The von Neumann entanglement entropy for Wigner-crystal states in one dimensional $N$-particle systems

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We study one-dimensional systems of $N$ particles in a one-dimensional harmonic trap with an inverse power law interaction $\sim |x|^{-d}$. Within the framework of the harmonic approximation we derive, in the strong interaction limit, the Schmidt decomposition of the one-particle reduced density matrix and investigate the nature of the degeneracy appearing in its spectrum. Furthermore, the ground-state asymptotic occupancies and their natural orbitals are derived in closed analytic form, which enables their easy determination for a wide range of values of $N$. A closed form asymptotic expression for the von Neumann entanglement entropy is also provided and its dependence on $N$ is discussed for the systems with $d = 1$ (charged particles) and with $d = 3$ (dipolar particles).
I. INTRODUCTION

Within the last few years, systems of confined particles have attracted considerable research attention because of the development of new technologies and experimental techniques that have opened up perspectives for their experimental fabrication. Besides the systems with short-range interactions, such as the Tonks–Girardeau (TG) gases [1], systems with particles exhibiting long-range interactions have also received a lot of attention in recent years. Among them, the best known are the systems of spatially confined particles with a Coulomb [2, 3] interaction or a dipole–dipole [4] interparticle interaction. Most recently, there has been a remarkable increase of interest in the study of quantum entanglement, as entangled systems play an essential role in quantum information technology [5]. In particular, a few attempts have been made recently towards understanding the entanglement in systems of interacting particles. For example, some light has been shed on entanglement both in quantum dot systems [6–15] and in systems of harmonically interacting particles in a harmonic trap (the so-called Moshinsky atom) [16–23]. Special attention has also been paid to the study of entanglement in the helium atoms and helium ions [24–32]. The effect of the confinement on the entanglement in the ground state of the helium atom has also been discussed in the literature [33]. For details on recent developments in entanglement studies of quantum composite systems, see [34] for an overview. However, there has been relatively little research so far on entanglement in systems with more than two particles. The reason for this lies in the fact that in most cases the determination of the wavefunction of a few-body state requires performing numerical calculations, which is a major problem in general. According to our best knowledge, the only N particle system of which the entanglement properties have been fully explored so far is the Moshinsky model system [17, 18].

The model on which we focus here is a system composed of N particles interacting via a long-range inverse power-law potential, which are confined by an external one-dimensional (1D) harmonic potential

\[
H = \frac{1}{2} \sum_{i=1}^{N} \partial_{x_i}^2 + V^g(x_1, x_2, \ldots, x_N), \tag{1}
\]

\[
V^g(x_1, x_2, \ldots, x_N) = \frac{1}{2} \sum_{i=1}^{N} x_i^2 + \sum_{i>j=1}^{N} \frac{g}{|x_i - x_j|^d}, \quad d > 0.
\tag{2}
\]

Due to the singular behaviour of the interaction potential \(|x_i - x_j|^{-d}\) at \(x_i = x_j\), the wavefunction of bosons (B) satisfies \(\psi_B(x_1, \ldots, x_N) = 0\) if \(x_i = x_j\), for any \(g \neq 0\) [1]. For example, when \(d = 1\) the system serves as a prototype for ions in electromagnetic traps and when \(d = 3\), as a model of confined dipolar particles. Here we address mainly the limit as \(g \rightarrow \infty\) in which the perfect linear Wigner molecule is formed [35–37], and the harmonic approximation (HA) is valid [11, 14, 38, 39]. Recently, within the framework of this approximation, we have derived when \(N = 3\) and \(d = 1\) an explicit integral representation for the asymptotic occupancies and their natural orbitals [11]. In the present paper, we extend the results of [11] and provide the Schmidt expansions of the asymptotic one-particle reduced density matrix (RDM) in the general case of \(N\) particles, investigating thereby the nature of the degeneracy appearing in its spectrum. Here we go even further and derive for the ground state of (1) closed form expressions for the asymptotic occupancies and their natural orbitals, which enables their easy determination for a wide range of values of \(N\) without the solution of the eigenvalue problem with the RDM. Moreover, we derive an asymptotic closed form expression for the von Neumann (vN) entropy and analyze its dependence on \(N\) for the systems with \(d = 1\) (charged particles) and with \(d = 3\) (dipolar particles). Additionally, in the first case, we address the question of how the changes in the parameter \(g\) affect the entanglement.

