum_i \frac{\partial^2}{\partial x_i^2} + g_{BB}\sum_{i>j}\delta(x_i - x_j)$$

As a reference state – the ground state at $g_{BB} = 0$



$N = 4$



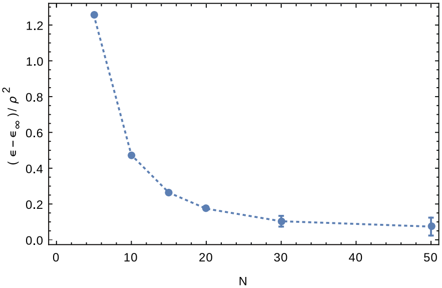
$N = 15$

$\gamma = \frac{g_{BB}}{\rho}, e = \frac{E}{\rho^2}, \rho = \frac{N}{L}$

With impurity

$$H = -\frac{1}{2}\sum_i \frac{\partial^2}{\partial x_i^2} - \frac{1}{2}\frac{\partial^2}{\partial y^2} + g_{BB}\sum_{i>j}\delta(x_i - x_j) + c\sum_i \delta(x_i - y)$$

Approach to the thermodynamic limit ($N = \rho L \to \infty$):



Weakly-interacting Bose gas with impenetrable impurity ($\gamma = \frac{g_{BB}}{\rho} = 0.1$, $\frac{1}{c} = 0$)

AGV and H. W. Hammer, PRA(R) **96**, 031601 (2017)

Gross-Pitaevski equation (without impurity)

GPE: Mean-field description of a weakly-interacting Bose gas

$$H = -\frac{\hbar^2}{2m_B}\sum_i \frac{\partial^2}{\partial x_i^2} + g_{BB}\sum_{i>j}\delta(x_i - x_j).$$

To derive it we assume that

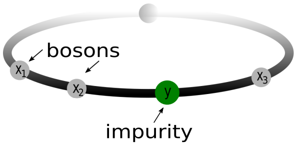
$$\Psi(x_1, ..., x_N) = \psi(x_1)...\psi(x_N),$$

which leads to the GPE

$$-\frac{\hbar^2}{2m_B}\frac{\partial^2}{\partial x^2}\psi(x) + g_{BB}N\psi(x)^3 = \mu\psi(x).$$

This equation has an analytic solution

Gross-Pitaevski equation (with impurity)



$$H = -\frac{\hbar^2}{2m_B}\sum_i \frac{\partial^2}{\partial x_i^2} - \frac{\hbar^2}{2m_I}\frac{\partial^2}{\partial y^2} + g_{BB}\sum_{i>j}\delta(x_i - x_j) + c\sum_i \delta(x_i - y)$$

- new coordinates $z_i = x_i - y$,
- Gross-Pitaevski-type equation for the bosons in new variables: $\Psi = \phi(z_1)...\phi(z_N)$

$$-\frac{\hbar^2(m_I + m_B)}{2m_B m_I}\frac{\partial^2}{\partial z^2}\phi(z) + g_{BB}N\phi(z)^3 + c\delta(z)\phi(z) = \mu\phi(z)$$

AGV and H. W. Hammer, PRA(R) **96**, 031601 (2017)

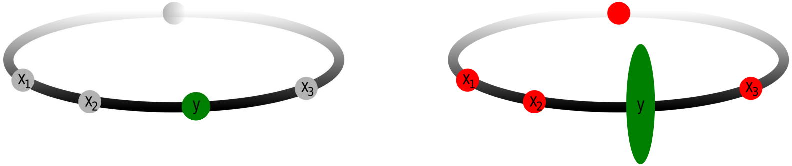
Gross-Pitaevski equation (with impurity)

This equation has also an analytical solution, but does it make sense?

