Entanglement in N-harmonium: bosons and fermions

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Received 22 May 2014, revised 22 August 2014
Accepted for publication 27 August 2014
Published 24 September 2014

Abstract

The ground-state entanglement of a single particle of the N-harmonium system (i.e., a completely integrable model of \(N\) particles where both the confinement and the two-particle interaction are harmonic) is shown to be analytically determined in terms of \(N\) and the relative interaction strength. For bosons, we compute the von Neumann entropy of the one-body reduced density matrix by using the corresponding natural occupation numbers. A critical number, \(N_c\), of particles exists, and below it, for positive values of the coupling constant, the entanglement grows when the number of particles increases; the opposite occurs for \(N > N_c\). For fermions, we compute the one-body reduced density matrix for the closed-shell spinned case. In the strong coupling regime, the linear entropy of the system decreases when \(N\) grows. For fixed \(N\), the entanglement is found (a) to decrease (increase) for negatively (positively) increases values of the coupling constant, and (b) to grow when the energy increases. Moreover, the spatial and spin contributions to the total entanglement are found to be of comparable size.

Keywords: many-body systems, quantum information, entanglement, harmonium

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

1. Introduction

The most precise determination of the properties of finite many-electron systems is usually calculated using a full configuration interaction (FCI) method, where the solution of the corresponding Schrödinger equation in a given one-electron basis is expressed in terms of a linear combination of all possible Slater determinants. Its application is naturally reduced to a bunch of small systems because of the enormous number of determinants involved \([1, 2]\).

Let us highlight that for all FCI approaches, the correlation effects, which remain solely in the wave function, are not described by any correlation operator. Moreover, these effects are usually numerically computed as a difference of two variational energy bounds. Thus, up to now the electron correlation has been widely and implicitly believed to be a purely methodical effect coming from the inadequate use of a multiconfiguration, Hartree–Fock-type trial wave function, which lacks physical reality.

The application of quantum information ideas and techniques in electronic structure theory has recently led to the conclusion that the electron correlation is closely related to the entanglement of electrons. Indeed, it has been proved that while the single Slater determinant in the monoconfigurational Hartree–Fock approximation is a disentangled state, the wave function of the multiconfiguration Hartree–Fock approximations (such as FCI) accounts for the entanglement effects. Therefore, entanglement plays an essential role not only in quantum communication between parties separated by macroscopic distances (see, e.g., \([3, 4]\)), but also in characterizing quantum correlations at short distances. The latter problem, where one should necessarily consider the indistinguishable character of the involved particles, has received relatively little attention until recently \([5–10]\). This has been a serious omission because of its relevance in quantum
information processing in various physical systems (see, e.g., [5, 11]) it also allows us to gain deeper insight into non-classical correlations of atomic and molecular systems, and to fully understand the course of their dissociation processes and chemical reactions [10–12].

The main difficulty, however, stems from the fact that the Schrödinger equation of most quantum many-body systems cannot be solved analytically. Even numerically, the determination of the wavefunction is, in general, a serious problem. In the last three years, an intense effort has been made to determine the entanglement of some real atomic and molecular species, such as helium-like atoms [13–17], a few processes of diatomic molecules [18], and elementary chemical reactions [19]. This research has basically focused on the entanglement of bipartite systems, mainly because the characterization of this phenomenon for systems of many indistinguishable constituents is much less known, even at the notional level of entanglement measurement [20].

Thus, the quantification of the entanglement of bound states for model systems enabling analytic solutions of the associated Schrödinger equation is a promising way to investigate correlation phenomena. Indeed, entanglement between the constituents of any bound system is most conveniently analyzed in such models, enabling us to relate it to bosonic or fermionic characteristics. Up to now, however, the entanglement of certain models of two bound electrons is all that has been determined. We refer to the two-harmonium (or Moshinsky) [21–25], Crandall, and Hooke [13] atoms. In all these models, the electron confinement is harmonic, and the electron-electron interaction is of a harmonic (two-harmonium), \( r_1^2 \) (Crandall), or Coulombic (Hooke) type. All of them show that when the spin degree of freedom and the indistinguishability of electrons are taken into account, new entanglement aspects [24] are encountered as compared to the model of distinguishable particles, although some further clarification is needed.

It is also worth noting that some entanglement features of the two-harmonium atom are also qualitatively reproduced by the other two models, which give a good description for certain two-fermion systems (e.g., two electrons in a quantum dot is approximately described by the Hooke model)—namely the growth of the entanglement when either the relative strength or the excitation energy is increases. It is most interesting that recently, the entanglement of some real helium-like atoms has been numerically shown to have an increases dependence on the energy. This has been done both by using very accurate one-electron Hylleraas–Kinosita type basis functions [14, 17] and some Gaussian or Slater-type orbital basis sets [6, 15]. It is also observed from the models that the entanglement decrease of these systems, in terms of the nuclear charge \( Z \), can also be understood as the result of the relative decrease of the electron-electron interaction.

In this paper, we will analytically study the entanglement of the one-body reduced density matrix of the N-harmonium model for bosons and fermions. Von Neumann (for bosons) and linear (for fermions) entropies will be used. The one-body reduced matrix for the spinless fermionic case has been previously computed [26]. We obtain for the first time an explicit expression of the one-body reduced density matrix for the closed-shell spinned fermionic case. This study will allow us to show that some entanglement features of finite many-particle systems can be understood to a certain extent by purely kinematical considerations. The N-particle harmonium is a completely integrable system with an arbitrary number of particles, \( N \), where both the confinement and the two-particle interaction are harmonic. This model has been implicitly used to a certain extent to study cold atoms [27], to determine area laws of the ground-state entanglement of some one-dimensional chains [28], and to gain further insight into numerous phenomena of a variety of physical systems up to black holes (see, e.g., [21, 29–35]).

The paper is structured as follows. First, in section 2 we briefly formulate the quantum-mechanical problem of the N-particle harmonium, showing its separability by using the appropriate set of normal coordinates [36] and fixing our notational settings. In section 3 we discuss the general mathematical structure of the one-body reduced density matrix in the bosonic case, obtaining its explicit expression. Moreover, we compute and discuss the analytical expression of the von Neumann entropy of the one-body reduced density matrix for the N-boson harmonium. Further, in sections 4 and 5, we obtain explicit expressions for the one-body reduced density matrix of the spinned N-fermion harmonium, and we analyze the linear entropy of the one-body reduced density matrix, both with and without the spin degree of freedom. The paper ends with concluding remarks and two appendices.