The structure of this letter is as follows. In Section II we derive, within the framework of the harmonic approximation, an asymptotic Schmidt decomposition of the RDM and provide closed-form asymptotic expressions for the ground state occupancies and the vN entropy. Section III focuses on these results and some concluding remarks are made in Section IV.

II. THE STRONG INTERACTION LIMIT

A. Harmonic approximation

The potential \(V^g\) given by Eq. (2) attains its minimum at points \(\vec{r}_{min} = (x_1^c, x_2^c, \ldots, x_N^c)\) which are determined by a set of equations \(\partial_{x_k} V^g(x_1, \ldots, x_N) = 0, \quad k = 1, \ldots, N\). As is easy to see, the potential (3) scales as

\[
V^g(\beta_1 g^{\frac{1}{2+d}}, \ldots, \beta_N g^{\frac{1}{2+d}}) = g^{\frac{d}{2+d}} V^{g=1}(\beta_1, \ldots, \beta_N), \tag{3}
\]
which means that the equilibrium positions of the particles \( x_i^c \) have the form \( x_i^c = \beta_i g^{\frac{1}{2(\beta_i - 1)}} \), where \( \beta_i \) are the solutions of \( \partial_{\beta_i} V^{g=1}(\beta_1, ..., \beta_N) = 0 \), \( k = 1, ..., N \). The values of \( \beta_i \) have simple analytic forms only in the cases \( N = 2, 3 \). For larger \( N \), we find them numerically.

If \( g \) is large enough, the particles crystallize around their classical equilibrium positions and the HA can be applied \([38, 39]\). From here on we refer to the point \( \vec{r}_{\text{min}} \) with \( x_1^c < x_2^c < ... < x_N^c \) without loss of generality. We denote it by \( \vec{r}_{\text{min}}^{(0)} \). In this case \( x_i^c = -x_{N-i+1}^c \) (\( x_{N+1}^c = 0 \) if \( N \) is odd), \( i = 1, 2, 3, ..., \frac{N}{2} \), where \( P = N \) if \( N \) is even but \( N - 1 \) for odd values of \( N \) \([38]\). As is well known, within the HA, the problem is equivalent to a set of \( N \) uncoupled oscillators \([38, 39]\).

\[
H_{\text{HA}} = \sum_{i=1}^{N} \left( -\frac{1}{2} d_{\beta_i}^2 + \frac{\omega_i^2 x_i^2}{2} \right),
\]

where the values of \( \omega_i^2 \) are the eigenvalues of the Hessian matrix \( H = \left( \frac{\partial^2 V^{g=1}}{\partial x_i \partial x_k} \right)_{i,N} \times_{N} \), and \( \vec{\zeta} = (\zeta_1, \zeta_2, ..., \zeta_N) \) are the so-called normal modes given by \( \vec{\zeta} = \mathbf{U} \vec{\zeta} \), where \( \mathbf{Z} = (z_1, z_2, ..., z_N) \), \( z_i = x_i - x_i^c \), and \( \mathbf{U} \) is the matrix of the corresponding eigenvectors of \( H \).

The transformation \( x_i = \beta_i g^{\frac{1}{2(\beta_i - 1)}} \) yields

\[
\frac{\partial^2 V^{g}(x_1, ..., x_N)}{\partial x_i \partial x_k} = g^{-\frac{1}{2(\beta_i - 1)}} \frac{\partial^2 V^{g}(\beta_1 g^{\frac{1}{2(\beta_1 - 1)}}, ..., \beta_N g^{\frac{1}{2(\beta_N - 1)}})}{\partial \beta_i \partial \beta_k},
\]

so that, due to \([39]\), we can readily conclude that the Hessian matrix does not depend on \( g \) but only on \( \{\beta_i\} \).