For example, We can derive the same equation for a heavy impurity and bosons of mass $m_B m_I/(m_I + m_B)$

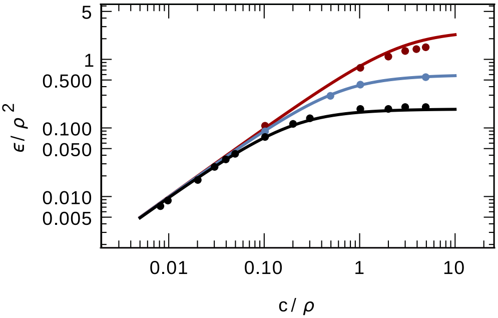
$$H = -\frac{\hbar^2(m_I + m_B)}{2m_B m_I}\sum_i \frac{\partial^2}{\partial x_i^2} + g_{BB}\sum_{i>j}\delta(x_i - x_j) + c\sum_i \delta(x_i - y) \to$$

$$-\frac{\hbar^2(m_I + m_B)}{2m_B m_I}\frac{\partial^2}{\partial x^2}\phi(x) + g_{BB}N\phi(x)^3 + c\delta(x - y)\phi(z) = \mu\phi(z)$$



Infinitely heavy impurity (thermodynamic limit)

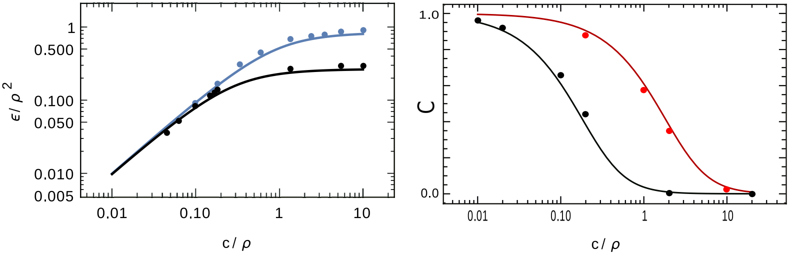
$$\epsilon = E(c) - E(c = 0),$$



$\frac{g_{BB}}{\rho} = 0.02, 0.2$ and 4 (from the bottom to the top)

Dots – quantum Monte-Carlo results: L. Parisi and S. Giorgini, PRA **95**, 023619 (2017)

Equal masses (thermodynamic limit)



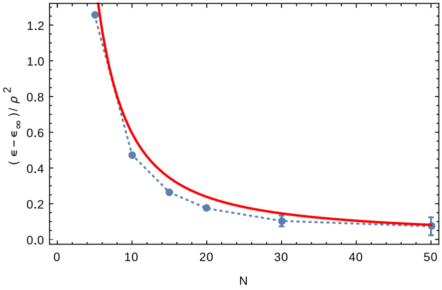
$\frac{g_{BB}}{\rho} = 0.02$ (bottom) and 0.2 (top) $\frac{g_{BB}}{\rho} = 0.02$ (bottom) and 2 (top)

Contact: $C = \frac{n_{BB}(z=0)}{\rho}$ – density of bosons at the impurity position.

Dots – quantum Monte-Carlo results: L. Parisi and S. Giorgini, PRA **95**, 023619 (2017)

Approach to the thermodynamic limit

$N \to \infty$, $L \to \infty$ with $\frac{N}{L} = \rho$



$\frac{g_{BB}}{\rho} = 0.1$, $\frac{1}{c} = 0$.

Dots – the flow equations, curve – the Gross-Pitaevski equation.

Outlook

- Combination of the analytical reference state with the similarity renormalization group.
- Two and three spatial dimensions:
  1. Numerical investigation.
  2. Can we use succesfully simple analytical ideas discussed here?
- Time dynamics of an impurity.
- Induced correlations between impurities. Effective impurity-impurity interactions.

Impurity-impurity interaction potential

Weakly-interacting regime ($c \to 0$) – attraction:

$$V(y_1 - y_2) \sim -\frac{c^2}{\sqrt{\gamma}} e^{-2\sqrt{\gamma}\rho|y_1 - y_2|}.$$

Impenetrable limit ($1/c = 0$) – attraction at small values of $|y_1 - y_2|$.
Repulsion at $|y_1 - y_2| \to \infty$:

$$V(y_1 - y_2) \sim \sqrt{\gamma} e^{-\sqrt{\gamma}\rho|y_1 - y_2|}.$$

A. Dehkharghani, AGV, and N. Zinner, arXiv:1712.01538

Collaboration

Hans-Werner Hammer, TU Darmstadt (Germany)

Amin Dehkharghani and Nikolaj Zinner, Aarhus University (Denmark)

Thank you