Many-particle systems in one dimension in the harmonic approximation

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Abstract
We consider the energetics and structural properties of a many-particle system in one dimension with pairwise contact interactions confined in a parabolic external potential. To render the problem analytically solvable, we use the harmonic approximation scheme at the level of the Hamiltonian. We investigate the scaling with particle number of the ground-state energies for systems consisting of identical bosons or fermions. We then proceed to focus on bosonic systems and make a detailed comparison with known exact results in the absence of the parabolic external trap for three-body systems. We also consider the thermodynamics of the harmonic model, which turns out to be similar for bosons and fermions due to the lack of degeneracy in one dimension.

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(Some figures may appear in colour only in the online journal)

1. Introduction

Exactly solvable models are key players in few- and many-body quantum mechanics and are indeed also fascinating creatures [1, 2]. The analytical intractability of general $N$-body systems makes it very important to have exact results to allow benchmark tests of complicated numerical methods. Unfortunately, exactly solvable models are few and far between and are more often found in low-dimensional systems. In the case of one spatial dimension, the famous Bethe ansatz [3] was successfully applied to models of bosons with zero-range interactions [4–6] and later on to interactions with a long range [7, 8].

In the field of cold atomic gases, an exciting direction has been taken aimed at the study of low-dimensional systems in general and one-dimensional (1D) setups in particular [9]. A notable highlight of this pursuit is the experimental realization of the so-called Tonks–Girardeau gas [10–12], where strongly interacting 1D bosons become impenetrable objects and behave similar to fermions [13, 14]. Very recently, it has even become possible to study this interesting regime in the limit of small particle number [15, 16].

Here we study an exactly solvable model of an $N$-body system in an external parabolic confinement. The outer trap is always present in cold atomic gas experiments but can often be neglected or treated in a local density approximation when large systems are studied. However, for small particle numbers the effect of the outer trap becomes important for the structure and dynamics of the system. To make the $N$-body problem tractable, we use a harmonic Hamiltonian approximation [8] with carefully chosen parameters that reproduce the essential features of two atoms interacting via short-range interactions in a parabolic trap [17].

This paper is organized as follows. After our discussion of the harmonic methods, we provide details of how the parameters of the harmonic interactions are obtained from knowledge of the exact solution to the two-body problem originally obtained by Busch et al [18]. We then present the results for the ground-state energies and the radii. Our focus is on bosonic systems, but we present a few results for fermions as well. A comparison with the exact results of MacGuire [6] is then made in relevant limits. We also compute the one-body density matrix and its largest eigenvalue to obtain the condensate fraction at zero temperature. Finally, we discuss the thermodynamics of our model and then proceed to the conclusions and the outlook for future work.

2. The method

We consider a system of $N$ quantum particles interacting pairwise via a delta function interaction and confined by a harmonic external potential in one spatial dimension.
The Hamiltonian for this system is
\[ H = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \frac{\partial^2}{\partial x_i^2} + \frac{1}{2} m \omega_0^2 \sum_{i=1}^{N} x_i^2 - \frac{2\hbar^2}{ma} \sum_{i,k} \delta^{(1)}(x_i - x_k), \]
(1)
where \( m \) is the mass of the particles, \( \omega_0 \) is the frequency of the external field and \( a \) is the 1D scattering length that parameters the strength of the two-body interaction (we will discuss below its relation to 3D scattering length). The external field \( \omega_0 \) defines the length scale of our system, \( l^2 = \hbar/(ma) \). For two particles, (1) has been solved in, e.g., [18, 19], and their results on two-body energies and wave functions for a given scattering length are used to determine the parameters of our model. We consider only the bound molecular branch of the system, i.e. \( a > 0 \).

In our general harmonic approximation scheme, we replace Hamiltonian (1) with
\[ H = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \frac{\partial^2}{\partial x_i^2} + \frac{1}{2} m \omega_0^2 \sum_{i} x_i^2 + \frac{1}{2} \mu \omega_0^2 \sum_{i,k} (x_i - x_k)^2 + V_S, \]
(2)
where \( \mu = m/2 \) is the reduced mass of the two-body system, \( \omega_0 \) is the interacting frequency and \( V_S \) is an energy shift. The solution to this equation for \( N \) particles for general systems is described in detail in [17] and, more specifically, for identical particles in [8, 20].