For transparency of presentation we concentrate on analyzing the spatially symmetric (+) and antisymmetric (−) ground states. The normalized eigenfunction of \( H \) with lowest energy is given by

\[
\psi(z_1, z_2, ..., z_N) = \prod_{i=1}^{N} \left( \frac{\omega_i}{\pi} \right)^{\frac{1}{2}} e^{-\frac{\omega_i^2 z_i^2}{2}},
\]

and provides an approximation to wavefunctions of \( H \) only around \( \vec{r}_{\text{min}} \). In terms of \( \vec{\zeta} \), approximations to the spatially symmetric (+) and antisymmetric (−) ground-state wavefunctions of \( H \) can be written in forms convenient for further analysis as \([11, 13]\).

\[
\Psi^{(\pm)}(x_1, x_2, ..., x_N) = \mathcal{N}^{(\pm)}(x_1, x_2, ..., x_N) \sum_p \{\text{sgn}(p)\} \psi(x(p_1) - x_1^c, x(p_2) - x_2^c, ..., x(p_N) - x_N^c),
\]

and the sum goes over all permutations, and \( \text{sgn}(p) \) is 1 for bosons while for fermions \( \text{sgn}(p) \) is 1 for even permutations and −1 for odd ones. The normalization factor \( \mathcal{N}^{(\pm)} \) tends to \( N!^{-1/2} \) as \( g \to \infty \) both in the bosonic and fermionic case, which is a fact that the classical distance between the classical equilibrium positions of any pair of particles tends to infinity as \( g \to \infty \), that is, \( \Delta_{ij} = |x_i^c - x_j^c| \to \infty \) for any \( i \neq j \) (note that the integral overlap between any pair of functions \( \psi(x(p_1) - x_1^c, x(p_2) - x_2^c, ..., x(p_N) - x_N^c) \) with different permutations of the coordinates vanishes). For the same reasons, the RDM of \( \Psi^{(\pm)} \),

\[
\rho^{(\pm)}(x, y) = \int_{\mathbb{R}^{N-1}} d\vec{x}_k \Psi^{(\pm)}(x, x_2, ..., x_N) \Psi^{(\pm)}(y, x_2, ..., x_N),
\]

reduces in the \( g \to \infty \) limit to

\[
\rho^{\to \infty}(x, y) = \sum_{i=1}^{N} \rho_i(x, y),
\]

with

\[
\rho_i(x, y) = \frac{1}{N} \int_{\mathbb{R}^{N-1}} \left( \prod_{k \neq i} d\mu_k \right) \psi(\mu_1, ..., \mu_{i-1}, x - x_i^c, \mu_{i+1}, ..., \mu_N) \times \psi(\mu_1, ..., \mu_{i-1}, y - x_i^c, \mu_{i+1}, ..., \mu_N).
\]
Note that $\mathcal{S}$ is properly normalized, namely $\text{Tr} \rho^{g \to \infty} = \int_\mathcal{R} \rho^{g \to \infty}(x, x) dx = 1$. The asymptotic behaviour for the RDM is thus the same for the case of bosons and fermions. It should be stressed that Eqs. (8)–(10) have already appeared before in [12]. Moreover, in [12], an asymptotic linear entropy $L$ of the ground state of the system (11) with $d = 1$ was computed directly from the integral representation $L = 1 - \int_{\mathbb{R}^2} [\rho^{g \to \infty}(x, y)]^2 dx dy$ (for $N$ up to $N = 10$).

The present paper goes substantially further as it discusses the Schmidt decomposition of $\mathcal{S}$ and provides closed form expressions for the occupancies, natural orbitals, and the vN entropy as well. Moreover, it provides the results for the entanglement both in the $d = 1$ and $d = 3$ case.

