Analytical and Machine Learning study of one-dimensional non-interacting spinless trapped fermionic systems

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In this work we study the ground-state properties of three different one-dimensional systems of N identical, non-interacting, spinless fermions trapped in a potential well. We consider a harmonic trap, an infinite potential well and a Morse potential, and for all of them we prove that the ground-state wavefunction can be written in terms of a Vandermonde determinant. We compute and plot the one-body density matrix and the pair correlation function for systems of 2 to 5 particles using two different analytical methods to check that both provide the same results. Moreover, we derive closed expressions for these functions in terms of polynomials for a general number of particles. These polynomials, in turn, can be expressed using Vandermonde vectors and square matrices. To complement the mathematical study of the systems, we reproduce and validate the analytical results using a Machine Learning approach. We use a Neural Quantum State as an ansatz for the ground-state wavefunction and a Variational Monte-Carlo method to find the best neural network parameters. Both the energies and the density matrices are correctly reproduced using Machine Learning.

Keywords: Vandermonde determinant, particles in a trap, ground state, one-body density matrix, pair correlation function, Hermite polynomials, Laguerre polynomials, Neural Quantum State.

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Contents

1 Introduction

The study of a collection of many particles can be remarkably complex when interactions are taken into account. The exploration of these many-body interacting systems lies within the domain of quantum many-body physics, with the objective of understanding emergent phenomena that appear due to the collective behavior [Col16].

The field of many-body physics has seen significant evolution and advancement over the past years, driven by both theoretical developments and technological progress. In particular, Machine Learning (ML) methods have been increasingly used to tackle the challenges of simulating and understanding complex quantum many-body systems. The first use of a variational representation of quantum states based on Artificial Neural Networks (ANNs) in the many-body context appears in [CT17]. These variational quantum states parametrized in terms of an ANN receive the name of Neural Network Quantum States or simply Neural Quantum States (NQS).

In this work we focus on non-interacting, one-dimensional, spinless (fully polarized) fermionic systems trapped in a potential well. Fermions have the peculiarity that they obey the Pauli exclusion principle, which states that no two fermions can occupy the same quantum state simultaneously, which determines how energy levels are filled. Although in our study fermions do not interact, the results we find in our work can be used as a tool in more complex many-body studies with interactions. Our investigation is structured around the analysis of three N-body quantum systems, the harmonic oscillator (HO), the infinite well (IW) and the Morse oscillator (MO), each characterized by a different well potential.

The work is divided into two main sections, one in which we present an extensive mathematical analysis of the systems under examination (Sec. 2) and another one where we benchmark the obtained results using ML techniques (Sec. 3). We start Sec. 2 by introducing the key concepts and the main mathematical tools we employ in our analysis, which comprise the definitions of VD, one-body density matrix (OBDM) and pair correlation function (PCF). Then we focus on each system to find its ground-state wavefunction in terms of a VD and we compute and plot the OBDM and the PCF using both integral formulae and uncorrelated formulae to corroborate that they give identical results. We finally find closed expressions for them in terms of polynomials, which can be represented as a matrix product involving Vandermonde vectors and square matrices. We find these matrices for $N = 2, 3, 4, 5$ and recalculate the OBDM and PCF using them to validate both the closed formulae and the obtained matrices. The original derivations and analytical findings are extensively discussed in the appendices.

In Sec. 3 we firstly provide a brief overview of the theoretical foundation underlying the computational analysis employing ML techniques. This is followed by the description of the methodology and the presentation of the results, which are compared to the analytical ones. We conclude the work with a summary of the obtained results and we also provide possible future lines of research.

2 Mathematical study of one-dimensional quantum systems

2.1 Vandermonde determinants

The Vandermonde matrix, mostly known for its determinant, is usually introduced in the interpolation domain when we want to interpolate n points $(x_1, y_1), \ldots, (x_n, y_n)$ by means of a polynomial of degree $n-1$, $P(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_{n-1} x^{n-1}$ [Kal18]. To determine the coefficients a_i of such polynomial, we can think of solving the following system of n equations:

$$\begin{cases} P(x_1) = a_0 + a_1 x_1 + a_2 x_1^2 + \cdots + a_{n-1} x_1^{n-1} = y_1 \\ P(x_2) = a_0 + a_1 x_2 + a_2 x_2^2 + \cdots + a_{n-1} x_2^{n-1} = y_2 \\ \quad \vdots \qquad\qquad\qquad\qquad\qquad\qquad \vdots \\ P(x_n) = a_0 + a_1 x_n + a_2 x_n^2 + \cdots + a_{n-1} x_n^{n-1} = y_n \end{cases}. \tag{1}$$

If we write it in matrix form, we have

$$\begin{pmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^{n-1} \\ 1 & x_2 & x_2^2 & \cdots & x_2^{n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & \cdots & x_n^{n-1} \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_{n-1} \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}. \tag{2}$$

The matrix that appears is called a Vandermonde matrix. In general, a Vandermonde matrix is an $n \times m$ matrix that contains the terms of a geometric progression in each row [Mey10]:

$$V_m(x_1, \ldots, x_n) = [x_i^{j-1}]_{i,j=1}^{n,m} = \begin{pmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^{m-1} \\ 1 & x_2 & x_2^2 & \cdots & x_2^{m-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & \cdots & x_n^{m-1} \end{pmatrix}. \tag{3}$$

Although this definition is commonly used, we can also find literature where a Vandermonde matrix is defined as the transpose of the above matrix [Muh20]. If the matrix is square ($n = m$), as in Eq. (2), we can define its determinant, the so called Vandermonde determinant, Vandermonde polynomial or Vandermondian [Muh20]:

$$\det V(x_1, ..., x_n) = \begin{vmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^{n-1} \\ 1 & x_2 & x_2^2 & \cdots & x_2^{n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & \cdots & x_n^{n-1} \end{vmatrix}. \tag{4}$$

Returning to the interpolation case, the system has a solution if the VD is different from zero. It happens that its value can be easily calculated by means of the following expression, which we prove in Appendix [A.1]:

$$\det V(x_1, ..., x_n) = \prod_{1 \le i < j \le n} (x_j - x_i). \tag{5}$$

One of the main advantages of this result is the reduction of the computational cost it represents. Calculating the VD using this formula has a time complexity of approximately $\mathcal{O}(n^2)$, which is significantly better than the $\mathcal{O}(n^3)$ complexity of standard determinant calculation methods [HLL+21].

The VD is primarily important in the context of quantum mechanics to satisfy the antisymmetry requirements for wavefunctions of indistinguishable fermions.

2.2 Many-body density matrices

2.2.1 Integral formulae for the density matrices

Many-body density matrices are a powerful tool in quantum mechanics that provide valuable information about the distribution and correlations of particles in a given state [Lö55]. In particular, in this dissertation we compute the OBDM and the PCF for the quantum systems under consideration. The latter is directly related to the two-body density matrix (TBDM), as we will now see.

The OBDM for a system of N particles describes the probability distribution of a particle's position and the correlations between different positions in the system [KQM22]. It is defined as

$$\rho^{(N)}(x, x') = N \int dx_2 \cdots dx_N \Psi^*(x, x_2, \ldots, x_N)\Psi(x', x_2, \ldots, x_N), \tag{6}$$

where $\Psi(x_1, \ldots, x_N)$ is the normalized many-body wavefunction and x and x' are two different positions of the same particle. If $x = x'$, we recover the expression for the density, $n^{(N)}(x)$:

$$\rho^{(N)}(x, x) = n^{(N)}(x) = N \int dx_2 \cdots dx_N |\Psi(x, x_2, \ldots, x_N)|^2. \tag{7}$$

On the other hand, the TBDM describes the probability distribution and correlations of two particles in a quantum system. It is defined as the following $N - 2$ integral:

$$\Gamma^{(N)}(x_1, x_2; x_1', x_2') = \binom{N}{2} \int dx_3 \cdots dx_N \Psi^*(x_1, x_2, \ldots, x_N)\Psi(x_1', x_2', \ldots, x_N). \tag{8}$$

Similarly, the three-body density matrix extends this concept to three particles, capturing the correlations and probability distribution among them. Higher-order density matrices continue this pattern for systems with more particles, providing insights into the correlations and statistics of multiple particles within a quantum system [Lö55]. The general formula for the k-body density matrix is given by

$$\begin{aligned}&\Gamma_k^{(N)}(x_1, x_2, \ldots, x_k; x_1', x_2', \ldots, x_k') \\ &= \binom{N}{k} \int dx_{k+1} \ldots dx_N \Psi^*(x_1, x_2, \ldots, x_k, \ldots, x_N)\Psi(x_1', x_2', \ldots, x_k', \ldots, x_N),\end{aligned} \tag{9}$$

from which we can retrieve Eqs. (6) and (8) by putting $k = 1$ and $k = 2$, respectively, i.e., $\Gamma_1^{(N)}(x_1; x_1') = \rho^{(N)}(x_1, x_1')$ and $\Gamma_2^{(N)}(x_1, x_2; x_1', x_2') = \Gamma^{(N)}(x_1, x_2; x_1', x_2')$. Note that for $k = N$ we have no integrals left:

$$\Gamma_N^{(N)}(x_1, x_2, \ldots, x_N; x_1', x_2', \ldots, x_N') = \Psi^*(x_1, x_2, \ldots, x_N)\Psi(x_1', x_2', \ldots, x_N'). \tag{10}$$

The expression for the PCF can be obtained from the TBDM by setting $x_1' = x_1$ and $x_2' = x_2$, which corresponds to the diagonal elements

$$g^{(N)}(x_1, x_2) = \Gamma^{(N)}(x_1, x_2; x_1, x_2). \tag{11}$$

Therefore, the PCF can be computed as

$$g^{(N)}(x_1, x_2) = \binom{N}{2} \int dx_3 \cdots dx_N |\Psi(x_1, x_2, \ldots, x_N)|^2. \tag{12}$$

We can see that $g^{(N)}(x_1, x_2) \geq 0$. The PCF is the probability of finding one particle at x_1 and another at x_2 in an N-body system [Lö55].

2.2.2 Uncorrelated formulae for the OBDM and the PCF

So far, we have shown integral expressions for the OBDM and the PCF. However, for the ground state of non-interacting systems and in the Hartree-Fock approximation (where the many-body wavefunction of a system is approximated as a single Slater determinant), we can find simplified formulae, which we refer to as uncorrelated formulae. In these two scenarios, the OBDM and the PCF can be calculated by sums of products of single-particle wavefunctions $\phi_n(x)$ that are solution of the one-body Schrödinger equation of the system under study. If the single-particle quantum number n takes the values $1, 2, 3, \ldots$, these formulae are:

$$\rho^{(N)}(x, x') = \sum_{n=1}^{N} \phi_n^*(x)\phi_n(x'), \tag{13}$$

$$g^{(N)}(x_1, x_2) = \frac{1}{2} \sum_{n,m=1}^{N} \Phi_{n,m}(x_1, x_2), \tag{14}$$

with

$$\Phi_{n,m}(x_1, x_2) = \phi_n^*(x_1)\phi_m^*(x_2)\left[\phi_n(x_1)\phi_m(x_2) - \phi_m(x_1)\phi_n(x_2)\right]. \tag{15}$$

We derive these expressions analytically in [A.2] starting from Eqs. (6) and (12). If the single-particle quantum number n starts from 0, we can use the same Eqs. (13) and (14) doing the sums from 0 to $N-1$.

With these formulae we do not require the full expression of the ground-state wavefunction, we just need the single-particle wavefunctions. Besides, the computational cost is greatly reduced by avoiding the calculation of integrals and determinants.

Combining Eqs. (13) and (14), we obtain a useful formula for the PCF in terms of the OBDM, as we discuss with detail at the end of Appendix [A.2],

$$g^{(N)}(x_1, x_2) = \frac{1}{2}\left(\rho^{(N)}(x_1, x_1)\rho^{(N)}(x_2, x_2) - \rho^{(N)}(x_1, x_2)\rho^{(N)}(x_2, x_1)\right). \tag{16}$$

This expression will make calculations easier when we find closed expressions for the PCF.

2.3 Harmonic oscillator

2.3.1 Description and ground-state wavefunction

We begin by considering N identical non-interacting spinless fermions of mass m trapped in a HO well of frequency ω. The Hamiltonian of the system can be written as

$$\mathcal{H} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\frac{d^2}{dx_i^2} + \frac{1}{2}m\omega^2\sum_{i=1}^{N}x_i^2 = \sum_{i=1}^{N}h_i, \tag{17}$$

where h_i is the single-particle Hamiltonian,

$$h_i = -\frac{\hbar^2}{2m}\frac{d^2}{dx_i^2} + \frac{1}{2}m\omega^2 x_i^2. \tag{18}$$

The analytical solutions of the eigenvalue problem $h_i\phi_n(x_i) = \epsilon_n\phi_n(x_i)$ are well known:

$$\phi_n(x) = N_n e^{-\frac{x^2}{2a_{ho}^2}} H_n\left(\frac{x}{a_{ho}}\right), \qquad \epsilon_n = \hbar\omega\left(n + \frac{1}{2}\right), \tag{19}$$

with $n = 0, 1, 2, \ldots$ the quantum number that characterizes both the single-particle energy level ϵ_n and the single-particle wavefunction $\phi_n(x)$. Here $a_{ho} = \sqrt{\frac{\hbar}{m\omega}}$ is the oscillator

length, $N_n = \frac{1}{\sqrt{2^n n! a_{ho}\sqrt{\pi}}}$ is a normalization constant and $H_n(x)$ is the Hermite polynomial of order n, which is a polynomial of degree n.

The Rodrigues' formula for the Hermite polynomials is

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}, \tag{20}$$

and, in particular, $H_0(x) = 1$ and $H_1(x) = 2x$. Additionally, these polynomials satisfy the recurrence relation

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x), \tag{21}$$

a property that we need in order to express the ground-state wavefunction compactly.

Due to the Pauli exclusion principle, fermions fill the lowest available energy states ensuring that no two fermions occupy the same quantum state simultaneously. Thus, since we have fully polarized fermions, the ground-state energy is simply the sum of single-particle energies:

$$E^{(N)} = \sum_{n=0}^{N-1} \epsilon_n = \hbar\omega \frac{N^2}{2}, \tag{22}$$

where the intermediate step is detailed in [E.1]. Besides, the ground-state wavefunction is a Slater determinant owing to the Pauli exclusion principle, ensuring anti-symmetry under the exchange of particle positions, as required for fermions.

Our objective is to find a general formula for the ground-state wavefunction. Before this, we analyze the 2-body case. It is not difficult to find that

$$\begin{aligned}\Psi(x_1, x_2) &= \frac{1}{\sqrt{2}} \begin{vmatrix} \phi_0(x_1) & \phi_1(x_1) \\ \phi_0(x_2) & \phi_1(x_2) \end{vmatrix} = \frac{1}{a_{ho}^2\sqrt{\pi}} e^{-\frac{x_1^2+x_2^2}{2a_{ho}^2}} (x_2 - x_1) \\ &= \frac{1}{a_{ho}^2\sqrt{\pi}} e^{-\frac{x_1^2+x_2^2}{2a_{ho}^2}} \prod_{1\le i<j\le 2} (x_j - x_i) = \frac{1}{a_{ho}^2\sqrt{\pi}} e^{-\frac{x_1^2+x_2^2}{2a_{ho}^2}} \det V(x_1, x_2),\end{aligned} \tag{23}$$

where in the last step we have identified $x_2 - x_1$ as a VD, Eq. (5). If we repeat the calculations for $N = 3$, we find that a VD appears again. This suggests that for the general N-particle case we should be able to express the ground-state wavefunction in terms of a VD. For the N-body case we obtain:

$$\begin{aligned}\Psi(x_1, \ldots, x_N) &= \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_0(x_1) & \phi_1(x_1) & \cdots & \phi_{N-1}(x_1) \\ \phi_0(x_2) & \phi_1(x_2) & \cdots & \phi_{N-1}(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_0(x_N) & \phi_1(x_N) & \cdots & \phi_{N-1}(x_N) \end{vmatrix} \\ &= \frac{1}{\sqrt{N!}} \left(\prod_{n=0}^{N-1} N_n \right) e^{-\frac{\sum_{i=1}^N x_i^2}{2a_{ho}^2}} \begin{vmatrix} H_0\left(\frac{x_1}{a_{ho}}\right) & H_1\left(\frac{x_1}{a_{ho}}\right) & \cdots & H_{N-1}\left(\frac{x_1}{a_{ho}}\right) \\ H_0\left(\frac{x_2}{a_{ho}}\right) & H_1\left(\frac{x_2}{a_{ho}}\right) & \cdots & H_{N-1}\left(\frac{x_2}{a_{ho}}\right) \\ \vdots & \vdots & \ddots & \vdots \\ H_0\left(\frac{x_N}{a_{ho}}\right) & H_1\left(\frac{x_N}{a_{ho}}\right) & \cdots & H_{N-1}\left(\frac{x_N}{a_{ho}}\right) \end{vmatrix}.\end{aligned} \tag{24}$$

In [B.1] we prove the hypothesis that this determinant of Hermite polynomials can be written in terms of a VD. We obtain the following result:

$$\det\left[H_{j-1}\left(\frac{x_i}{a_{ho}}\right) \right]_{i,j=1,\ldots,N} = \left[\prod_{i=1}^{N-1} \left(\frac{2}{a_{ho}}\right)^i \right] \det V(x_1, \ldots, x_N). \tag{25}$$

Therefore, the N-body wavefunction is

$$\Psi(x_1,\ldots,x_N) = \frac{1}{\sqrt{N!}}\left[\prod_{n=0}^{N-1}\left(\frac{2}{a_{ho}}\right)^n N_n\right] e^{-\frac{\sum_{i=1}^N x_i^2}{2a_{ho}^2}} \det V(x_1,\ldots,x_N)$$
$$= \frac{1}{\sqrt{N!}}\left[\prod_{n=0}^{N-1}\left(\frac{2}{a_{ho}}\right)^n N_n\right] e^{-\frac{\sum_{i=1}^N x_i^2}{2a_{ho}^2}} \prod_{1\le i<j\le N}(x_j - x_i). \tag{26}$$

We have thus proven that the ground-state wavefunction in a harmonic trap can be written in terms of a VD.

2.3.2 Plots of the OBDM and the PCF

Having found the general expression for the ground-state wavefunction of the HO, Eq. (26), we can now use it to compute and plot the OBDM and the PCF with the integral formulae (6) and (12) using the SymPy library in Python. In Figs. 1, 2 we show the plots for $N = 2, 3, 4, 5$. We work with HO units, with which lengths are measured in terms of $a_{ho} = 1$. We also repeat the calculations using the uncorrelated formulae (13) and (14), and as expected the obtained plots are identical to Figs. 1, 2. We postpone the discussion of the plots to Sec. 2.6, where we will analyze them together with those of other systems.

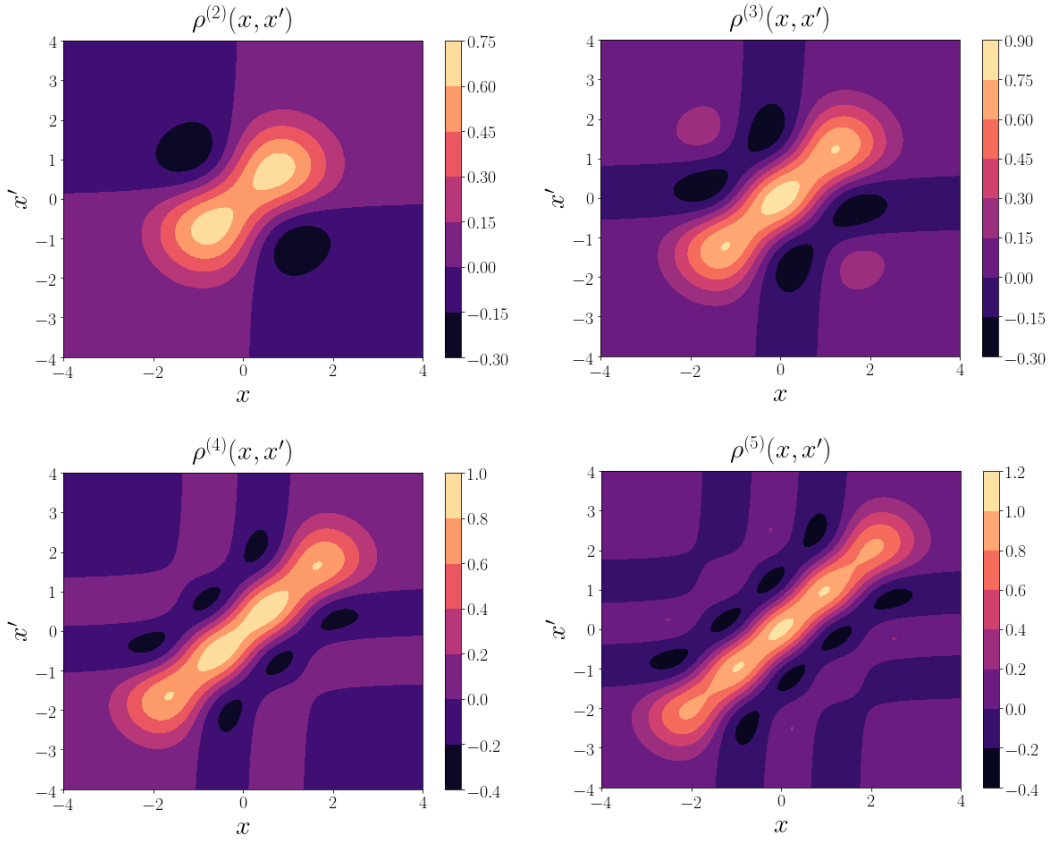

Figure 1: OBDM $\rho^{(N)}(x,x')$ in terms of the positions x and x' for $N = 2$ to 5 particles in a HO well We use HO units.

