Quantum Statistics and Thermodynamics in the Harmonic Approximation

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We describe a method to compute thermodynamic quantities in the harmonic approximation for identical bosons and fermions in an external confining field. We use the canonical partition function where only energies and their degeneracies enter. The number of states of given energy and symmetry is found by separating the center of mass motion, and counting the remaining states of given symmetry and excitation energy of the relative motion. The oscillator frequencies that enter the harmonic Hamiltonian can be derived from realistic model parameters and the method corresponds to an effective interaction approach based on harmonic interactions. To demonstrate the method, we apply it to systems in two dimensions. Numerical calculations are compared to a brute force method that is considerably more computationally intensive.

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I. INTRODUCTION

The many-body problem cannot be solved exactly for realistic interactions and systems. Numerous approximations have been formulated and applied over the years. One of the problems is that many particles require a large Hilbert space to allow for the many possible correlations. In fact, the space typically grows exponentially with the particle number. The necessary reduction of the Hilbert space to obtain a tractable problem has to be accompanied by a corresponding transformation of the interaction which in turn has to be used in the smaller space. This is the method of effective interactions in reduced spaces.

A different approach starts by an approximation applied to the interaction itself. In many physical fields, the two-body interaction is a complicated entity, and therefore it is desirable to reduce this complexity. One such direction is to perform a harmonic approximation of the interaction Hamiltonian which leaves all terms (one- and two-body) as a polynomial of at most second order in the coordinates of all particles. This yields an exactly soluble model for the many-body system [1, 2]. However, to utilize such an approach, the input parameters must be adjusted to reproduce properties of realistic systems for low particle numbers. This could be two-body binding and scattering information and structural expectation values.

This sort of approach has been pursued in nuclear and condensed-matter physics for many years [3, 4] as a source of exact insight into many-body problems [5] when numerics are either intractable or hard to interpret. More recently, cold atomic gases have emerged as an arena and testing ground for various models due to their solvability. Of course, as mentioned above, the parameters have to be meaningfully related to realistic physical systems. This can be done through fits to two-body properties as described previously in Ref. [2]. Here we take a parametric approach and study the details of the harmonic approximation for identical quantum particles as function of the two relevant frequencies for such a system: the (internal) interaction frequency and the (external) trapping frequencies, both of which are described by (isotropic) harmonic terms. Deformation can be easily implemented and will not be considered here.

The objective of the present paper is to describe a method for calculating thermodynamical quantities for systems of identical bosons and fermions, a problem of relevance for any subfield of physics concerned with quantum mechanical behavior of multiparticle system in equilibrium. This requires full access to the partition function and the thermodynamic quantities that can be derived.
from it. The quantum statistics of ensemble of particles is needed here, and we present a general method for obtaining such information for harmonic Hamiltonians that works for any number of particles in principle.

There is great interest in the universal thermodynamics of strongly interacting Fermi gases [13], and measurements have determined the equation of state of the system [14]. Those studies are mostly concerned with trap-averaged quantities that are less sensitive to sudden changes in thermodynamic behavior as expected near phase transitions. However, recently it has become possible to determine local properties of the gas by density fluctuation measurements [15]. Quantities that involve derivatives of the energy or pressure like heat capacity and compressibility can thus be used to study for instance superfluid properties of both fermionic [16] and bosonic systems [17]. In addition, the same experiments are also able to explore effects of changing the dimensionality of the system through optical lattice potentials.

In the current presentation we focus on extending th harmonic approximation into the statistical regime, and more particularly on the technicalities of the method used to achieve this. To demonstrate our method we consider the case of a two-dimensional system of identical bosons or fermions for different ratios of interaction to external trapping frequencies. The paper is organized as follows. In Sec. II we briefly recap the harmonic method and then discuss the partition function in the harmonic approximation. The most important part of the method is the counting of the degeneracies in the partition function which we discuss in extended detail. The thermodynamic quantities are briefly outlined and a discussion of how to related the parameters in the harmonic Hamiltonian to the model by Busch et al. [10] is given. Practical numerical results are obtained and discussed in Sec. III for a system of cold atoms confined to two spatial dimensions. Both bosons and fermions are explicitly investigated. Finally, give a summary and an outlook in Sec. IV.

II. METHOD

We consider a system of $N$ identical quantum particles, fermions or bosons, that have two-body interactions, all of which are confined by an external field. All interactions are substituted by carefully chosen harmonic oscillators. The solutions of the Hamiltonian can then be found explicitly and treatment of thermodynamic properties is possible. We first present the necessary ingredients of the model, and continue to develop the method for calculating the partition function. This includes the key discussion of how to obtain the degeneracies of the many-body states.

A. Formulation of the model

The $N$-body Hamiltonian contains kinetic energy, one- and two-body interaction terms, all of which we assume can be written in terms of second order polynomials in the particle coordinates when proper choice of effective interaction parameters have been made. The resulting harmonic oscillator structure can be separated into terms related to each of the Cartesian coordinates and the Hamiltonian in one, two, and three dimensions is a sum of terms from each coordinate. For example, in the $x$-direction, the effective Hamiltonian is

$$
\begin{align*}
\hat{H}_x &= -\frac{\hbar^2}{2m} \sum_{k=1}^{N} \frac{d^2}{dx_k^2} + \frac{1}{2} m \sum_{k=1}^{N} \omega_0^2 x_k^2 \\
&+ \frac{1}{4} \mu \sum_{i,k} \omega_{\text{int}}^2 (x_i - x_k)^2 + V_{x0},
\end{align*}
$$

where $m$ is the mass of the identical particles and $\mu = m/2$ is the reduced mass. The one-body (external) harmonic trap frequency is $\omega_0$, while the two-body interaction frequency between all pairs is denoted $\omega_{\text{int}}$ (internal). $V_{x0}$ is a constant energy shift which is included for generality. Double counting of interactions account for the factor $1/4$. For two and three dimensions, the total Hamiltonian is $H = H_x + H_y$ and $H = H_x + H_y + H_z$. We will assume that the external harmonic trap is isotropic, extension to the deformed case are straightforward and will be addressed in future work. All particles are identical and interact in the same way which means that $\omega_{\text{int}}$ is independent of $i$ and $k$. Also the one-body frequency, $\omega_0$, is independent of $k$.