2. The N-harmonium problem

The N-harmonium model is a system of \( N \) interacting particles (fermions or bosons) which interact harmonically in a three-dimensional harmonic well. It is characterized by the Hamiltonian

\[
H = \frac{1}{2} \sum_{i=1}^{N} p_i^2 + \frac{k}{2} \sum_{i=1}^{N} r_i^2 + \frac{\delta}{2} \sum_{j<i}^{N} r_{ij}^2,
\]

(1)

where \( r_{ij} := |r_i - r_j| \), \( k \) is the coupling constant of the harmonic well, and \( \delta \) is the coupling of the harmonic interaction between the particles. The treatment of harmonically interacting bosons by means of this Hamiltonian represents the first exact solution of an N-particle system using only conditions on the reduced space of two-particle density matrices [37]. This system can be expressed in a separable form (i.e., as a system of uncoupled oscillators) using the set of normal coordinates \( \{\xi_1, \ldots, \xi_N\} \), given by

\[
\xi_N := \frac{1}{\sqrt{N}} \sum_{i=1}^{N} r_i \quad \text{and} \quad \xi_m := \frac{1}{\sqrt{m(m+1)}} \sum_{i=1}^{m} (r_i - r_{m+1}),
\]

(2)

with \( m \in \{1, \ldots, N - 1\} \). This is an orthogonal transformation of the position variables. A similar change of coordinates
for momenta results in a canonical transformation, preserving the symplectic form. Let us call the new set of momenta \( \{ \mathcal{E}_m \} \).

A direct calculation shows that
\[
\sum_{m=1}^{N-1} \mathcal{E}_m^2 = \frac{1}{N} \sum_{i<j} r_{ij}^2 = \sum_{m=1}^{N} r_m^2 - \delta_N^2, \tag{3}
\]
so that the Hamiltonian (1) can be expressed in the following separable form:
\[
H = H_N + \sum_{m=1}^{N-1} H_m, \quad \text{where} \quad H_N = \frac{1}{2} \mathcal{E}_N^2 + \frac{1}{2} \alpha^2 \delta_N^2
\]
and
\[
H_m = \frac{1}{2} \mathcal{E}_m^2 + \frac{1}{2} \mu^2 \delta_m^2, \tag{4}
\]
where \( \alpha^2 := k \) and \( \mu^2 := k + N\delta \), depending on the number of particles. Then, the physical solutions of the associated Schrödinger equation (i.e., the wave functions \( \Psi(x_1, \ldots, x_N) \)), can be readily obtained. Here, let us first note that (a) there is a ground state whenever \( \mu^2 > 0 \), and (b) the particles are no longer bound if the relative interaction strength
\[
\delta < - \frac{1}{N}. \tag{5}
\]

On the other hand, let us comment here that the entanglement problem is formulated in terms of reduced density matrices. Either directly from the resulting one-particle reduced density matrix or, since the particles are assumed to interact pairwise, in terms of the two-particle density matrix,
\[
\rho(x_1, x_2; y_1, y_2) := \int \text{d}x_3 \ldots \text{d}x_N \left\{ \Psi(x_1, x_2, x_3, \ldots, x_N) \right\}^* \times \left\{ \Psi(y_1, y_2, \ldots, x_N) \right\}. \tag{6}
\]
which carries all the necessary information required for calculating the quantum-mechanical properties of the whole system. The symbol \( x \) stands for spatial and spin coordinates, \( x := (r, \zeta) \). In particular, the ground-state energy of the system can be computed by minimizing a simple linear functional of \( \rho \). In passing, let us mention that the N-representability problem for this matrix has proved to be a major challenge for quantum chemistry [38]. The one-body density matrix, which is the basic variable in reduced density matrix functional theory [39], is then given as
\[
\rho_i(x; y) := \int \rho(x_1, x_2; y_1, x_2) \text{d}x_2. \tag{7}
\]
By means of the spectral theorem, \( \rho_i(x; y) \) can be decomposed in terms of its natural spin orbitals, \( \{ \phi_i(x) \} \), and its eigenvalues, \( \{ \epsilon_i \} \); the natural occupation numbers:
\[
\rho_i(x; y) = \sum \epsilon_i n_i \phi_i(x) \phi_i(y), \quad \text{where} \quad \sum \epsilon_i n_i = 1, \quad \text{(for fermions)} \quad 0 \leq n_i \leq 1/N.
\]
For the case of an assembly of bosons, we will compute the von Neumann entropy of the one-body reduced density matrix, explicitly finding the occupation numbers of the system, as described in the next section. Recently, there has been a renewed interest in formulating the reduced density matrix theory using Wigner quasidistributions [25, 40, 41]. Our treatment for bosons will use the Wigner function in phase space, which is a natural procedure for these systems.

Let us propose that a critical value exists for the number of particles. Below this critical value (around 3.5), we will show that for positive values of the coupling constant, \( \delta \), the first occupation number decreases (and consequently the von Neumann entropy grows) as the number of particles increases. Above this value, the first occupation number increases as the number of particles increases. Moreover, the first occupation number tends to 1 (and the entropy tends to 0) in the limit when the number of particles tends to infinity.

For fermions, we use the one-body reduced density matrix to compute an explicit expression for both its purity and its linear entropy. Let us propose that we will show that, in the region of negative coupling \( \delta \), the entropy grows when the number of particles increases. A similar situation is observed in the attractive case for small values of the coupling constant. For large values of \( \delta/k \), the situation is the opposite: When particles are added to the system, the entropy decreases. In both bosonic and fermionic cases, we will show that it is possible to calculate these two measures of entanglement as a function of the coupling constant, \( \delta/k \), and the number of particles.

3. The N-boson harmonium: von Neumann entropy

In this section, we determine the von Neumann entropy of the N-boson harmonium ground state in terms of \( N \) and the relative interaction strength, \( \delta/k \). Taking into account the Gaussian character of the ground-state oscillator wave function, the ground state distribution on phase space is characterized by the Wigner N-body density function,
\[
W_{N/gs}(n_1, \ldots, r_N; p_1, \ldots, p_N) \quad = \quad \frac{1}{\pi^{3N}} \exp \left[ \frac{1}{4} \sum_{m=1}^{N} H_m \delta N \right] \times \prod_{m=2}^{N} \exp \left[ \frac{1}{4} \sum_{i=1}^{N} p_i^2 \right]. \tag{8}
\]

The energy of the ground state is the total sum of the contributions of each individual oscillator (i.e., \( E_{gs} = \sum_i \omega_i + (N - 1)\mu) \)). On the other hand, the one-body density factorizes as a product of two separable quantities:
\[
d_{1B}(r; p) \quad := \quad \int W_{N/gs}(r, r_2, \ldots, r_N; p, p_2, \ldots, p_N) \quad \times \quad \prod_{m=2}^{N} \delta m \text{d}p_m \quad = \quad e^{-\mu^2 r^2 - \mu^2} \quad \Delta^2 (r; \mu, \omega, N) \Delta^2 (p, \mu, \omega, N). \tag{9}
\]

It can be shown that the \( \Delta \)-function fulfills the following recursion relation:
\[
\Delta^{2}(r; \mu, \omega, N) \quad := \quad \frac{1}{\pi^{3N/2}} \int \exp \left[ \frac{1}{N} \frac{\omega - \mu}{\pi} r^2 + \sum_{m=2}^{N} p_m \right] \text{d}r \text{d}p_m. \tag{10}
\]
Then, the one-body quasidensity function can be rewritten in the Gaussian way as

\[ d_{N}^{1}(U) = \frac{\lambda_{N}^{3}}{\pi^{3}} e^{-\lambda_{N} U^{2}}, \tag{16} \]

showing that it is actually a Gibbs state. Note that \( \lambda_{N} \leq 1 \) for all \( N \), since \( \omega + \mu \geq 2\sqrt{\omega \mu} \) and \( A_{N} \geq N^{2} \omega \mu \); also note that \( \lambda_{N} \to 1 \) when \( N \to \infty \).