The parameters \( \omega_0 \) and \( V_S \) are now chosen to fit pertinent properties of the original Hamiltonian at the two-body level in the usual spirit of constructing descriptions of \( N \)-body systems based on two-body interactions. Here we impose the condition that at the two-body level the harmonic oscillator reproduces the energy and average square radius of the exact two-body solution. In order to fulfill these constraints, we use the size of the system to determine the interaction frequency through the relation
\[ \langle \psi | x^2 | \psi \rangle = \frac{\hbar}{2\mu \sqrt{\omega_0^2 + \alpha_0^2}}. \]
(3)
where \( x = x_1 - x_2 \) is the relative coordinate in the two-body system. The energy shift is determined by requiring that the model reproduces the energy of the two-body system
\[ E_2 = \frac{1}{2} \hbar \sqrt{\omega_0^2 + \alpha_0^2} + V_S. \]
(4)
The quantities \( E_2 \) and \( \langle x^2 \rangle \) can be easily obtained by numerically solving the transcendental equations fulfilled by the exact solution for two bosons (or two fermions in different spin states) interacting via a zero-range interaction in a parabolic trap [18]. Note that when we consider identical fermions below, there can, in principle, only be a non-zero two-body interaction in states that are odd under exchange of the two fermions. In this paper, we are mostly interested in the scaling behaviour with particle number of the fermions as the interaction frequency is varied (through the scattering length), and we therefore ignore this point and use the same input for fermions as for bosons. The most important difference is, of course, the quantum statistics, which is fully taken into account.

We note that in cold atoms, effective 1D setups are created by using a tightly confining potential in two transverse directions, usually through the application of an optical lattice [9]. In a deep transverse lattice, the atoms are then effectively occupying only the lowest transverse motional degree of freedom. This transverse degree of freedom, however, has an influence on the effective 1D scattering length that described the inter-atomic interaction in the system. A mapping exists between the true 3D scattering length and the effective 1D scattering length that takes the transverse degrees of freedom explicitly into account [21]. This mapping should thus be applied before making a comparison with realistic experiments.

Once the parameters have been determined, (2) can be solved. The ground-state energy for identical bosons is
\[ E_{g}^{(b)} = \frac{1}{2} N(N - 1) V_S + \frac{1}{2} (N - 1) \hbar \omega_0 + \frac{1}{2} \hbar \omega_0, \]
(5)
where
\[ \omega_0^2 = N \omega_m^2 / 2 + \omega_0^2 \]
(6)
is the \( (N - 1) \)-degenerate frequency that comes from the solution of (2) [17]. The last term in (5) is the energy related to the centre-of-mass motion and will be ignored as we are interested in the internal dynamics of the system.

Although most of this work is about bosons, input for identical fermions is also possible. Since fermions obey the Pauli principle, \( N - 1 \) particles must be placed at higher oscillator levels as there are no degeneracies in one dimension. We can obtain the amount of energy in the ground state by filling consecutive oscillator levels, i.e.
\[ \hbar \omega_0 \sum_{k=0}^{N-1} \left( k + \frac{1}{2} \right) = \frac{N^2}{2} \hbar \omega_0. \]
(7)
The complete ground-state energy is then
\[ E_{g}^{(f)} = \frac{1}{2} N(N - 1) V_S + \frac{N^2}{2} \hbar \omega_0 + \frac{1}{2} \hbar \omega_0. \]
(8)
This is a different scaling from that for the bosons in (5). In the fermion case, the energy is dominated by the \( N^2 \hbar \omega_0 / 2 \) term, which scales as \( N^{3/2} \).