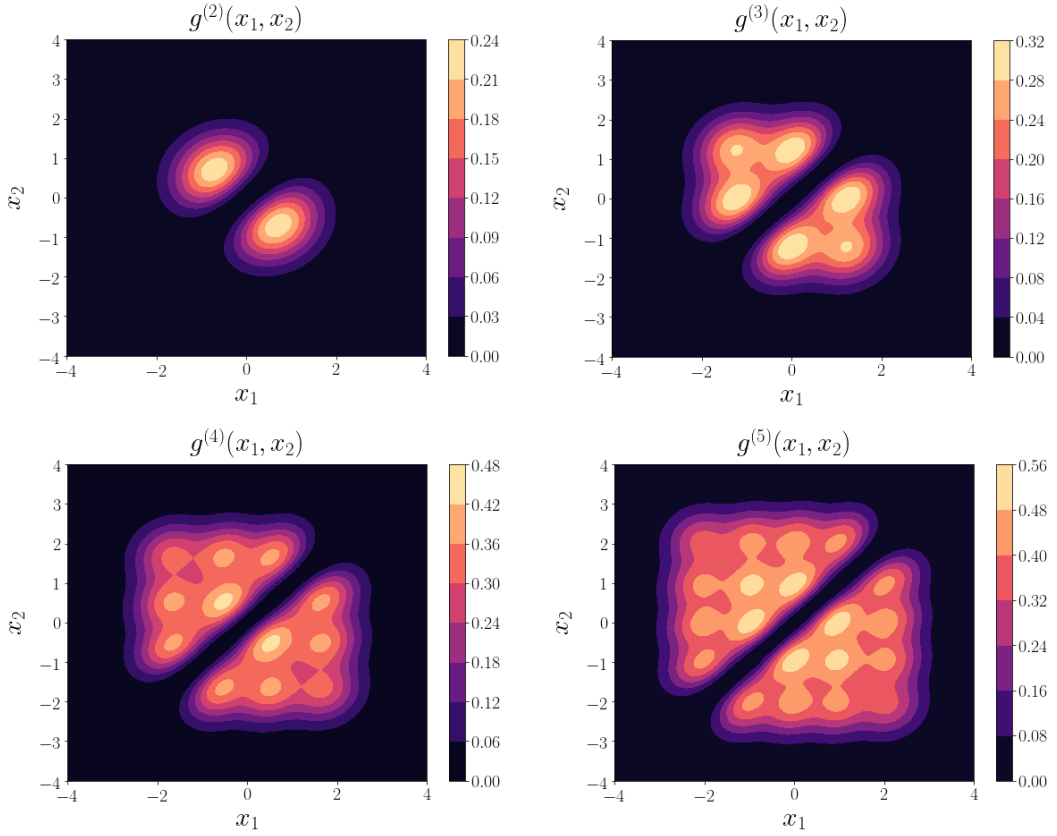

Figure 2: PCF $g^{(N)}(x_1, x_2)$ in terms of the positions x_1 and x_2 for $N = 2$ to 5 particles in a HO well. We use HO units.

2.3.3 Closed expressions for the OBDM and the PCF

After computing the integrals of Eq. (6), we see that the OBDM can be compactly expressed as

$$\rho^{(N)}(x, x') = \frac{1}{a_{ho}\sqrt{\pi}} e^{-\frac{x^2+x'^2}{2a_{ho}^2}} \mathcal{R}^{(N)}(x, x'), \tag{27}$$

where $\mathcal{R}^{(N)}(x, x')$ is a polynomial of order $N-1$ in both x and x'. This polynomial can be represented in terms of the so called Vandermonde vector $\boldsymbol{x}^{(N)} = (1, x, x^2, \ldots, x^{N-1})^T$ and an $N \times N$ matrix $R^{(N)}$:

$$\mathcal{R}^{(N)}(x, x') = \boldsymbol{x}^{(N),T} R^{(N)} \boldsymbol{x'}^{(N)}. \tag{28}$$

These $N \times N$ matrices can be easily found looking at the coefficients of the expressions of $\rho^{(N)}(x, x')$ obtained by integration, Eq. (6). For example, for $N = 3$ we obtain

$$\rho^{(3)}(x, x') = \frac{1}{a_{ho}\sqrt{\pi}} e^{-\frac{x^2+x'^2}{2a_{ho}^2}} \left(2x^2x'^2 - x^2 + 2xx' - x'^2 + \frac{3}{2}\right). \tag{29}$$

Comparing with the expression of $\mathcal{R}^{(3)}(x, x')$, with unknown coefficients a_{ij},

$$\begin{aligned}\mathcal{R}^{(3)}(x, x') = \begin{pmatrix}1 & x & x^2\end{pmatrix} \begin{pmatrix}a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33}\end{pmatrix} \begin{pmatrix}1 \\ x' \\ x'^2\end{pmatrix} = a_{11} + x'a_{12} + x'^2a_{13} \\ + xa_{21} + xx'a_{22} + xx'^2a_{23} + x^2a_{31} + x^2x'a_{32} + x^2x'^2a_{33},\end{aligned} \tag{30}$$

we see that the coefficients of the first row are multiplied by x^0, the ones of the second row are multiplied by x and the ones in the third row are multiplied by x^2, adding in each row x'^0, x' and x'^2 from the left column to the right one. Knowing this, it is immediate to write Eq. (29) using Eq. (28) with the matrix

$$R^{(3)} = \begin{pmatrix} 3/2 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 2 \end{pmatrix}. \tag{31}$$

We can do the same for all N. For example, the results for $N = 2, 4$ are:

$$R^{(2)} = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}, \quad R^{(4)} = \begin{pmatrix} 3/2 & 0 & -1 & 0 \\ 0 & 5 & 0 & -2 \\ -1 & 0 & 2 & 0 \\ 0 & -2 & 0 & 4/3 \end{pmatrix}. \tag{32}$$

Similarly, after computing the integrals in Eq. (12) we find that the PCF can be expressed as

$$g^{(N)}(x_1, x_2) = \frac{1}{2a_{ho}^2\pi} e^{-\frac{x_1^2+x_2^2}{a_{ho}^2}} \frac{(x_1 - x_2)^2}{a_{ho}^2} \mathcal{G}^{(N)}(x_1, x_2), \tag{33}$$

where $\mathcal{G}^{(N)}(x_1, x_2)$ is a polynomial of order $2(N-2)$ in both x_1 and x_2 that can be represented in terms of matrix products,

$$\mathcal{G}^{(N)}(x_1, x_2) = \boldsymbol{x}_1^{(2N-3),T} G^{(2N-3)} \boldsymbol{x}_2^{(2N-3)}. \tag{34}$$

Here, $G^{(2N-3)}$ is a $(2N-3) \times (2N-3)$ matrix. Following the same procedure as before, we find these matrices identifying the coefficients obtained by integration. For $N = 2, 3, 4$, for example, we obtain:

$$G^{(1)} = \begin{pmatrix} 2 \end{pmatrix}, \quad G^{(3)} = \begin{pmatrix} 3 & 0 & 2 \\ 0 & 8 & 0 \\ 2 & 0 & 4 \end{pmatrix}, \quad G^{(5)} = \frac{1}{6} \begin{pmatrix} 45 & 0 & -24 & 0 & 12 \\ 0 & 48 & 0 & 0 & 0 \\ -24 & 0 & 96 & 0 & 0 \\ 0 & 0 & 0 & 64 & 0 \\ 12 & 0 & 0 & 0 & 16 \end{pmatrix}. \tag{35}$$

Note that, up to this point, we have derived the closed expressions for the OBDM and the PCF by generalizing from some particular cases. However, these closed expressions can also be derived mathematically by using the uncorrelated formulae, Eqs. (13) and (14). We do this with all detail in [B.2]. For the OBDM, we arrive at the same result that we have found by generalization, Eq. (27), and additionally we obtain an analytical expression of $\mathcal{R}^{(N)}(x, x')$ in terms of Hermite polynomials,

$$\mathcal{R}^{(N)}(x, x') = \sum_{n=0}^{N-1} \frac{1}{2^n n!} H_n\left(\frac{x}{a_{ho}}\right) H_n\left(\frac{x'}{a_{ho}}\right). \tag{36}$$

Once obtained the closed expression for the OBDM, we can find that of the PCF from Eq. (16). In this manner, not only do we retrieve the formula we have obtained by generalization, Eq. (33), but we also find an analytical expression for the polynomial $\mathcal{G}^{(N)}(x_1, x_2)$,

$$\begin{aligned} \mathcal{G}^{(N)}(x_1, x_2) = \frac{a_{ho}^2}{(x_1 - x_2)^2} \sum_{n,m=0}^{N-1} \frac{1}{2^{n+m} n! m!} \Bigg[& H_n^2\left(\frac{x_1}{a_{ho}}\right) H_m^2\left(\frac{x_2}{a_{ho}}\right) \\ & - H_n\left(\frac{x_1}{a_{ho}}\right) H_n\left(\frac{x_2}{a_{ho}}\right) H_m\left(\frac{x_2}{a_{ho}}\right) H_m\left(\frac{x_1}{a_{ho}}\right) \Bigg]. \end{aligned} \tag{37}$$

In [B.2] we prove that this is indeed a polynomial and not just a rational fraction, as it could seem at first glance. Also, in [B.2] we show the matrices $R^{(N)}$ and $G^{(2N-3)}$ for $N = 5$, which are too large to include here. We have repeated the plots of the OBDM and the PCF for $N = 2, 3, 4, 5$ using their closed expressions and have obtained the same results, Figs. 1 and 2, as expected.

2.4 Infinite well

2.4.1 Description and ground-state wavefunction

In this section, we proceed to study a system of N identical, non-interacting, spinless fermions trapped in an infinite square well potential. Colloquially, it is said that the particles are trapped in a box, since this potential reminds us of a box of size L:

$$V(x) = \begin{cases} 0 & 0 \leq x \leq L \\ \infty & \text{otherwise} \end{cases}. \tag{38}$$

The Hamiltonian of the system is thus

$$\mathcal{H} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\frac{d^2}{dx_i^2} + \sum_{i=1}^{N}V(x_i) = \sum_{i=1}^{N}h_i, \tag{39}$$

with h_i the single-particle Hamiltonian. The single-particle energies and wavefunctions can be found by solving the eigenvalue problem $h_i\phi_n(x_i) = \epsilon_n\phi_n(x_i)$ inside the box, where there is no potential and the single-particle Hamiltonian is just the kinetic term. We then impose the boundary conditions, $\phi_n(0) = \phi_n(L) = 0$. We obtain

$$\phi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right), \qquad \epsilon_n = \frac{\hbar^2\pi^2}{2mL^2}n^2, \tag{40}$$

with $n = 1, 2, 3...$ With the single-particle energies we can compute the ground-state energy of the system,

$$E^{(N)} = \sum_{n=1}^{N}\epsilon_n = \frac{\hbar^2\pi^2}{12mL^2}N(N+1)(2N+1), \tag{41}$$

as discussed in [E.1].

To compute the ground-state wavefunction, we proceed as in the HO case, first computing the Slater determinant for a particular case to see if we can write it in terms of a VD. For the two-body case, we obtain the result

$$\Psi(x_1, x_2) = \frac{1}{\sqrt{2}}\begin{vmatrix}\phi_1(x_1) & \phi_2(x_1)\\ \phi_1(x_2) & \phi_2(x_2)\end{vmatrix} = \frac{4}{\sqrt{2}L}\sin\frac{\pi x_1}{L}\sin\frac{\pi x_2}{L}\left(\cos\frac{\pi x_2}{L} - \cos\frac{\pi x_1}{L}\right), \tag{42}$$

where we have used the sine double angle formula, $\sin 2\alpha = 2\sin\alpha\cos\alpha$. Notice that we can indeed detect the presence of a VD of the variables $\cos\frac{\pi x_i}{L}$ $(i = 1, 2)$,

$$\cos\frac{\pi x_2}{L} - \cos\frac{\pi x_1}{L} = \prod_{1\leq i<j\leq 2}\left(\cos\frac{\pi x_j}{L} - \cos\frac{\pi x_i}{L}\right) = \det V\left(\cos\frac{\pi x_1}{L}, \cos\frac{\pi x_2}{L}\right). \tag{43}$$

This suggests that we should be able to write the general expression of the ground-state

wavefunction in terms of a VD of cosines. Starting from the definition,

$$\begin{aligned}\Psi(x_1,...,x_N) &= \frac{1}{\sqrt{N!}}\det[\phi_m(x_n)]_{n,m=1,...,N}\\ &= \frac{1}{\sqrt{N!}}\det\left[\sqrt{\frac{2}{L}}\sin\frac{m\pi x_n}{L}\right]_{n,m=1,...,N}\\ &= \left(\frac{1}{2i}\right)^N\frac{1}{\sqrt{N!}}\left(\sqrt{\frac{2}{L}}\right)^N\det\left[e^{\frac{im\pi x_n}{L}}-e^{-\frac{im\pi x_n}{L}}\right]_{n,m=1,...,N},\end{aligned} \tag{44}$$

where we have used that $\sin\alpha = \frac{e^{i\alpha}-e^{-i\alpha}}{2i}$. Using the so called Vandermonde formula [Pro88],

$$\det\left[z_j^k - z_j^{-k}\right]_{j,k=1,...,N} = \prod_{l=1}^{N}(z_l - z_l^{-1})\prod_{1\le j<k\le N}(z_k - z_j)\left(1-\frac{1}{z_j z_k}\right), \tag{45}$$

we can transform the determinant in Eq. (44) to

$$\begin{aligned}&\det\left[\left(e^{\frac{i\pi x_n}{L}}\right)^m - \left(e^{\frac{i\pi x_n}{L}}\right)^{-m}\right]_{n,m=1,...,N}\\ &= \prod_{l=1}^{N}\left(e^{\frac{i\pi x_l}{L}}-e^{-\frac{i\pi x_l}{L}}\right)\prod_{1\le j<k\le N}\left(e^{\frac{i\pi x_k}{L}}-e^{\frac{i\pi x_j}{L}}\right)\left(1-e^{-\frac{i\pi(x_j+x_k)}{L}}\right)\\ &= \prod_{l=1}^{N}2i\sin\frac{\pi x_l}{L}\prod_{1\le j<k\le N}\left(e^{\frac{i\pi x_k}{L}}-e^{\frac{i\pi x_j}{L}}-e^{-\frac{i\pi x_j}{L}}+e^{-\frac{i\pi x_k}{L}}\right)\\ &= \prod_{l=1}^{N}2i\sin\frac{\pi x_l}{L}\prod_{1\le j<k\le N}2\left(\cos\frac{\pi x_k}{L}-\cos\frac{\pi x_j}{L}\right).\end{aligned} \tag{46}$$

The general expression for the ground-state wavefunction is then

$$\begin{aligned}\Psi(x_1,...,x_N) &= \left(\frac{1}{2i}\right)^N\frac{1}{\sqrt{N!}}\left(\sqrt{\frac{2}{L}}\right)^N\prod_{l=1}^{N}2i\sin\frac{\pi x_l}{L}\prod_{1\le j<k\le N}2\left(\cos\frac{\pi x_k}{L}-\cos\frac{\pi x_j}{L}\right)\\ &= \frac{1}{\sqrt{N!}}2^{\frac{N(N-1)}{2}}\left(\sqrt{\frac{2}{L}}\right)^N\prod_{l=1}^{N}\sin\frac{\pi x_l}{L}\prod_{1\le j<k\le N}\left(\cos\frac{\pi x_k}{L}-\cos\frac{\pi x_j}{L}\right),\end{aligned} \tag{47}$$

where we have used that there are $\binom{N}{2} = \frac{N(N-1)}{2}$ terms in the second product. Thus, for the IW, a VD appears in the ground-state wavefunction:

$$\Psi(x_1,...,x_N) = \frac{1}{\sqrt{N!}}2^{\frac{N(N-1)}{2}}\left(\sqrt{\frac{2}{L}}\right)^N\left[\prod_{l=1}^{N}\sin\frac{\pi x_l}{L}\right]\det V\left(\cos\frac{\pi x_1}{L},\ldots,\cos\frac{\pi x_N}{L}\right). \tag{48}$$

2.4.2 Plots of the OBDM and the PCF

In the same way as we did with the HO case, we have computed and plotted the OBDM and the PCF for $N = 2, 3, 4, 5$ with both the integral formulae, Eqs. (6) and (12), and the uncorrelated formulae, (13) and (14), and we have found the same results. The plots are shown below (Figs. 3, 4), with the range of the particle positions going from 0 to 1 in the natural units of this system (lengths measured in units of $L = 1$).

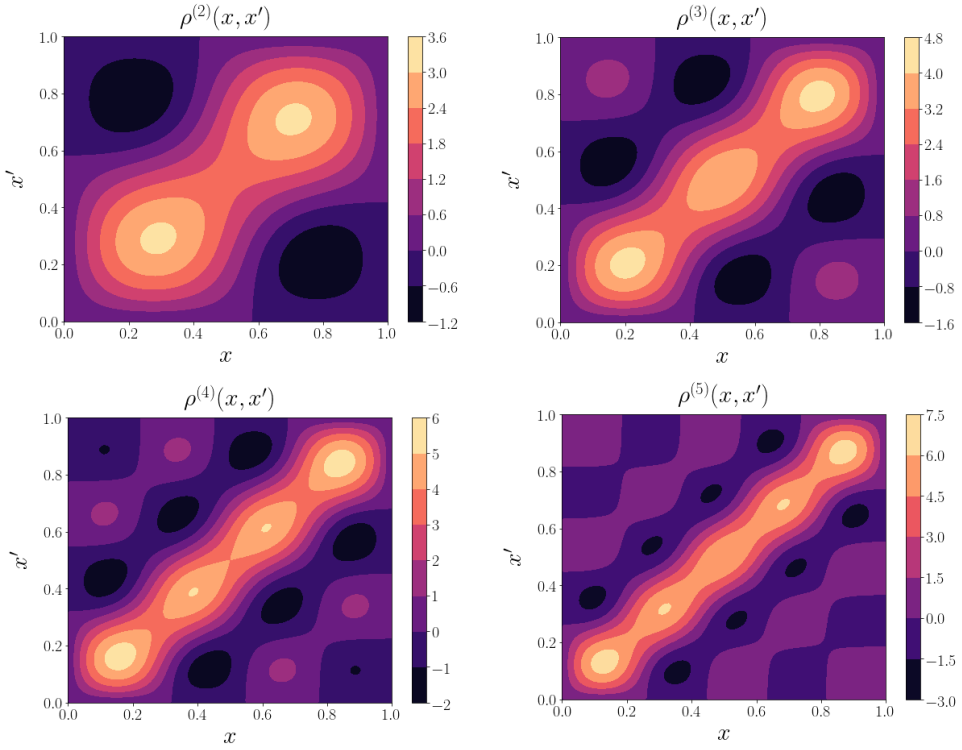

Figure 3: OBDM $\rho^{(N)}(x, x')$ in terms of the positions x and x' for $N = 2$ to 5 particles in an IW. We use IW natural units.

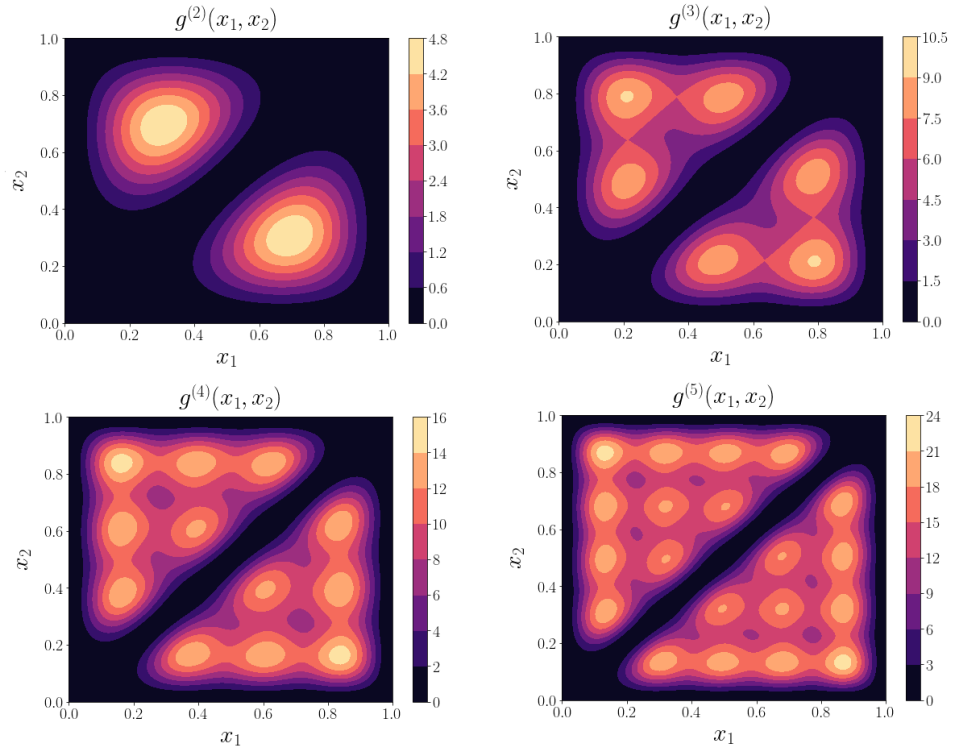

Figure 4: PCF $g^{(N)}(x_1, x_2)$ in terms of the positions x_1 and x_2 for $N = 2$ to 5 particles in an IW. We use IW natural units.

2.4.3 Closed expressions for the OBDM and the PCF

Similarly as we have done in the HO case, we can find a closed expression for the OBDM and the PCF in terms of polynomials, which in turn can be found from a matrix product involving Vandermonde vectors. The detailed mathematical procedure is discussed in [C], here we summarize and gather the obtained results. To find the closed expression for the OBDM, we use the following identity [SLL14],

$$\begin{aligned}\sin nA &= \sin A \sum_{i=1}^{\lfloor \frac{n+1}{2} \rfloor} (-1)^{i+1} \binom{n-i}{i-1} (2\cos A)^{n-(2i-1)} \\ &= \sin A \left\{ (2\cos A)^{n-1} - \binom{n-2}{1} (2\cos A)^{n-3} + \binom{n-3}{2} (2\cos A)^{n-5} - \cdots \right\}, \end{aligned} \tag{49}$$

where the notation $\lfloor x \rfloor$ denotes the largest integer N such that $N \leq x$. After some calculations, starting from the uncorrelated formula of the OBDM, Eq. (13), we find that

$$\rho^{(N)}(x,x') = \frac{2}{L} \sin\frac{\pi x}{L} \sin\frac{\pi x'}{L} \mathcal{R}^{(N)}(y,y'), \tag{50}$$

where $y = \cos\frac{\pi x}{L}$, $y' = \cos\frac{\pi x'}{L}$ and

$$\mathcal{R}^{(N)}(y,y') = \sum_{n=1}^{N} \sum_{i,j=1}^{\lfloor \frac{n+1}{2} \rfloor} (-1)^{i+j} \binom{n-i}{i-1} \binom{n-j}{j-1} (2y)^{n-(2i-1)} (2y')^{n-(2j-1)} \tag{51}$$

is a polynomial of order $N-1$ in both y and y' that can be written in terms of Vandermonde vectors and an $N \times N$ matrix, $R^{(N)}$:

$$\mathcal{R}^{(N)}(y,y') = \boldsymbol{y}^{(N),T} R^{(N)} \boldsymbol{y'}^{(N)}. \tag{52}$$

These matrices can be easily found computing the polynomial in Eq. (51) and recognizing the coefficients in a similar fashion as we did in Sec. 2.3.3. As an example, for $N = 2, 3$ we obtain

$$R^{(2)} = \begin{pmatrix} 1 & 0 \\ 0 & 4 \end{pmatrix}, \quad R^{(3)} = \begin{pmatrix} 2 & 0 & -4 \\ 0 & 4 & 0 \\ -4 & 0 & 16 \end{pmatrix}. \tag{53}$$

The closed expression of the PCF can be found from Eqs. (16) and (50):

$$g^{(N)}(x_1,x_2) = \frac{2}{L^2} \sin^2\frac{\pi x_1}{L} \sin^2\frac{\pi x_2}{L} \mathcal{G}^{(N)}(y_1,y_2), \tag{54}$$

where

$$\mathcal{G}^{(N)}(y_1,y_2) = \mathcal{R}^{(N)}(y_1,y_1)\mathcal{R}^{(N)}(y_2,y_2) - \mathcal{R}^{(N)}(y_1,y_2)\mathcal{R}^{(N)}(y_2,y_1) \tag{55}$$

is a polynomial of order $2(N-1)$ in both y_1 and y_2 that can also be represented as a matrix product,

$$\mathcal{G}^{(N)}(y_1,y_2) = \boldsymbol{y_1}^{(2N-1),T} G^{(2N-1)} \boldsymbol{y_2}^{(2N-1)}, \tag{56}$$

with $G^{(2N-1)}$ a $(2N-1) \times (2N-1)$ matrix. These matrices can be found computing the polynomial in Eq. (55) and identifying the coefficients. As an example, for $N = 2, 3$, we have

$$G^{(3)} = \begin{pmatrix} 0 & 0 & 4 \\ 0 & -8 & 0 \\ 4 & 0 & 0 \end{pmatrix}, \quad G^{(5)} = \begin{pmatrix} 0 & 0 & 8 & 0 & 16 \\ 0 & -16 & 0 & 32 & 0 \\ 8 & 0 & -96 & 0 & 64 \\ 0 & 32 & 0 & -128 & 0 \\ 16 & 0 & 64 & 0 & 0 \end{pmatrix}. \tag{57}$$

All the matrices $R^{(N)}$ and $G^{(2N-1)}$ for $N = 2, 3, 4, 5$ are found in [C] from Eqs. (51) and (55). To facilitate the calculations, we have used a Python code that receives the not simplified polynomials, makes the pertinent simplifications and groupings, and returns the desired matrices.