It is known that there is a unitary operator, associated with any symplectic transformation (say, \( S_{0} \)), which acts on the Hilbert space \( [42] \). Let us use this transformation to find the set of occupation numbers on the basis of the Wigner eigenfunctions of the harmonic oscillator. Since the one-body quasidensity function factorizes completely, from now on we will work in one dimension. From the series formula

\[ (1 - t) \sum_{r=0}^{\infty} L_{r}(x) e^{-x/2} t^{r} = e^{-\frac{1 + x t}{1 - t}}, \tag{17} \]

where \( L_{r}(x) \) is the Laguerre polynomial, it follows that

\[ d_{N}^{1}(U) = \sum_{r=0}^{\infty} \frac{(-1)^{r}}{\pi} L_{r}(2U^{2}) e^{-U^{2}} n_{r}, \tag{18} \]

where the occupation numbers are equal to

\[ n_{r} = \frac{2\lambda_{N}}{1 + \lambda_{N}} \left( \frac{1 - \lambda_{N}}{1 + \lambda_{N}} \right)^{r} = (1 - \frac{t_{N}}{t_{r}}) t_{r}^{r}, \tag{19} \]

fulfilling \( \sum_{r} n_{r} = 1 \), as one should expect.

For the sake of completeness in figure 1 we plot the numerical behavior of the one-body quasidensity function of the N-boson hamiltonian for different values of the number of bosons. We observe that, as the number of bosons grows, the profiles of the position and momentum densities become narrower and wider, respectively. This clearly indicates that the more precisely the particles are localized in position space, the larger the localization in momentum space, as one should expect, according to the position-momentum uncertainty principle. There is no relevant difference for negative values of the coupling constant, \( \delta \), except that in this case, it can be plotted only when \( \delta/k \geq -1/N \).

Finally, we can compute the von Neumann entropy of the N-boson hamiltonian explicitly in terms of \( N \) and the relative interaction strength \( \delta/k \), obtaining the value

\[ S(N) := -\sum_{r=0}^{\infty} n_{r} \log n_{r} = -\log (1 - t_{N}) - t_{N} \log \left( 1 - \frac{t_{N}}{1 - t_{N}} \right) \]

\[ = -\frac{N^{2} \sqrt{\omega \mu}}{2N^{2} \sqrt{\omega \mu} + 2N \sqrt{\omega \mu} - \sqrt{A_{N} + N \sqrt{\omega \mu}}} \log \left( \frac{2N^{2} \sqrt{\omega \mu}}{2N^{2} \sqrt{\omega \mu} + 2N \sqrt{\omega \mu} - \sqrt{A_{N} + N \sqrt{\omega \mu}}} \right), \tag{20} \]

which complements and extends a similar formula encountered by other means in a black-hole context \([31]\). This entanglement measure is numerically examined in figure 2 in terms of the number of bosons, \( N \), and the relative interaction strength, \( \delta/k \). As stated in (5), the minimum value of this relative strength is \(-1/N\). There is a critical point around \( N_{c} \sim 3.5 \) where the entanglement acquires its maximum value. This is more clearly seen in figure 3, where the explicit dependence of the von Neumann entropy on \( N \) is
shown. To investigate it more closely, we study the dependence of the occupation numbers on the number of bosons and the relative interaction strength. In particular, in figure 4 we plot the first occupation number separately in terms of $N$ and the relative strength. Therein, we note that below a critical value of number of particles (around $\sim N^{3.5}$), for positive values of the coupling constant $\delta/k$, the first occupation number decreases as the number of particles increases. Beyond this value, the situation is reversed: The value of the first occupation number increases as the number of particles increases. This implies that $n_0 \sim 1$ in the limit when the number of particles tends to infinite, which is a necessary condition for the existence of a Bose-Einstein condensation [43].

In summary, the critical point around $N \sim 3.5$, where the von Neumann entropy is maximum, is closely connected with the minimum of the first occupation number occurring at this position. We found that above this critical value, the spatial entanglement decreases when we add more and more particles to the system, so that the degrowth rate increases when the coupling constant increases. Moreover, it can be shown that the entropy vanishes when $N$ goes to infinite.
4. The spinless N-fermion harmonium: linear entropy

In this section, we study the spatial entanglement of the N-fermion harmonium (i.e., entanglement without taking into account the spin degree of freedom of the constituents) using the linear entropy of the one-particle density matrix as a measure of the entanglement of one particle. This measure is a first-order approximation of the von Neumann entropy of the reduced one-body density of the system. In fact, it is a lower bound of this entropy. We will consider the case in which the reduced one-body density of the system is

\[ \rho_{1\text{N}}(\omega_{\mu}) = \sum_{n=0}^{N} \phi_{1n}^{\dagger}(\omega_{\mu}) \phi_{1n}(\omega_{\mu}) \]

where \( \phi_{1n}(\omega_{\mu}) \) is a single-particle wave function given by a Hermite function of degree \( n \) and frequency \( \mu \). The collective mode, \( \xi_{\mathbf{n}} \), is symmetric under any exchange of the position coordinates. Therefore, one has \( n_{N} = 0 \); otherwise one would have \( n_{m} = 0 \) for some \( m \neq N \), and the wave function would not be totally antisymmetric. This eigenfunction can be rewritten as

\[ \Psi_{N}^{f}(\xi_{1}, \ldots, \xi_{N}) = (\text{const.}) \sum_{J \in S_{N}} (-1)^{J} \]

\[ \times \left[ \psi(\xi) e^{-\frac{1}{2}(\xi_{1}^{2} + \xi_{1}^{2} + \cdots + \xi_{N}^{2})} \right] \]

where \( H_{m} \) is the Hermite polynomial of degree \( n \), and now \( n_{m} \in \{1, \ldots, N-1\} \). The exponential power of (23) is the bosonic wave function, which is the counterpart of the Wigner function in (8).