The Schrödinger equation for the Hamiltonian in Eq. (1) can be solved analytically for any particle number (details can be found in [2]) The pertinent properties in the present context are that the energies, $E_j$, of the excited states have oscillator character. Here $E_j$ denotes the $j$th many-body excited state, i.e. the energy of all $N$ particles when they are distributed in a certain way in the oscillator levels that come out of the diagonalization of the full Hamiltonian. In this paper we will concentrate mostly on the case of a two-dimensional system, and we therefore specialize to this case now. The energy of a many-body state, $E_j$, can be written

$$
E_j = \hbar \omega_r (N_{\text{rel}} + N - 1) + \hbar \omega_0 (N_{\text{cm}} + 1),
$$

$$
N_{\text{rel}} = \sum_{k=1}^{N-1} (n_{x}^k + n_{y}^k),
$$

$$
N_{\text{cm}} = n_{x}^{\text{cm}} + n_{y}^{\text{cm}},
$$

where $n_{x}^k$ and $n_{x}^{\text{cm}}$ are quanta in the $x$-direction related to the relative and center-of-mass excitations with the former carrying the index $k$ running over all $N$ particles (and similar terms for the $y$-direction). The total number of relative and center-of-mass quanta in the many-body state $j$ are denoted $N_{\text{rel}}$ and $N_{\text{cm}}$ respectively. Note that
The constants, \( h\omega_r(N - 1) \) and \( h\omega_0 \) in the formula for \( E_j \), are from the two-dimensional zero-point energy of intrinsic and center of mass parts, respectively. The one-body frequency, \( \omega_0 \), corresponds to center of mass motion. The other frequency, \( \omega_r \), is \( N - 1 \) times degenerate for identical particles. It is given by the relation \[ \omega_r^2 = \omega_0^2 \frac{N}{2} + \omega_0^2. \]

If the two-body interaction goes to zero (\( \omega_{\text{int}} \to 0 \)), \( \omega_r \to \omega_0 \), and the resulting eigenvalues and eigenfunctions converge to those of the external one-body trapping potential. The solutions are \( N \) non-interacting identical particles occupying \( N \) states in a harmonic oscillator. For interacting particles, we obtain instead \( N - 1 \) identical frequencies with value given by Eq. \[2\].

The extension of the above discuss to three dimensions involves also the \( z \)-direction and is straightforward, although the extra quantum numbers makes the degeneracy larger and the counting of many-body states more involved.

With the harmonic Hamiltonian, the exact spectrum of excited many-body states, \( E_j \), are thus available for a given number of particles. For the thermodynamic calculations, the natural choice is to use the canonical ensemble applicable for a definite number of particles. The canonical partition function is

\[ Z = \sum_j g_j \exp(-E_j/T), \]

where \( g_j \) is the degeneracy of the \( j \)th many-body state and \( T \) is the temperature measured in energy units (the Boltzmann constant, \( k_B = 1 \)). Once \( Z \) is obtained, all thermodynamic quantities can be derived from it. The most involved question is how to obtain \( g_j \) for a given energy of the many-body system. This will now be discussed.

**B. Symmetry constraints on degeneracies**

The only quantities in the partition function are the energies, \( E_j \), and their degeneracies, \( g_j \). The energies are appropriate multiples of the harmonic oscillator frequencies introduced above. The degeneracies depend strongly on which symmetry restriction is imposed. Problems arise when all, or a group of, particles cannot be distinguished because they are identical and allow occupation of the same states. We then have to count the number of (anti-)symmetric states for the indistinguishable particles of a given excitation energy, \( E_j \), and the corresponding degeneracies, \( g_j \), of each many-body state of energy \( E_j \).

We now describe our procedure to obtain \( g_j \). It is based on knowledge of the non-interacting system, a recursive procedure, and the fact that when the two-body interaction vanishes, the degeneracies remain the same as we will now explain.

We start with \( N \) identical particles without any two-body interaction (\( \omega_{\text{int}} \to 0 \)), and all in the same external trap with frequency \( \omega_0 \). This Hamiltonian will have \( N \) degenerate solutions of frequency \( \omega_0 \) per spatial dimension (so \( 2N \) for the two dimensional case). The many-body solutions are the products of \( N \) combinations of the single-particle harmonic oscillator wave functions. For identical fermions, the Pauli principle, or equivalently the antisymmetrization, requires that each of the single-particle states at most is occupied by one particle. In addition, if this condition of occupancy by at most one particle for each state is fulfilled, then one and only one antisymmetric state is uniquely constructed as the Slater determinant of the \( N \) singly occupied single-particle states.

Importantly, the energy can be characterized by the sum, \( N_{_{\text{tot}}} = N_{_{\text{rel}}} + N_{_{\text{cm}}} \), of single-particle oscillator quantum numbers for all particles in the state \( E_j \), as seen in Eqs. \[3\] and \[4\]. Assume that we have computed the number, \( g_{\text{non}}(N_{\text{tot}}) \), of properly symmetrized states of non-interacting identical particles in the external potential. The quantity \( g_{\text{non}}(N_{\text{tot}}) \) can be computed in a simple manner by trail-and-error, i.e. taking all possible permutations and testing which are completely symmetric and which are completely antisymmetric. This is, however, notoriously difficult since the computational effort is exponentially increasing with particle number. Also, it does not distinguish between center of mass motion and relative motion and this needs to be disentangled. This can be done by recalling the symmetry of the center of mass as we now discuss.

The center of mass motion is a symmetric mode in all permutations of the particle coordinates, simply because the center of mass coordinate is the sum of the individual particle coordinates. This motion is always symmetric, independent of the number of quanta in this mode, \( N_{\text{cm}} \). Therefore, the relative motion determines the symmetry of the total wave function. The excited states consist of a combination of two distinctly different types of excitations. They are characterized by the number of quanta in the center of mass motion, \( N_{\text{cm}} \), and the number of quanta in the relative motion, \( N_{\text{rel}} \).