Using the obtained matrices to plot the OBDM and the PCF with Eqs. (50) and (54), we obtain the same figures as in Sec. 2.4.2 (Figs. 3, 4), thus validating that the matrices are correct.

2.5 Morse oscillator

2.5.1 Description and ground-state wavefunction

The last system we study consists of N identical non-interacting spinless fermions in a Morse oscillator well. The Morse potential is a model for the potential energy of a vibrating diatomic molecule. It takes into account the effects of bond breaking and includes the anharmonicity of real bonds, thus becoming a better approximation of the vibrational motion of a molecule than the HO [Fid16]. The Morse potential is represented as:

$$V(x) = D\left(1 - e^{-ax}\right)^2, \quad -\infty < x < \infty, \tag{58}$$

where D is the dissociation energy (or equivalently, the depth of the potential well), a is a positive parameter that controls the width of the well, and $x = r - r_e$, with r the distance between the two atoms (or internuclear separation) and r_e the equilibrium separation between atoms, the choice of which is arbitrary. The actual domain of x is from $-r_e$ to ∞, but it has been found that the physical effects of changing $-r_e$ for $-\infty$ are completely negligible [Mor29, Haa46]. Notice that this potential is not parity symmetric, so it is different from the HO or the IW.

The effective force constant of the bond, k_e, is given by the second derivative of the potential (58) at the minimum of the well ($x = 0$): $k_e = \left(d^2V/dx^2\right)_{x=0} = 2a^2D$, from where we can also find the effective oscillator frequency of a particle with mass m by comparison with a HO:

$$\omega_e = \sqrt{\frac{k_e}{m}} = a\sqrt{\frac{2D}{m}}. \tag{59}$$

For our system of N particles, the Hamiltonian can be written as

$$\mathcal{H} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\frac{d^2}{dx_i^2} + D\sum_{i=1}^{N}\left(1 - e^{-ax_i}\right)^2 = \sum_{i=1}^{N} h_i, \tag{60}$$

where h_i is the single-particle Hamiltonian. Thus, the Schrödinger equation for the single-particle states of the MO is

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + D\left(1 - e^{-ax}\right)^2\right]\phi_n(x) = \epsilon_n\phi_n(x). \tag{61}$$

Defining a new dimensionless variable, $y = ax$, we obtain

$$\left[-\frac{\hbar^2a^2}{2m}\frac{d^2}{dy^2} + D\left(1 - e^{-y}\right)^2\right]\phi_n(y) = \epsilon_n\phi_n(y). \tag{62}$$

Dividing the equation by D and defining $\varepsilon_n = \frac{\epsilon_n}{D}$ and $\lambda^2 = \frac{2mD}{\hbar^2a^2}$, we get the equation

$$\frac{d^2\phi_n(y)}{dy^2} + \lambda^2\left[\varepsilon_n - (1 - e^{-y})^2\right]\phi_n(y) = 0, \tag{63}$$

which can be solved exactly, giving the following normalized states and energies [DS88]:

$$\phi_n(z) = N_n z^{\lambda-n-\frac{1}{2}} e^{-z/2} L_n^{2\lambda-2n-1}(z), \qquad \epsilon_n = \left[\left(n+\frac{1}{2}\right) - \frac{1}{2\lambda}\left(n+\frac{1}{2}\right)^2\right]\hbar\omega_e, \tag{64}$$

where we have defined

$$z = 2\lambda e^{-y}, \;\; N_n = \sqrt{\frac{n!(2\lambda-2n-1)a}{\Gamma(2\lambda-n)}}. \tag{65}$$

In [DS88] there is a mistake and a is missing in the numerator of N_n.

If we consider bound states, the quantum number n can only take values $n = 0, 1, 2 \ldots, \lfloor \lambda - \frac{1}{2} \rfloor$. On the other hand, the functions $L_n^\alpha(x)$ are the associated (or generalized) Laguerre polynomials. The Rodrigues' formula for these polynomials of degree n is

$$L_n^\alpha(x) = \frac{x^{-\alpha}e^x}{n!}\frac{d^n}{dx^n}(x^{n+\alpha}e^{-x}), \tag{66}$$

where $\alpha > -1$. The closed form for these polynomials can be derived from the Rodrigues' formula [SHP16]:

$$L_n^\alpha(x) = \sum_{i=0}^{n}(-1)^i \binom{n+\alpha}{n-i}\frac{x^i}{i!} \equiv \sum_{i=0}^{n} C_{n,i}^\alpha x^i, \tag{67}$$

with

$$\binom{\delta}{m} = \frac{1}{m!}\prod_{k=0}^{m-1}(\delta-k) = \frac{1}{m!}\delta(\delta-1)(\delta-2)\cdots(\delta-m+1) \tag{68}$$

a binomial coefficient for $m \in \mathbb{N}$ and $\delta \in \mathbb{R}$. In particular, the first two associated Laguerre polynomials are $L_0^\alpha(x) = 1$ and $L_1^\alpha(x) = 1 + \alpha - x$.

From Eq. (64) we can find the ground-state energy of the system. This is done in detail in Appendix [E.1]. The result is

$$E^{(N)} = \sum_{n=0}^{N-1}\epsilon_n = \left[\frac{N^2}{2} - \frac{1}{24\lambda}N\left(4N^2-1\right)\right]\hbar\omega_e. \tag{69}$$

To compute the ground-state wavefunction and see if it can be written in terms of a VD, we define for simplicity $\beta = \lambda - \frac{1}{2}$, obtaining $\phi_n(x) = N_n z^\beta e^{-\frac{z}{2}} z^{-n} L_n^{2\beta-2n}(z)$, where $z = z(x) = 2\lambda e^{-ax}$. Thus, we have

$$\begin{aligned}\Psi(x_1,\ldots,x_N) &= \frac{1}{\sqrt{N!}}\det[\phi_{j-1}(x_i)]_{i,j=1,\ldots,N} \\ &= \frac{1}{\sqrt{N!}}\left[\prod_{i=0}^{N-1} N_i z_{i+1}^\beta\right] e^{-\frac{\sum_{i=1}^N z_i}{2}} \det\left[z_i^{-(j-1)} L_{j-1}^{2\beta-2(j-1)}(z_i)\right]_{i,j=1,\ldots,N}.\end{aligned} \tag{70}$$

In [D.1] we find the non trivial mathematical relation:

$$\det\left[z_i^{-(j-1)} L_{j-1}^{2\beta-2(j-1)}(z_i)\right]_{i,j=1,\ldots,N} = \left[\prod_{i=1}^{N-1}\binom{2\beta-i}{i}\right]\det V\left(\frac{1}{z_1},\ldots,\frac{1}{z_N}\right). \tag{71}$$

This enables us to write the ground-state wavefunction in terms of a VD, as we wanted:

$$\Psi(x_1,\ldots,x_N) = \frac{1}{\sqrt{N!}}\left[\prod_{i=0}^{N-1} N_i z_{i+1}^\beta\right] e^{-\frac{\sum_{i=1}^N z_i}{2}} \left[\prod_{i=1}^{N-1}\binom{2\beta-i}{i}\right] \prod_{1\le i<j\le N}\left(\frac{1}{z_j}-\frac{1}{z_i}\right). \tag{72}$$

2.5.2 Plots of the OBDM and PCF

As we did with the other systems, we have computed and plotted the OBDM and the PCF for $N = 2, 3, 4, 5$ with both the integral formulae, Eqs (6) and (12), and the uncorrelated formulae, Eqs. (13) and (14), obtaining identical results. The plots are shown below (Figs. 5, 6), with the range of the particle positions going from -1 to 2 in the natural units of this system (lengths in units of $\frac{1}{a} = 1$). We use $\lambda = 11.5$, which corresponds to 12 bound states. We discuss this choice in Sec. 2.6.

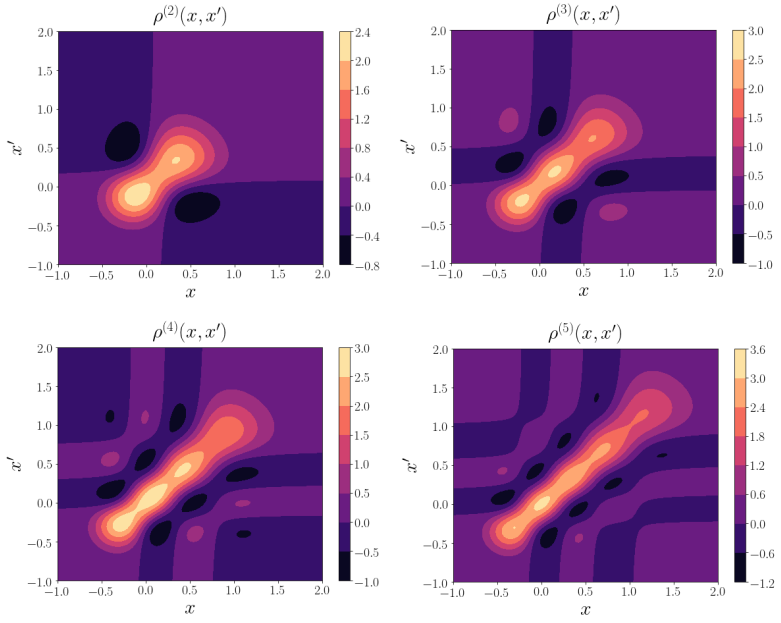

Figure 5: OBDM $\rho^{(N)}(x, x')$ in terms of the positions x and x' for $N = 2$ to 5 particles in a MO, with $\lambda = 11.5$. We use MO natural units.

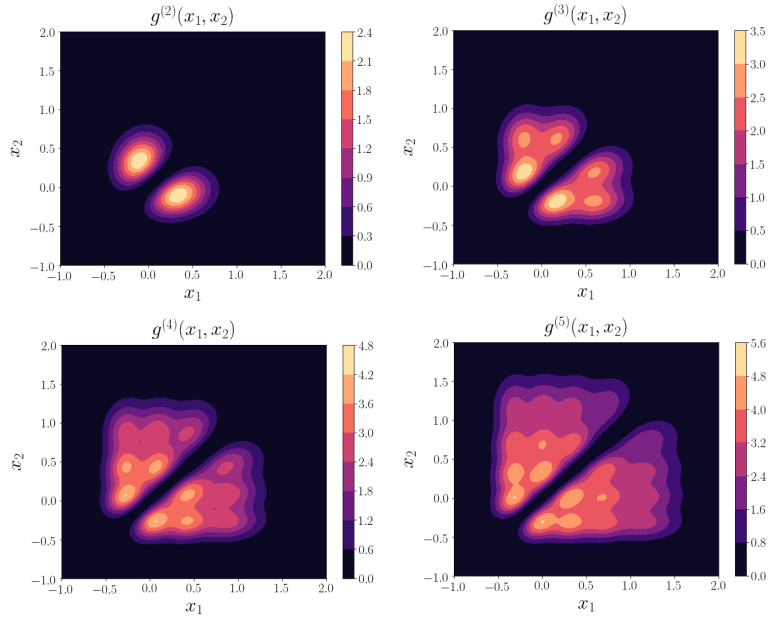

Figure 6: PCF $g^{(N)}(x_1, x_2)$ in terms of the positions x_1 and x_2 for $N = 2$ to 5 particles in a MO, with $\lambda = 11.5$. We use MO natural units.

2.5.3 Closed expressions for the OBDM and the PCF

In this section, we want to find a closed expression for the OBDM and the PCF in a MO. The analytical calculations are found in detail in [D.2]. We find that the OBDM can be written as

$$\rho^{(N)}(z,z') = (zz')^{\beta-N+1} e^{-\frac{z+z'}{2}} \mathcal{R}^{(N)}(z,z'), \tag{73}$$

where

$$\mathcal{R}^{(N)}(z,z') = \sum_{n=0}^{N-1} N_n^2 (zz')^{N-1-n} \sum_{i,j=0}^{n} C_{n,i}^{2\beta-2n} C_{n,j}^{2\beta-2n} z^i z'^j \tag{74}$$

is a polynomial of order $N-1$ in both z and z' that can be written in terms of Vandermonde vectors and an $N \times N$ matrix $R^{(N)}$ as

$$\mathcal{R}^{(N)}(z,z') = \boldsymbol{z}^{(N),T} R^{(N)} \boldsymbol{z'}^{(N)}. \tag{75}$$

From Eqs. (73) and (16), it follows that the closed expression of the PCF is

$$g^{(N)}(z_1,z_2) = \frac{1}{2}(z_1 z_2)^{2\beta-2N+2} e^{-(z_1+z_2)} \mathcal{G}^{(N)}(z_1,z_2), \tag{76}$$

where $\mathcal{G}^{(N)}(z_1,z_2)$ is simply

$$\mathcal{G}^{(N)}(z_1,z_2) = \mathcal{R}^{(N)}(z_1,z_1)\mathcal{R}^{(N)}(z_2,z_2) - \mathcal{R}^{(N)}(z_1,z_2)\mathcal{R}^{(N)}(z_2,z_1), \tag{77}$$

that is, a polynomial of order $2(N-1)$ in both z_1 and z_2 that can be represented in terms of matrix products as

$$\mathcal{G}^{(N)}(z_1,z_2) = \boldsymbol{z_1}^{(2N-1),T} G^{(2N-1)} \boldsymbol{z_2}^{(2N-1)}, \tag{78}$$

with $G^{(2N-1)}$ a $(2N-1)\times(2N-1)$ matrix. In contrast to the HO or the IW, where the elements of the matrices were rational numbers, here the matrices contain real numbers. For example, for $N=2$, we have

$$R^{(2)} = \begin{pmatrix} N_1^2 \left(C_{1,0}^{2\beta-2}\right)^2 & N_1^2 C_{1,0}^{2\beta-2} C_{1,1}^{2\beta-2} \\ N_1^2 C_{1,1}^{2\beta-2} C_{1,0}^{2\beta-2} & N_0^2 + N_1^2 \left(C_{1,1}^{2\beta-2}\right)^2 \end{pmatrix}, \; G^{(3)} = N_0^2 N_1^2 \left(C_{1,0}^{2\beta-2}\right)^2 \begin{pmatrix} 0 & 0 & 1 \\ 0 & -2 & 0 \\ 1 & 0 & 0 \end{pmatrix}. \tag{79}$$

In [D.2] we compute all the matrices $R^{(N)}$ and $G^{(2N-1)}$ for $N=2,3,4,5$ and use them to calculate and plot the OBDM and the PCF with the closed expressions. The results obtained are the identical to Figs. 5, 6, thus validating the formulae we have found.

2.6 Discussion and comparison of the different plots

Now that we have obtained the plots of the OBDM and the PCF for all the systems (Figs. 1, 2, 3, 4, 5, 6), we examine them together and discuss their similarities and differences. Starting for the OBDM, all the plots show that the diagonal $x = x'$ and its near surroundings present positive values. This is because $\rho^{(N)}(x,x) = n^{(N)}(x)$ is the density, which is positive definite, Eq. (7). In the diagonal we find as many peaks as particles. We observe a clear localization of the single-particle states. For the HO, the peaks in the diagonal are more intense at the central part, and as we move away from the center, they become less intense. In contrast, for the IW, the most intense peaks are the ones further from the center. For the MO, the most intense peak is located near the origin of coordinates $x = x' = 0$, as expected from Eq. (64). Moreover, as we move away from the

diagonal, in all three systems there start to appear undulate areas with alternating sign. This pattern of alternating positive and negative values arises from the nodal structure of the single-particle states [E.2]. In particular, there are $2(N-1)$ changes of sign along the off-diagonal direction as reflected in Eq. (13).

If we now examine the plots of the PCF, we see at first glance that $g^{(N)}(x_1, x_2)$ is a non-negative function, as we already knew, and also that in the diagonal region, where x_1 and x_2 take close values, the PCF vanishes. This characteristic is a result of the Pauli exclusion principle, and we can also see it in Eq. (16), where clearly $g^{(N)}(x_1, x_1) = 0$. We see that the PCF is squared-shape, formed by two triangular parts separated by the diagonal. Similarly as it happens with the OBDM, for the HO the peaks are more intense in the internal part of the triangles, while for the IW the most intense peaks are those in the borders of the square. For the MO, the two most intense peaks are found when x or x' are near to zero.

Finally, while for the HO and the IW the OBDM and the PCF are symmetric with respect to the off-diagonal, thit is not the case for the MO. This stems from the anharmonicity of the Morse potential, which breaks the parity symmetry, making it less likely to find particles away from the minimum of the potential.

Overall, we see that the OBDM is similar for all the systems regardless of the potential, and the same happens with the PFC. This suggests some kind of universality for non-interacting 1D systems of confined spinless fermions.

Note that the plots for the MO depend on the dimensionless parameter λ. We have chosen $\lambda = 11.5$ arbitrarily, bearing in mind that $\lambda \geq 4.5$, since we do the plots for $N = 2$ to 5, so at least we need 5 bound states (recall that the quantum number goes from $n_{min} = 0$ to $n_{max} = \lfloor \lambda - \frac{1}{2} \rfloor$). In our case we have 12 bound states, so it is enough. We have repeated the plots for other values of lambda ($\lambda = 4.5$, $\lambda = 8$, $\lambda = 16.2$, etc.) and we obtain the same patterns. The difference is that as λ increases, the absolute values of the OBDM and the PCF increase while the range of particle positions decrease.

3 Study of the ground state using Machine Learning

In the preceding sections, our investigation has been exclusively focused on analytical methods to derive all pertinent outcomes. However, now we take a different approach by incorporating ML to reproduce and validate these findings. This approach will not only strengthen our results, but also show that ML techniques are capable of solving the three quantum systems under examination.

In particular, in this section, we will use an ANN as an ansatz for the ground-state wavefunction (i.e. a NQS) and apply ML techniques to variationally minimize the energy of the quantum systems, thus obtaining appropriate parameters for the ANN. Once we obtain the wavefunction, we will compute the OBDM and the PCF of the systems for $N = 2, 3, 4, 5$ and check if the results agree with the analytical ones.

3.1 Artificial Neural Networks

An ANN is a ML algorithm inspired by networks of biological neurons that consists of interconnected nodes, called neurons, arranged in layers [JTR10]. In a similar way as neurons in our nervous system can learn from data, an ANN can learn from input data and produce an output. The input layer is the first layer of an ANN, and is the one that receives the raw input data. In the middle of the ANN there can be one or more hidden layers, where each neuron performs a weighted sum of the inputs (from the previous layer

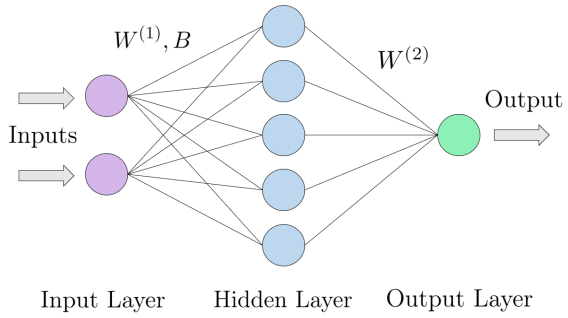

Figure 7: Architecture of a one-layer ANN with two neurons in the input layer, five neurons in the hidden layer and one neuron in the output layer (i.e. this ANN will produce one output).There is only one hidden layer, and the weights and biases are represented by the matrices $W^{(1)} = [w^{(1)}_{i,j}]_{1\leq i\leq 5, 1\leq j\leq 2}$, $W^{(2)} = [w^{(2)}_{i,j}]_{i=1, 1\leq j\leq 5}$ and $B = [b_{i,j}]_{1\leq 1\leq 5, j=1}$. In this case the formula for the output would be $y = \sum_{i=1}^{N_{hid}} w^{(2)}_{1,i}\sigma\left(\sum_{j=1}^{N_{inp}} w^{(1)}_{i,j}x_j + b_{i,1}\right)$, where N_{inp} and N_{hid} are the number of neurons in the input layer and the hidden layer, respectively, and $\sigma(x)$ is the activation function.

or directly from the input layer), adds an additional parameter called bias (associated with each neuron) and applies an activation function to produce an output. These weights represent the connections between two neurons, and the activation function introduces non-linearity to the network. Common choices of nonlinear activation functions are the sigmoid function or the hyperbolic tangent [Bon11]. Finally, the outputs from the last hidden layer are passed to the output layer, which produces the final outputs. The number of neurons in the output layer corresponds to the number of possible outputs. Fig. 7 shows an example of ANN to better understand its structure.

An important property of ANNs is that they are universal function approximators, in the sense that with a sufficient number of neurons and appropriate parameters (weights and biases), they can approximate any continuous function to arbitrary accuracy [GC12]. This statement is known as the Universal Approximation Theorem.

We use an ANN as the trial ground-state wavefunction in a variational method. In our case, the input to our ANN are the positions of the N fermions $\{x_i\}_{i=1,\dots,N}$ and the output is the ground-state wavefunction, $\Psi_{\mathcal{W}}(x_1, \dots, x_N)$, where $\mathcal{W}$ is a multidimensional variable containing the weights and biases[1]. The ANN needs to be trained by adjusting its weights and biases in such a way that the ANN output becomes closer to the desired output. One of the most widely used training methods is back-propagation, which involves computing the gradient of a chosen loss function (LF) with respect to the ANN parameters so that the parameters can be adjusted in such a way to minimize the LF.

We use the ANN elaborated by J. W. T. Keeble ([Kee19], [KDRF+23], [Kee22]), which has two hidden layers with 64 hidden neurons per layer and uses the hyperbolic tangent as the activation function. To impose anti-symmetry of the wavefunction, permutation equivariance is maintained throughout the ANN. The library used to implement this ANN is PyTorch, an open-source machine learning library.