As an illustrative case, let us consider the three-harmonium system. To produce an antisymmetric wave function, there is only one possibility for the degree of the polynomials, namely \( n_{1} = 1 \) and \( n_{2} = 2 \). Then, the ground-state eigenfunction is

\[ \Psi_{gs}(\xi_{1}, \xi_{2}, \xi_{3}) = (\text{const.}) \sum_{J \in S_{3}} (-1)^{J} \]

\[ \times \left[ \psi(\xi) e^{-\frac{1}{2}(\xi_{1}^{2} + \xi_{1}^{2} + \xi_{2}^{2} + \xi_{2}^{2} + \cdots + \xi_{3}^{2})} \right] \]

where \( \psi(\xi) := H_{1}(\sqrt{\mu} \xi_{1}) H_{2}(\sqrt{\mu} \xi_{2}) \) and \( \xi := (\xi_{1}, \xi_{2}) \). Note that the six elements of the permutation group \( S_{3} \) are

\[ p_{1} = (1 \ 2 \ 3), \quad p_{2} = (2 \ 1 \ 3), \quad p_{3} = (2 \ 3 \ 1), \]

\[ p_{4} = (1 \ 3 \ 2), \quad p_{5} = (3 \ 1 \ 2), \quad p_{6} = (3 \ 2 \ 1). \]

The coordinate, \( \xi \), transforms under the representation of the permutation group in the following form:

\[ R(p_{1}) \xi = \xi, \quad R(p_{2}) \xi = M_{1} \xi, \quad R(p_{3}) \xi = M_{1} M_{2} \xi, \]

\[ R(p_{4}) \xi = M_{2} \xi, \quad R(p_{5}) \xi = M_{1} M_{3} \xi, \quad R(p_{6}) \xi = M_{3} \xi, \]

where

\[ M_{1} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad M_{2} = \begin{pmatrix} \cos \pi/3 & \sin \pi/3 \\ -\sin \pi/3 & \cos \pi/3 \end{pmatrix} \]

\[ M_{3} = \begin{pmatrix} \cos \pi/3 & -\sin \pi/3 \\ -\sin \pi/3 & \cos \pi/3 \end{pmatrix}. \]
Note that $\det M = -1$ and $M' M = 1$. Any matrix

$$M_\phi = \begin{pmatrix} \cos \phi & \sin \phi \\ \sin \phi & -\cos \phi \end{pmatrix}$$

is a reflection in the axis $\theta = \phi/2$. In our case, this means $\theta = \pi/2$, $\pi/6$, and $-\pi/6$ (i.e., three reflection axes at 60-degree angles to each other). The rotations $R(p_i)$ and $R(p_j)$ are products of two reflections each. Thus, the eigenfunction transforms as follows:

$$\Psi'_\xi (\xi_1, \xi_2, \xi_3) = (\text{const.}) e^{-\sum\xi_i^2} \left( \frac{2}{\mu^{3/2}} \right) \sum_{i=1}^{N} (-1)^{i+1} \psi \left( R(p_i) \xi \right)$$

is a Vandermonde determinant. This three-fermion result can be extended to the N-fermion system. In fact, the general results of the theory of antisymmetric functions ensure that the wave function of a system of spinless fermions is equal to the wave function of the corresponding bosonic system, multiplied by the $N$-variable Vandermonde determinant (see section 3.1 of [44]). So, the ground-state wave function of the spinless N-fermion hamiltonian described by the Hamiltonian

$$\Psi'_f (\eta_1, \ldots, \eta_N) = (\text{const.}) \prod_{i<j} (\eta_i - \eta_j)$$

where the product-like symbol on the right-hand side of this expression denotes the Vandermonde determinant,

$$\mathcal{V}_{(\eta_1, \ldots, \eta_N)} := \begin{vmatrix} 1 & \cdots & 1 \\ \eta_1 & \cdots & \eta_N \\ \vdots & \ddots & \vdots \\ \eta_{N-1} & \cdots & \eta_N \end{vmatrix}$$

$$= \prod_{1 \leq i < j \leq N} (\eta_i - \eta_j).$$

Concrete calculations [30, 34] have borne out this fact several times. On the other hand, it has been pointed out by several authors that this function is actually a generalization of Laughlin’s wave function for the fractional quantum Hall effect [45]. This is not surprising since, in the Hall effect, the magnetic field can be understood as a harmonic potential acting on the electrons. Let us also point out that the Wigner function corresponding to the Gaussian one on the right-hand side of (27) is nothing but the Wigner N-body quasidensity given by (8).

Let us now calculate the one-body density of the one-dimensional spinless N-fermion hamiltonian, which is defined by

$$\rho_1(r; r') = \int d\eta_2 \cdots d\eta_N \Psi'_f (r, \eta_2, \ldots, \eta_N) \Psi'_f$$

(29)

For this purpose, it is convenient to rewrite the eigenfunction (27) as

$$\Psi'_f (\eta_1, \ldots, \eta_N) = (\text{const.}) \times \mathcal{V}_{(\eta_1, \ldots, \eta_N)} e^{-a(\eta_1^2 + \cdots + \eta_N^2) + b_1(r + r' + 2z)^2}$$

(30)

where $\zeta = r_1 + \cdots + r_N$ and $a = 2b_1N$. Then, the one-body density reads

$$\rho_1(r; r') = k_N e^{-(\alpha - \beta)(r^2 + r'^2)} \int d\zeta e^{-2b_1z^2 - 2\alpha z} \prod_{j=2}^{N} e^{-\zeta_j^2}$$

(32)

where $k_N$ denotes the normalization constant (to be calculated later), and $z_j := \sqrt{2a} \left[ r_j - \frac{b_1}{2a} (r + r' + 2z) \right]$ is a convenient change of coordinates. A key observation [26] is that the last expression on the right-hand side is the multiplication of two Slater determinants, and therefore the computation of the reduced density matrix can be completed using well-known methods in quantum chemistry. Indeed, with the notation

$$\beta_N := \sqrt{\frac{(\mu - \omega)(N - 1)\omega + \mu}{2N}}, \quad q(r; r') := \frac{1}{\sqrt{\beta} \left[ r-r' \right]}$$

(33)

one can express the one-body density as

$$\rho_1(r; r') = k_N e^{-\omega (r^2 + r'^2) + 2c_N r r'} \int du e^{-\omega (u^2)} \frac{1}{2^{j}} H_j$$

(34)

with $a_N := a - b_N - c_N$. This expression can be calculated analytically with the help of the following general formula,
derived in appendix A:
\[
\int_{-\infty}^{\infty} e^{-u^2} H_k(q_{(r,r')}) - \beta_N u] H_k(q_{(r,r')}) - \beta_N u\] du
= \sum_{n_{1,2}=0 \text{ even}}^{k} (2\beta_N)^{n_{1}+n_{2}} (k) \binom{k}{n_{1}} (k) \binom{k}{n_{2}} H_{k-n_{1}} \times (-q_{(r,r')}) H_{k-n_{2}} (-q_{(r,r')}) \Gamma \left( \frac{n_{1}+n_{2}+1}{2} \right).
\]
(35)