### B. Schmidt decomposition of the RDM

To start with, let us note that the equilibrium positions in Eq. (9) can be eliminated by translating the coordinates by $x \rightarrow \hat{x} + x^c_i$, $y \rightarrow \hat{y} + y^c_i$, $\rho_i(x, y) \rightarrow \tilde{\rho}_i(\hat{x}, \hat{y})$. Being normalizable, real, and symmetric under permutations of coordinates, the function $\tilde{\rho}_i$ has a Schmidt decomposition in the form

$$
\tilde{\rho}_i(\hat{x}, \hat{y}) = \sum_{l=0}^{\infty} \lambda^{(i)}_l v^{(i)}_l (\hat{x}) v^{(i)}_l (\hat{y}),
$$

(10)

$$
\langle v^{(i)}_l | v^{(i)}_k \rangle = \delta_{lk}, \text{ where } v^{(i)}_l \text{ and } \lambda^{(i)}_l \text{ satisfy the integral eigensystem}
$$

$$
\int_{-\infty}^{\infty} \tilde{\rho}_i(\hat{x}, \hat{y}) v^{(i)}_l (\hat{y}) d\hat{y} = \lambda^{(i)}_l v^{(i)}_l (\hat{x}).
$$

(11)

By changing the variables back in (10), namely by $\hat{x} \rightarrow x - x^c_i$, $\hat{y} \rightarrow y - y^c_i$, one gets

$$
\rho_i(x, y) = \sum_{l=0}^{\infty} \lambda^{(i)}_l v^{(i)}_l (x - x^c_i) v^{(i)}_l (y - y^c_i),
$$

(12)

and substituting the above into $\mathcal{S}$, we arrive at

$$
\rho^{g \to \infty}(x, y) = \sum_{i=1}^{N} \sum_{l=0}^{\infty} \lambda^{(i)}_l v^{(i)}_l (x - x^c_i) v^{(i)}_l (y - x^c_i).
$$

(13)

One can easily infer that in the limit as $g \to \infty$, where $\Delta_{ij} \to \infty$ ($i \neq j$), the integral overlap $\langle v^{(i)}_k (x - x^c_i) v^{(j)}_l(x - x^c_j) \rangle$ vanishes for any $k, l$ as long as $i \neq j$. Hence, bearing in mind that $\langle v^{(i)}_l (x - x^c_i) v^{(j)}_k(x - x^c_j) \rangle = \delta_{lk}$, we can conclude that the family $\{v^{(i)}_l (x - x^c_i)\}_{i=1,l=0}^{N,\infty}$ forms an orthonormal set as $g \to \infty$. In this limit the expansion (13) is therefore nothing else but the Schmidt decomposition of the asymptotic RDM $\mathcal{S}$, which means $v^{(i)}_l (x - x^c_i)$ are its eigenvectors (natural orbitals) and $\lambda^{(i)}_l$ are its eigenvalues (occupancies).

The normal-mode coordinates have the form $\tilde{\zeta}_i = U_{i,1} \tilde{z}_1 + U_{i,2} \tilde{z}_2 + \ldots + U_{i,N} \tilde{z}_N$, where the $U_{i,j}$, being the elements of the matrix $U$, satisfy $U_{i,j} = -U_{i,N-j+1}$ (here $U_{i,(N+1)/2} = 0$ if $N$ is odd) or $U_{i,j} = U_{i,N-j+1}$, for all indices $j$ at fixed $i$. One can readily infer from the above that $\tilde{\rho}_i = \tilde{\rho}_{N-i+1}$ and, as a result, we have $v^{(i)}_l (\hat{x}) = v^{(N-i+1)}_l (\hat{x})$ and $\lambda^{(i)}_l = \lambda^{(N-i+1)}_l$. Thus, conservation of probability gives ($M_i = \sum_{l=0}^{\infty} \lambda^{(i)}_l$): $2 \sum_{i=1}^{N/2} M_i = 1$ and $2 \sum_{i=1}^{(N-1)/2} M_i + M_{(N+1)/2} = 1$, for even and odd values of $N$, respectively. All the asymptotic occupancies except those corresponding to $\rho_{(N+1)/2}$ ($N$ odd) are thus two-fold degenerate.