3. Results
We now present numerical results obtained for systems with \( N = 3 \sim 30 \) particles studying their energetics, the radial behaviour of the systems and the one-body density matrix. Here we focus on the case of identical bosons. A particular issue is the ratio of the three-body energy to the two-body energy. The exact formula of MacGuire [6] applies to 1D systems of bosons with zero-range interactions, and we make a comparison of the harmonic results with that model in the strongly bound limit where the two-body energy is large and negative. Finally, we also consider the thermodynamics of the system within the harmonic approximation.
3.1. Energies and radii

The ground-state energy for bosons is shown in figure 1 and that for fermions is shown in figure 2 for different particle numbers and scattering lengths. Note that the upper panels show the energy per particle, while in the lower panels the energy is divided by a different power that we will discuss below. A striking feature to note is the positivity of the energy for fermions, while that of the bosons can have both signs. This is a consequence of the Pauli principle, which implies that the fermions will have to occupy higher orbitals for lack of degeneracies in one dimension as discussed above. Even in the case of very small scattering lengths (and thus large negative two-body binding energies) the contribution from the higher orbits renders the overall ground-state energy positive.

Once the two-body problem is solved and the parameters are determined, they follow the behaviour of (5). As seen in figure 1, the sign of the energy of the Bose system is mostly negative, but for small systems at large scattering lengths, the energy turns positive. This can be understood from the fact that the energy shift, $V_S$, is negative and the shift term in the energy of (5) scales with $N^2$, while the positive oscillator frequency term scales with the lower power $N^{3/2}$. For bosons, the energy is positive for all the particle numbers examined for $a/l = 100$. Using equation (5), one can derive the critical number for bosons where the energy changes sign. It is given by

$$N_{\text{crit}} = \frac{\hbar^2 \omega^2_{\text{cm}} + 2\sqrt{\hbar^2 \omega^4_{\text{cm}}/4 + 4V^2_S \omega^6_0}}{4V^2_S}.$$  \hspace{1cm} (9)

From this relation one can calculate that for bosons the energy becomes negative at $a/l = 100$ when $N \geq 116$.

The bottom panels of figures 1 and 2 show the energies divided by the relevant scaling factor ($N^2$ for bosons and $N^{5/2}$ for fermions) to emphasize the scaling behaviour at large $N$. In the figures we can see that the asymptotic scalings are nicely approached when the scattering length is not too small. For the case of small scattering length, the two-body energy will, in general, behave as $E_2 \sim -1/a^2$ while $\langle x^2 \rangle \sim a^2$, since in this limit the trap can be ignored on the bound state branch in the spectrum that we study here. However, the relations in (3) and (4) that we use to determine our oscillator parameters now imply that both $V_S$ and $\omega_0$ must scale with $a^{-2}$ to be fulfilled (note that $E_2$ is negative). This means that there will be competition between the terms in the ground-state energies given by (5) and (8). The asymptotic behaviour for large $N$ is therefore approached more slowly for small $a$.

We also calculate the relative size of the bosonic ground-state wave functions, $\langle (X - X_{\text{CM}})^2 \rangle$, as a function of particle number for several different scattering lengths. Note here that $X$ denotes the single-particle coordinate of one of the bosons and that no index is needed since the particles are identical. The results are shown in figure 3. One can see for the large scattering lengths that the radius increases before eventually decreasing for larger particle numbers (more than 20 for $a/l = 100$). For scattering lengths of 2 and smaller, the size decreases monotonically with increasing particle number. Again this is connected to the fact that the small $a$ regime has very strong two-body binding and thus small $\langle x^2 \rangle$ which is imprinted on the $N$-body system, which tends to be very compact and presumably leads to strong clusterization in the real system followed by loss of atoms from the trap.