Then, the integral on the right-hand side of (34) can be expressed as the following power sum:
\[
\int du e^{-u^2} \sum_{j=0}^{N-1} \frac{1}{2^j j!} H_j[q_{(r,r')}] - \beta_N u \] \[H_j[q_{(r,r')}] - \beta_N u\]
= \sqrt{\pi} \sum_{j=0}^{N-1} \sum_{i=0}^{N-1} c_{i,j}^{(N)} a_{2i-2j-1},
\]
(36)

where the expansion coefficients, \(c_{i,j}^{(N)}\), depend on both the frequencies \(\omega, \mu\) and the number of particles. When \(r + s\) is an odd number or is larger than \(2(N - 1)\), \(c_{i,0}^{(N)} = 0\). By symmetry it is clear that \(c_{i,j}^{(N)} = c_{i,j}^{(N)}\). In the one-fermion case, there is only one coefficient \(c_{0,0}^{(N)} = 1\). For \(N\) fermions, the rank of the quadratic form of the \(c_{i,j}\) is \(2N - 1\). In particular, when \(N = 2\), we have the expansion coefficients:
\[
c_{0,0}^{2} = \frac{2\mu}{\omega + \mu }, \quad c_{1,0}^{2} = \frac{\mu(\omega^2 + 2\omega \mu + 5\mu^2)}{(\omega + \mu)^2} \quad \text{and}
\]
\[
c_{2,0}^{2} = \frac{\mu(\omega - \mu)(3\omega + \mu)}{2(\omega + \mu)^2}.
\]
(37)

For completeness, let us mention that the reader will have no difficulty in verifying that \(p_{\rho}(r, r')\) —the diagonal of (29)—coincides (except for the difference in the normalization conventions) with the one obtained in [25 Section V] by the Wigner function method. Moreover, for \(N = 3\) the non-vanishing expansion coefficients are
\[
c_{0,0}^{3} = \frac{3}{2} \left[ 1 + \frac{(\omega - \mu)^2}{(2\omega + \mu)^2} \right],
\]
\[
c_{1,1}^{3} = \frac{\mu(-15\omega^3 + 51\mu^2\omega + 15\mu^2\omega + 3\mu^3)}{(2\omega + \mu)^3},
\]
\[
c_{2,2}^{3} = \frac{\mu^2(363\omega^4 + 168\mu^2\omega + 90\mu^2\omega + 24\mu^3\omega + 3\mu^3)}{4(2\omega + \mu)^4},
\]
\[
c_{0,2}^{3} = -\frac{\mu(39\omega^3 - 3\mu^2\omega + 15\mu^2\omega + 3\mu^3)}{2(2\omega + \mu)^3},
\]
\[
c_{1,0}^{3} = c_{3,4} = \frac{\mu^2(5\omega + \mu)^2(\omega - \mu)^2}{8(2\omega + \mu)^3} \quad \text{and} \quad c_{3,1} = c_{1,3} = \frac{\mu^2(\omega - \mu)(65\omega^3 + 33\mu^2\omega + 9\mu^2\omega + 3\mu^3)}{2(2\omega + \mu)^3}.
\]
(38)

Except for the difference in the normalization and notation conventions, these coefficients coincide with the ones found in [26].

Keeping all this in mind and determining the normalization constant, \(k_N\), by imposing that \(\int \rho_1(r, r) \ dr = 1\), one finally has the expression
\[
\rho_1(r, r') = \frac{1}{\sqrt{\pi} \sqrt{N}} \frac{\mu}{\omega + \mu} e^{-\alpha(r^2 + r'^2)} \times \sum_{j=0}^{N-1} \sum_{i=0}^{N-1} c_{i,j}^{(N)} a_{2i-2j-1},
\]
(39)

for the one-body density of the one-dimensional spinless N-fermion harmonium.

Let us now quantify the entanglement of the system by means of the linear entropy associated with the one-body density [46]:
\[
S_L = 1 - N \text{Tr} \left[ \rho_1^2 \right],
\]
(40)

where \(\Pi_N = N \text{Tr} \left[ \rho_1^2 \right]\) is the purity of the system. This entanglement measure, which is a non-negative quantity that vanishes if and only if the state has Slater rank 1 and is therefore separable, has been recently used in various two-fermion systems [13, 24] as well as for various helium-like systems [14, 16, 17] in both ground and excited states. Moreover, in our systems it turns out that
\[
\text{Tr} \left[ \rho_1^2 \right] = \int \rho_1(r, r') \rho_1(r', r) \ dr' dr
\]
\[
= k_N^2 \sum_{i,m=0}^{N-1} \sum_{j=0}^{N-1} c_{i,n}^{(N)} c_{j,m}^{(N)} I_{(2i+m,2j+m)}(2r+|y),
\]
(41)

where, as shown in appendix B,
\[
I_{(n,m)} = I_{(m,n)} \int_{-\infty}^{\infty} r^n e^{-\alpha(r^2 + r'^2)} c_s e^{r'r'} \ dx \ dy
\]
\[
= 2 \sum_{i,j=0}^{n} \binom{n}{i} \binom{m}{j} (-1)^j \frac{1}{2} \left[ 1 + (-1)^{i+j} \right] \left[ 1 + (-1)^{i+j} \right].
\]
(42)

with \(\lambda_1 = 4(a_N - c_N)\) and \(\lambda_2 = 4(a_N + c_N)\).

Using expressions (40), (41), and (42), we have investigated the dependence of the linear entropy of the system on the relative interaction strength \(\delta/k\), as well as on the energy. The results are given in figure 5. A first basic observation is that for fixed N, the entanglement decreases (increases) when the relative interaction strength increases in the negative (positive) region. Moreover, for negative values of the coupling constant, the spatial entanglement of the N-fermion harmonium grows when \(N\) increases. For small positive values of the coupling constant (i.e., when the fermions attract each other), we find that for very small values of \(\delta/k\), the entanglement grows again with increases \(N\). In general, we observe that for positive values of the strength, we have various regimes of dependence on \(N\). In the strong-coupling regime, the linear entropy grows as the number of particles
increases since the purity decreases with an increase number of particles. For instance, for $\delta/k = 10$, the purity is 0.92 for $N = 2$ and 0.94 for $N = 10$, whereas for $\delta/k = 1$, the purity is 0.998 and 0.992, respectively.

Figure 6 displays the dependence of the linear entropy of the system on the ground-state energy, $E_{gs}/\omega$, for various values of the number of fermions, $N$. We should keep in mind that the relation between the relative interaction strength and the energy is given by

$$\delta/k = \left[ \frac{2E_{gs}/\omega - 1}{N^2 - 1} \right]^2 - 1. \quad (43)$$

We find that the entanglement grows when the energy increases. For $N = 2$, this behavior has been recently observed not only in the Moshinsky or two-fermion harmonium atom, but also in other two-fermion systems [13–17]. The novelty is that this behavior appears to also be true for heavier N-fermion harmonium atoms.