Since the asymptotic RDM possesses a degenerate spectrum, its Schmidt decomposition fails to be unique. For the sake of completeness, we derive below another form of the Schmidt decomposition of the asymptotic RDM. Accordingly, for each double-point of degeneracy, $\lambda^{(i)}_l = \lambda^{(N-i+1)}_l$, we define from the corresponding orbitals $v^{(i)}_l$ and $v^{(N-i+1)}_l$, the new ones as

$$
v^{(i)}_l (z) = \frac{v^{(i)}_l (z - x^c_i) + v^{(N-i+1)}_l (z - x^c_{N-i+1})}{\sqrt{2}},
$$

(14)

and

$$
v^{(i)}_l (z) = \frac{v^{(i)}_l (z - x^c_i) - v^{(N-i+1)}_l (z - x^c_{N-i+1})}{\sqrt{2}},
$$

(15)
that fulfill \( \langle \eta^i_l | \tau^i_l \rangle = 0 \). As is easy to check in terms of (13–15), Eq. (15) can be rearranged to

\[
\rho^{g \to \infty}(x, y) = \sum_{i=1}^{\infty} \sum_{l=0}^{\infty} \lambda^i_l [\eta^i_l(x)\nu^i_l(y) + \tau^i_l(x)\tau^i_l(y)],
\]

(16)

for even and odd values of \( N \), respectively. In the limit as \( g \to \infty \), we have \( \langle \eta^i_l | \tau^i_k \rangle = \delta_{lk} \delta_{ij} \) and the integral overlaps \( \langle \eta^i_l | r_{k,j} \rangle , (\nu^i_l | r_{k,j} \rangle , (\nu^i_l | r_{k,j} \rangle \), vanish for any \( l, k, i, j \). (\( i, j = 1, 2, 3, ..., \frac{P}{2} \) with \( P \) as before). We therefore can recognize (16–17) as a Schmidt for \( m \) of the asymptotic RDM different from that given by (15).

C. Occupancies

By inspection, the integrals (14) can be performed explicitly:

\[
\tilde{\rho}_i(\tilde{x}, \tilde{y}) = A_i e^{-a_i(\tilde{x}^2 + \tilde{y}^2) - b_i \tilde{x} \tilde{y}}, a_i > 0, b_i < 0,
\]

(18)

where, however, due to the reasons mentioned at the beginning of the section (11A) the coefficients \( A_i, a_i, b_i \) can be found in closed analytic forms only in the cases \( N = 2 \) and \( N = 3 \). Nonetheless, it turns out that even in the former case they have quite complicated forms:

\[
A_i = \frac{\sqrt{d^2 + 2}}{\sqrt{2\pi (\sqrt{d^2 + 1})}},
\]

\[
a_i = \frac{d + 6\sqrt{d^2 + 2} + 3}{8(1 + \sqrt{d^2 + 2})},
\]

\[
b_i = -\frac{d - 2\sqrt{d^2 + 2} + 3}{4(1 + \sqrt{d^2 + 2})},
\]

(\( i = 1, 2 \)). We have noted that the Schmidt decomposition of the function \( (18) \), thereby the asymptotic occupancies \( \lambda^i_l \) and their natural orbitals \( \nu^i_l \), can be found in closed form. Here we proceed similarly to (21), wherein the occupancies of the analytically solvable two-particle Moshinsky model were derived by the use of Mehler’s formula:

\[
e^{-(u^2 + v^2) / 1 - u^2 + uv / 1 - v^2} = \sum_{l=0}^{\infty} \frac{1}{\sqrt{2\pi}} \frac{1}{l!} \sqrt{1 - y^2 / 2} \frac{H(l; u)H(l; v)}{l!},
\]

(19)

where \( H(l; \cdot) \) is the \( l \)th order Hermite polynomial. Indeed, by matching Eq. (18) with (19), one arrives, after performing some tedious algebra, at

\[
\tilde{\rho}_i(\tilde{x}, \tilde{y}) = A_i e^{-a_i(\tilde{x}^2 + \tilde{y}^2) - b_i \tilde{x} \tilde{y}} = \sum_{l=0}^{\infty} \lambda^i_l \nu^i_l(\tilde{x}) \nu^i_l(\tilde{y}),
\]