For fermions (not shown), the Pauli principle and the subsequent need to occupy higher orbitals mean that the system will, in general, be larger for the same scattering length and will not show a decreasing behaviour when $N$ is increased but rather a slight increase. This can be seen from the energetics of the ground state in (8), which is dominated by the positive term containing the oscillator frequency for large $N$. This implies that the radius will remain large, constrained solely by the external trap.
two and three dimensions [17]. In the present 1D study, we see a non-monotonic behaviour in the radii as a function of $N$ which can also be seen in two dimensions but which is almost completely absent in the corresponding 3D system. The scattering lengths for which the maximum in the size occurs are roughly those where the three-body energy comes out positive. This implies an increased radial size, although still restricted by the external trapping potential. For large $N$, however, the bosons will always become negative in energy as the shift term dominates in (3) and the radius goes down again. The fact that lower dimensions show a more pronounced non-monotonicity of the size can then be traced to the fact that the positive energy contribution from zero-point motion grows with dimension and washes out the behaviour. For fermions, as discussed above, the energy is positive from the start and the radius stays large. However, the degeneracies allowed in higher dimensions add extra ingredients and shell structure to both the energy and the radial size.

3.2. Three boson energies

We now consider the case of three bosons within our harmonic approximation scheme in order to make a comparison with the results obtained by MacGuire [6] in the absence of external confinement. The exact bound state energy, $E_N$, of $N$ bosons interacting via attractive pairwise zero-range interactions in a homogeneous 1D space can be expressed in terms of the two-body energy, $E_2$, as

$$E_N = \frac{1}{6} N (N^2 - 1) E_2. \quad (10)$$

For the case of three particles this becomes $E_3 = 4E_2$. Since we have an external trap, we do not expect to reproduce this result. However, in the limit $a \to 0$ where $E_2 \to -\infty$ the external trap should become negligible and a comparison can be made.

We plot the ratio $E_3/E_2$ as a function of scattering length in figure 4 and as a function of $E_2$ in figure 5. The plot ends at $a/l \approx 0.25$ at which point it becomes numerically very challenging to compute the wave function based on the exact solution of Busch et al [18]. However, beyond that we can use the exact solution as discussed below.

One can see in figure 4 that as the scattering length decreases (more clearly seen as $E_2 \to -\infty$ in figure 5), the ratio approaches a limit. Using (5) and (4) in the limit where $a \to 0$ and $\omega_r \to \omega_{in}$ (see (6)), we find that

$$\frac{E_3}{E_2} = 3 + \left( \frac{3}{2} - \frac{3}{2} \right) \frac{\omega_{in}}{E_2}. \quad (11)$$

Relating $\omega_{in}$ to $\langle x^2 \rangle$ through (3), we obtain

$$\frac{E_3}{E_2} = 3 + \left( \frac{3}{2} - \frac{3}{2} \right) \frac{\hbar^2}{2\mu E_2 \langle x^2 \rangle}. \quad (12)$$

We can now use the exact wave function for a delta function potential in one dimension, $\psi(x) = Ae^{-\kappa x}$ where $\kappa = \sqrt{-2\mu E_2/\hbar^2}$, to obtain $\hbar^2/(2\mu E_2 \langle x^2 \rangle) = 2$. Our limit thus becomes $E_3/E_2 \approx 3.55$. This is also the number we find numerically for the smallest value of $a$ that we could access. Comparing with the exact value of MacGuire, $E_3/E_2 = 4$, this implies that the energetics of our model is accurate to about 10% for small scattering lengths. The wave function in
the harmonic model is a Gaussian, which in the limit $a \to 0$
will tend to a delta function, similar to the exact solution, so
we also expect the harmonic model to provide an accurate
structural description in this limit.

On the other hand, when $a$ becomes very large (the
unitarity limit) the trap plays an important role. Looking back
at the basic Hamiltonian in (1), we see that when $a \to \infty$, the
interaction term tends to zero and we should be dominated by
the trap only. However, the exact result always shows that there
is a shift of energy in this limit so that $E_2 \equiv \hbar \omega / 2$ for $a \to \infty$
the non-interacting system has twice the energy since there is
zero-point motion from both particles). Within our model we
have $\omega_o \to \omega_0$ and $\langle \chi^2 \rangle \to \hbar^2 / 2$ when $a \to \infty$ as the external
field provides the only length scale left in the problem. We have

$$\frac{E_1}{E_2} = 3 - \frac{\hbar \omega_0}{2E_2}, \quad (13)$$

and in the large $a$ limit, $E_2 \to \hbar \omega_0 / 2$, so we obtain a limiting
value of $E_1 \to 2$. At $a / l = 100$, we numerically obtain 1.98
for this ratio, so we reproduce this limit. The wave function
becomes essentially exact in this limit, and we thus expect the
structure to be well reproduced.