We denote the number of properly (anti)symmetric \( N \)-body states by \( g_{\mu}(N_{\text{rel}}) \), which is the number of states that have the proper symmetry in terms of the relative coordinates. It can be computed from knowledge of the total number of non-interacting many-body states, \( g_{\text{non}}(N_{\text{rel}}) \), for all values of \( N_{\text{tot}} = N_{\text{rel}} + N_{\text{cm}} \). To do so, one must subtract the number of states of different center of mass quanta from the total number of non-interacting
many-body states in a recursive manner, i.e.
\[ g_p(N_{\text{tot}}) = g_{\text{non}}(N_{\text{rel}}) - \sum_{N_{\text{cm}}=1}^{N_{\text{rel}}} d_{N_{\text{cm}}} g_p(N_{\text{rel}} - N_{\text{cm}}), \quad (7) \]

where the degeneracy, \( d_{N_{\text{cm}}} \), of the center of mass state depends on the spatial dimension of the oscillator; \( d_{N_{\text{cm}}} = 1 \) for one, \( d_{N_{\text{cm}}} = N_{\text{cm}} + 1 \) for two, and \( d_{N_{\text{cm}}} = (N_{\text{cm}} + 1)(N_{\text{cm}} + 2)/2 \) for three dimensions, respectively. The formula comes from the fact that we know only the total number of quanta, \( N_{\text{tot}} \), but not \( N_{\text{rel}} \) and \( N_{\text{cm}} \) individually. We need to recursively subtract the states that correspond to \( N_{\text{cm}} = 1, 2, \ldots, N_{\text{tot}} \) as the formula prescribes. The factor \( d_{N_{\text{cm}}} \) is due to the degeneracy of the center of mass motion itself for given number of quanta, \( N_{\text{cm}} \). Note that \( g_p(0) \) is well-defined and corresponds to a state with no quanta of excitation, i.e. the ground state. It can be zero or non-zero depending on \( N \) and whether the particles are bosons or fermions. Eq. (7) determines the degeneracy of an \( N \)-body state in a harmonic system and is one of the main results of this work.

The degeneracy can now be calculated iteratively from Eq. (7) for any number of quanta, \( N_{\text{tot}} \) from a starting point based on a non-interacting system of identical particles in a trap. These states must then be either completely symmetric or antisymmetric with respect to interchange of all coordinates of any pair of particles to obey either bosonic or fermionic statistics. Now we add the two-body interaction on top of the external one-body potential. The external frequency, \( \omega_0 \), remains in the spectrum corresponding to the center of mass motion, and an \( N-1 \) times degenerate frequency, \( \omega_r \), appears corresponding to relative motion. The absolutely crucial point is that the degeneracies do not depend on the two-body interaction strength which will only influence the value of the degenerate frequency. The counting remains completely unchanged, because the number of states of a given symmetry is a discrete number which does not change with continuous variation of the interaction.

Mathematically, this corresponds to a continuous map (the scheme for counting degeneracies) from a continuous interval (the interaction frequency, \( \omega_r \)) to a discrete set (number of states, \( g_j \), with given energy). Such a map must necessarily be a constant map. The underlying point here is that our splitting into \( N_{\text{cm}} \) and \( N_{\text{rel}} \) is done in a way that moves the states that are related to the relative motion when \( \omega_r \) is increased from zero to its full value, while the states that are related to center of mass motion remain constant in energy since \( \omega_0 \) remains a solutions.

We confirmed this simple counting method by an elaborate and computationally very slow brute force procedure which is much worse than computing \( g_{\text{non}}(N_{\text{tot}}) \) above. The (anti-)symmetrization of each of the computed wave functions is performed by permutations of all the coordinates followed by extraction of a basis with a size equal to the smallest number of linearly independent states. For sufficiently small \( N \) this can be computed in reasonable time and comparison can be made. In all cases considered below we found perfect agreement between the numerics and the procedure outlined above. The procedure above is, however, far superior since it needs only counting of states with given energy, not the full wave functions.

C. Thermodynamic quantities

We can now use Eq. (7) to get the number of center of mass states and the number of relative states as functions of the sum of corresponding quanta. Along with the frequencies, this is all we need to calculate the partition function in Eq. (6). This simplification occurs since the structure of the wave functions do not enter in the partition function.

The center of mass mode of frequency \( \omega_0 \) separates in Eq. (6) because both the exponential function and the degeneracy factorizes, that is \( g_j = g_{\text{as}}(N_{\text{rel}})d_{N_{\text{cm}}} \) where the center of mass contribution is analytical and given below Eq. (7). We have

\[ Z(N,T) = Z_{\text{cm}}(N,T) \times Z_{\text{rel}}(N,T), \quad (8) \]
\[ Z_{\text{cm}}(N,T) = \left( \exp\left(-E_{g_0}/(2T)\right) \right)^D, \]
\[ Z_{\text{rel}}(N,T) = \sum_{N_{\text{rel}}=0}^{N_{\text{tot}}} g_{\text{as}}(N_{\text{rel}}) \exp\left(-N_{\text{rel}}\hbar \omega_r/T\right), \]

where \( D \) is the dimension, \( E_{g_0} = \hbar \omega_0 \), and \( E_{g_s} = E_0 + (2N-1)\hbar \omega_r + V_0 \). In practice, the infinite sum over relative quanta has to be limited by a cut-off value which is chosen sufficiently high to achieve the required accuracy. Certain quantities are more sensitive to the cut-off than others, such as those with more derivatives of the partition function (heat capacity, compressibility, etc.). For all the results presented below we have checked convergence by increasing the cut-off and identifying the value of \( T \) below which the relevant quantities remain unchanged. From the canonical partition function, Eqs. (6) or (8), we get immediately the basic quantities of energy, \( E \) and free energy, \( F = E - TS \), that is

\[ F = -T \ln Z, \quad E = T^2 \frac{\partial \ln Z}{\partial T}, \quad C_V = \frac{\partial E}{\partial T}, \quad (9) \]

where \( S \) is the entropy, and \( C_V \) is the heat capacity [18, 19].