(20)

with

\[
\nu^i_l(\tilde{x}) = \frac{w^i_l}{\pi^{1/4}} e^{-\frac{1}{2} w^i_l \tilde{x}^2} H(l; \sqrt{w^i_l \tilde{x}}),
\]

(21)
and
\[ \lambda_{i}^{(i)} = A_i \sqrt{\frac{\pi(1-y_i^2)}{w_i} y_i}, \]  \hspace{1cm} (22)

where
\[ w_i = \sqrt{4a_i^2 - b_i^2}, \]
\[ y_i = \frac{\sqrt{2a_i - b_i} - \sqrt{2a_i + b_i}}{\sqrt{2a_i - b_i} + \sqrt{2a_i + b_i}}. \]

We found that the values of two lowest asymptotic occupancies computed by means of (22) for \( N = 3, d = 1: \)
\[ \lambda_{0}^{(1)} \cong 0.324905, \lambda_{0}^{(2)} \cong 0.319336 \]
are in agreement with the values of [11] (0.3249, 0.3193), where they were determined by the numerical solution of [11], which confirms the correctness of (21)–(22).

D. The von Neumann entropy

The entanglement vN entropy is given by [40]
\[ S = -\text{Tr}[\rho \log_2 \rho], \]  \hspace{1cm} (23)
and in terms of the occupancies, it takes the form \( S = -\sum \lambda_i \log_2 \lambda_i. \) In view of (16)–(17), it follows that the asymptotic vN entropy can be decomposed for even and odd values of \( N \) as
\[ S_{g \to \infty} = 2 \sum_{i=1}^{N} S_i, \]  \hspace{1cm} (24)
and
\[ S_{g \to \infty} = 2 \sum_{i=1}^{N-1} S_i + S_{N+1}, \]  \hspace{1cm} (25)
respectively, where the components \( S_i \) are given by \( S_i = -\sum \lambda_i^{(i)} \log_2 \lambda_i^{(i)}. \) Next, using the analytical formula obtained by us for \( \lambda_i^{(i)}, \) Eq. (22), we attempt to derive a closed form expression for \( S_i. \) We found that for this purpose it is convenient to rewrite \( S_i \) as
\[ S_i = -\lim_{q \to 1} \sum_{i=0}^{\infty} [\lambda_i^{(i)}]^q \frac{d}{dq} \log_2 \left( \sum_{i=0}^{\infty} [\lambda_i^{(i)}]^q \right), \]  \hspace{1cm} (26)
which can be easily verified by referring to the derivative formulas \( (\log_a x)' = \frac{1}{x \ln a}, (a^x)' = a^x \ln a. \) By performing the summation in (26), we obtain
\[ \sum_{i=0}^{\infty} [\lambda_i^{(i)}]^q = \frac{\pi^{q/2} \left( A_i \sqrt{\frac{1-y_i^2}{w_i}} \right)^q}{1-y_i^q}. \]  \hspace{1cm} (27)
Substituting this into (26) and then taking the limit as \( q \to 1, \) we get
\[ S_i = -\frac{A_i \sqrt{\frac{\pi(y_i+1)}{y_i}} \ln \left( y_i^2 \left( \frac{\pi A_i^2 (1-y_i^2)}{w_i} \right)^{1-y_i} \right)}{(1-y_i)^{3/2} \ln(4)}. \]  \hspace{1cm} (28)
III. NUMERICAL RESULTS

In our research for finding the ground-state approximate wavefunction of (1) for finite values of \(g\), we apply a simple trial wave function given by a Jastrow-type wavefunction:

\[
\chi(x_1, x_2, ..., x_N) \propto \prod_{k=1}^{N} e^{-\frac{x_k^2}{2}} \prod_{i>j}^{N} f(\alpha \frac{x_i - x_j}{\sqrt{2}}),
\]  

(29)

with

\[
f(x) = e^{x^2/2} \phi(x),
\]