3.2 Methodology

Now that we have an ansatz for the ground-state wavefunction, we solve the Schrödinger equation for each system using a Variational Monte-Carlo approach with two phases. The

[1]In fact, we obtain the sign of the wavefunction, $\text{sgn}(\Psi_{\mathcal{W}})$ and the logarithm of the absolute value of the wavefunction, $\log(|\Psi_{\mathcal{W}}|)$. This is done for numerical stability.

first one is the pre-training phase, which is designed to obtain a first ANN that reproduces the HO single-particle wavefunctions. After this phase, we have a physical state that bears some resemblance to the targeted ground-state wavefunction. This step, although expendable, helps to avoid beginning the energy-minimization phase from scratch. In this phase, we minimize the expectation value of the energy to adapt the weights and biases of the ANN in order to find the ground-state wavefunction. This expectation value can be expressed as a statistical average over local energies, as it is usually done in Monte-Carlo approaches:

$$E = \frac{\langle \Psi_{\mathcal{W}} | \, \mathcal{H} \, | \Psi_{\mathcal{W}} \rangle}{\langle \Psi_{\mathcal{W}} | \Psi_{\mathcal{W}} \rangle} = \mathbb{E}_{X \sim |\Psi_{\mathcal{W}}|^2} \left[\Psi_{\mathcal{W}}(X)^{-1} \, \mathcal{H} \, \Psi_{\mathcal{W}}(X) \right], \tag{80}$$

where $E_L(X) = \Psi_{\mathcal{W}}(X)^{-1} \, \mathcal{H} \, \Psi_{\mathcal{W}}(X)$ is the local energy and $X = (x_1, \ldots, x_N)$ is an N-dimensional random variable (or walker) that follows the Born probability distribution, $|\Psi_{\mathcal{W}}|^2$. To obtain variables distributed in such a way, we do a sampling using the Metropolis-Hastings algorithm [Miy23]. During this second phase, we use back-propagation to minimize the energy LF until our NQS converges to the ground-state wavefunction. However, for numerical stability and precision, instead of directly implementing Eq. (80), we use an auxiliary LF [KDRF+23].

Both phases use $N_w = 4096$ walkers and are iterated a determined number of epochs, the second phase needing more epochs than the first one (here we talk about pre-epochs). For the HO, we need much less epochs than with the IW or the MO because we start the energy-minimization phase with an ansatz that is already close to the HO wavefunction. Nevertheless, the epochs needed in all cases stay in the order of 10^4, and the pre-epochs are around 10^3. The potentials are implemented according to the theory, but for the IW we cannot put a well of infinite height. Instead, we use a finite well of height $V_0 = 1000$.

3.3 Comparison with the analytical results

To compare the obtained ground-state energies with the analytical ones [Eqs. (22), (41) and (69)], we have made a summary table for $N = 2, 3, 4, 5$ (Tab. 1). To do all the numerical computations we have used the natural units of each system, so the theoretical values also need to be in these units. The formulae in natural units are gathered in [E.1]. Energies are written with an error of $\delta E^{(N)}_{\text{ML}} = 2\sigma$, where σ is the standard deviation, computed as

$$\sigma = \sqrt{\frac{1}{N_w - 1} \sum_{i=0}^{N_w - 1} (E_{L_i} - \langle E_L \rangle)^2}, \tag{81}$$

where we have included the Bessel correction. We can see in Tab. 1 that the results for the HO and the MO are in agreement with the theoretical values, since they satisfy

$$\left| E^{(N)}_{\text{ML}} - E^{(N)}_{\text{theory}} \right| < 2\delta E^{(N)}_{\text{ML}}. \tag{82}$$

However, for the IW we find discrepancies, which may be a consequence of the finite height of the well. To quantify these discrepancies, we compute the relative errors as $\epsilon_r^{(N)} = \left(\left| E^{(N)}_{\text{theory}} - E^{(N)}_{\text{ML}} \right| / E^{(N)}_{\text{theory}} \right) \cdot 100$. We find $\epsilon_r^{(2)} = 7.2\%$, $\epsilon_r^{(3)} = 5.7\%$, $\epsilon_r^{(4)} = 2.0\%$ and $\epsilon_r^{(5)} = 2.5\%$. We obtain relative errors below 10%, so we can say that, although the discrepancies are significant (because Eq. (82) is not satisfied), we have not obtained excessively large values in the relative errors. Thus, we conclude that the IW results are improvable but still acceptable. We investigated if the differences could be attributed to the discontinuity of the potential, so we tried to reproduce this potential using the Fermi-Dirac function, but we obtained worse results. Thus, the discrepancies may be a natural

	HO		IW		MO	
N	ML	Theory	ML	Theory	ML	Theory
2	1.99997 ± 0.00002	2	$(2.32 \pm 0.08)\,\pi^2$	$(5/2)\pi^2$	21.746 ± 0.004	21.75
3	4.49996 ± 0.00004	4.5	$(6.6 \pm 0.1)\,\pi^2$	$7\pi^2$	47.38 ± 0.02	47.375
4	8.0001 ± 0.0003	8	$(14.7 \pm 0.2)\,\pi^2$	$15\pi^2$	81.52 ± 0.02	81.5
5	12.4998 ± 0.0002	12.5	$(26.8 \pm 0.3)\,\pi^2$	$(55/2)\pi^2$	123.13 ± 0.01	123.125

Table 1: Comparison of the ML results with the theoretical values of the ground-state energy for the HO, IW and MO ($N = 2, 3, 4, 5$).

consequence of the potential approximation. Also, we have to take into account that if we plot the energy as a function of the epochs, we see that it is continuously oscillating, so it is unsurprising to encounter slight discrepancies.

Additionally, we have calculated the OBDM and the PCF with the obtained ground-state wavefunction. We obtain similar plots as the ones found analytically in the first part of the work [F]. They present the same pattern and intensities, although we can find minor differences that can be attributed to the limitations of any approximation method. Overall, we conclude that a NQS is able to reproduce the ground-state wavefunction of the systems quite accurately.

4 Conclusions

In this work we have studied the ground-state properties of three confined 1D fermionic systems totally polarized with no interactions (HO, IW and MO). In the first place we have done this exploration from an analytical point of view. We have proven our initial hypothesis that all the systems under consideration have a ground-state wavefunction that can be expressed in terms of a VD. We have provided their analytical formulae, as well as the ones for the ground-state energy, taking into account the Fermi exclusion principle. We have also computed and plotted the OBDM and the PCF of the systems for $N = 2, 3, 4, 5$ with both the integral and the uncorrelated formulae and validated that they lead to the same results. Finally, we have found closed expressions of the OBDM and the PCF in terms of polynomials for a general number N of particles and we have also computed the associated matrices for $N = 2, 3, 4, 5$. Computing and plotting the OBDM and the PCF for a third time, we have checked the veracity of the closed expressions and matrices.

In the second part of the work, we have used ML techniques to validate our results and see if they are capable to solve the systems. We have used a NQS to find an approximate representation of the ground-state wavefunction by minimizing the variational energy of the systems, thus finding the neural network weights and biases. The obtained energies of the HO and the MO are compatible with the theoretical values, but for the IW, although the ML values are very close to the theoretical ones, we obtain significant discrepancy. This could be attributed to the use of a finite (but still high) well or to energy oscillations during the minimization process. Apart from this, the plots of the OBDM and the PCF computed using our NQS are in line with our analytical results with minor differences. Overall, we can conclude that ML is able to solve these systems with good accuracy.

Further studies could include interactions between particles to find differences with respect to the non-interacting case. It could also be investigated if in these cases the many-body wavefunction can still be written in terms of VDs. A more complex study could even incorporate spin. Another path to follow would be to analyze other 1D systems such as the double well potential or the Pöschl–Teller potential, or even consider 2D or 3D systems.

Bibliography

[Bon11] Jeffrey A. Bonnell. *Implementation of a New Sigmoid Function in Backpropagation Neural Networks*. East Tennessee State University, August 2011.

[Col16] Piers Coleman. *Introduction to Many-Body Physics*. Cambridge University Press, February 2016.

[CT17] Giuseppe Carleo and Matthias Troyer. Solving the Quantum Many-Body Problem with Artificial Neural Networks. *Science*, 355(6325):602–606, February 2017.

[DM15] Kathy Driver and Martin E. Muldoon. Common and interlacing zeros of families of Laguerre polynomials. *Journal of Approximation Theory*, 193(1):89–98, May 2015.

[DS88] Jens P. Dahl and Michael Springborg. The Morse oscillator in position space, momentum space, and phase space. *Journal of Chemical Physics*, 88(7):4535–4547, April 1988.

[Fid16] Elok Fidiani. Modeling of Diatomic Molecule using The Morse Potential and The Verlet Algorithm. *AIP Conference Proceedings*, 1719(1):030001, March 2016.

[GC12] Naveen K. Gupta and Vinay Chandwani. Artificial Neural Networks as Universal Function Approximators. *International Journal of Emerging Trends in Engineering and Development*, 4(2):456–464, May 2012.

[GM48] Robert E. Greenwood and J. J. Miller. Zeros of the Hermite polynomials and weights for Gauss' mechanical quadrature formula. *Bulletin of the American Mathematical Society*, 54(8):765–769, August 1948.

[Haa46] Dirk T. Haar. The Vibrational Levels of an Anharmonic Oscillator. *Physical Review*, 70(3-4):222–223, August 1946.

[HLL+21] Jiequn Han, Yingzhou Li, Lin Lin, Jianfeng Lu, Jiefu Zhang, and Linfeng Zhang. Universal approximation of symmetric and anti-symmetric functions. *Communications in Mathematical Sciences*, 20(5):1397–1408, December 2021.

[JTR10] Jianmin Jiang, Paul R. Trundle, and Jinchang Ren. Medical image analysis with artificial neural networks. *Computerized medical imaging and graphics: the official journal of the Computerized Medical Imaging Society*, 34(8):617–631, December 2010.

[Kal18] Dan Kalman. The Generalized Vandermonde Matrix. *Mathematics Magazine*, 57(1):15–21, February 2018.

[KDRF+23] James W. T. Keeble, Mehdi Drissi, Abel Rojo-Francàs, Bruno Juliá-Díaz, and Arnau Rios. Machine learning one-dimensional spinless trapped fermionic systems with neural-network quantum states. *arXiv: nucl-th/2304.04725*, April 2023.

[Kee19] James W. T. Keeble. Machine learning one-dimensional spinless trapped fermionic systems with neural-network quantum states. https://github.com/jwtkeeble/SpinlessFermions, January 2019.

[Kee22] James W. T. Keeble. *Neural Network Solutions to the Fermionic Schrödinger Equation*. University of Surrey, September 2022.

[KQM22] Mitchell J. Knight, Harry M. Quiney, and Andy M. Martin. Reduced density matrix approach to ultracold few-fermion systems in one dimension. *New Journal of Physics*, 24(5):053004, May 2022.

[Lö55] Per-Olov Löwdin. Quantum Theory of Many-Particle Systems. I. Physical Interpretations by Means of Density Matrices, Natural Spin-Orbitals, and

Convergence Problems in the Method of Configurational Interaction. *Physical Review*, 97(6):1474–1489, March 1955.

[Mey10] Carl D. Meyer. *Matrix Analysis and Applied Linear Algebra*. SIAM, May 2010.

[Miy23] Koichi Miyamoto. Quantum Metropolis-Hastings algorithm with the target distribution calculated by quantum Monte Carlo integration. *Physical Review Research*, 5(3):033059, July 2023.

[Mor29] Philip M. Morse. Diatomic molecules according to the wave mechanics. II. Vibrational levels. *Physical Review*, 34(1):57–64, July 1929.

[Muh20] Asaph K. Muhumuza. *Extreme points of the Vandermonde determinant in numerical approximation, random matrix theory and financial mathematics*. Mälardalen University Sweden, December 2020.

[Pro88] Robert A. Proctor. Odd symplectic groups. *Invent Math*, 92(2):307–332, June 1988.

[SHP16] Wen-Kai Shao, Yuan He, and Jing Pan. Some identities for the generalized Laguerre polynomials. *Journal of Nonlinear Science and Applications*, 9(5):3388–3396, February 2016.

[SLL14] Murray R. Spiegel, Seymour Lipschutz, and John Liu. *Mathematical Handbook of Formulas and Tables*. Mc Grau Hill Education, May 2014.

A Derivation of useful formulae

A.1 Vandermonde determinant formula

Here we provide a proof by induction of the VD formula, given by

$$\det V(x_1,...,x_n) = \begin{vmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^{n-1} \\ 1 & x_2 & x_2^2 & \cdots & x_2^{n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & \cdots & x_n^{n-1} \end{vmatrix} = \prod_{1\le i<j\le n} (x_j - x_i). \tag{83}$$

Following the steps of an induction proof, we first prove the formula for $n = 2$:

$$\det V(x_1,x_2) = \begin{vmatrix} 1 & x_1 \\ 1 & x_2 \end{vmatrix} = x_2 - x_1 = \prod_{1\le i<j\le 2} (x_j - x_i). \tag{84}$$

Having seen that the formula is true for this case, we assume (induction hypothesis) that it is true for an arbitrary $n \in \mathbb{Z}^+$, and we verify if it is true for $n+1$. That is, we want to prove that

$$\det V(x_1,\ldots,x_{n+1}) = \begin{vmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^{n-1} & x_1^n \\ 1 & x_2 & x_2^2 & \cdots & x_2^{n-1} & x_2^n \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & x_n & x_n^2 & \cdots & x_n^{n-1} & x_n^n \\ 1 & x_{n+1} & x_{n+1}^2 & \cdots & x_{n+1}^{n-1} & x_{n+1}^n \end{vmatrix} = \prod_{1\le i<j\le n+1} (x_j - x_i). \tag{85}$$

If we subtract to each column the previous column multiplied by x_1 (starting from the right side of the determinant and moving to the left), i.e., $C_i \to C_i - x_1 C_{i-1}$, with $i = 2,\ldots,n+1$, we obtain:

$$\begin{aligned} \det V(x_1,\ldots,x_{n+1}) &= \begin{vmatrix} 1 & 0 & 0 & \cdots & 0 & 0 \\ 1 & x_2-x_1 & x_2(x_2-x_1) & \cdots & x_2^{n-2}(x_2-x_1) & x_2^{n-1}(x_2-x_1) \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & x_n-x_1 & x_n(x_n-x_1) & \cdots & x_n^{n-2}(x_n-x_1) & x_n^{n-1}(x_n-x_1) \\ 1 & x_{n+1}-x_1 & x_{n+1}(x_{n+1}-x_1) & \cdots & x_{n+1}^{n-2}(x_{n+1}-x_1) & x_{n+1}^{n-1}(x_{n+1}-x_1) \end{vmatrix} \\ &= \begin{vmatrix} x_2-x_1 & x_2(x_2-x_1) & \cdots & x_2^{n-2}(x_2-x_1) & x_2^{n-1}(x_2-x_1) \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ x_n-x_1 & x_n(x_n-x_1) & \cdots & x_n^{n-2}(x_n-x_1) & x_n^{n-1}(x_n-x_1) \\ x_{n+1}-x_1 & x_{n+1}(x_{n+1}-x_1) & \cdots & x_{n+1}^{n-2}(x_{n+1}-x_1) & x_{n+1}^{n-1}(x_{n+1}-x_1) \end{vmatrix}, \end{aligned} \tag{86}$$

where we have developed the determinant by the first row. Putting the repeated factors in each row outside of the determinant and then using the induction hypothesis, we have:

$$\begin{aligned} \det V(x_1,\ldots,x_{n+1}) &= (x_2-x_1)\cdots(x_n-x_1)(x_{n+1}-x_1) \begin{vmatrix} 1 & x_2 & x_2^2 & \cdots & x_2^{n-1} \\ 1 & x_3 & x_3^2 & \cdots & x_3^{n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n+1} & x_{n+1}^2 & \cdots & x_{n+1}^{n-1} \end{vmatrix} \\ &= (x_2-x_1)\cdots(x_n-x_1)(x_{n+1}-x_1) \prod_{2\le i<j\le n+1} (x_j - x_i) = \prod_{1\le i<j\le n+1} (x_j - x_i). \end{aligned} \tag{87}$$

Thus, it is true for $n+1$, thereby proving the formula true $\forall\, n \in \mathbb{Z}^+$.

A.2 Uncorrelated formulae for the OBDM and the PCF

In this section we derive the uncorrelated formulae for the OBDM and the PCF. We start for the OBDM and then we proceed with the PCF.

First of all, we want to show that, for the ground state of non-interacting systems and in the Hartree-Fock approximation, the integral expression of the OBDM,

$$\rho^{(N)}(x,x') = N\int dx_2\dots dx_N \Psi^*(x,x_2,\dots,x_N)\Psi(x',x_2,\dots,x_N), \tag{88}$$

can be written as a sum of products of the single-particle wavefunctions $\phi_n(x)$, for $n = 1,2,3\dots$, that are solution of the one-body Schrödinger equation of the system under study (for example, N particles in an IW):

$$\rho^{(N)}(x,x') = \sum_{n=1}^{N}\phi_n^*(x)\phi_n(x'). \tag{89}$$

The first step is to write the many-body wavefunction as a Slater determinant using the Leibniz formula[2]

$$\Psi(x_1,\dots,x_N) = \frac{1}{\sqrt{N!}}\sum_P (-1)^P \phi_{P1}(x_1)\cdots\phi_{PN}(x_N), \tag{90}$$

where P is a permutation, $P1, P2, \dots, PN$ are its labels and $(-1)^P$ is its sign, i.e.

$$(-1)^P = \begin{cases} 1 \text{ for an even number of transpositions} \\ -1 \text{ for an odd number of transpositions} \end{cases}. \tag{91}$$

Thus,

$$\begin{aligned}
\rho^{(N)}(x,x') &= \frac{N}{N!}\int dx_2\dots dx_N \sum_P (-1)^P \phi_{P1}^*(x)\cdots\phi_{PN}^*(x_N)\sum_Q (-1)^Q \phi_{Q1}(x')\cdots\phi_{QN}(x_N) \\
&= \frac{N}{N!}\sum_{P,Q}(-1)^P(-1)^Q\phi_{P1}^*(x)\phi_{Q1}(x')\int\phi_{P2}^*(x_2)\phi_{Q2}(x_2)dx_2\cdots\int\phi_{PN}^*(x_N)\phi_{QN}(x_N)dx_N \\
&= \frac{N}{N!}\sum_{P,Q}(-1)^P(-1)^Q\phi_{P1}^*(x)\phi_{Q1}(x')\delta_{P2,Q2}\cdots\delta_{PN,QN} = \frac{N}{N!}(N-1)!\sum_{n=1}^{N}\phi_n^*(x)\phi_n(x') \\
&= \frac{N!}{N!}\sum_{n=1}^{N}\phi_n^*(x)\phi_n(x') = \sum_{n=1}^{N}\phi_n^*(x)\phi_n(x'),
\end{aligned} \tag{92}$$

where we have used the orthonormality condition of the single-particle wavefunctions,

$$\int \phi_n^*(x)\phi_m(x)\,dx = \delta_{n,m}, \tag{93}$$

and also that

$$\sum_{P,Q}(-1)^P(-1)^Q\phi_{P1}^*(x)\phi_{Q1}(x')\delta_{P2,Q2}\cdots\delta_{PN,QN} = (N-1)!\sum_{n=1}^{N}\phi_n^*(x)\phi_n(x'). \tag{94}$$

[2]The Leibniz formula expresses the determinant of an $n\times n$ matrix A in terms of permutations of its elements a_{ij} as $\det A = \sum_P (-1)^P a_{1,P1}a_{2,P2}\cdots a_{n,Pn}$.

This may not be immediate to see, but here we put an example for $N = 3$ to see it clearer. Since in this case $P = \{123, 132, 213, 231, 312, 321\}$, we have:

$$\begin{aligned}
&\sum_{P,Q}(-1)^P(-1)^Q\phi^*_{P1}(x)\phi_{Q1}(x')\delta_{P2,Q2}\delta_{P3,Q3} = \sum_{Q}(-1)^Q\left[\phi^*_1(x)\phi_{Q1}(x')\delta_{2,Q2}\delta_{3,Q3}\right.\\
&-\phi^*_1(x)\phi_{Q1}(x')\delta_{3,Q2}\delta_{2,Q3} - \phi^*_2(x)\phi_{Q1}(x')\delta_{1,Q2}\delta_{3,Q3} + \phi^*_2(x)\phi_{Q1}(x')\delta_{3,Q2}\delta_{1,Q3}\\
&\left.+\phi^*_3(x)\phi_{Q1}(x')\delta_{1,Q2}\delta_{2,Q3} - \phi^*_3(x)\phi_{Q1}(x')\delta_{2,Q2}\delta_{1,Q3}\right]\\
&= 2\phi^*_1(x)\phi_1(x') + 2\phi^*_2(x)\phi_2(x') + 2\phi^*_3(x)\phi_3(x') = (3-1)!\sum_{n=1}^{3}\phi^*_n(x)\phi_n(x'). \qquad (95)
\end{aligned}$$

The generalization of the multiplying factor $(N-1)!$ can be better understood if we focus on the term $\phi^*_1(x)\phi_1(x')$. If we had had $N = 4$, the multiplying term would have been 3! instead of 2!, because these are the number of times that number 1 is in the first position $(1234, 1243, 1324, 1342, 1423, 1432)$, i.e., the number of permutations of three elements (2,3,4), which is 3!.

In case n starts from 0, as it happens with the HO or the MO, none of the calculations would have changed, except that instead of writing $1, \ldots, N$ we would have written $0, \ldots, N-1$ throughout all the derivation. Thus, the result is the same as in Eq. (92) but with the change $n_{min} = 0$ and $n_{max} = N - 1$.