In thermodynamic formulations of macroscopic systems, both temperature and volume is usually external parameters. Both the energy, \( E \), and heat capacity, \( C_V \), defined above, are in principle the derivatives for a fixed volume, \( V \) (and also fixed \( T \) and \( N \)). In our case with an externally confined \( N \)-body system the volume is not the fixed quantity, but rather it is the external trapping frequency, \( \omega_0 \), that is fixed. The derivatives above are thus taken for fixed \( \omega_0 \). Usually, variation of the volume
allows information about pressure and compressibility. \break
Definitions of these quantities and connection to their \break
thermodynamic counterparts require a precise translation \break
between \( \omega_0 \) and volume. Here we employ the simplest \break
choice and define the volume via the length parameter \break
related to the external trap, \( b \), which is defined by \( b^2 = \frac{\hbar}{m_0 \omega_0} \). We now have \( V = s_d b^D \), where \( s_2 = \pi \) and \( s_3 = 4\pi/3 \) are the two and three dimensional angular surface areas. Derivatives of any quantity, \( Q \), with respect to volume can now be written
\[
\frac{\partial Q}{\partial V} = \frac{\partial Q}{\partial \omega_0} \frac{\partial \omega_0}{\partial V} = \frac{2\omega_0}{D \omega_0} \frac{\partial Q}{\partial \omega_0},
\]
(10)

For the pressure, \( P \), we find
\[
P = -\frac{\partial F}{\partial V} = \frac{2\omega_0}{D \omega_0} \frac{\partial F}{\partial \omega_0},
\]
(11)

which, from the definition in Eq. (6), gives
\[
P = P_{cm} + P_{rel},
\]
(12)
\[
P_{cm} = \frac{2T}{m_0} \frac{\partial \ln Z_{cm}}{\partial \omega_0},
\]
(13)
\[
P_{rel} = \frac{2T}{m_0} \frac{\partial \ln Z_{rel}}{\partial \omega_0}.
\]
(14)

The derivatives are easily worked out since they only contain \( \partial \omega_0 / \partial \omega_0 = \omega_0 / \omega_0 \).

Continuation to the second derivative with respect to \( V \) produce the isothermal bulk modulus, \( B_T \), defined as
\[
B_T = \frac{1}{\kappa_T} = -V \frac{\partial P}{\partial V} = \frac{2\omega_0}{D \omega_0} \frac{\partial P}{\partial \omega_0},
\]
(15)

which is the reciprocal of the isothermal compressibility, \( \kappa_T \). Again two terms arise related to center of mass and relative degrees of freedom. Several terms appear by carrying out the two derivatives. This kind of compressibility, that of a response of a system to an applied pressure, is different to the compressibility of a self-bound system such as a nucleus \cite{20}. For self-bound systems, the compressibility refers to resistance to density fluctuations. This can be written as the second derivative of the energy per particle with respect to the Fermi momentum for fermionic systems.

Before we present results for degeneracies and various thermodynamic properties, we discuss how one can fix the two-body interaction term to capture the properties of the realistic system which have interactions that are not harmonic. In the case of identical bosons, the procedure was already presented in Ref. \cite{2} but we repeat the arguments here for completeness.

We assume that we are in the situation that the real two-body interaction is of much shorter range than the external trap length \( b \) above. In this case, we can use the zero-range model of Busch et al. \cite{10} to obtain the solutions in the trap. The effective two-body interaction that we want to use is a harmonic oscillator, which in general contains two parts; an oscillator frequency, \( \omega_{\text{int}} \), and a shift, \( V_0 \). To fix these parameters we employ the conditions that the two-body harmonic interaction should reproduce the correct two-body binding energy of the ground state in the Busch model, and also the spatial extend of the wave function. The latter condition is implemented by calculating the root-mean-square radius, \( \langle r^2 \rangle \), in the exact solution and fixing the oscillator parameter to reproduce value. The energy shift is subsequently tuned so as to also reproduce the two-body binding energy.

Clearly, since the Busch model uses a zero-range interaction, the only scale left is the external trap frequency, \( \omega_0 \). Therefore what we obtain from this is the quantity \( \omega_{\text{int}} / \omega_0 \). We ignore the shift from now on since it merely provides an overall shift in the \( N \)-body harmonic Hamiltonian which is not of interest in the current paper. The next step is to insert this value into Eq. (5) to obtain \( \omega_r / \omega_0 \), which will now naturally depend on \( N \). In the upper panel in Fig. 1 we show the result of this procedure for the case of bosons in two dimensions (more detail for bosons in both two and three dimensions can be found in Ref. \cite{2}). The results are plotted as function of the two-dimensional scattering length \( a \). Note that when \( a \) is small, the ground state becomes strongly bound, while for large \( a \) it goes to the non-interacting limit. This is clearly reflected in the behavior of \( \omega_r / \omega_0 \).

The result of this procedure agrees rather well with predictions from the well-studied problem of bosons interacting through a zero-range interaction \cite{21} in the strong and weak coupling limits \cite{2}, also in the case where higher-order interaction terms are included \cite{22}. Recently, a very similar procedure has been used to study
polar molecules in layered system 23 where excellent agreement with exact methods has been found both for isotropic 24 and anisotropic potentials 25 which have reasonably large potential pockets. Incidentally, one-dimensional dipolar system also turn out to have such potential pockets 26 and applying the harmonic approximation to these systems is an interesting direction for future research.