In the limit of large $N$, we can also estimate the scalings
and make a comparison with the exact results when $a \to 0$.
From (5) we have that the bosons scale as $E_N \sim N(N-1)E_2$,
which means that we have an underbinding by a factor of
$N + 1$. Fermions in (8) are different since here we have $E_N \sim
N^{5/2}E_2$, i.e. the underbinding is only by a factor of about
$\sqrt{N}$. Note, however, that in the opposite limit of $a \to \infty$,
the dominant term in (5) and (8) changes as $V_5 \to 0$ and
$\omega_o \to \omega_0$. This is an essentially non-interacting situation and
we have the intuitively obvious result $E_N \sim \hbar \omega_0 / 2$, which is
just the scaling dictated by the trap. For the values of $a$
away from these two limits, the scaling is an interplay of both
terms, and we obtain a more complicated behaviour. We note
that one could also turn these arguments upside down and
use the exact results for $N$ particles in the $a \to 0$ limit to fit
the parameters of the model, for instance by using $E_1 = 4E_2$
instead of either the frequency or radius condition we impose
on the two-body problem. Overall, we expect this to provide
only minor quantitative changes in the harmonic model and
its predictions.

3.3. One-body density

The one-body density matrix, $\rho(x_1, x'_1) = N \int \psi^* \langle x_1, \ldots, x_N \rangle \psi(x_1, \ldots, x_N) \; dx_1 \ldots dx_N$, is the most basic
correlation function and is the starting point of statistical
property calculations. It contains information on the
mean-field nature of the wave function for a bosonic system.
It is of interest in itself, but we will focus on its largest
eigenvalue, $\lambda$, which directly measures how much a given
state has the structure of a coherent state. Figure 6 shows $\lambda$
as a function of the number of bosons for several scattering
lengths. We mainly see an increase with particle number,
although there are slight decreases for small particle numbers
and large scattering lengths. In contrast with our previous
results in [17] for higher dimensions, only scattering lengths
of the order of unity or smaller show a $\lambda$ much different from
1, showing that the persistence of the mean-field structure

3.4. Thermodynamics

The energy spectrum can be built by considering excitations
in the internal oscillator frequency. To address the
thermodynamics of the systems, one can proceed as
described in detail in [20]. One naturally starts with the
partition function

$$Z(T) = \sum_i g_i \exp[-E_i / (k_B T)], \quad (14)$$

where $E_i$ is the energy of the $i$th state, $g_i$ is the degeneracy
of that state and $k_B$ is Boltzmann’s constant. 1D systems
are simpler since there is no degeneracy in energy levels in
contrast to higher dimensions. With the sequence of energies
and single-particle degeneracies, thermodynamic quantities
can be calculated. Once the spectrum and degeneracies of
our systems have been worked out, we can calculate basic
thermodynamic quantities in the canonical ensemble. In 1D,
the number of states grows much more slowly than in higher
dimensions, although one does have to climb somewhat high
in the spectrum due to the lack of degeneracy. In fact, in
1D there is no difference between bosons and fermions in
the sequence of the degeneracies of the $N$-body excited
states. This comes from the fact that all that the Pauli
principle implies for fermions is that the ground state has
them occupying higher orbit, which increases the ground-state
energy, in comparison to bosons which can all go into the
lowest orbital. Excitations on top of these ground states will
now cost the same amount of energy and they will all have the
same degeneracy since it is simply a matter of distribution of
a number of particles in levels to obtain a specific total energy
cost (the energy of the excitation above the ground state).

The latter fact implies that some thermodynamic quantities such as the entropy and heat capacity are identical
The heat capacity per particle at several boson numbers and scattering lengths, identified as $N$ and $a$ as a function of temperature.