Following a similar procedure, now we want to show that, for the ground state of non-interacting systems and in the Hartree-Fock approximation, the integral expression of the PCF,

$$g^{(N)}(x_1, x_2) = \binom{N}{2}\int dx_3 \ldots dx_N \Psi^*(x_1, x_2, \ldots, x_N)\Psi(x_1, x_2, \ldots, x_N), \qquad (96)$$

can be written as

$$g^{(N)}(x_1, x_2) = \frac{1}{2}\sum_{n,m=1}^{N}\Phi_{n,m}(x_1, x_2), \qquad (97)$$

thus avoiding to compute an $N-2$ integral. Here,

$$\Phi_{n,m}(x_1, x_2) = \phi^*_n(x_1)\phi^*_m(x_2)\left[\phi_n(x_1)\phi_m(x_2) - \phi_m(x_1)\phi_n(x_2)\right]. \qquad (98)$$

The first step is to write the many-body wavefunction as a Slater determinant, Eq. (90). Substituting it in Eq. (96), we obtain:

$$\begin{aligned}
g^{(N)}(x_1, x_2) &= \binom{N}{2}\frac{1}{N!}\int dx_3 \ldots dx_N \sum_{P,Q}(-1)^{P+Q}\phi^*_{P1}(x_1)\cdots\phi^*_{PN}(x_N)\phi_{Q1}(x_1)\cdots\phi_{QN}(x_N)\\
&= \binom{N}{2}\frac{1}{N!}\sum_{P,Q}(-1)^{P+Q}\phi^*_{P1}(x_1)\phi^*_{P2}(x_2)\phi_{Q1}(x_1)\phi_{Q2}(x_2)\prod_{i=3}^{N}\int dx_i\phi^*_{Pi}(x_i)\phi_{Qi}(x_i)\\
&= \binom{N}{2}\frac{1}{N!}\sum_{P,Q}(-1)^{P+Q}\phi^*_{P1}(x_1)\phi^*_{P2}(x_2)\phi_{Q1}(x_1)\phi_{Q2}(x_2)\delta_{P3,Q3}\cdots\delta_{PN,QN}. \qquad (99)
\end{aligned}$$

To see that this can be expressed as in Eq. (97), we derive a specific case with $N = 3$ and

then explain it for a general N. For $N = 3$,

$$
\begin{aligned}
g^{(3)}(x_1, x_2) &= \binom{3}{2} \frac{1}{3!} \sum_{P,Q} (-1)^Q (-1)^P \phi^*_{P1}(x_1)\phi^*_{P2}(x_2)\phi_{Q1}(x_1)\phi_{Q2}(x_2)\delta_{P3,Q3} \\
&= \binom{3}{2} \frac{1}{3!} \sum_{Q} (-1)^Q \left[\phi^*_1(x_1)\phi^*_2(x_2)\phi_{Q1}(x_1)\phi_{Q2}(x_2)\delta_{3,Q3}\right. \\
&- \phi^*_1(x_1)\phi^*_3(x_2)\phi_{Q1}(x_1)\phi_{Q2}(x_2)\delta_{2,Q3} - \phi^*_2(x_1)\phi^*_1(x_2)\phi_{Q1}(x_1)\phi_{Q2}(x_2)\delta_{3,Q3} \\
&+ \phi^*_2(x_1)\phi^*_3(x_2)\phi_{Q1}(x_1)\phi_{Q2}(x_2)\delta_{1,Q3} + \phi^*_3(x_1)\phi^*_1(x_2)\phi_{Q1}(x_1)\phi_{Q2}(x_2)\delta_{2,Q3} \\
&\left.-\phi^*_3(x_1)\phi^*_1(x_2)\phi_{Q1}(x_1)\phi_{Q2}(x_2)\delta_{2,Q3}\right] = \frac{1}{2}\left\{\phi^*_1(x_1)\phi^*_2(x_2)\left[\phi_1(x_1)\phi_2(x_2) - \phi_2(x_1)\phi_1(x_2)\right]\right. \\
&- \phi^*_1(x_1)\phi^*_3(x_2)\left[-\phi_1(x_1)\phi_3(x_2) + \phi_3(x_1)\phi_1(x_2)\right] - \phi^*_2(x_1)\phi^*_1(x_2)\left[-\phi_2(x_1)\phi_1(x_2) + \phi_1(x_1)\phi_2(x_2)\right] \\
&+ \phi^*_2(x_1)\phi^*_3(x_2)\left[\phi_2(x_1)\phi_3(x_2) - \phi_3(x_1)\phi_2(x_2)\right] + \phi^*_3(x_1)\phi^*_1(x_2)\left[\phi_3(x_1)\phi_1(x_2) - \phi_1(x_1)\phi_3(x_2)\right] \\
&\left.-\phi^*_3(x_1)\phi^*_2(x_2)\left[-\phi_3(x_1)\phi_2(x_2) + \phi_2(x_1)\phi_3(x_2)\right]\right\} = \frac{1}{2}\sum_{n,m=1}^{3} \Phi_{n,m}(x_1, x_2).
\end{aligned} \tag{100}
$$

For $N \geq 4$ it is easier if we classify the permutations in N sets G_N determined by the initial number, that is, the permutations that start with 1 belong to the first set, the ones that start with 2 belong to the second one, and so on:

$$
\begin{aligned}
G_1 &= (\{12P(34\ldots N)\}; \{13P(24\ldots N)\}; \{14P(23\ldots N)\}, ...) \\
G_2 &= (\{21P(34\ldots N)\}; \{23P(14\ldots N)\}; \{24P(13\ldots N)\}, ...) \\
&\vdots \\
G_N &= (\{N1P(23\ldots N)\}; \{N2P(13\ldots N)\}; \{N3P(12\ldots N)\}, ...)
\end{aligned} \tag{101}
$$

The elements of each set are separated by a semicolon and are all the permutations with fixed first and second position, as we can see. For example, the first element of G_1 is the set of permutations $\{12P(34\ldots N)\}$, where $P(i\ldots j)$ are all the permutations of $i, \ldots, j$.

Due to the product of Kronecker deltas, each element of G_i only combines with itself and with its opposite element (anti-element), i.e., the permutations that have the first two numbers exchanged. For example, the second element of G_1 starts with $1, 3$, so it only combines with itself and also with the first element of G_3, which starts by $3, 1$, and any other combination is zero. Note that each element consists of $(N-2)!$ permutations, so from each group we obtain $(N-2)!$ equal terms, $\phi^*_n(x_1)\phi^*_m(x_2)[\phi_n(x_1)\phi_m(x_2) - \phi_m(x_1)\phi_n(x_2)]$. The positive sign appears when the permutation of each element combines with itself, because $(-1)^P = (-1)^Q$ so $(-1)^P(-1)^Q = 1$, and the negative sign appears when it combines with the same permutation of the anti-element (thus differing just from the transposition of the first two numbers, e.g. 12 instead of 21), so if $(-1)^P = 1$, $(-1)^Q = -1$, and vice versa.

As an example, for $N = 5$, the first element of G_1 is $\{12345; 12354; 12435; 12453; 12534; 12543\}$, and it only combines with the first element of G_2, that is $\{21345; 21354; 21435; 21453; 21534; 21543\}$. In particular, 12345 only combines with 12345 and with 21345 (because the permutation of 3,4,5 is the same), thus giving $\phi^*_1(x_1)\phi^*_2(x_2)[\phi_1(x_1)\phi_2(x_2) - \phi_2(x_1)\phi_1(x_2)]$. Similarly, 12354 only combines with itself and 21354, again giving as a result $\phi^*_1(x_1)\phi^*_2(x_2)[\phi_1(x_1)\phi_2(x_2) - \phi_2(x_1)\phi_1(x_2)]$. At the end, we have $(N-2)! = 3! = 6$ times the same result, thus, $(N-2)!\phi^*_1(x_1)\phi^*_2(x_2)[\phi_1(x_1)\phi_2(x_2) - \phi_2(x_1)\phi_1(x_2)]$. The process is repeated for each element of each group, and since for each element there always appear

$(N-2)!$ equal terms $\Phi_{n,m}$, we have that, in general,

$$g^{(N)}(x_1,x_2) = \binom{N}{2}\frac{1}{N!}(N-2)!\sum_{n,m=1}^{N}\Phi_{n,m}(x_1,x_2) = \frac{N!}{2!(N-2)!}(N-2)!\sum_{n,m=1}^{N}\Phi_{n,m}(x_1,x_2)$$
$$= \frac{1}{2}\sum_{n,m=1}^{N}\Phi_{n,m}(x_1,x_2), \tag{102}$$

as we wanted to show.

In case n starts from 0, as it happens with the HO or the MO, the result is the same but with the change $n_{min} = m_{min} = 0$ and $n_{max} = m_{max} = N-1$.

Note that Eq. (97) can also be written in terms of the OBDM:

$$g^{(N)}(x_1,x_2) = \frac{1}{2}\sum_{n=1}^{N}\phi_n^*(x_1)\phi_n(x_1)\sum_{m=1}^{N}\phi_m^*(x_2)\phi_m(x_2) - \sum_{n=1}^{N}\phi_n^*(x_1)\phi_n(x_2)\sum_{m=1}^{N}\phi_m^*(x_2)\phi_m(x_1)$$
$$= \frac{1}{2}\left(\rho^{(N)}(x_1,x_1)\rho^{(N)}(x_2,x_2) - \rho^{(N)}(x_1,x_2)\rho^{(N)}(x_2,x_1)\right). \tag{103}$$

B Derivations for the harmonic oscillator

B.1 Slater determinant of Hermite polynomials as a VD

Here we prove that the Slater determinant of Hermite polynomials is proportional to a VD. In particular,

$$\begin{vmatrix} H_0\left(\frac{x_1}{a_{ho}}\right) & H_1\left(\frac{x_1}{a_{ho}}\right) & \cdots & H_{N-1}\left(\frac{x_1}{a_{ho}}\right) \\ H_0\left(\frac{x_2}{a_{ho}}\right) & H_1\left(\frac{x_2}{a_{ho}}\right) & \cdots & H_{N-1}\left(\frac{x_2}{a_{ho}}\right) \\ \vdots & \vdots & \ddots & \vdots \\ H_0\left(\frac{x_N}{a_{ho}}\right) & H_1\left(\frac{x_N}{a_{ho}}\right) & \cdots & H_{N-1}\left(\frac{x_N}{a_{ho}}\right) \end{vmatrix} = \prod_{i=1}^{N-1} \left(\frac{2}{a_{ho}}\right)^i \det V(x_1, \ldots, x_N). \tag{104}$$

For this proof, we need the recurrence relation of the Hermite polynomials,

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x), \tag{105}$$

and the property of the determinants that says that if the elements of a row or a column are expressed as a sum of two terms, then the determinant can be expressed as the sum of two determinants:

$$\begin{vmatrix} a & b+x \\ c & d+y \end{vmatrix} = \begin{vmatrix} a & b \\ c & d \end{vmatrix} + \begin{vmatrix} a & x \\ c & y \end{vmatrix}. \tag{106}$$

This can be interpolated to cases with more sums.

First of all, we do the demonstration for $N = 3$ to facilitate the understanding of the N-particle case[3]. For the 3-particle case, we have the following Slater determinant of Hermite polynomials:

$$\begin{vmatrix} H_0(x_1) & H_1(x_1) & H_2(x_1) \\ H_0(x_2) & H_1(x_2) & H_2(x_2) \\ H_0(x_3) & H_1(x_3) & H_2(x_3) \end{vmatrix}. \tag{107}$$

Using the recurrence relation for $n = 1$ ($H_2(x) = 2xH_1(x) - 2H_0(x)$) and the aforementioned property of the determinants, we can write

$$\begin{aligned} \begin{vmatrix} H_0(x_1) & H_1(x_1) & H_2(x_1) \\ H_0(x_2) & H_1(x_2) & H_2(x_2) \\ H_0(x_3) & H_1(x_3) & H_2(x_3) \end{vmatrix} &= \begin{vmatrix} H_0(x_1) & H_1(x_1) & 2x_1H_1(x_1) - 2H_0(x_1) \\ H_0(x_2) & H_1(x_2) & 2x_2H_1(x_2) - 2H_0(x_2) \\ H_0(x_3) & H_1(x_3) & 2x_3H_1(x_3) - 2H_0(x_3) \end{vmatrix} \\ &= 2\begin{vmatrix} H_0(x_1) & H_1(x_1) & x_1H_1(x_1) \\ H_0(x_2) & H_1(x_2) & x_2H_1(x_2) \\ H_0(x_3) & H_1(x_3) & x_3H_1(x_3) \end{vmatrix} - 2\begin{vmatrix} H_0(x_1) & H_1(x_1) & H_0(x_1) \\ H_0(x_2) & H_1(x_2) & H_0(x_2) \\ H_0(x_3) & H_1(x_3) & H_0(x_3) \end{vmatrix} \\ &= 2\begin{vmatrix} H_0(x_1) & H_1(x_1) & x_1H_1(x_1) \\ H_0(x_2) & H_1(x_2) & x_2H_1(x_2) \\ H_0(x_3) & H_1(x_3) & x_3H_1(x_3) \end{vmatrix}, \end{aligned} \tag{108}$$

where we have put outside the multiplying 2 in the third column and the second determinant has been set to zero because we have two equal columns (these are two widely known properties of the determinants). Finally, using that $H_0(x) = 1$ and $H_1(x) = 2x$, we obtain:

$$\begin{vmatrix} H_0(x_1) & H_1(x_1) & H_2(x_1) \\ H_0(x_2) & H_1(x_2) & H_2(x_2) \\ H_0(x_3) & H_1(x_3) & H_2(x_3) \end{vmatrix} = 2 \cdot 2^2 \begin{vmatrix} 1 & x_1 & x_1^2 \\ 1 & x_1 & x_2^2 \\ 1 & x_1 & x_3^2 \end{vmatrix} = \left(\prod_{i=1}^{3-1} 2^i\right) \det V(x_1, x_2, x_3). \tag{109}$$

[3] We do the derivations without a_{ho} and at the end we will change x_i for $\frac{x_i}{a_{ho}}$

For the N-particle case the methodology is analogous. Notice that the second term of Eq. (105) will never appear because there will always be an equal column inside the determinant, so the latter will be zero. We write explicitly more terms to better see the procedure. In the first step, we change all the columns except the first two ones using the recurrence relation. As we have said, only the first term appears, so basically we have to reduce an order of the Hermite polynomials and add a multiplying $2x$ factor. We also put outside the factor of 2, and since it appears in $N-2$ columns, we have a 2^{N-2} outside:

$$\begin{aligned} H &\equiv \begin{vmatrix} H_0(x_1) & H_1(x_1) & H_2(x_1) & H_3(x_1) & \cdots & H_{N-2}(x_1) & H_{N-1}(x_1) \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ H_0(x_N) & H_1(x_N) & H_2(x_N) & H_3(x_N) & \cdots & H_{N-2}(x_N) & H_{N-1}(x_N) \end{vmatrix} \\ &= 2^{N-2} \begin{vmatrix} H_0(x_1) & H_1(x_1) & x_1H_1(x_1) & x_1H_2(x_1) & \cdots & x_1H_{N-3}(x_1) & x_1H_{N-2}(x_1) \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ H_0(x_N) & H_1(x_N) & x_NH_1(x_N) & x_NH_2(x_N) & \cdots & x_NH_{N-3}(x_N) & x_NH_{N-2}(x_N) \end{vmatrix}. \end{aligned}$$

Now we repeat the same procedure for all the columns except the first three ones, so a factor of 2^{N-3} is put outside:

$$H = 2^{N-2}2^{N-3} \begin{vmatrix} H_0(x_1) & H_1(x_1) & x_1H_1(x_1) & x_1^2H_1(x_1) & \cdots & x_1^2H_{N-4}(x_1) & x_1^2H_{N-3}(x_1) \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ H_0(x_N) & H_1(x_N) & x_NH_1(x_N) & x_N^2H_1(x_N) & \cdots & x_N^2H_{N-4}(x_N) & x_N^2H_{N-3}(x_N) \end{vmatrix}.$$

If we continue with this process $N-4$ more times, we will have a first order Hermite polynomial in the last column (and in the rest columns except the first one, where we will have $H_0(x)$), since $N-3-(N-4)=1$. Thus, we have:

$$H = 2^{N-2}2^{N-3}\cdots 2^1 \begin{vmatrix} H_0(x_1) & H_1(x_1) & x_1H_1(x_1) & x_1^2H_1(x_1) & \cdots & x_1^{N-3}H_1(x_1) & x_1^{N-2}H_1(x_1) \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ H_0(x_N) & H_1(x_N) & x_NH_1(x_N) & x_N^2H_1(x_N) & \cdots & x_N^{N-3}H_1(x_N) & x_N^{N-2}H_1(x_N) \end{vmatrix}.$$

Finally, we write $H_0(x)=1$ and $H_1(x)=2x$ and put outside the factors of 2, thereby obtaining a 2^{N-1} (we have a multiplying 2 in all columns except in the first one):

$$H = \left(\prod_{i=1}^{N-1} 2^i\right) \begin{vmatrix} 1 & x_1 & x_1^2 & x_1^3 & \cdots & x_1^{N-2} & x_1^{N-1} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & x_N & x_N^2 & x_N^3 & \cdots & x_N^{N-2} & x_N^{N-1} \end{vmatrix} = \left(\prod_{i=1}^{N-1} 2^i\right) \det V(\{x_i\}_{i=1}^N). \quad (110)$$

If we change x_i for $\frac{x_i}{a_{ho}}$, we can put outside the determinant the a_{ho} dividing as $a_{ho}\cdot a_{ho}^2\cdots a_{ho}^{N-1} = \prod_{i=1}^{N-1} a_{ho}$. Thus, we obtain the desired expression:

$$\begin{vmatrix} H_0\left(\frac{x_1}{a_{ho}}\right) & H_1\left(\frac{x_1}{a_{ho}}\right) & \cdots & H_{N-1}\left(\frac{x_1}{a_{ho}}\right) \\ H_0\left(\frac{x_2}{a_{ho}}\right) & H_1\left(\frac{x_2}{a_{ho}}\right) & \cdots & H_{N-1}\left(\frac{x_2}{a_{ho}}\right) \\ \vdots & \vdots & \ddots & \vdots \\ H_0\left(\frac{x_N}{a_{ho}}\right) & H_1\left(\frac{x_N}{a_{ho}}\right) & \cdots & H_{N-1}\left(\frac{x_N}{a_{ho}}\right) \end{vmatrix} = \prod_{i=1}^{N-1}\left(\frac{2}{a_{ho}}\right)^i \begin{vmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^{N-1} \\ 1 & x_2 & x_2^2 & \cdots & x_2^{N-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_N & x_N^2 & \cdots & x_N^{N-1} \end{vmatrix}, \quad (111)$$

as we wanted to show.

B.2 Closed expressions for the harmonic oscillator OBDM and PCF

In this section, we want to find analytically the closed expressions for the OBDM and the PCF in a HO potential. We do the calculations using the uncorrelated formulae of these functions, Eqs. (13), (14). In this case, the single-particle wavefunctions are

$$\phi_n(x) = N_n e^{-\frac{x^2}{2a_{ho}^2}} H_n\left(\frac{x}{a_{ho}}\right), \qquad n = 0, 1, 2, \ldots, \tag{112}$$

with $N_n = \frac{1}{\sqrt{2^n n! a_{ho}\sqrt{\pi}}}$. Starting for the OBDM, we have that

$$\begin{aligned}
\rho^{(N)}(x, x') &= \sum_{n=0}^{N-1} N_n^2 e^{-\frac{x^2+x'^2}{2a_{ho}^2}} H_n\left(\frac{x}{a_{ho}}\right) H_n\left(\frac{x'}{a_{ho}}\right) \\
&= \frac{1}{a_{ho}\sqrt{\pi}} e^{-\frac{x^2+x'^2}{2a_{ho}^2}} \sum_{n=0}^{N-1} \frac{1}{2^n n!} H_n\left(\frac{x}{a_{ho}}\right) H_n\left(\frac{x'}{a_{ho}}\right) \\
&= \frac{1}{a_{ho}\sqrt{\pi}} e^{-\frac{x^2+x'^2}{2a_{ho}^2}} \mathcal{R}^{(N)}(x, x'),
\end{aligned} \tag{113}$$

where we have defined

$$\mathcal{R}^{(N)}(x, x') = \sum_{n=0}^{N-1} \frac{1}{2^n n!} H_n\left(\frac{x}{a_{ho}}\right) H_n\left(\frac{x'}{a_{ho}}\right), \tag{114}$$

which is a polynomial of degree $N-1$ in both x and x', since the n^{th} Hermite polynomial has degree n.

For the PCF it is easier to derive its closed expression, because it can be computed in terms of the OBDM as shown in Eq. (16):

$$\begin{aligned}
&g^{(N)}(x_1, x_2) = \frac{1}{2}\left(\rho^{(N)}(x_1, x_1)\rho^{(N)}(x_2, x_2) - \rho^{(N)}(x_1, x_2)\rho^{(N)}(x_2, x_1)\right) \\
&= \frac{1}{2}\frac{1}{a_{ho}^2\pi} e^{-\frac{x_1^2+x_2^2}{a_{ho}^2}} \left[\left(\sum_{n=0}^{N-1} \frac{1}{2^n n!} H_n^2\left(\frac{x_1}{a_{ho}}\right)\right)\left(\sum_{m=0}^{N-1} \frac{1}{2^m m!} H_m^2\left(\frac{x_2}{a_{ho}}\right)\right)\right. \\
&\left. - \left(\sum_{n=0}^{N-1} \frac{1}{2^n n!} H_n\left(\frac{x_1}{a_{ho}}\right) H_n\left(\frac{x_2}{a_{ho}}\right)\right)\left(\sum_{m=0}^{N-1} \frac{1}{2^m m!} H_m\left(\frac{x_2}{a_{ho}}\right) H_m\left(\frac{x_1}{a_{ho}}\right)\right)\right] \\
&= \frac{1}{2}\frac{1}{a_{ho}^2\pi} e^{-\frac{x_1^2+x_2^2}{a_{ho}^2}} \sum_{n,m=0}^{N-1} \frac{1}{2^{n+m} n! m!} \left[H_n^2\left(\frac{x_1}{a_{ho}}\right) H_m^2\left(\frac{x_2}{a_{ho}}\right)\right. \\
&\left. - H_n\left(\frac{x_1}{a_{ho}}\right) H_n\left(\frac{x_2}{a_{ho}}\right) H_m\left(\frac{x_2}{a_{ho}}\right) H_m\left(\frac{x_1}{a_{ho}}\right)\right] = \frac{1}{2}\frac{1}{a_{ho}^2\pi} e^{-\frac{x_1^2+x_2^2}{a_{ho}^2}} \mathcal{P}^{(N)}(x_1, x_2),
\end{aligned} \tag{115}$$

where

$$\begin{aligned}
\mathcal{P}^{(N)}(x_1, x_2) = \sum_{n,m=0}^{N-1} \frac{1}{2^{n+m} n! m!} &\left[H_n^2\left(\frac{x_1}{a_{ho}}\right) H_m^2\left(\frac{x_2}{a_{ho}}\right)\right. \\
&\left. - H_n\left(\frac{x_1}{a_{ho}}\right) H_n\left(\frac{x_2}{a_{ho}}\right) H_m\left(\frac{x_2}{a_{ho}}\right) H_m\left(\frac{x_1}{a_{ho}}\right)\right]
\end{aligned} \tag{116}$$

is a polynomial of degree $2N-2$ in both x_1 and x_2. However, as we discuss in Sec. 2.3.3, we have seen in SymPy that we can further factorize this polynomial and get a factor

$(x_1 - x_2)^2$. Let us see if this is true for all the values of N (in SymPy we can just try a finite number of cases, so actually it does not serve as a proof). We define the function

$$f_{n,m}(y_1, y_2) = H_n^2(y_1)H_m^2(y_2) - H_n(y_1)H_n(y_2)H_m(y_2)H_m(y_1), \tag{117}$$

with $y_i = \frac{x_i}{a_{ho}}$ $(i = 1, 2)$. This function is inside a sum that goes from $n, m = 0$ to $N - 1$. Notice that when $n = m$, $f_{n,m}(y_1, y_2) = 0$. Thus, to make the sum we can always sum in groups of two, $f_{n,m}(y_1, y_2) + f_{m,n}(y_1, y_2)$. To make it more clear, all the combinations can be put inside a square matrix, and when we do the sum in n, m, we can sum all the pairs of transposed elements. For example, for $n, m = 0, \ldots, 2$, we have the elements

$$\begin{pmatrix} 0 & f_{01}(y_1, y_2) & f_{02}(y_1, y_2) \\ f_{10}(y_1, y_2) & 0 & f_{12}(y_1, y_2) \\ f_{20}(y_1, y_2) & f_{21}(y_1, y_2) & 0 \end{pmatrix}. \tag{118}$$