For identical (spin-polarized) fermions a complication arises from the fact that the original Busch model applies to particles interacting through an isotropic s-wave interaction only. The Pauli principle dictates that s-wave interactions are zero for identical fermions, and therefore the interactions must have p-wave (or higher odd partial wave) character. In two dimensions, the equivalent of the Busch model with p-waves can be solved and the spectrum turns out to be very similar to the s-wave case except for (unimportant) shifts 27. However, a further complication arises since the corresponding ground state wave function is singular at the origin in a manner that does not allow it to be normalized 28. This can be fixed by a properly defined scalar product as discussed for the three-dimensional case in Ref. 29. We will not pursue this approach here but instead we note that any higher order structural average of the type \( \langle r^n \rangle \) with \( n \) an integer is still perfectly convergent. We thus consider a higher order average, \( \langle r^4 \rangle / \langle r^2 \rangle \), in order to fix the oscillator parameter for identical fermions. We are thus tacitly using that the p-wave spectrum is very similar to the s-wave one and assume that the wave function should be so as well. Of course, it must be kept in mind that this is not at odds with the Pauli principle since the two-body wave function in the p-wave channel is still zero at the origin. In any case, the Pauli principle is exactly enforced on the \( N \)-body system as discussed above.

The results for \( \omega_r / \omega_0 \) are shown in the lower panel of Fig. 1. The similarity to s-waves and bosons is quite clear, and the only difference seems to be slightly lower overall values for the fermionic case. Below we will illustrate our method by calculating thermodynamic quantities for both fermions and bosons. Here the only thing that matters is the ratio \( \omega_r / \omega_0 \). One can then reverse the process and use Fig. 1 to obtain a corresponding value of the scattering length and thus compare to a realistic system with trapped bosons or single-component fermions. Since this is mainly a discussion of method, we will not dwell on this any further. An important thing to note, however, is that since the ratios \( \omega_r / \omega_0 \) are similar for bosons and fermions, the results below will truly isolate the statistical behavior coming from the exchange requirements in the different cases.

### III. THERMODYNAMIC RESULTS

We now proceed to demonstrate our methods by computing the density of states and the thermodynamic quantities that have been introduced above. They depend on particle mass, dimension, number of particles and their quantum statistics, temperature, one- and two-body frequencies. If we measure all energies in units of \( \hbar \omega_0 \), all results for given particles in \( D \) dimensions, depend only on the two ratios, \( T / \hbar \omega_0 \) and \( \omega_r / \omega_0 \). This implies that any kind of interaction model used to define the effective harmonic hamiltonian only has to provide these two quantities as pointed out above.

#### A. Degeneracies

First we discuss the degeneracies themselves which are found by the procedure discussed above, essentially through the recursive formula Eq. (7). While the number of non-interacting (anti-)symmetric states increases exponentially as function of excitation energy, the numbers can, however, be tremendously reduced by the symmetry requirements. A simple example indicating this tendency is that for bosons all particles are allowed to occupy the

![FIG. 2: The number of completely symmetric (bosons) and antisymmetric (fermions) states as function of excitation energy for different numbers of particles in a two-dimensional harmonically trapped system. The particle numbers are indicated on the plots. Notice that the horizontal axis for bosons is \( N^{1/2} \), while it is \( N^{1/4} N_{rel}^{1/2} \) for fermions.](image)
lowest level with zero quanta, \( N_{tot} = 0 \). In contrast, a given number of fermions has a minimum sum of quanta, \( N_{gs} \), in the ground state, that is \( N_{tot} \geq N_{gs} \neq 0 \). We show the numbers of given symmetry as functions of excitation energy in Fig. 2

Since we are dealing with harmonic oscillators, a given energy corresponds to a given total number of quanta. The starting point for the ground state is naturally \( N_{cm} = 0 \) and \( N_{tot} = N_{rel} \), which is larger for fermions than for bosons due to the requirement that at most one fermion can occupy each state. The corresponding higher degeneracy implies therefore that the number of states of given excitation energy is larger for fermions than for bosons because the latter do not need to obey the Pauli Principle. For bosons, the lowest excited state consisting of one quantum added to zero quanta in the ground state can only be a center of mass excitation, since one quantum in the relative motion would be antisymmetric in one pair of coordinates (it would have to be a state of \( p \)-wave/parity-odd symmetry). The lowest completely symmetric excited state of the relative motion appear for \( N_{rel} = 2 \). In conclusion, there is always a gap in the excitation spectrum for bosons corresponding to \( 2\hbar\omega_r \) where fermions only have a gap of \( \hbar\omega_r \). This will be reflected in the temperature dependence below.

For bosons (upper part of Fig. 2) the same degeneracy is found for low energy (small total number of quanta) for all particle numbers. In the upper plot of Fig. 2, the horizontal axis is \( N_{rel}^{1/2} \) since we have found that this is a good measure for the excitation energy in the system. For fermions, one can give a qualitative argument for the exponential behavior which we discuss below. The similarity of degeneracies at low energy for bosons can be understood by the direct counting procedure where a given number of particles, \( N \), has to be distributed to add up to the total number of quanta, \( N_{rel} \). First, \( N - 1 \) particles are placed in the lowest oscillator level, and the one remaining particle then has to be placed in the level with total number of quanta equal to \( N_{rel} \). Then we move the single particle one step down to \( N_{rel} - 1 \), and simultaneously compensating by moving one particle one step up from the lowest level. We continue with these combinations until we have \( N_{rel} \) particles in the second oscillator level and all others in the lowest level. Adding one particle and repeating the counting process we realize that their is a one-to-one correspondence between the configurations of \( N \) and \( N + 1 \) particles. Going from one to the other is simply by removing or adding one particle in the lowest oscillator level with zero contribution to the total number of quanta.

For \( N \) bosons, the deviation from this universal curve starts for \( N_{rel} = N + 1 \). The reason is again found by following the counting procedure. The configurations with all particles in the lowest two levels are only possible when \( N_{rel} \leq N \). This implies that we find fewer states when \( N_{rel} \geq N + 1 \) for \( N \) than for \( N + 1 \) particles. The curves break away from the universal curve for increasing \( N \) when \( N_{rel} = N + 1 \).