(30)

where \(\phi\) is a relative motion wavefunction for the ground state of the two-particle system and \(\alpha\) is a variational parameter that is optimized in order to minimize the expectation value of the energy. Such a form of \(\phi\) was recently suggested in [42] and its applicability to the case of charged particles has been demonstrated. We recall at this point that in the limit as \(g \to 0\), the system (1) forms a TG gas and its exact ground-state wave function is given by (29) with \(f = |x|\). In the case of \(N = 2\), the Hamiltonian (1) separates in terms of

\[x = \frac{x_2 - x_1}{\sqrt{2}}, \quad X = \frac{x_1 + x_2}{\sqrt{2}},\]

into \(H = H^z + H^X\), where \(H^X = -1/2d\chi^2 + 1/2X^2\) is exactly solvable and \(H^z\) is given by

\[H^z = \frac{1}{2}d^2 + \frac{1}{2}x^2 + \frac{g}{2\pi|x|d}.
\]

(31)

Because the interaction \(|x|^{-d}\) (\(d > 0\)) diverges when \(x \to 0\), the ground-state even wavefunction \(\phi(+)\) of (21) is given by \(\phi(+) = |\phi(-)|\), where \(\phi(-)\) (\(\phi(-)(0) = 0\)) is the lowest energy odd wavefunction. Note that the function (29) with \(\phi = |\phi(-)|\) is properly defined for the 1D bosons, i.e., it is symmetric and \(\chi(x_1, x_2, ..., x_N) = 0\) if \(x_i = x_j\).

| \(N\) | 3  | 4  |
|-----|----|----|
| \(g\) | 0.546 | 0.551(0.9) | 0.628 | 0.636(0.833) |
| \(g = 2\) | 0.609 | 0.616(0.88) | 0.685 | 0.694(0.8) |
| \(g = 7\) | 0.682 | 0.679(0.87) | 0.765 | 0.758(0.78) |

TABLE I. Linear entropies obtained as discussed in the text and compared with those obtained in [12] (Fig. 6 in it) by means of the CI method. The optimal values of \(\alpha\) are placed in brackets. Here in each case \(\Delta y = 0.25\) was used.

The occupancies and their natural orbitals are determined by the following integral eigenequation \(\int_{-\infty}^{\infty} \rho(x, y) v_i(y) dy = \lambda_i v_i(x)\), which can be turned into an algebraic problem by discretizing the variables \(x\) and \(y\) with equal subintervals of length \(\Delta y\) (see, for example, [14]). Thus, the eigenvalues of the matrix \(B = [\Delta y \rho(m_i, m_j)]_{K \times K}\), where \(m_i = -c+\Delta y, \Delta y = 2c/(K - 1), i, j = 0, ..., K - 1\), provide approximations to the \(K\) largest occupancies. The method produces reasonable approximations to the lowest occupancies if only the value of \(\Delta y\) is small enough and the value of \(2c\) is at least as large as the side of a square in which \(\rho(x, y)\) is mainly confined. A good criterion for convergence is the closeness of the sum of approximate occupancies to the theoretical value 1. In this paper, both for the optimization of [29] with respect to \(\alpha\) and for the determination of \(B\), Monte Carlo techniques are used (for \(N > 3\)). An exception is the case of \(g \to 0\) (the TG limit), where an effective algorithm presented by Pezer and Buljan [43] is used to determine the occupancies.

In order to gain insight into the effectiveness of the ansatz (20), we first determine the occupancies \(\lambda_i\) of the ground states of three- and four-particle systems with \(g = 0.5, 2, 7\) (\(d = 1\)) and assess their accuracy by comparing the linear entropies \(L = 1 - \sum_i \lambda_i^2\) with the numerical results of [12], wherein the corresponding values of \(L\) were determined by the CI method. In each case, we solve Eq. (21) for the corresponding function \(\phi(-)\) by the Rayleigh–Ritz method with a set of the ten lowest odd eigenfunctions of 1D harmonic oscillator. Our numerical results, together with the ones of [12] are summarized in Table I, where, for the sake of completeness, we also give the optimal values of \(\alpha\). It is apparent from the results that the ansatz (20) gives a reasonable estimate of the linear entropy, which allows us to expect that it also provides good approximations to the true values of the occupancies.