In this case, the sum would be $(f_{01}(y_1, y_2) + f_{10}(y_1, y_2)) + (f_{02}(y_1, y_2) + f_{20}(y_1, y_2)) + (f_{12}(y_1, y_2)+f_{21}(y_1, y_2))$, that is $\sum_{n,m=0}^{N-1} f_{n,m}(y_1, y_2) = \sum_{n<m=0}^{N-1} (f_{n,m}(y_1, y_2) + f_{m,n}(y_1, y_2))$ and in particular for Eq. (116), since the multiplying factor does not change if we exchange n and m, we have that

$$\sum_{n,m=0}^{N-1} \frac{1}{2^{n+m}n!m!} f_{n,m}(y_1, y_2) = \sum_{n<m=0}^{N-1} \frac{1}{2^{n+m}n!m!} \left(f_{n,m}(y_1, y_2) + f_{m,n}(y_1, y_2)\right). \tag{119}$$

We are doing the sum like this because it turns out that $f_{n,m}(y_1, y_2)$ cannot be factored in $(y_1 - y_2)^2$, but the sum $f_{n,m}(y_1, y_2) + f_{m,n}(y_1, y_2)$ can. Indeed:

$$f_{m,n}(y_1, y_2) = H_m^2(y_1)H_n^2(y_2) - H_m(y_1)H_m(y_2)H_n(y_2)H_n(y_1), \tag{120}$$

so we have that

$$\begin{aligned} F_{n,m}(y_1, y_2) \equiv f_{n,m}(y_1, y_2) + f_{m,n}(y_1, y_2) = H_n^2(y_1)H_m^2(y_2) + H_n^2(y_2)H_m^2(y_1) \\ - 2H_n(y_1)H_n(y_2)H_m(y_2)H_m(y_1) = \left[H_n(y_1)H_m(y_2) - H_n(y_2)H_m(y_1)\right]^2. \end{aligned} \tag{121}$$

Now, if $y_1 = y_2$, $H_n(y_1)H_m(y_2) - H_n(y_2)H_m(y_1) = 0$. That means that we can write

$$H_n(y_1)H_m(y_2) - H_n(y_2)H_m(y_1) = (y_1 - y_2)\mathcal{Q}^{(N)}(y_1, y_2), \tag{122}$$

where $\mathcal{Q}^{(N)}$ is a polynomial of degree $N - 2$ in both y_1 and y_2. Thus,

$$F_{n,m}(y_1, y_2) = \left[(y_1 - y_2)\mathcal{Q}^{(N)}(y_1, y_2)\right]^2 = (y_1 - y_2)^2\mathcal{Q}'^{(N)}(y_1, y_2), \tag{123}$$

with $\mathcal{Q}'^{(N)}(y_1, y_2)$ a polynomial of degree $2N - 4$ in both y_1 and y_2. Therefore,

$$\begin{aligned} \mathcal{P}^{(N)}(x_1, x_2) = \sum_{n<m=0}^{N-1} \frac{1}{2^{n+m}n!m!} F_{n,m}(y_1, y_2) = \sum_{n<m=0}^{N-1} \frac{1}{2^{n+m}n!m!} (y_1 - y_2)^2\mathcal{Q}'^{(N)}(y_1, y_2) \\ = (y_1 - y_2)^2 \sum_{n<m=0}^{N-1} \frac{1}{2^{n+m}n!m!} \mathcal{Q}'^{(N)}(y_1, y_2) = \frac{1}{a_{ho}^2}(x_1 - x_2)^2\mathcal{G}^{(N)}(x_1, x_2), \end{aligned} \tag{124}$$

with

$$\mathcal{G}^{(N)}(x_1, x_2) = \sum_{n<m=0}^{N-1} \frac{1}{2^{n+m}n!m!} \mathcal{Q}'^{(N)}(y_1, y_2) \tag{125}$$

also a polynomial of degree $2N-4$ in both y_1 and y_2. We can also write this polynomial in terms of the Hermite polynomials. Since from Eq. (123) $\mathcal{Q}'^{(N)}(y_1,y_2) = \frac{F_{n,m}(y_1,y_2)}{(y_1-y_2)^2}$, we have that

$$\mathcal{G}^{(N)}(x_1,x_2) = \frac{1}{(y_1-y_2)^2}\mathcal{P}^{(N)}(x_1,x_2), \tag{126}$$

and from Eq. (116), we have that

$$\begin{aligned}\mathcal{G}^{(N)}(x_1,x_2) = \frac{a_{ho}^2}{(x_1-x_2)^2}\sum_{n,m=0}^{N-1}\frac{1}{2^{n+m}n!m!}\Bigg[H_n^2\left(\frac{x_1}{a_{ho}}\right)H_m^2\left(\frac{x_2}{a_{ho}}\right)\\ - H_n\left(\frac{x_1}{a_{ho}}\right)H_n\left(\frac{x_2}{a_{ho}}\right)H_m\left(\frac{x_2}{a_{ho}}\right)H_m\left(\frac{x_1}{a_{ho}}\right)\Bigg].\end{aligned} \tag{127}$$

Finally, combining Eq. (115) and (124), we obtain the desired closed expression for the PCF:

$$g^{(N)}(x_1,x_2) = \frac{1}{2a_{ho}^2\pi}e^{-\frac{x_1^2+x_2^2}{a_{ho}^2}}\frac{(x_1-x_2)^2}{a_{ho}^2}\mathcal{G}^{(N)}(x_1,x_2). \tag{128}$$

To finish this section, we also discuss the matrices $R^{(N)}$ and $G^{(2N-3)}$ for $N=5$, which were too large to add in Sec. 2.3.3. In this case we found them using SymPy as detailed in the aforementioned section, yielding:

$$R^{(5)} = \begin{pmatrix} 15/8 & 0 & -5/2 & 0 & 1/2 \\ 0 & 5 & 0 & -2 & 0 \\ -5/2 & 0 & 8 & 0 & -2 \\ 0 & -2 & 0 & 4/3 & 0 \\ 1/2 & 0 & -2 & 0 & 2/3 \end{pmatrix}, \tag{129}$$

$$G^{(7)} = \frac{1}{72}\begin{pmatrix} 675 & 0 & 90 & 0 & -180 & 0 & 72 \\ 0 & 2520 & 0 & -1440 & 0 & 288 & 0 \\ 90 & 0 & 2340 & 0 & -1080 & 0 & 144 \\ 0 & -1440 & 0 & 1920 & 0 & -384 & 0 \\ -180 & 0 & -1080 & 0 & 1200 & 0 & -96 \\ 0 & 288 & 0 & -384 & 0 & 384 & 0 \\ 72 & 0 & 144 & 0 & -96 & 0 & 64 \end{pmatrix}. \tag{130}$$

C Closed expressions for the infinite well OBDM and PCF

In this section, we want to find a closed expression for the OBDM and the PCF in an IW. We do the calculations analytically using the uncorrelated formulae of the functions, Eqs. (13), (14). In this case, the single-particle wavefunctions are

$$\phi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right), \qquad n = 1, 2, 3, \dots \tag{131}$$

For the OBDM, we do some particular cases to familiarize ourselves with the expressions and then we derive the general closed expression. Let us start with $N = 2$. Since the single-particle wavefunctions are real, we have that $\phi_n^*(x) = \phi_n(x)$, so we can write that

$$\begin{aligned}\rho^{(2)}(x, x') &= \phi_1(x)\phi_1(x') + \phi_2(x)\phi_2(x') = \frac{2}{L}\left(\sin\frac{\pi x}{L}\sin\frac{\pi x'}{L} + \sin\frac{2\pi x}{L}\sin\frac{2\pi x'}{L}\right) \\ &= \frac{2}{L}\sin\frac{\pi x}{L}\sin\frac{\pi x'}{L}\left(1 + 4\cos\frac{\pi x}{L}\cos\frac{\pi x'}{L}\right),\end{aligned} \tag{132}$$

where we have used that $\sin 2\alpha = 2\sin\alpha\cos\alpha$. Similarly, for $N = 3$

$$\begin{aligned}\rho^{(3)}(x, x') &= \phi_1(x)\phi_1(x') + \phi_2(x)\phi_2(x') + \phi_3(x)\phi_3(x') \\ &= \frac{2}{L}\left(\sin\frac{\pi x}{L}\sin\frac{\pi x'}{L} + \sin\frac{2\pi x}{L}\sin\frac{2\pi x'}{L} + \sin\frac{3\pi x}{L}\sin\frac{3\pi x'}{L}\right).\end{aligned}$$

Here, we use the identity [SLL14]

$$\begin{aligned}\sin nA &= \sin A \sum_{i=1}^{\lfloor\frac{n+1}{2}\rfloor} (-1)^{i+1}\binom{n-i}{i-1}(2\cos A)^{n-(2i-1)} \\ &= \sin A\left\{(2\cos A)^{n-1} - \binom{n-2}{1}(2\cos A)^{n-3} + \binom{n-3}{2}(2\cos A)^{n-5} - \cdots\right\}.\end{aligned} \tag{133}$$

Thus,

$$\begin{aligned}\rho^{(3)}(x, x') = \frac{2}{L}\sin\frac{\pi x}{L}\sin\frac{\pi x'}{L}\Bigg[1 + 4\cos\frac{\pi x}{L}\cos\frac{\pi x'}{L} \\ + \left(4\cos^2\frac{\pi x}{L} - 1\right)\left(4\cos^2\frac{\pi x'}{L} - 1\right)\Bigg].\end{aligned} \tag{134}$$

Therefore, we can see that the OBDM can be written as

$$\rho^{(N)}(x, x') = \frac{2}{L}\sin\frac{\pi x}{L}\sin\frac{\pi x'}{L}\mathcal{R}^{(N)}\left(\cos\frac{\pi x}{L}, \cos\frac{\pi x'}{L}\right), \tag{135}$$

with $\mathcal{R}^{(N)}\left(\cos\frac{\pi x}{L}, \cos\frac{\pi x'}{L}\right)$ a polynomial of order $N-1$ in both $\cos\frac{\pi x}{L}$ and $\cos\frac{\pi x'}{L}$.

We can state this more formally by seeing that

$$\begin{aligned}\rho^{(N)}(x, x') &= \frac{2}{L}\sum_{n=1}^{N}\sin\frac{n\pi x}{L}\sin\frac{n\pi x'}{L} \\ &= \frac{2}{L}\sin\frac{\pi x}{L}\sin\frac{\pi x'}{L}\sum_{n=1}^{N}\sum_{i,j=1}^{\lfloor\frac{n+1}{2}\rfloor}(-1)^{i+j}\binom{n-i}{i-1}\binom{n-j}{j-1}(2y)^{n-(2i-1)}(2y')^{n-(2j-1)},\end{aligned}$$

where we have defined $y = \cos\frac{\pi x}{L}$ and $y' = \cos\frac{\pi x'}{L}$. The function

$$\mathcal{R}^{(N)}\left(y, y'\right) = \sum_{n=1}^{N} \sum_{i,j=1}^{\lfloor \frac{n+1}{2} \rfloor} (-1)^{i+j} \binom{n-i}{i-1} \binom{n-j}{j-1} (2y)^{n-(2i-1)} \left(2y'\right)^{n-(2j-1)} \tag{136}$$

is a polynomial whose order is found when n is maximum ($n = N$) and $2i-1$ and $2j-1$ are minimum ($i, j = 1$), that is, it is of order $N-(2-1) = N-1$ in both y and y'. Hence, the closed expression of the OBDM is

$$\rho^{(N)}(x, x') = \frac{2}{L} \sin\frac{\pi x}{L} \sin\frac{\pi x'}{L} \mathcal{R}^{(N)}\left(y, y'\right). \tag{137}$$

On the other hand, $\mathcal{R}^{(N)}\left(y, y'\right)$ can also be written in terms of Vandermonde vectors and an $N \times N$ matrix, $R^{(N)}$:

$$\mathcal{R}^{(N)}(y, y') = \boldsymbol{y}^{(N),T} R^{(N)} \boldsymbol{y'}^{(N)} = \begin{pmatrix} 1 & y & y^2 & \cdots & y^{N-1} \end{pmatrix} R^{(N)} \begin{pmatrix} 1 \\ y' \\ y'^2 \\ \vdots \\ y'^{N-1} \end{pmatrix}. \tag{138}$$

For example, for the two particular cases we have discussed, we see that the matrices are:

$$R^{(2)} = \begin{pmatrix} 1 & 0 \\ 0 & 4 \end{pmatrix}, \quad R^{(3)} = \begin{pmatrix} 2 & 0 & -4 \\ 0 & 4 & 0 \\ -4 & 0 & 16 \end{pmatrix}. \tag{139}$$

For the PCF it is easier to derive its closed expression, because it can be computed in terms of the OBDM:

$$\begin{aligned} g^{(N)}(x_1, x_2) &= \frac{1}{2}\left(\rho^{(N)}(x_1, x_1)\rho^{(N)}(x_2, x_2) - \rho^{(N)}(x_1, x_2)\rho^{(N)}(x_2, x_1)\right) \\ &= \frac{2}{L^2} \sin^2\frac{\pi x_1}{L} \sin^2\frac{\pi x_2}{L} \left[\mathcal{R}^{(N)}\left(y_1, y_1\right) \mathcal{R}^{(N)}\left(y_2, y_2\right) - \mathcal{R}^{(N)}\left(y_1, y_2\right) \mathcal{R}^{(N)}\left(y_2, y_1\right)\right]. \end{aligned} \tag{140}$$

Recall that $\mathcal{R}^{(N)}(y_1, y_1)$ and $\mathcal{R}^{(N)}(y_2, y_2)$ are polynomials of order $2(N-1)$ in y_1 and y_2, respectively, and $\mathcal{R}^{(N)}(y_1, y_2)$ and $\mathcal{R}^{(N)}(y_2, y_1)$ are of order $N-1$ in both y_1 and y_2, so $\mathcal{G}^{(N)}(y_1, y_2) \equiv \mathcal{R}^{(N)}(y_1, y_1)\mathcal{R}^{(N)}(y_2, y_2) - \mathcal{R}^{(N)}(y_1, y_2)\mathcal{R}^{(N)}(y_2, y_1)$ is a polynomial of order $2(N-1)$ in both y_1 and y_2. Thus, the closed expression of the PCF is

$$g^{(N)}(x_1, x_2) = \frac{2}{L^2} \sin^2\frac{\pi x_1}{L} \sin^2\frac{\pi x_2}{L} \mathcal{G}^{(N)}(y_1, y_2), \tag{141}$$

where $\mathcal{G}^{(N)}(y_1, y_2)$ can be represented in terms of matrix products as

$$\mathcal{G}^{(N)}(y_1, y_2) = \boldsymbol{y_1}^{(2N-1),T} G^{(2N-1)} \boldsymbol{y_2}^{(2N-1)}, \tag{142}$$

being $G^{(2N-1)}$ a $(2N-1) \times (2N-1)$ matrix.

As said, here we show the rest of the matrices that we did not show in Sec. 2.4.3, that is, $N = 4, 5$. These matrices, as well as the ones for $N = 2, 3$, have been found calculating the polynomials that appear in the closed expressions of the OBDM and the PCF, Eqs. (51) and (55), and identifying the coefficients as we explained in Sec. 2.3.3. As N increases, the simplification of the polynomials (doing all the multiplications and groupings of terms)

becomes more difficult. That is why we have used a Python code that receives the not simplified polynomial, makes the pertinent simplifications and groupings, and returns the desired matrix. This is easy to do with the `expand()` function of SymPy. The results are shown below:

$$R^{(4)} = \begin{pmatrix} 2 & 0 & -4 & 0 \\ 0 & 20 & 0 & -32 \\ -4 & 0 & 16 & 0 \\ 0 & -32 & 0 & 64 \end{pmatrix}, \quad R^{(5)} = \begin{pmatrix} 3 & 0 & -16 & 0 & 16 \\ 0 & 20 & 0 & -32 & 0 \\ -16 & 0 & 160 & 0 & -192 \\ 0 & -32 & 0 & 64 & 0 \\ 16 & 0 & -192 & 0 & 256 \end{pmatrix},$$

$$G^{(7)} = \begin{pmatrix} 0 & 0 & 40 & 0 & -112 & 0 & 128 \\ 0 & -80 & 0 & 288 & 0 & -256 & 0 \\ 40 & 0 & -352 & 0 & 832 & 0 & -256 \\ 0 & 288 & 0 & -1408 & 0 & 1536 & 0 \\ -112 & 0 & 832 & 0 & -2560 & 0 & 1024 \\ 0 & -256 & 0 & 1536 & 0 & -2048 & 0 \\ 128 & 0 & -256 & 0 & 1024 & 0 & 0 \end{pmatrix},$$

$$G^{(9)} = \begin{pmatrix} 0 & 0 & 60 & 0 & 32 & 0 & -448 & 0 & 512 \\ 0 & -120 & 0 & 832 & 0 & -1664 & 0 & 1024 & 0 \\ 60 & 0 & -1728 & 0 & 6528 & 0 & -8448 & 0 & 3072 \\ 0 & 832 & 0 & -8832 & 0 & 20992 & 0 & -14336 & 0 \\ 32 & 0 & 6528 & 0 & -28160 & 0 & 38912 & 0 & -12288 \\ 0 & -1664 & 0 & 20992 & 0 & -55296 & 0 & 40960 & 0 \\ -448 & 0 & -8448 & 0 & 38912 & 0 & -57344 & 0 & 16384 \\ 0 & 1024 & 0 & -14336 & 0 & 40960 & 0 & -32768 & 0 \\ 512 & 0 & 3072 & 0 & -12288 & 0 & 16384 & 0 & 0 \end{pmatrix}.$$

D Derivations for the Morse oscillator

D.1 Slater determinant of associated Laguerre polynomials as a VD

The ground-state wavefunction in a MO is a Slater determinant that contains associated Laguerre polynomials. We want to rewrite this determinant as a VD as we did in the HO case. In particular, we prove that

$$\det\left[z_i^{-(j-1)}L_{j-1}^{2\beta-2(j-1)}(z_i)\right]_{i,j=1,\dots,N}=\left[\prod_{i=1}^{N-1}\binom{2\beta-i}{i}\right]\det V\left(\frac{1}{z_1},\dots,\frac{1}{z_N}\right), \tag{143}$$

being

$$\binom{2\beta-i}{i}=\frac{1}{i!}\prod_{j=i}^{2i-1}(2\beta-j)=\frac{1}{i!}(2\beta-i)(2\beta-i-1)\cdots(2\beta-2i+1), \tag{144}$$

with $\beta\in\mathbb{R}$.

We need to use the explicit formula of the associated Laguerre polynomials,

$$L_n^\alpha(x)=\sum_{i=0}^{n}(-1)^i\binom{n+\alpha}{n-i}\frac{x^i}{i!}, \tag{145}$$

where the binomial coefficient is defined as

$$\binom{\delta}{m}=\frac{1}{m!}\prod_{k=0}^{m-1}(\delta-k)=\frac{1}{m!}\delta(\delta-1)(\delta-2)\cdots(\delta-m+1), \tag{146}$$

with $m\in\mathbb{N}$ and $\delta\in\mathbb{R}$. The first two associated Laguerre polynomials are $L_0^\alpha(x)=1$ and $L_1^\alpha(x)=1+\alpha-x$. Let us start proving Eq. (143) for $N=3$, to see how the procedure works:

$$\begin{aligned}\det\left[z_i^{-(j-1)}L_{j-1}^{2\beta-2(j-1)}(z_i)\right]_{i,j=1,\dots,3}&=\begin{vmatrix}L_0^{2\beta}(z_1) & z_1^{-1}L_1^{2\beta-2}(z_1) & z_1^{-2}L_2^{2\beta-4}(z_1)\\ L_0^{2\beta}(z_2) & z_2^{-1}L_1^{2\beta-2}(z_2) & z_2^{-2}L_2^{2\beta-4}(z_2)\\ L_0^{2\beta}(z_3) & z_3^{-1}L_1^{2\beta-2}(z_3) & z_3^{-2}L_2^{2\beta-4}(z_3)\end{vmatrix}\\ &=\begin{vmatrix}1 & z_1^{-1}L_1^{2\beta-2}(z_1) & z_1^{-2}L_2^{2\beta-4}(z_1)\\ 1 & z_2^{-1}L_1^{2\beta-2}(z_2) & z_2^{-2}L_2^{2\beta-4}(z_2)\\ 1 & z_3^{-1}L_1^{2\beta-2}(z_3) & z_3^{-2}L_2^{2\beta-4}(z_3)\end{vmatrix}.\end{aligned} \tag{147}$$

Notice that $L_1^\alpha(x)$, according to Eq. (145), can be written as a sum of a term with x^0 and a term with x^1. This means that in the second column of the above determinant, only the term with z_i^0 of $L_1^{2\beta-2}(z_i)$ survives, since the term with z_i becomes a constant after being multiplied by z_i^{-1}, thus being proportional to the first column (remember that the determinant can be separated in two determinants according to Eq. (106)). The same happens with the third column: $L_2^\alpha(x)$ can be written as a sum of three terms, one with x^0, the second with x^1 and the last one with x^2. Only the term with z_i^0 of $L_2^{2\beta-4}(z_i)$ survives, since after multiplying by z_i^{-2}, the terms with $z_i^{-2}z_i^2$ and with $z_i^{-2}z_i$ become proportional to the first and second columns, respectively. Thus,

$$\begin{aligned}\det\left[z_i^{-(j-1)}L_{j-1}^{2\beta-2(j-1)}(z_i)\right]_{i,j=1,\dots,3}&=\binom{1+(2\beta-2)}{1}\binom{2+(2\beta-4)}{2}\begin{vmatrix}1 & z_1^{-1} & z_1^{-2}\\ 1 & z_2^{-1} & z_2^{-2}\\ 1 & z_3^{-1} & z_3^{-2}\end{vmatrix}\\ &=\binom{2\beta-1}{1}\binom{2\beta-2}{2}\det V\left(\frac{1}{z_1},\frac{1}{z_2},\frac{1}{z_3}\right).\end{aligned} \tag{148}$$