![Fig. 3: Helmholtz free energies of a two-dimensional system, divided by particle number, \( N \), for several boson (upper) and fermion (lower) systems, identified by the number of particles and frequency ratio, \( (N, \omega_r/\omega_0) \). The ground state energy is subtracted, and the energy unit is \( \hbar\omega_0 \) for both energies and temperatures. The ground state energy, \( E_{gs} \), has been substracted.](image)

The degeneracies for fermions have very different behavior, as seen in the lower part of Fig. 2. Notice that the horizontal axis is different in the two plots. We notice a regime of linear dependence which has the same origin as the exponential square root dependence of excitation energy of the free Fermi gas level density [4]. For two dimensions, the particle number dependence is roughly \( N^{1/4} \) as reflected on the axis in the fermion plot. This holds for intermediate excitation energies and for relatively large particle numbers. A qualitative understanding of the behavior can be obtained in a manner following Ref. [4]. The density of single-particle states at the Fermi level in a two-dimensional harmonic trap is roughly \( g_F \sim (2N)^{1/2}/\hbar\omega_0 \), while the typical excitation energy in the system is \( E^* = \hbar\omega_0 N_{rel} \). The many-body level density in this situation is then proportional to \( \exp \left[ \sqrt{\pi^2(2N)^{1/2}/N_{rel}/6} \right] \). This explains the choice of horizontal axis for fermions in Fig. 2. The suggested linear dependence is not very clear but the assumptions are not well fulfilled. The requirements is that the excitation energy has to be sufficiently large to allow statistical treatment and sufficiently small not to exhaust particles at the bottom of the potential. This is not true for the relatively small particle numbers that we must necessarily work with to make the problem tractable by both brute force symmetrization and the counting scheme developed here.

### B. Energy and free energy

We are now in a position to explore the thermodynamics and to compare bosonic and fermionic behavior in de-
fermions. We measure energy in units of $N k_B T$ to isolate the high temperature behavior which is $2 N k_B T$ for two dimensional harmonic system by the equipartition theorem. Again, we subtract the uninteresting constant ground state energy. The increase from zero at zero temperature is rather steep for both types of particles. All curves continue to increase with temperature but much slower after a few units of $\hbar \omega_0$. The largest energy per $N k_B T$ is for the system with the least particles and the smallest frequency ratio. This can be understood from the fact that for large $\omega_r/\omega_0$, only the center of mass modes (twice degenerate in two dimensions) are active. However, since we divide by $N$, the values become smaller for larger $N$, but the behavior remains the same (self-similar lines for $\omega_r/\omega_0 = 10$ in Fig. 4). This is similar for both bosons and fermions. We also observe that the equipartition limit at high temperature is reached for substantially larger temperatures, a clear sign of the interaction effects.

The low-temperature behavior is, however, different for bosons and fermions. The low-energy $2 \hbar \omega_r$ gap in the boson spectra arises due to a ground state with all particles with zero oscillator quanta of excitation. Then there are no states with one quanta of excitation. For fermions, there are only $\hbar \omega_r$ gaps. Therefore the energy exhibits flat regions at relatively low temperature, but these features are observed first for fermions and later for bosons due to the difference in energy gap which is related to the activation energy. This demonstrates a clear signature of quantum statistics in the harmonic model, but which should be expected in generic interacting systems with identical particles.

Next, we show the entropy, $S$, in Fig. 5. We note the increase of available states per particle as function of temperature goes from zero to values around a few times the temperature in units of $\hbar \omega_0$. For lower ratios $\omega_r/\omega_0$, the increase with temperature is faster since less energy
is required to excite the internal modes of the system and more states are available, correspondingly increasing $S$. Again, for larger values of $\omega_r/\omega_0$, the center of mass is the only active mode at low temperature and the division by $N$ in the plots explains the lower value of $S$ for larger $N$. Only at substantially larger temperatures will both internal and center of mass modes become active. The effect of symmetry is not very pronounced, although it is noticeable that the entropy is larger for fermionic than for bosonic systems due to the larger degeneracy.

An interesting feature of the fermion plot is that for $N = 8$ the limit of $S/N$ for $T \to 0$ is non-vanishing. The number of available states is finite reflecting that the ground state itself is degenerate. This is seen by simply counting of oscillator degeneracy for a two-dimensional harmonic oscillator. The lowest three quantum levels can hold 6 identical fermions (1, 2, and 3, respectively), and the fourth can hold additionally four particles. This means that eight particles only occupy half of the last level, leaving the ground state as six times degenerate. This behavior at zero temperature then nicely indicate the presence of shell structure.

C. Heat capacity and compressibility

We now consider some derived thermodynamic quantities that are of experimental interest in many fields of physics. The heat capacity and the compressibility are two such quantities that can be obtained from second derivatives of the partition function as discussed above. In Fig. 6 we show the heat capacity per particle, $C_V/N$, defined in Eq. (9) as function of temperature for both bosons and fermions. They both start with an initial activation of the external trap mode, since the degenerate relative degrees of freedom all require higher temperature to be excited. After a delay, these internal modes are activated, and the heat capacity increases with temperature. The delay and the rate of increase depend strongly on $\omega_r/\omega_0$ with a slower increase of $C_V$ for larger interaction ratios.

The tendency to increase slower and in steps is related to gaps in the energy spectrum. At high excitation energy, the spectrum becomes denser, and gap sizes larger than the temperature cannot appear. However, the presence of a gap in the low-energy spectrum is important for the heat capacity in general. In fact, this is clearly seen by the fact that bosons have a flat profile for a region of low temperature, while the fermions have two flat plateaus. Fermions rise faster initially, and always approach the equipartition heat capacity from below ($C_V/N \to 2$ for two dimensions). The larger gap causes a delay in the boson systems. The heat capacity slightly overshoots the equipartition value, oscillate back below the equipartition value (at a temperature outside the scale in Fig. 6), and eventually approach the limit from below. The curve marked COM shows the heat capacity when assuming that only the center of mass mode is excited. All the other curves will approach this at very large temperatures when the internal structure is washed out. However, as the plots clearly show, the approach is very different for different particle numbers and interaction strengths.