It is worth noting that our results can be considered as a generalization of previous results for the entanglement entropy of the fractional quantum Hall effect, based on an exact matrix-product representation of the Laughlin wave function [47–49]. This well-known wave function, formulated by R Laughlin to explain the fractional quantum Hall effect, consists of a lone Slater determinant and reads as in (27), except that there is no coupling between the electrons; that is, $\omega = \mu$ or $\delta = 0$, and the domain is the complex space.

5. Total entanglement of the spinned N-fermion harmonium

So far, we have considered only spinless particles. This means that in the two previous sections, we have determined the spatial entanglement of the N-boson and N-fermion harmonia. Nevertheless, our conclusions for the bosonic system also apply to the total entanglement from a qualitative point of view, because the spin part of the ground-state eigenfunction fully factorizes. For fermionic systems this is no longer true, at least when they are isolated. In fact, the ground state of two fermions is the product of a two-boson state and an antisymmetric spin state. For a system of fermions with spin in the presence of a strong magnetic field, the spin part of the eigenfunction factorizes, so the spatial part must be antisymmetric [26]. In general, however, for the isolated fermionic system, the spatial and spin parts of the ground-state wave function are not separable, and antisymmetry must take into consideration both spin and position coordinates.

Let us now calculate the total entanglement of the N-fermion harmonium (i.e., the entanglement of both spatial and spin degrees of freedom) using the linear entropy as a measure of entanglement. For simplicity, we consider one-dimensional models with an even number (say, $N$) of spinned electrons from now on. The total spin of the system is zero, and all the spatial orbitals are doubly occupied (restricted configuration). This will eventually allow for an easy generalization to closed-shell three-dimensional systems. We define the set of spin natural orbitals in the following way:

$$\varphi_j(x) = \begin{cases} \phi_\uparrow(r) \uparrow, & \text{if } j \text{ is odd}, \\ \phi_\downarrow(r) \downarrow, & \text{if } j \text{ is even}. \end{cases}$$

The symbols $\uparrow$ and $\downarrow$ mean spin up and spin down, respectively, and we denote $x := (r, \varsigma)$, $\varsigma$ as the spin coordinate.
Let us begin with the consideration of the simpler, non-interacting case; that is, when \( \delta = 0 \), and hence \( \mu = \omega \). The corresponding ground-state eigenfunction is then given by the expression

\[
\Psi^J(x_1, \ldots, x_N) = \frac{1}{\sqrt{2N!}} \sum_{J \in S_N} (-)^J \prod_{i=1}^{2N} \phi_{\mu-1}(x_{J(i)}) \times \prod_{i=1}^{N} \prod_{j=1}^{2} \phi_{\omega-1}^{-1}(p_{2i-1}) \phi_{\omega-1}^i(p_{2i}) \]  

(44)

In the noninteracting case, the basis of the one-particle Hilbert space is the set of Hermite functions whose degree is less than \( N \). Moreover, let us define

\[
H = \{ j \in S_{2N} : j \text{ fixes } 1, \ldots, N \} \approx S_N
\]

\[
K = \{ j \in S_{2N} : j \text{ fixes } N+1, \ldots, 2N \} \approx S_N,
\]

where \( S_N = H \times K \) is the direct product of these two subgroups. The set \( S_{2N} = S_{2N} / S_N \) is the set of right cosets in \( S_{2N} \), giving the following equivalence relation:

\[
J \sim J' \text{ if and only if } \exists (j, j') \in S_N \text{ such that } J' = (j, j')J.
\]

Therefore, we can reorganize the expression (44) in the following form:

\[
\Psi^J(x_1, \ldots, x_N) = \frac{1}{\sqrt{2N!}} \sum_{J \in S_N} (-)^J \prod_{i=1}^{N} \prod_{j=1}^{2} \phi_{\omega-1}^{-1}(p_{2i-1}) \phi_{\omega-1}^i(p_{2i}) \]

where the sum runs over a representative of each coset. The choice of the representative \( J \in \{ J \} \in S_{2N} / S_N \) is immaterial. The number of summands is

\[
|S_{2N} / S_N| = \frac{|S_{2N}|}{|S_N|} = \frac{(2N)!}{(N!)^2} = \binom{2N}{N}. \]

Moreover, it is clear that

\[
\rho^J_1(x', r') = \rho^J_1(x, r) = \int \sum_{J \in S_N} (-)^J \prod_{i=1}^{N} \prod_{j=1}^{2} \phi_{\omega-1}^{-1}(p_{2i-1}) \phi_{\omega-1}^i(p_{2i}) \]

(46)

The occupation numbers appear twice, which is a well-known result for atomic and molecular scientists.

Let us now consider the general interacting case, for which \( \delta \neq 0 \), and hence \( \mu \neq \omega \). The ground-state eigenfunction for the Hamiltonian (1) is similar to (22), except that each spatial orbital is doubly occupied. For the same reasons as in the spinless case, the collective mode, \( \xi_{2N} \), occupies the Hermite function of degree zero. The other coordinates, \( \{ \xi_m \}_{m=1}^{2N-1} \), occupy the other spatial orbitals in such a way that the total wave function is totally antisymmetric under interchange with coordinates \( \{ \xi_m \}_{m=1}^{2N-1} \).

The one-body reduced density matrix corresponding to the wave function (45) is diagonal in spin space and is given by the expression

\[
\rho_1(x, x') = \begin{pmatrix}
\rho^{11}_1(x, r) & 0 \\
0 & \rho^{11}_1(x, r)
\end{pmatrix}.
\]

(47)

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\[
\Psi^J(x_1, \ldots, x_{2N}) = \frac{1}{\sqrt{2N!}} \sum_{J \in S_{2N}} (-)^J \prod_{i=1}^{N} \prod_{j=1}^{2} \phi_{\omega-1}^{-1}(p_{2i-1}) \phi_{\omega-1}^i(p_{2i}) \]

(48)

For instance, in the particular case, \( N = 4 \), the eigenfunction has the form

\[
\Psi^J(x_1, x_2, x_3, x_4) = \frac{1}{\sqrt{4!}} \sum_{J \in S_4} (-)^J \prod_{i=1}^{4} \prod_{j=1}^{2} \phi_{\omega-1}^{-1}(p_{2i-1}) \phi_{\omega-1}^i(p_{2i}) \]

(49)

The expression

\[
\rho^J_1(x', r') = \rho^J_1(x, r) = \int \sum_{J \in S_N} (-)^J \prod_{i=1}^{N} \prod_{j=1}^{2} \phi_{\omega-1}^{-1}(p_{2i-1}) \phi_{\omega-1}^i(p_{2i}) \]