Now, it is immediate to solve the general case for N particles. As we have seen, only the fist term of the sum in Eq. (145), which is given by $\binom{n+\alpha}{n}$, survives in each case. Therefore, we take these constants out of the determinant:

$$
\begin{aligned}
&\det\left[z_i^{-(j-1)} L_{j-1}^{2\beta-2(j-1)}(z_i)\right]_{i,j=1,\dots,N} \\
&= \begin{vmatrix} 1 & z_1^{-1} L_1^{2\beta-2}(z_1) & z_1^{-2} L_2^{2\beta-4}(z_1) & \cdots & z_1^{-(N-1)} L_{N-1}^{2\beta-2N+2}(z_1) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & z_N^{-1} L_1^{2\beta-2}(z_N) & z_N^{-2} L_2^{2\beta-4}(z_N) & \cdots & z_N^{-(N-1)} L_{N-1}^{2\beta-2N+2}(z_N) \end{vmatrix} \\
&= \binom{1+(2\beta-2)}{1}\binom{2+(2\beta-4)}{2}\cdots\binom{N-1+(2\beta-2N+2)}{N-1} \begin{vmatrix} 1 & z_1^{-1} & z_1^{-2} & \cdots & z_1^{-(N-1)} \\ 1 & z_2^{-1} & z_2^{-2} & \cdots & z_2^{-(N-1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & z_N^{-1} & z_N^{-2} & \cdots & z_N^{-(N-1)} \end{vmatrix} \\
&= \binom{2\beta-1}{1}\binom{2\beta-2}{2}\cdots\binom{2\beta-(N-1)}{N-1} \det V\left(\frac{1}{z_1},\dots,\frac{1}{z_N}\right) \\
&= \left[\prod_{i=1}^{N-1}\binom{2\beta-i}{i}\right] \det V\left(\frac{1}{z_1},\dots,\frac{1}{z_N}\right). \qquad (149)
\end{aligned}
$$

We have thus proven Eq. (143). To write the binomial coefficient as in Eq. (144), we use the definition in Eq. (146) with $\delta = 2\beta - i$ and $m = i$. We obtain

$$\binom{2\beta-i}{i} = \frac{1}{i!}\prod_{k=0}^{i-1}(2\beta-i-k) = \frac{1}{i!}(2\beta-i)(2\beta-i-1)\cdots(2\beta-2i+1). \qquad (150)$$

Defining the new variable $j = i + k$, we can rewrite it as

$$\binom{2\beta-i}{i} = \frac{1}{i!}\prod_{j=i}^{2i-1}(2\beta-j) = \frac{1}{i!}(2\beta-i)(2\beta-i-1)\cdots(2\beta-2i+1). \qquad (151)$$

D.2 Closed expressions for the Morse oscillator OBDM and PCF

Following the same steps as in Secs. [B.2, C], we want to find a closed expression for the OBDM and the PCF in a MO. Again, we do the calculations analytically using the uncorrelated formula of the functions, Eqs. (13), (14). In this case, the single-particle wavefunctions are

$$\phi_n(z) = N_n z^\beta e^{-z/2} z^{-n} L_n^{2\beta-2n}(z), \qquad n = 0, 1, 2 \ldots, \lfloor \lambda - \frac{1}{2} \rfloor, \tag{152}$$

being $\beta = \lambda - \frac{1}{2}$ and

$$N_n = \sqrt{\frac{n!(2\beta - 2n)a}{\Gamma(2\lambda - n)}}. \tag{153}$$

Additionally, we use the closed form of the associated Laguerre polynomials:

$$L_n^\alpha(x) = \sum_{i=0}^{n} (-1)^i \binom{n+\alpha}{n-i} \frac{x^i}{i!} \equiv \sum_{i=0}^{n} C_{n,i}^\alpha x^i. \tag{154}$$

We start for the OBDM. For $N = 2$, we have

$$\begin{aligned}
\rho^{(2)}(z, z') &= \phi_0(z)\phi_0(z') + \phi_1(z)\phi_1(z') = \frac{2\beta a}{\Gamma(2\lambda)} z^\beta z'^\beta e^{-\frac{z+z'}{2}} L_0^{2\beta}(z) L_0^{2\beta}(z') \\
&+ \frac{(2\beta-2)a}{\Gamma(2\lambda-1)} (zz')^{-1} z^\beta z'^\beta e^{-\frac{z+z'}{2}} L_1^{2\beta-2}(z) L_1^{2\beta-2}(z') \\
&= (zz')^\beta e^{-\frac{z+z'}{2}} \left\{ \frac{2\beta a}{\Gamma(2\lambda)} + \frac{(2\beta-2)a}{\Gamma(2\lambda-1)} (zz')^{-1} \left(C_{1,0}^{2\beta-2} + C_{1,1}^{2\beta-2} z \right) \left(C_{1,0}^{2\beta-2} + C_{1,1}^{2\beta-2} z' \right) \right\}.
\end{aligned}$$

Notice that the expression inside the braces can be written as $\frac{1}{zz'}\mathcal{R}^{(2)}(z, z')$, with $\mathcal{R}^{(2)}(z, z') = a + bz' + cz + dzz'$ a polynomial of order $N - 1 = 1$ in both z and z'. This can also be written in terms of Vandermonde vectors and a 2×2 matrix:

$$\mathcal{R}^{(2)}(z, z') = \boldsymbol{z}^{(2),T} R^{(2)} \boldsymbol{z'}^{(2)} = \begin{pmatrix} 1 & z \end{pmatrix} R^{(2)} \begin{pmatrix} 1 \\ z' \end{pmatrix}, \tag{155}$$

with

$$R^{(2)} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \frac{(2\beta-2)a}{\Gamma(2\lambda-1)} \begin{pmatrix} \left(C_{1,0}^{2\beta-2}\right)^2 & C_{1,0}^{2\beta-2} C_{1,1}^{2\beta-2} \\ C_{1,1}^{2\beta-2} C_{1,0}^{2\beta-2} & \left(C_{1,1}^{2\beta-2}\right)^2 + \frac{2\beta\Gamma(2\lambda-1)}{(2\beta-2)\Gamma(2\lambda)} \end{pmatrix}, \tag{156}$$

so finally we can write

$$\rho^{(2)}(z, z') = (zz')^\beta e^{-\frac{z+z'}{2}} \frac{1}{zz'} \mathcal{R}^{(N)}(z, z'). \tag{157}$$

Similarly, for $N = 3$ we obtain

$$\begin{aligned}
&\rho^{(3)}(z, z') = \rho^{(2)}(z, z') + \phi_2(z)\phi_2(z') = \rho^{(2)}(z, z') \\
&+ (zz')^\beta e^{-\frac{z+z'}{2}} \frac{2(2\beta-4)a}{\Gamma(2\lambda-2)} (zz')^{-2} \left(C_{2,0}^{2\beta-4} + C_{2,1}^{2\beta-4} z + C_{2,2}^{2\beta-4} z^2 \right) \left(C_{2,0}^{2\beta-4} + C_{2,1}^{2\beta-4} z' + C_{2,2}^{2\beta-4} z'^2 \right).
\end{aligned}$$

Again, we can take a common factor of $\frac{1}{(zz')^2}$ and we obtain a polynomial of order 2 in z and z'.

For any N, we will always have the same structure, because each time we increase the n in $(zz')^{-n}$, an extra term of order n appears in the sum of the Laguerre polynomials. Thus, we can write that

$$\rho^{(N)}(z,z') = (zz')^{\beta} e^{-\frac{z+z'}{2}} \frac{1}{(zz')^{N-1}} \mathcal{R}^{(N)}(z,z'), \tag{158}$$

where $\mathcal{R}^{(N)}(z,z')$ is a polynomial of order $N-1$ in both z and z'. This is the closed expression for the OBDM in a MO. More compactly,

$$\rho^{(N)}(z,z') = (zz')^{\beta-N+1} e^{-\frac{z+z'}{2}} \mathcal{R}^{(N)}(z,z'). \tag{159}$$

Actually, we can derive the above expression more formally:

$$\begin{aligned}
\rho^{(N)}(z,z') &= \sum_{n=0}^{N-1} \phi_n^*(z)\phi_n(z') = \sum_{n=0}^{N-1} N_n^2 (zz')^{\beta} e^{-\frac{z+z'}{2}} (zz')^{-n} L_n^{2\beta-2n}(z) L_n^{2\beta-2n}(z') \\
&= (zz')^{\beta} e^{-\frac{z+z'}{2}} \sum_{n=0}^{N-1} N_n^2 (zz')^{-n} \sum_{i,j=0}^{n} C_{n,i}^{2\beta-2n} C_{n,j}^{2\beta-2n} z^i z'^j \\
&= (zz')^{\beta} (zz')^{-(N-1)} e^{-\frac{z+z'}{2}} \sum_{n=0}^{N-1} N_n^2 (zz')^{N-1-n} \sum_{i,j=0}^{n} C_{n,i}^{2\beta-2n} C_{n,j}^{2\beta-2n} z^i z'^j,
\end{aligned} \tag{160}$$

where in the last step we have divided and multiplied by $(zz')^{N-1}$. The reason for this is that in the second sum there will always be a constant term corresponding to $i=j=0$, which in turn is multiplied by $(zz')^{-n}$. If we multiply this by $(zz')^{n_{max}}$, with $n_{max} = N-1$, we obtain a polynomial in z and z':

$$\begin{aligned}
\mathcal{R}^{(N)}(z,z') &= \sum_{n=0}^{N-1} N_n^2 (zz')^{N-1-n} \sum_{i,j=0}^{n} C_{n,i}^{2\beta-2n} C_{n,j}^{2\beta-2n} z^i z'^j \\
&= \sum_{n=0}^{N-1} N_n^2 (zz')^{N-1-n} \sum_{i,j=0}^{n} \frac{1}{i!j!} (-1)^{i+j} \binom{2\beta-n}{n-i} \binom{2\beta-n}{n-j} z^i z'^j.
\end{aligned} \tag{161}$$

This way we retrieve Eq. (159). This polynomial can be written in terms of Vandermonde vectors and an $N \times N$ matrix, $R^{(N)}$, as

$$\mathcal{R}^{(N)}(z,z') = \boldsymbol{z}^{(N),T} R^{(N)} \boldsymbol{z'}^{(N)}. \tag{162}$$

On the other hand, we can find the closed expression of the PCF from the OBDM as

$$\begin{aligned}
g^{(N)}(z_1,z_2) &= \frac{1}{2}\left(\rho^{(N)}(z_1,z_1)\rho^{(N)}(z_2,z_2) - \rho^{(N)}(z_1,z_2)\rho^{(N)}(z_2,z_1)\right) \\
&= \frac{1}{2}\Big(z_1^{2\beta-2N+2} e^{-z_1} \mathcal{R}^{(N)}(z_1,z_1) z_2^{2\beta-2N+2} e^{-z_2} \mathcal{R}^{(N)}(z_2,z_2) \\
&- (z_1 z_2)^{\beta-N+1} e^{-\frac{z_1+z_2}{2}} \mathcal{R}^{(N)}(z_1,z_2) (z_1 z_2)^{\beta-N+1} e^{-\frac{z_1+z_2}{2}} \mathcal{R}^{(N)}(z_2,z_1)\Big) \\
&= \frac{1}{2}(z_1 z_2)^{2\beta-2N+2} e^{-(z_1+z_2)} \left[\mathcal{R}^{(N)}(z_1,z_1)\mathcal{R}^{(N)}(z_2,z_2) - \mathcal{R}^{(N)}(z_1,z_2)\mathcal{R}^{(N)}(z_2,z_1)\right].
\end{aligned} \tag{163}$$

Since $\mathcal{R}^{(N)}(z_1,z_1)$ and $\mathcal{R}^{(N)}(z_2,z_2)$ are polynomials of order $2(N-1)$ in z_1 and z_2, respectively, and $\mathcal{R}^{(N)}(z_1,z_2)$ and $\mathcal{R}^{(N)}(z_2,z_1)$ are of order $N-1$ in both z_1 and z_2,

$\mathcal{G}^{(N)}(z_1,z_2) = \mathcal{R}^{(N)}(z_1,z_1)\mathcal{R}^{(N)}(z_2,z_2) - \mathcal{R}^{(N)}(z_1,z_2)\mathcal{R}^{(N)}(z_2,z_1)$ is a polynomial of order $2(N-1)$ in both z_1 and z_2. Thus, the closed expression of the PCF is

$$g^{(N)}(z_1,z_2) = \frac{1}{2}(z_1 z_2)^{2\beta-2N+2} e^{-(z_1+z_2)} \mathcal{G}^{(N)}(z_1,z_2), \tag{164}$$

where $\mathcal{G}^{(N)}(z_1,z_2)$ can be represented in terms of a matrix product as

$$\mathcal{G}^{(N)}(z_1,z_2) = \boldsymbol{z_1}^{(2N-1),T} G^{(2N-1)} \boldsymbol{z_2}^{(2N-1)}, \tag{165}$$

with $G^{(2N-1)}$ a $(2N-1)\times(2N-1)$ matrix.

As mentioned in Sec. 2.5.3, we have found all the matrices for $N = 2,3,4,5$ by using Eqs. (74) and (77). Similarly as in Appendix [C], we have used a Python code that receives the not simplified polynomial and returns the desired matrix, because doing the groupings manually would become very laborious. The $R^{(N)}$ matrices are shown below:

$$R^{(2)} = \begin{pmatrix} N_1^2 \left(C_{1,0}^{2\beta-2}\right)^2 & N_1^2 C_{1,0}^{2\beta-2} C_{1,1}^{2\beta-2} \\ N_1^2 C_{1,1}^{2\beta-2} C_{1,0}^{2\beta-2} & N_0^2 + N_1^2 \left(C_{1,1}^{2\beta-2}\right)^2 \end{pmatrix},$$

$$R^{(3)} = \begin{pmatrix} N_2^2 \left(C_{2,0}^{2\beta-4}\right)^2 & N_2^2 C_{2,0}^{2\beta-4} C_{2,1}^{2\beta-4} & N_2^2 C_{2,0}^{2\beta-4} C_{2,2}^{2\beta-4} \\ N_2^2 C_{2,1}^{2\beta-4} C_{2,0}^{2\beta-4} & N_1^2 \left(C_{1,0}^{2\beta-2}\right)^2 + N_2^2 \left(C_{2,1}^{2\beta-4}\right)^2 & N_1^2 C_{1,0}^{2\beta-2} C_{1,1}^{2\beta-2} + N_2^2 C_{2,1}^{2\beta-4} C_{2,2}^{2\beta-4} \\ N_2^2 C_{2,2}^{2\beta-4} C_{2,0}^{2\beta-4} & N_1^2 C_{1,1}^{2\beta-2} C_{1,0}^{2\beta-2} + N_2^2 C_{2,2}^{2\beta-4} C_{2,1}^{2\beta-4} & N_0^2 + N_1^2 \left(C_{1,1}^{2\beta-2}\right)^2 + N_2^2 \left(C_{2,2}^{2\beta-4}\right)^2 \end{pmatrix},$$

For $N=4$, the matrices are so big that we have to separate them into blocks for ease of presentation:

$$R^{(4)} = \begin{pmatrix} R_1^{(4)} & R_2^{(4)} & R_3^{(4)} & R_4^{(4)} \end{pmatrix},$$

where

$$R_1^{(4)} = \begin{pmatrix} N_3^2 \left(C_{3,0}^{2\beta-6}\right)^2 \\ N_3^2 C_{3,0}^{2\beta-6} C_{3,1}^{2\beta-6} \\ N_3^2 C_{3,0}^{2\beta-6} C_{3,2}^{2\beta-6} \\ N_3^2 C_{3,0}^{2\beta-6} C_{3,3}^{2\beta-6} \end{pmatrix}, \quad R_2^{(4)} = \begin{pmatrix} N_3^2 C_{3,0}^{2\beta-6} C_{3,1}^{2\beta-6} \\ N_2^2 \left(C_{2,0}^{2\beta-4}\right)^2 + N_3^2 \left(C_{3,1}^{2\beta-6}\right)^2 \\ N_2^2 C_{2,0}^{2\beta-4} C_{2,1}^{2\beta-4} + N_3^2 C_{3,1}^{2\beta-6} C_{3,2}^{2\beta-6} \\ N_2^2 C_{2,0}^{2\beta-4} C_{2,2}^{2\beta-4} + N_3^2 C_{3,1}^{2\beta-6} C_{3,3}^{2\beta-6} \end{pmatrix},$$

$$R_3^{(4)} = \begin{pmatrix} N_3^2 C_{3,0}^{2\beta-6} C_{3,2}^{2\beta-6} \\ N_2^2 C_{2,0}^{2\beta-4} C_{2,1}^{2\beta-4} + N_3^2 C_{3,1}^{2\beta-6} C_{3,2}^{2\beta-6} \\ N_1^2 \left(C_{1,0}^{2\beta-2}\right)^2 + N_2^2 \left(C_{2,1}^{2\beta-4}\right)^2 + N_3^2 \left(C_{3,2}^{2\beta-6}\right)^2 \\ N_1^2 C_{1,0}^{2\beta-2} C_{1,1}^{2\beta-2} + N_2^2 C_{2,1}^{2\beta-4} C_{2,2}^{2\beta-4} + N_3^2 C_{3,2}^{2\beta-6} C_{3,3}^{2\beta-6} \end{pmatrix},$$

$$R_4^{(4)} = \begin{pmatrix} N_3^2 C_{3,0}^{2\beta-6} C_{3,3}^{2\beta-6} \\ N_2^2 C_{2,0}^{2\beta-4} C_{2,2}^{2\beta-4} + N_3^2 C_{3,1}^{2\beta-6} C_{3,3}^{2\beta-6} \\ N_1^2 C_{1,0}^{2\beta-2} C_{1,1}^{2\beta-2} + N_2^2 C_{2,1}^{2\beta-4} C_{2,2}^{2\beta-4} + N_3^2 C_{3,2}^{2\beta-6} C_{3,3}^{2\beta-6} \\ N_0^2 + N_1^2 \left(C_{1,1}^{2\beta-2}\right)^2 + N_2^2 \left(C_{2,2}^{2\beta-4}\right)^2 + N_3^2 \left(C_{3,3}^{2\beta-6}\right)^2 \end{pmatrix}.$$

Similarly, for $N=5$ we have:

$$R^{(5)} = \begin{pmatrix} R_1^{(5)} & R_2^{(5)} & R_3^{(5)} & R_4^{(5)} & R_5^{(5)} \end{pmatrix},$$

where

$$R_1^{(5)} = \begin{pmatrix} N_4^2 \left(C_{4,0}^{2\beta-8}\right)^2 \\ N_4^2 C_{4,0}^{2\beta-8} C_{4,1}^{2\beta-8} \\ N_4^2 C_{4,0}^{2\beta-8} C_{4,2}^{2\beta-8} \\ N_4^2 C_{4,0}^{2\beta-8} C_{4,3}^{2\beta-8} \\ N_4^2 C_{4,0}^{2\beta-8} C_{4,4}^{2\beta-8} \end{pmatrix}, \quad R_2^{(5)} = \begin{pmatrix} N_4^2 C_{4,0}^{2\beta-8} C_{4,1}^{2\beta-8} \\ N_3^2 \left(C_{3,0}^{2\beta-6}\right)^2 + N_4^2 \left(C_{4,1}^{2\beta-8}\right)^2 \\ N_3^2 C_{3,0}^{2\beta-6} C_{3,1}^{2\beta-6} + N_4^2 C_{4,1}^{2\beta-8} C_{4,2}^{2\beta-8} \\ N_3^2 C_{3,0}^{2\beta-6} C_{3,2}^{2\beta-6} + N_4^2 C_{4,1}^{2\beta-8} C_{4,3}^{2\beta-8} \\ N_3^2 C_{3,0}^{2\beta-6} C_{3,3}^{2\beta-6} + N_4^2 C_{4,1}^{2\beta-8} C_{4,4}^{2\beta-8} \end{pmatrix},$$

$$R_3^{(5)} = \begin{pmatrix} N_4^2 C_{4,0}^{2\beta-8} C_{4,2}^{2\beta-8} \\ N_3^2 C_{3,0}^{2\beta-6} C_{3,1}^{2\beta-6} + N_4^2 C_{4,1}^{2\beta-8} C_{4,2}^{2\beta-8} \\ N_2^2 \left(C_{2,0}^{2\beta-4}\right)^2 + N_3^2 \left(C_{3,1}^{2\beta-6}\right)^2 + N_4^2 \left(C_{4,2}^{2\beta-8}\right)^2 \\ N_2^2 C_{2,0}^{2\beta-4} C_{2,1}^{2\beta-4} + N_3^2 C_{3,1}^{2\beta-6} C_{3,2}^{2\beta-6} + N_4^2 C_{4,2}^{2\beta-8} C_{4,3}^{2\beta-8} \\ N_2^2 C_{2,0}^{2\beta-4} C_{2,2}^{2\beta-4} + N_3^2 C_{3,1}^{2\beta-6} C_{3,3}^{2\beta-6} + N_4^2 C_{4,2}^{2\beta-8} C_{4,4}^{2\beta-8} \end{pmatrix},$$

$$R_4^{(5)} = \begin{pmatrix} N_4^2 C_{4,0}^{2\beta-8} C_{4,3}^{2\beta-8} \\ N_3^2 C_{3,0}^{2\beta-6} C_{3,2}^{2\beta-6} + N_4^2 C_{4,1}^{2\beta-8} C_{4,3}^{2\beta-8} \\ N_2^2 C_{2,0}^{2\beta-4} C_{2,1}^{2\beta-4} + N_3^2 C_{3,1}^{2\beta-6} C_{3,2}^{2\beta-6} + N_4^2 C_{4,2}^{2\beta-8} C_{4,3}^{2\beta-8} \\ N_1^2 \left(C_{1,0}^{2\beta-2}\right)^2 + N_2^2 \left(C_{2,1}^{2\beta-4}\right)^2 + N_3^2 \left(C_{3,2}^{2\beta-6}\right)^2 + N_4^2 \left(C_{4,3}^{2\beta-8}\right)^2 \\ N_1^2 C_{1,0}^{2\beta-2} C_{1,1}^{2\beta-2} + N_2^2 C_{2,1}^{2\beta-4} C_{2,2}^{2\beta-4} + N_3^2 C_{3,2}^{2\beta-6} C_{3,3}^{2\beta-6} + N_4^2 C_{4,3}^{2\beta-8} C_{4,4}^{2\beta-8} \end{pmatrix},$$

$$R_5^{(5)} = \begin{pmatrix} N_4^2 C_{4,0}^{2\beta-8} C_{4,4}^{2\beta-8} \\ N_3^2 C_{3,0}^{2\beta-6} C_{3,3}^{2\beta-6} + N_4^2 C_{4,1}^{2\beta-8} C_{4,4}^{2\beta-8} \\ N_2^2 C_{2,0}^{2\beta-4} C_{2,2}^{2\beta-4} + N_3^2 C_{3,1}^{2\beta-6} C_{3,3}^{2\beta-6} + N_4^2 C_{4,2}^{2\beta-8} C_{4,4}^{2\beta-8} \\ N_1^2 C_{1,0}^{2\beta-2} C_{1,1}^{2\beta-2} + N_2^2 C_{2,1}^{2\beta-4} C_{2,2}^{2\beta-4} + N_3^2 C_{3,2}^{2\beta-4} C_{3,3}^{2\beta-6} + N_4^2 C_{4,3}^{2\beta-8} C_{4,4}^{2\beta-8} \\ N_0^2 + N_1^2 \left(C_{1,1}^{2\beta-2}\right)^2 + N_2^2 \left(C_{2,2}^{2\beta-4}\right)^2 + N_3^2 \left(C_{3,3}^{2\beta-6}\right)^2 + N_4^2 \left(C_{4,4}^{2\beta-8}\right)^2 \end{pmatrix}.$$

The expressions for $G^{(2N-1)}$ are even more difficult and large. We can only write here the case for $N = 2$ because for the other cases the matrices become excessively big:

$$G^{(3)} = N_0^2 N_1^2 \left(C_{1,0}^{2\beta-2}\right)^2 \begin{pmatrix} 0 & 0 & 1 \\ 0 & -2 & 0 \\ 1 & 0 & 0 \end{pmatrix}.$$

For $N = 3, 4, 5$ the results are excessively large, so we do not include these cases in this document. However, we have computed and plotted the OBDM and the PCF with all the matrices for $N = 2, 3, 4, 5$ and we have obtained the same results as in Sec. 2.5.2, thus checking the derived closed expressions matrices.