In Fig. 6 we show the isothermal compressibility per particle, $\kappa_T/N$, as defined in Eq. (15). The high temperature behavior of a harmonic system is $1/T$. The compressibility shows a small increase through a maximum at very small temperature followed by steady decrease towards zero at large temperature with a $1/T$ slope. The compressibility indicates how easy it is to squeeze the system and a large value indicates that the system is very susceptible to compression. We see that the more strongly interacting systems (larger $\omega_r/\omega_0$) have larger $\kappa_T$. This comes from the fact that the attraction in these systems will make it energetically favourable to contract, due to the larger degeneracy of the interaction frequency, $\omega_r$.

This also explains why $\kappa_T$ increases with $N$. Comparing bosons and fermions we find the same qualitative behavior. The fermions are slightly less compressible,
with a sharper dependence on particle number and interaction strength. This is a common feature of Fermi systems and usually attributed to the Pauli principle. For comparison, Fig. \ref{fig:compressibility} shows the compressibility for fermions in three spatial dimensions, which shows the same qualitative behavior. The results for bosons are similar and we do not show them here. Notice that the peak features in the compressibility are sharper in the three-dimensional case. Our system is similar to an attractively interacting Fermi gas where superfluidity is expected to show a signature in the compressibility \cite{16}. Our results are consistent with the fact that phase transitions are less pronounced in lower dimensions.

\section{Summary and Conclusions}

The harmonic approximation is extremely useful because its simplicity allows transparent calculations of otherwise complicated properties. The only approximation lies in the choice of harmonic potentials acting on each particle and between pairs of particles. One can therefore think of the harmonic approximation as an effective interaction scheme and subsequently investigate the behavior of its predictions under changes in the input parameters. The latter should naturally be connected to whatever realistic physical system one is interested in studying.

In this paper, we explore the harmonic approximation scheme by considering the Hamiltonian for a many-body system consisting of a given number of identical particles. In particular, we explore the consequences of symmetry requirements on the properties of the system. This is done with thermodynamic applications in mind since this is a venue where the quantum statistics plays a decisive role at low temperatures. We develop a new method for counting the number of correctly symmetrized many-body states that reduces the complications that arise from this fundamental problem of statistical mechanics and thermodynamics.

The advantage of the harmonic approach is obviously that the energy spectrum is analytically known. However, the degeneracy of each many-body state of given total energy still remains to be determined before the partition function is fully defined and possible to compute numerically. We design a novel procedure to obtain the degeneracy of each state, subject to requirements of symmetry and antisymmetry appropriate for bosons and fermions, respectively. We separate the completely permutation symmetric center of mass motion from the relative motion, which then has to carry the symmetry corresponding to bosons or fermions. We count by subtracting the number of states of different quanta in the center of mass motion from the total number of non-interacting states of given symmetry.

To demonstrate the method, we consider the case of a two-dimensional system with identical bosons or fermions (with no internal degrees of freedom). Within the canonical ensemble, we compute the partition function, and from it the free energy, entropy, heat capacity, and compressibility of the system. This is done for a relatively small number of particles (up to 20). The method is a considerable improvement over the brute force method where one explicitly checks for symmetry properties by exchanging all pairs of particles one by one. However, it is still computationally involved when going beyond the particle numbers considered here. However, as is known from for instance the virial expansion \cite{30}, it is often enough to consider small particle numbers and then extrapolate to large system sizes from this information.

The effective harmonic interaction can be related to quantities in realistic systems and we discuss a case of great usefulness within the realm of ultracold atomic gases, that of two particles interaction in a harmonic
bosons can interact in the s-wave channel originally considered by Busch et al. [10] identical fermions must have an antisymmetric relative wave function and thus an s-wave interaction of zero-range. While considered by Busch [10], identical fermions must have an antisymmetric relative wave function and thus an s-wave interaction of zero-range. While we have to consider the p-wave channel, but we find that the effective harmonic interaction frequencies are very similar to the s-wave case in the two-dimensional setup that we consider here. Therefore we have chosen to parametrize the discussion of the thermodynamic quantities by the harmonic oscillator frequency of the two-body interaction itself. One can then make the connection to a realistic system by working backwards through the model of Busch et al.

Our numerical results show that the low-temperature behavior reflects shell structure for the particle numbers we study. The large-temperature equipartition limits are recovered for energy and heat capacity, and the transition from small to large temperature is fastest for smaller two-body interaction strength. The qualitative behavior is rather similar for bosons and fermions. However, bosons always have a gap in the low-energy spectrum since one quantum of excitation of the relative motion must be antisymmetric and therefore forbidden. This leads to a slower variation with temperature, since this gap has to be overcome before the number of available states goes up. Our results for the density of states turn out to scale with the number of relative excitation quanta in a manner that is very similar to the treatment of the many-body density of states for a uniform Fermi gas. Surprisingly, the bosonic many-body level density scales similarly to the fermionic one, although the particle number enters differently in our interpolation formulas.

In future studies it will be interesting to consider also multi-component systems, something which is simply done within the harmonic approach since the level counting can be factorized in the different components. Also, a study of the virial expansion based on the harmonic approach is currently on-going, both in two and three dimensions. In addition, we note that one dimensional system have attracted a lot of attention recently due to their realization in ultracold atomic physics [28]. It would be interesting to test our prediction against some of the models that are being explored in the experiments and for which a number of exactly solvable many-body models are known [28]. Furthermore, recent experiments studying ultracold few-body two-component Fermi systems (particle numbers of ten or less) [28] would be an interesting comparison for the harmonic approximation.