(46)

Moreover, it is clear that

\[
\rho^J_1(x', r') = \rho^J_1(x, r) = \int \sum_{J \in S_N} (-)^J \prod_{i=1}^{N} \prod_{j=1}^{2} \phi_{\omega-1}^{-1}(p_{2i-1}) \phi_{\omega-1}^i(p_{2i}) \]

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\[
\Psi^J(x_1, \ldots, x_{2N}) = \frac{1}{\sqrt{2N!}} \sum_{J \in S_{2N}} (-)^J \prod_{i=1}^{N} \prod_{j=1}^{2} \phi_{\omega-1}^{-1}(p_{2i-1}) \phi_{\omega-1}^i(p_{2i}) \]

(48)

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\[
\Psi^J(x_1, x_2, x_3, x_4) = \frac{1}{\sqrt{4!}} \sum_{J \in S_4} (-)^J \prod_{i=1}^{4} \prod_{j=1}^{2} \phi_{\omega-1}^{-1}(p_{2i-1}) \phi_{\omega-1}^i(p_{2i}) \]
\[ \Psi^f(x_1, \ldots, x_{2N}) = (\text{const.}) e^{-\frac{1}{2} \sum_{i=1}^{2N} r_i^2} \times \prod_{i=1}^{2N} \int \prod_{j \neq i} \left[ \prod_{J \in S_N} (-1)^J \sum_{i=1}^{2N} i \right] \times \int_{\mathbb{R}^N} \prod_{j=1}^{2N} e^{-\frac{1}{2} \sum_{i=1}^{2N} (r_i^2 \pm r_j^2) + b_{2N}(\eta \pm \eta')^2} \times V_{r_1, \ldots, r_N} \left( \prod_{j=2}^{2N} z_j \right) \]

The corresponding energy is \( E_{gs} = \frac{1}{2} (\omega + \mu) + \mu (N^2 - 1) \).

Let us define \( \eta = r + r_2 + \cdots + r_N \) and \( \eta' = r' + r_2 + \cdots + r_N \). To compute the one-density, we use twice the Hubbard-Stratonovich identity, both to compute \( N \) integrals with \( \zeta = N_N + \cdots + r_N \), and also to compute \( N - 1 \) integrals with \( \zeta = r_2 + \cdots + r_N \). Each diagonal element of the one-body density matrix reads

\[ \rho^{11}(r, r') = \rho_1^{11}(r, r') = (\text{const.}) e^{-\frac{1}{2} (r^2 + r'^2)} \times \int_{\mathbb{R}^N} \prod_{j=1}^{2N} e^{-\frac{1}{2} \sum_{i=1}^{2N} (r_i^2 \pm r_j^2) + b_{2N}(\eta \pm \eta')^2} \times V_{r_1, \ldots, r_N} \left( \prod_{j=2}^{2N} z_j \right) \times \prod_{j=N+1}^{2N} e^{-z_j^2}, \]

where \( z_j = \sqrt{2a} \left[ r_j - \frac{\eta}{2a} (\eta + \eta') + 2z \right] \). Once again, the expression on the right is the total integral of the product of two Slater determinants; that is,

\[ \int_{\mathbb{R}^N} \prod_{j=1}^{2N} e^{-z_j^2} \times \prod_{j=N+1}^{2N} e^{-z_j^2} \]

is a real constant. Therefore,

\[ \rho^{11}(r, r') = \rho_1^{11}(r, r') = (\text{const.}) e^{-\frac{1}{2} (r^2 + r'^2)} \]

Assuming again that an antisymmetric polynomial is equal to a symmetric polynomial multiplied by a Vandermonde determinant [44], we can write the ground-state eigenfunction of the general interacting spinless N-fermion system as

\[ \times J \left[ \phi^a_0(\xi_1) \phi^b_0(\xi_2) \phi^c_0(\xi_3) \phi^d_0(\xi_4) \right] = (\text{const.}) \sum_{J \in S_N} (-1)^J \sum_{i=1}^{2N} i = + \cdots + \sum_{i=1}^{2N} i \]

\[ \times J \left[ \sum_{\xi} e^{\frac{i}{\xi} + \xi - (\xi + \xi')^2} \right] = (\text{const.}) \sum_{S_N} (-1)^J \sum_{i=1}^{2N} i \]

\[ \times \nu_{J(1), J(2)} \nu_{J(3), J(4)} e^{-\frac{1}{2} \sum_{\xi} (\xi + \xi')^2 - (\xi + \xi')^2}. \]

Figure 7. Linear entropy of the spinless N-fermion harmonium as a function of the relative coupling constant for various values of \( N \). Qualitatively, it is similar to the spinless case in figure 5.

\[ \times J \left[ \phi^a_0(\xi_1) \phi^b_0(\xi_2) \phi^c_0(\xi_3) \phi^d_0(\xi_4) \right] = (\text{const.}) \sum_{J \in S_N} (-1)^J \sum_{i=1}^{2N} i = + \cdots + \sum_{i=1}^{2N} i \]

\[ \times J \left[ \sum_{\xi} e^{\frac{i}{\xi} + \xi - (\xi + \xi')^2} \right] = (\text{const.}) \sum_{S_N} (-1)^J \sum_{i=1}^{2N} i \]

\[ \times \nu_{J(1), J(2)} \nu_{J(3), J(4)} e^{-\frac{1}{2} \sum_{\xi} (\xi + \xi')^2 - (\xi + \xi')^2}. \]
entanglements. Figure 8 exhibits the results for $\delta/k \in \{-1/15, 2, 4, 22\}$. In the spinned case, the behavior is similar to the spinless system, so that the total entanglement behaves similar to the spatial entanglement. In fact, for small values of the coupling, the entropy grows when the number of particles increases, while in the strong-coupling regime the opposite is true. The inclusion of the spin tends to enhance the entropy of the system; this phenomenon is most important for small values of the coupling constant. Note that in turn, the contributions of the spin and the spatial entropy are of comparable size.

Finally, let us investigate the relative behavior of entanglement and energy. This is done in figure 9, where the linear entropy as a function of the ground-state energy is shown for some values of the number of particles. Let us recall here that the relation between the relative coupling and the energy is given by

$$\delta/k = \left[ \frac{2E_{gs}/\omega - 1}{2N^2 - 1} \right]^2 - 1. \quad (54)$$

As in the spinless case, the entropy grows when the ground-state energy increases. For very large values of the dimensionless energy, $E_{gs}/\omega$ (i.e., very large values of the relative strength $\delta/k$), the gap between the spinless and spinned cases decreases.

Figure 8. Linear entropy of the one-body reduced density matrix for the spinless and spinned N-fermion harmonium as a function of the number of particles for different values of $\delta/k$.