Figure 7. The heat capacity per particle at several boson numbers and scattering lengths, identified as $N$ and $a$ as a function of temperature.

C/NkB vs $T/(\hbar \omega_0)$

For bosons and fermions at the same scattering length. Working in the canonical ensemble, in figure 7 we show the heat capacity $C$, which is the same for bosons and fermions. The heat capacity is related to the partition function by

$$C = \frac{\partial E}{\partial T},$$

$$E = -k_B T^2 \frac{\partial \log Z}{\partial T}.$$  \hspace{1cm} (15)

(16)

For all particle numbers, we see an initial increase, which then slows down at higher temperatures. This initial increase is the saturation of the centre-of-mass mode. The temperature where the slope changes depends on particle number since more particles being present in the system implies that the centre-of-mass mode constitutes a smaller share of the overall excitation energy. At larger scattering lengths, the heat capacity gradually increases towards the equipartition limit value of 1. At small scattering lengths, the large size of the excitation frequency sharply delays the approach to the equipartition limit. For the same scattering length, more particles mean a slower approach to the high-temperature limit. This is clear from (6), which shows that the excitation frequency increases with particle number.

4. Summary and outlook

We have presented the results for an $N$-body system of particles moving in one dimension and interacting via pairwise zero-range interactions under the influence of an external harmonic oscillator trap. The Hamiltonian is solved analytically within the harmonic approximation where the parameters of the model are adjusted to reproduce the properties of the exact solution to the corresponding two-body problem. This is along the lines of the standard approach to many-body problems in many fields of physics.

The ground-state energies for both bosonic and fermionic systems were obtained and we have discussed the scaling of these quantities with the particle number. We also obtained the radial size of the bosonic systems and made a comparison with previous findings in 2D and 3D setups. A careful study of the energy of three bosons in the harmonic model reveals that in the limit of high two-body binding energy where the external trap can be neglected, the harmonic model results are about 10% lower than the exact result obtained by MacGuire [6], whereas in the opposite limit of negligible two-body binding energy (large scattering length) the model becomes essentially exact. For larger particle numbers, the harmonic approximation tends to underbind the system compared with the exact results when the two-body system is strongly bound.

In addition, we studied the one-body density matrix. The main goal was to compute its largest eigenvalue for characterizing the degree of coherence in the system. The results turn out to be similar to those obtained in two and three dimensions, except that the 1D coherence turns out to be more robust except for large two-body binding energies. Finally, we studied the thermodynamics of the 1D system. The specific heat was found to behave in a manner that is quite similar to higher dimensions. However, it is worth noting that within the harmonic model, the spectrum of excitation for bosons and fermions turns out to be exactly the same. Due to the lack of degeneracy of the levels in one dimension, the only difference found is therefore in the ground-state energy.

The 1D setup studied here provides a very valuable benchmark for the harmonic models that have been used in higher dimensions in different contexts [8, 22–24]. Another good testing ground for the harmonic models is systems that have long-range interaction. In particular, systems of dipolar molecules in 1D tubes have been recently studied owing to their interesting few- and many-body structure [25–34]. The dipole–dipole interaction in two different 1D tubes is typically characterized by having a pocket that becomes deep when the dipolar interaction is strong [31]. This implies that a harmonic approximation is a good starting point. This approach has been studied in the case of 2D layers with dipolar particles [35–38] and compares very well with exact results [39–41] away from the weak-coupling limit. The application of the harmonic approximation to 1D arrays containing dipolar particles is a topic left for future work.

Another interesting direction in which the harmonic model can be used is for the study of higher-order terms in the interaction such as those coming from effective-range corrections to the model of Busch et al [18, 42]. Recent experiments have shown the potential need for such corrections in both 2D [43] and 3D cold atomic gas systems [44]. A possible way to account for such corrections would be by including quartic interaction terms and then carefully fitting the additional parameter to few-body properties. Within the harmonic model, the quartic interactions can be computed quite straightforwardly through Gaussian integrals. This could then be compared with mean-field results that include effective-range corrections in the limit of large particle numbers [45–48].

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