E Ground-state calculations

E.1 Ground-state energy of the systems

In this section we find the ground-state energy for each one of the systems of N spinless fermions, taking into account the Pauli exclusion principle. For the calculations, we need the following formulae:

$$\sum_{i=0}^{M} i = \frac{1}{2}M(M+1), \tag{166}$$

$$\sum_{i=0}^{M} i^2 = \frac{1}{6}M(M+1)(2M+1). \tag{167}$$

Let us start for the HO, which has the following single-particle energy:

$$\epsilon_n = \hbar\omega\left(n+\frac{1}{2}\right), \quad n = 0, 1, 2\dots \tag{168}$$

Thus, the ground-state energy is

$$\begin{aligned} E^{(N)} &= \sum_{n=0}^{N-1}\epsilon_n = \hbar\omega\sum_{n=0}^{N-1}\left(n+\frac{1}{2}\right) = \hbar\omega\left[\frac{1}{2}(N-1)N+\frac{1}{2}N\right] \\ &= \hbar\omega\left(\frac{N^2}{2}-\frac{N}{2}+\frac{N}{2}\right) = \hbar\omega\frac{N^2}{2}. \end{aligned} \tag{169}$$

Using HO units, since $\hbar\omega = 1$, the energy is just $E^{(N)} = \frac{N^2}{2}$.

For the IW,

$$\epsilon_n = \frac{\hbar^2\pi^2}{2mL^2}n^2, \quad n = 1, 2, 3\dots \tag{170}$$

Therefore

$$E^{(N)} = \sum_{n=1}^{N}\epsilon_n = \frac{\hbar^2\pi^2}{2mL^2}\sum_{n=1}^{N}n^2 = \frac{\hbar^2\pi^2}{12mL^2}N(N+1)(2N+1). \tag{171}$$

In the natural units of the system, we have that $\frac{\hbar^2}{mL^2} = 1$, so $E^{(N)} = \frac{\pi^2}{12}N(N+1)(2N+1)$.

Finally, for the MO the single-particle energies are given by

$$\epsilon_n = \left[\left(n+\frac{1}{2}\right)-\frac{1}{2\lambda}\left(n+\frac{1}{2}\right)^2\right]\hbar\omega_e, \quad n = 0, 1, 2\dots \tag{172}$$

so the ground-state energy is

$$\begin{aligned} E^{(N)} &= \sum_{n=0}^{N-1}\epsilon_n = \left[\frac{N^2}{2}-\frac{1}{2\lambda}\sum_{n=0}^{N-1}\left(n^2+n+\frac{1}{4}\right)\right]\hbar\omega_e \\ &= \left[\frac{N^2}{2}-\frac{1}{2\lambda}\left(\frac{1}{6}(N-1)N(2N-1)+\frac{1}{2}(N-1)N+\frac{1}{4}N\right)\right]\hbar\omega_e \\ &= \left[\frac{N^2}{2}-\frac{1}{2\lambda}\left(\frac{1}{6}(2N^3-3N^2+N)+\frac{N^2}{2}-\frac{N}{2}+\frac{N}{4}\right)\right]\hbar\omega_e \\ &= \left[\frac{N^2}{2}-\frac{1}{2\lambda}\left(\frac{1}{6}(2N^3+N)-\frac{N}{4}\right)\right]\hbar\omega_e = \left[\frac{N^2}{2}-\frac{1}{24\lambda}N\left(4N^2-1\right)\right]\hbar\omega_e. \end{aligned} \tag{173}$$

In the natural units of the MO, $\frac{a^2\hbar^2}{m} = 1$, so $\hbar\omega_e = \lambda$ and $E^{(N)} = \frac{N^2}{2}\lambda - \frac{1}{24}N\left(4N^2-1\right)$.

E.2 Nodal structure of the single-particle wavefunctions

The single-particle wavefunctions of the three systems have a number of nodes directly related to the principal quantum number n. Here we show which is the exact relation.

For the HO, the single-particle wavefunctions vanish only in the roots of the Hermite polynomials, as we can see:

$$\phi_n(x) = N_n e^{-\frac{x^2}{2a_{ho}^2}} H_n\left(\frac{x}{a_{ho}}\right), \qquad n = 0, 1, 2, \ldots \tag{174}$$

However, a Hermite polynomial of degree n has n distinct real nodes or zeros [GM48], so $\phi_n(x)$ has n distinct real nodes.

For the MO we encounter a similar case, since the single-particle wavefunctions vanish only in the roots of the associated Laguerre polynomials:

$$\phi_n(z) = N_n z^{\beta} e^{-z/2} z^{-n} L_n^{2\beta-2n}(z), \qquad n = 0, 1, 2 \ldots, \lfloor \lambda - \frac{1}{2} \rfloor. \tag{175}$$

Recall that $z = 2\lambda e^{-ax}$ is strictly positive, so only the Laguerre term can make the wavefunction to vanish. On the other hand, an associated Laguerre polynomial of degree n has n distinct real and positive nodes or zeros [DM15], so the single-particle wavefunctions have exactly n nodes, because z is also positive. In Fig. 8 we plot the Hermite and associated Laguerre polynomials for $n = 0$ to 4.

For the IW, the single-particle states vanish in the zeros of the sine:

$$\phi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right), \qquad n = 1, 2, 3, \ldots \tag{176}$$

This happens when $\sin\left(\frac{n\pi x}{L}\right) = 0$, that is, $\frac{n\pi x}{L} = m\pi$, or equivalently $x = \frac{m}{n}L$, with $m = 0, 1, 2, \ldots, n$ because x goes from 0 to L. Therefore, without counting $x = 0$ and $x = L$, there are $n - 1$ nodes. For example, for $n = 4$, $x = 0, \frac{1}{4}L, \frac{2}{4}L, \frac{3}{4}L, L$, we have three nodes. Notice though that for the IW n starts from 1, so in fact for the three systems we have the same number of nodes for a particular energy level. For example, for the first level to be filled by fermions, we have 0 nodes in all cases.

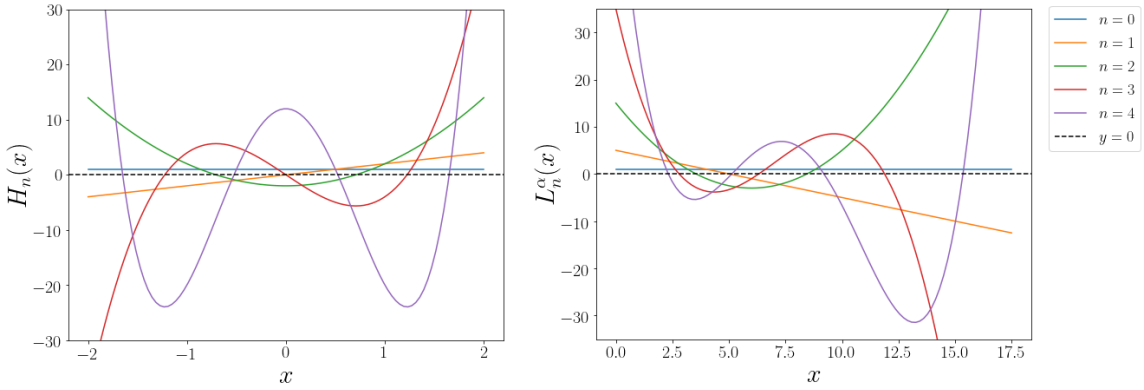

Figure 8: Plot of Hermite polynomials and the associated Laguerre polynomials for $\alpha = 4$ and $n = 0, 1, 2, 3, 4$, which are the n values used in this work. We can see that these polynomials have n zeros and, in particular, for the associated Laguerre polynomials these zeros are positive.

F Plots of the OBDM and the PCF obtained with ML

Here we show the plots of the OBDM and the PCF for the HO (Figs. 9, 10), the IW (Figs. 11, 12) and the MO (Figs. 13, 14) obtained using ML techniques.

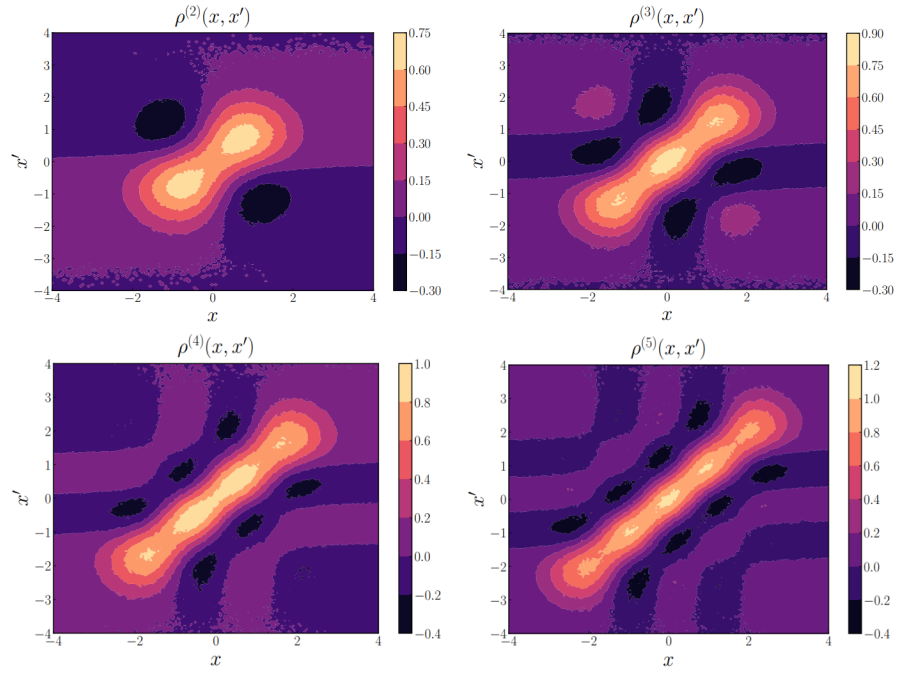

Figure 9: OBDM $\rho^{(N)}(x,x')$ obtained with ML techniques in terms of the positions x and x' for $N=2$ to 5 particles in a HO well. We use HO units.

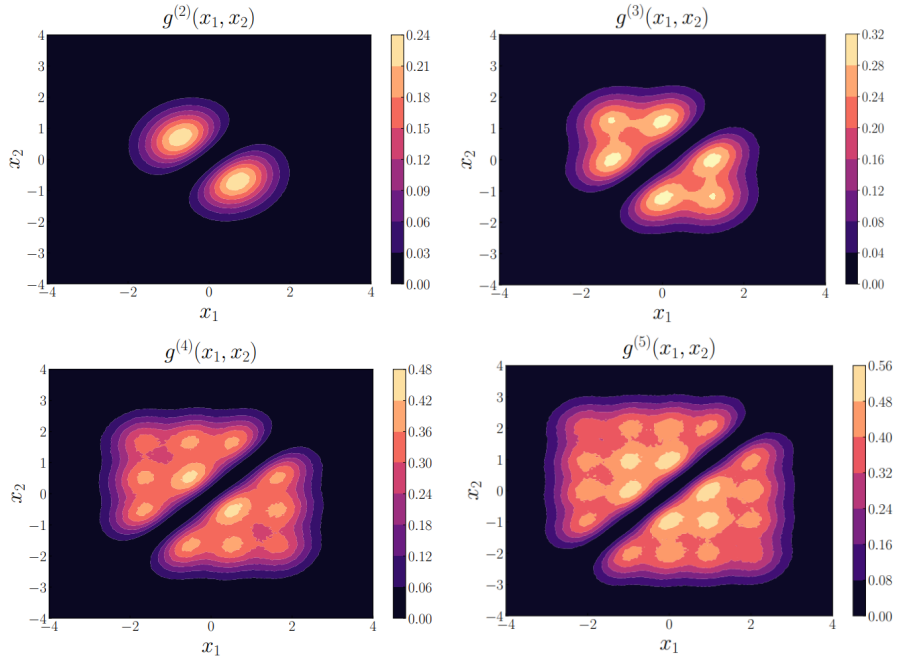

Figure 10: PCF $g^{(N)}(x_1,x_2)$ obtained with ML techniques in terms of the positions x_1 and x_2 for $N=2$ to 5 particles in a HO well. We use HO units.

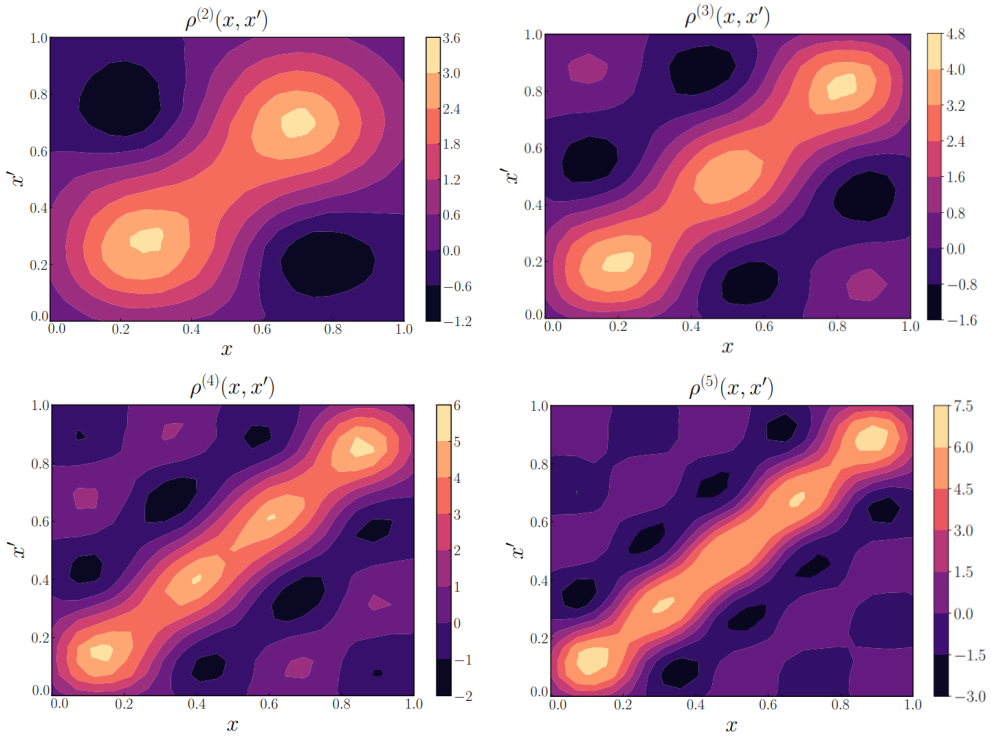

Figure 11: OBDM $\rho^{(N)}(x, x')$ obtained with ML techniques in terms of the positions x and x' for $N = 2$ to 5 particles in an IW. We use IW natural units.

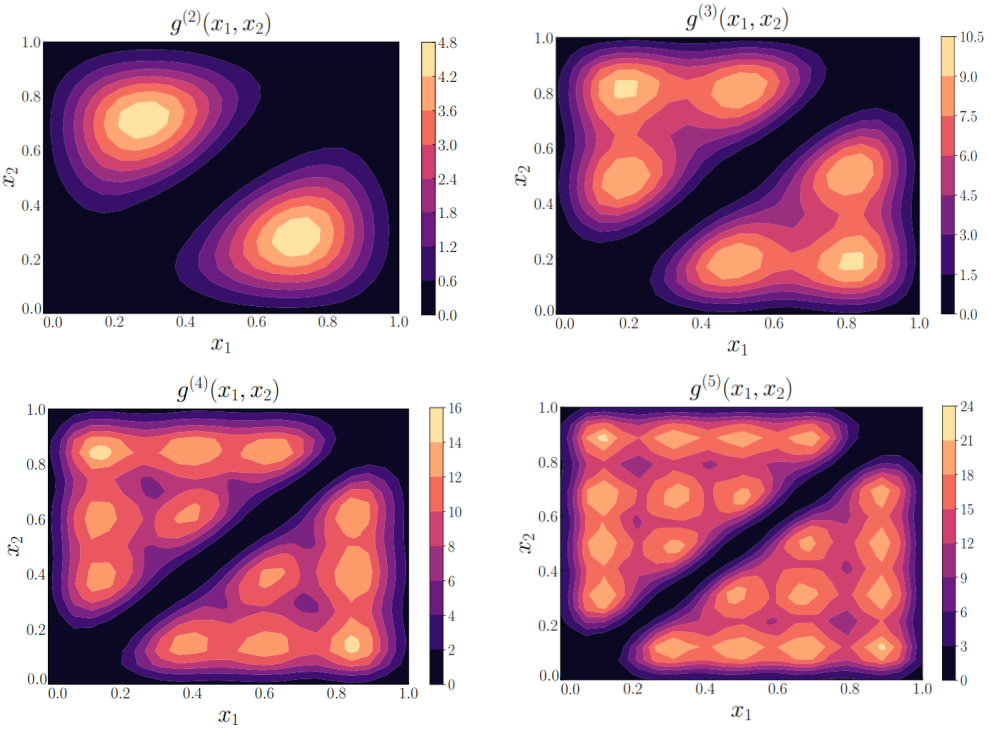

Figure 12: PCF $g^{(N)}(x_1, x_2)$ obtained with ML techniques in terms of the positions x_1 and x_2 for $N = 2$ to 5 particles in an IW. We use IW natural units.

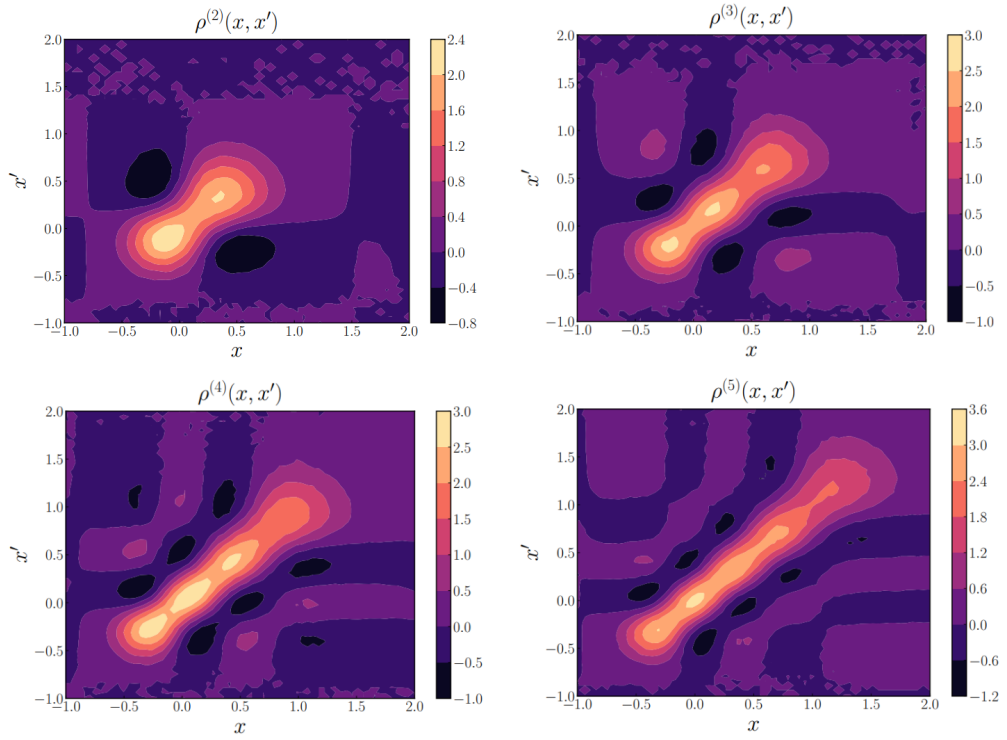

Figure 13: OBDM $\rho^{(N)}(x, x')$ obtained with ML techniques in terms of the positions x and x' for $N = 2$ to 5 particles in a MO, with $\lambda = 11.5$. We use MO natural units.

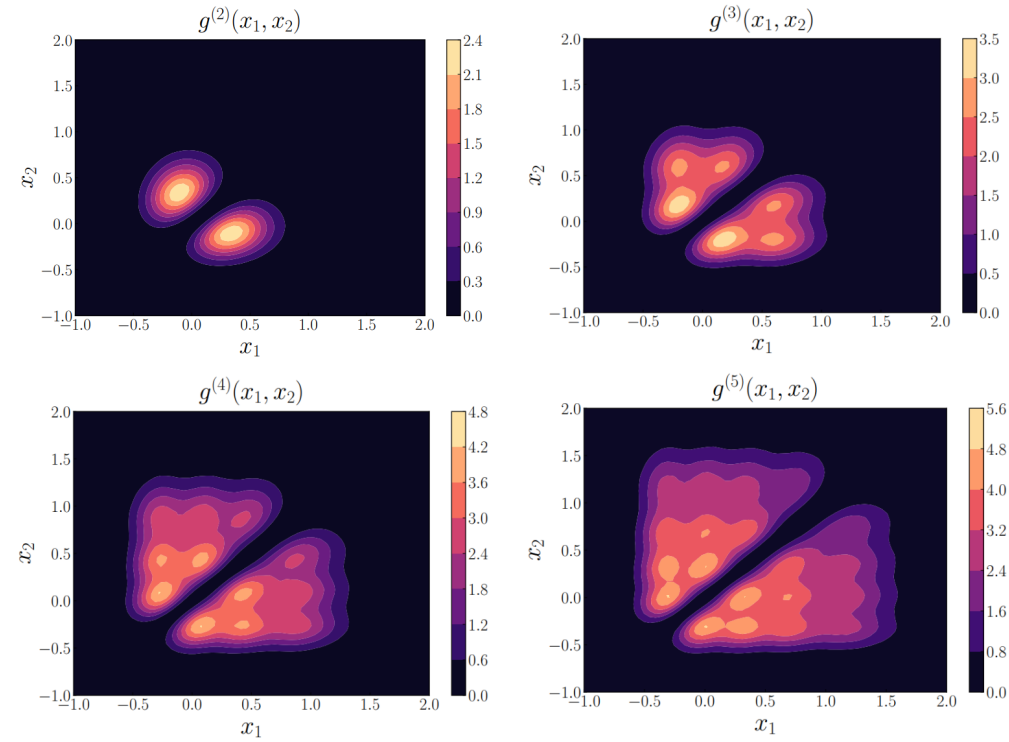

Figure 14: PCF $g^{(N)}(x_1, x_2)$ obtained with ML techniques in terms of the positions x_1 and x_2 for $N = 2$ to 5 particles in a MO, with $\lambda = 11.5$. We use MO natural units.