[1] M. A. Zaluska-Kotur, M. Gajda, A. Orlowski, and J. Mostowski, Phys. Rev. A 61, 033613 (2000); J. Yan, J. Stat. Phys. 113, 623 (2003); M. Gajda, Phys. Rev. A 73, 023603 (2006);
[2] J. R. Armstrong, N. T. Zinner, D. V. Fedorov, and A. S. Jensen, J. Phys. B: At. Mol. Opt. Phys. 44 (2011)055303.
[3] A. L. Fetter and J. D. Walecka: Quantum Theory of Many-Particle Systems, (McGraw-Hill, San Francisco, 1971).
[4] A. Bohr and B. R. Mottelson: Nuclear Structure, Vol 1, (Benjamin, New York, 1969).
[5] B. Sutherland: Beautiful Models, (World Scientific Publishing Co., Singapore, 2004); R. J. Baxter: Exactly Solved Models in Statistical Mechanics, (Academic Press, New York, 1982); V. E. Korepin: Exactly Solvable Models of Strongly Correlated Electrons, (World Scientific Publishing Co., Singapore, 1994).
[6] I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. 80, 885 (2008).
[7] C. Chin, R. Grimm, P. S. Julienne, and E. Tiesinga, Rev. Mod. Phys. 82, 1225 (2010).
[8] F. Serwane, G. Zürn, T. Lompe, T. B. Ottenstein, A. N. Wenz, and S. Jochim, Science 332, 6027 (2010); G. Zürn, F. Serwane, T. Lompe, A. N. Wenz, M. G. Ries, J. E. Bohn, S. Jochim, arXiv:1111.2727v2.
[9] H. A. Bethe, Phys. Rev. 76, 38 (1949).
[10] T. Busch, B. G. Englert, K. Rzadzinski, and M. Wilkens, Found. Phys. 28, 548 (1998).
[11] T. Stöferle, H. Moritz, K. Günter, M. Köhl, and T. Esslinger, Phys. Rev. Lett. 96, 030401 (2006); T. Volz et al., Nature Phys. 2, 692 (2006); G. Thalhammer et al., Phys. Rev. Lett. 96, 050402 (2006); C. Ospelkaus et al., Phys. Rev. Lett. 97, 120402 (2006).
[12] W. C. Haxton and T. Luu, Phys. Rev. Lett. 89, 182503 (2002); I. Stetcu, B. R. Barrett, and U. van Kolck, Phys. Lett. B 653, 358 (2007); I. Stetcu, B. R. Barrett, U. van Kolck, and J. P. Vary, Phys. Rev. A 76, 063613 (2007); Y. Alhassid, G. F. Bertsch, and L. Fang, Phys. Rev. Lett. 100, 230401 (2008); N. T. Zinner, K. Mølmer, C. Özen, D. J. Dean, and K. Langanke, Phys. Rev. A 80, 013613 (2009); I. Stetcu, J. Rotureau, B. R. Barrett, and U. van Kolck, Ann. Phys. 325, 1644 (2010); T. Luu, M. J. Savage, A. Schwenk, and J. P. Vary, Phys. Rev. C 82, 034003 (2010); J. Rotureau, I. Stetcu, B. R. Barrett, M. C. Birse, and U. van Kolck, Phys. Rev. A 82, 032711 (2010).
[13] H. Hu , P. D. Drummond, and X.-J. Liu, Nature Phys. 3, 469 (2007).
[14] M. Horikoshi, S. Nakajima, M. Ueda, and T. Makiyama, Science 327, 442 (2010); N. Navon, S. Nascimento, F. Chevy, and C. Salomon, Science 328, 729 (2010); C. Cao et al., Science 331, 58 (2011).
[15] C. Sanner et al., Phys. Rev. Lett. 105, 040402 (2010); T. Müller et al., Phys. Rev. Lett. 105, 040401 (2010).
[16] M. J. H. Ku, A. T. Sommer, L. W. Clark, and M. W. Zwierlein, arXiv:1110.3309v1.
[17] C. L. Hung, X. Zhang, N. Gemelke, and C. Chin, Nature 470, 236 (2011).
[18] D. A. McQuarrie: Statistical Mechanics, (HarperCollins, New York, 1976).
[19] K. Huang: Statistical Mechanics, 2nd ed. (John Wiley & Sons, New York, 1987).
[20] S. S. M. Wong: Introductory Nuclear Physics, (Wiley Interscience, New York, 1998).
[21] R. V. E. Lovelace and T. J. Tommila, Phys. Rev. A 35, 3597 (1987); G. Baym and C. J. Pethick, Phys. Rev. Lett. 76, 6 (1996).

[22] H. Fu, Y. Wang, and B. Gao, Phys. Rev. A 67, 053612 (2003); N. T. Zinner and M. Thogersen, Phys. Rev. A 80, 023607 (2009); M. Thogersen, N. T. Zinner, and A. S. Jensen, Phys. Rev. A 80, 043625 (2009).

[23] J. R. Armstrong, N. T. Zinner, D. V. Fedorov, and A. S. Jensen, Europhys. Lett. 91, 16001 (2010); N. T. Zinner, B. Wunsch, D. Pekker, and D.-W. Wang, arXiv:1009.2030v3; N. T. Zinner et al., arXiv:1105.6264v1.

[24] J. R. Armstrong, N. T. Zinner, D. V. Fedorov, and A. S. Jensen, [arXiv:1106.2102v1]; A. G. Volosniev, D. V. Fedorov, A. S. Jensen, and N. T. Zinner, arXiv:1109.4602v1.

[25] A. G. Volosniev et al., J. Phys. B: At. Mol. Opt. Phys. 44, 125301 (2011); A. G. Volosniev, D. V. Fedorov, A. S. Jensen, and N. T. Zinner, Phys. Rev. Lett. 106, 250401 (2011); A. G. Volosniev et al., [arXiv:1112.2541v1].

[26] B. Wunsch et al., Phys. Rev. Lett. 107, 073201 (2011); N. T. Zinner et al., Phys. Rev. A 84, 063606 (2011).

[27] N. T. Zinner, [arXiv:1111.1565v1].

[28] K. Kanjilal and D. Blume, Phys. Rev. A 73, 060701(R) (2006).

[29] L. Pricoupenko, Phys. Rev. A 73, 012701 (2006).

[30] T.-L. Ho and E. J. Mueller, Phys. Rev. Lett. 92, 160404 (2004); X.-J. Liu, H. Hu, and P. D. Drummond, Phys. Rev. Lett. 102, 160401 (2009); Phys. Rev. A 82, 023619 (2010); S.-G. Peng, S.-Q. Li, P. D. Drummond, and X.-J. Liu, Phys. Rev. A 83, 063618 (2011).