Figure 9. Linear entropy, $S_L$, of the N-fermion spinned harmonium versus the ground-state energy, $E_{gs}/\omega$, for different values of $N$. The relation between the relative strength, $\delta/k$, and the energy is stated in (54).

6. Concluding remarks

In this work, we have shown that some entanglement features of finite many-particle systems can be understood, to a certain extent, by purely kinematical considerations. This is done by explicitly analyzing the entanglement of the N-boson and N-fermion harmonium systems. This has been possible because
for these harmonic systems, we have been able to analytically calculate not only the one-body reduced matrix for bosons and fermions, but also the von Neumann entropy in the bosonic case and the linear entropy in the fermionic case. In doing so, we complement and extend to harmonic systems with an arbitrary number of particles the study of entanglement recently done for various two-electron models [13, 21–25], as well as some helium-like systems [6, 14, 15, 17] and certain quantum complex networks [50].

We have analytically determined the entanglement of these harmonic systems for both spatial and spin degrees of freedom in terms of the number of particles and the relative interaction strength (or coupling constant). We have used the von Neumann entropy and the linear entropy as entanglement quantifiers in the bosonic and fermionic systems, respectively. We have found that for positive couplings, the entanglement of the three-boson harmonium atom is bigger than the one in the two-boson system, but in general the entanglement of the N-boson harmonium decreases when \( N \) increases. Moreover, the entanglement of a given N-boson system grows when the positive coupling constant increases that is, when the positive value of the strength of the interparticle interaction relative to the confinement well increases. On the other hand, globally speaking, the spatial entanglement of the N-fermion harmonium grows when \( N \) increases for both negative and sufficiently small positive values of the coupling constant. Moreover, the entanglement behavior is opposite in the positive strong-coupling regime. On the other hand, entanglement of a given N-fermion system grows when the coupling constant increases. The contribution of the spin degree of freedom to the entanglement of the N-fermion system is shown to be of positive comparable size to the contribution of the spatial degrees of freedom.

In summary, we have shown that in the repulsive and attractive cases for relatively small values of the coupling constant, the entanglement of both bosonic and fermionic N-harmonium atoms grows when the number of particles increases, basically because purity decreases. However, in the regime of strong coupling, the situation is exactly the opposite: purity increases (and hence entanglement decreases) by adding particles to the system.

### Acknowledgments

CLBR was supported by a Francisco José de Caldas scholarship, funded by Colciencias. He very much appreciates the warm atmosphere of the Departamento de Física Atómica Molecular y Nuclear at the Universidad de Granada. IVT and JSB gratefully acknowledge the MINECO grant FIS2011–24540 and the excellence grant FQM-7276 of the Junta de Andalucía. In addition, the authors are most grateful to A R Plastino, J L Alonso, A Botero, J M Gracia-Bondía, and J C Várilly for helpful and illuminating discussions.

### Appendix A. Calculation of the integral \( \int_{-\infty}^{\infty} e^{-u^2} H_k(a - cu) H_k(b - cu) du \)

In this section, we calculate the integral

\[
\int_{-\infty}^{\infty} e^{-u^2} H_k(a - cu) H_k(b - cu) du, \tag{A.1}
\]

where \( a, b, \) and \( c \) are real numbers and \( H_k(x) \) is the Hermite polynomial of degree \( k \). We use the following property of the Hermite polynomials:

\[
H_n(-z) = (-1)^n H_n(z),
\]

as well as the power series of these polynomials around \( z = z_0 \),

\[
H_n(z) = \sum_{k=0}^{n} \binom{n}{k} H_{n-k}(z_0)(z - z_0)^k.
\]

This expression allows us to rewrite each Hermite polynomial in the following form:

\[
H_k(a - cu) = (-1)^k \times \sum_{n_k=0}^{k} (2c)^{n_k} \left( \binom{k}{n_k} \right) H_{k-n_k}(-a) u^{n_k}. \tag{A.2}
\]

Inserting (A.2) into (A.1) we obtain

\[
\int_{-\infty}^{\infty} e^{-u^2} H_k(a - cu) H_k(b - cu) du = \int_{-\infty}^{\infty} e^{-u^2} (-1)^k \sum_{n_k=0}^{k} (2c)^{n_k} \left( \binom{k}{n_k} \right) H_{k-n_k}(-a) u^{n_k}(-1)^k \\
\times \sum_{n_2=0}^{k} (2c)^{n_2} \binom{k}{n_2} H_{k-n_2}(-b) u^{n_2} \\
= \sum_{n_1+n_2 \text{ even}} (2c)^{n_1+n_2} \binom{k}{n_1} \binom{k}{n_2} H_{k-n_1}(-a) H_{k-n_2}(-b) \Gamma \left( \frac{n_1 + n_2 + 1}{2} \right). \tag{A.3}
\]

### Appendix B. The Gaussian integral, \( I_{(n,m)} \)

In the following, we calculate the integral

\[
I_{(n,m)} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} x^n y^m e^{-(x^2+y^2)/2} dx dy. \tag{B.1}
\]

Here, we perform the change of coordinates

\[
x = u + v \quad \text{and} \quad y = u - v, \tag{B.2}
\]
and the integral now reads
\[
I_{(n,m)} = 2 \sum_{i=0}^{n} \sum_{j=0}^{m} \binom{n}{i} \binom{m}{j} (-1)^{i+j} 
\times \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} u^{n+m-i-j} \rho_{\lambda_1}^{-i} \rho_{\lambda_2}^{j} du dv, \quad (B.3)
\]
with \( \lambda_1 = 2(a - c) \) and \( \lambda_2 = 2(a + c) \). From the form of the (double) integral, on using polar coordinates in the \((u,v)\)-plane, \( u = R \cos \phi \) and \( v = R \sin \phi \), the double integral vanishes if \( i + j \) is odd, since the exponential is an even function of \( \phi \). Switching \( u \) and \( v \) in the polar coordinates, we likewise see that it vanishes if \( (m + n) - (i + j) \) is odd.

The integral thus becomes
\[
I_{(n,m)} = \sum_{i=0}^{n} \sum_{j=0}^{m} \binom{n}{i} \binom{m}{j} (-1)^{i+j} \rho_{\lambda_1}^{-i} \rho_{\lambda_2}^{j} \times 
\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} u^{n+m-i-j} v^{i+j} du dv
\]
\[
= 2 \sum_{i=0}^{n} \sum_{j=0}^{m} \binom{n}{i} \binom{m}{j} (-1)^{i+j} \rho_{\lambda_1}^{-i} \rho_{\lambda_2}^{j} \times 
\int \frac{n + m - i - j + 1}{2} f \left( \frac{n + m + 1}{2} \right)
\times \frac{1}{4} \left[ 1 + (-1)^{n+m-i-j} \right] \left[ 1 + (-1)^{i+j} \right]. \quad (B.4)
\]

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