Introduction

- When a system has reached sufficient size for it to be properly described by thermodynamic theory, it is a complicated question to answer.
- This project has been motivated by a recent experiment [1].
- The system considered is a one-dimensional system composed by one impurity interacting with a bosonic bath in the presence of an external harmonic potential.
- We address the question by studying the binding energy of an impurity interacting with a one-dimensional bosonic system of increasing size for different coupling strengths.
- In order to simplify the problem, we assume the coupling strength between the bosons and between the impurity and the bosons to be the same (\(g_{gb} = g_{bb} = g_0\)).
- Then, the problem reduces to, solve system

\[
\hat{H} = \frac{\hbar^2}{2m} \sum_{n=1}^{N} \frac{d^2}{dx^2} \sum_{j=1}^{N} \frac{1}{2} \phi_j^2 + \sum_{\langle i,j \rangle} g_0 \delta(x_i-x_j)
\]

(1)

and to compute the binding energy (i.e., chemical potential) using the ground-state energy of a Bose gas \(E_0\).

\[
\mu = E_0(N+1) - E_0(N)
\]

(2)

- Results of solving (1) are compared to the thermodynamic predictions. From this, we can determine when the system has reached a sufficiently large size for the thermodynamical theory to apply.

Theoretical predictions

Two interacting bosons in an external harmonic field (\(N = 2\))

The equation describing the energy levels of the system (1) with \(N = 2\) is

\[
E = E_{CM} + E_r = 0.5 + E_r,
\]

where \(E_r\) depends on the scattering length and has the expression,

\[
\frac{2}{\Gamma(-E_r/2 + 3/4)} - \frac{2}{\Gamma(-E_r/2 + 1/4)} = \sqrt{2} \frac{a_{\infty}}{a}
\]

(3)

Bath of interacting bosons in an external harmonic field (\(N \to \infty\))

Lieb-Liniger theory solves the problem of an homogeneous gas of interacting bosons when \(N \to \infty\) [2]. After finding \(\mu(r_0)\), we derive the chemical potential expression for a bath of interacting bosons in an harmonic trap by means of the local density approximation (LDA),

\[
\mu_0 = \mu_l(n(x)) + V_{ext}(x), \quad N = \int n(x) dx
\]

(4)

Results

The binding energy of one impurity interacting with a Bose gas of increasing size is computed for five different values of \(g\) thanks to the DMC method.

Conclusions

For intermediate values of the coupling strength \(g\), we determine for which \(N\) the system can be described using thermodynamic theory.

<table>
<thead>
<tr>
<th>(g)</th>
<th>(N)</th>
<th>crossing (N)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>≈</td>
<td>30</td>
</tr>
<tr>
<td>2</td>
<td>≈</td>
<td>45</td>
</tr>
<tr>
<td>20</td>
<td>≈</td>
<td>50</td>
</tr>
</tbody>
</table>

Table 1: values of \(N\) at which the crossover occurs for different \(g\).

- Tonks-Girardeau limit, \(g \to \infty\): In this case, the gas exhibits Fermi-like features. Interestingly enough, an analytical expression exists for the chemical potential:

\[
\mu_F(N+1) = \hbar(N + \frac{1}{2})
\]

(6)

Let the binding energy be defined as,

\[
e_r = \frac{\mu_{\text{DMC}} - \mu_{\text{LDA}}}{\mu_{\text{LDA}}}
\]

(5)

where \(\mu_{\text{DMC}}\) stands for the exact BE computed using DMC.

In the following figure, the decrease of the relative error in function of \(N\) can be appreciated.

State of art

Here we present the results reported in Science by [1] that motivated our work.

- The authors of [1] studied the crossover from few- to many-body physics in the case of a quasi 1D system consisting of one impurity interacting with an increasing number of fermions.
- Impurity and fermions are in different hyperfine states. Thus, only impurity and fermions will be able to interact.

Fig. 1: Orange line: \(N \to \infty\), blue line: \(N = 2\). Dots ranging from blue to orange represent systems from \(N = 1\) to 5.

Fig. 2: Relative error in function of \(N\)

Methodology

- In order to compute (2), the ground-state energy of the system described in (1) has to be computed.
- We will solve analytically the limiting cases \(N = 1\), \(N = 2\) and \(N \to \infty\). \(N \to \infty\) corresponds to the thermodynamical limit and it will be solved by means of Lieb-Liniger theory and local density approximation.
- Values \(E_0\) for systems of intermediate sizes have to be obtained numerically using variational and diffusion Monte Carlo methods.

State of art

References