Let us now move to the point where we explore the effects of changing the control parameters of the system (1) on the behavior of the ground state vN entropy. As it comes down to the effect of \(g\), we restrict our study to the...
case \( d = 1 \). In order to make our calculations as efficient as possible, we perform them for some values of \( g \) for which the functions \( f \) can be derived in closed exact forms (see Appendix). Here we consider the cases \( g = \sqrt{2} \) (\( n = 1 \)), \( g \approx 5.231 \) (\( n = 3 \)), \( g \approx 10.2176 \) (\( n = 5 \)), \( g \approx 26.640 \) (\( n = 10 \)) where an especially simple form of \( f \) is obtained in the first case, \( f = |x| + x^2 \). Our numerical results for \( S \), including the limiting case of \( g \to 0 \), are depicted in Fig. 1 together with the results obtained for \( S^{g \to \infty} \) by means of (24)–(25) and (28). Moreover, in order to gain some insight into how the parameter \( d \) influences the entanglement, the variation of \( S^{g \to \infty} \) for \( d = 3 \) is also shown in this figure. We can observe how \( S \) converges to the values predicted by the HA as \( g \) is increased, which confirms both the correctness of our theoretical derivations and the effectiveness of (28). As can be seen, for all cases considered, the \( \text{vN} \) entropy \( S \) shows a monotonic increase with \( N \). We conclude from the results that the range of values of \( g \) in which \( S \) makes its most rapid variation also increases with \( N \). In other words, the larger is \( N \), the larger is the value of \( g \) at which \( S \) starts to approach its asymptotic value. For example, as one can infer from Fig. 1 the systems with \( N = 4 \) and with \( N = 6 \) start to reach their asymptotic behaviors practically when \( g \) exceeds the values of about \( g = 10 \) and \( g = 26 \), respectively.

We found that if \( N \) is relatively small and \( g \to \infty \), then only the occupancies with \( l = 0 \), that is \( \lambda_0^{(i)} \), contribute considerably to the conservation of the probability. More precisely, as we have verified, their sum over \( i \) generally decreases as \( N \) increases. For example, in the case of \( d = 1 \) considered in Fig 1 we found that it falls off from 0.982 at \( N = 2 \) to 0.947 at \( N = 6 \). We have thus a qualitative result that in the expansions of the RDM of Wigner molecule state (Eq. (24) and Eqs. (16)–(17)) formed by a small \( N \), only the terms with \( l = 0 \) are substantial. Finally, by comparing the asymptotic results obtained for \( d = 1 \) and for \( d = 3 \), we arrive at the conclusion that strongly interacting charged bosons are less entangled than the strongly interacting dipolar ones.

![Image](image_url)

**FIG. 1.** The \( \text{vN} \) entropy as a function of \( N \) for the systems with \( d = 1 \) for \( g \to 0 \), \( g = \sqrt{2} \), \( g \approx 5.23 \), \( g \approx 10.21 \), \( g \approx 26.64 \), \( g \to \infty \), and for the system with \( d = 3 \) for \( g \to \infty \).

**IV. SUMMARY**

We studied the asymptotic entanglement properties of systems composed of \( N \) particles trapped in a 1D harmonic potential with the inverse power law interparticle interaction \( \sim |x|^{-d} \). We focused mainly on the strong interaction limit of \( g \to \infty \) in which Wigner crystal states are formed. Based on the harmonic approximation, we investigated the nature of the degeneracy appearing in this limit in the spectrum of the RDM, by providing its asymptotic Schmidt expansions. Moreover, we obtained closed form expressions for the ground-state asymptotic natural orbitals and their occupancies by use of Mehler’s formula. Furthermore, based on this finding, we also derived an analytical expression for the corresponding asymptotic von Neumann entropy and provided the results for its dependence on \( N \) for the systems of charged (\( d = 1 \)) and dipolar (\( d = 3 \)) particles. It turned out that the Wigner molecule states formed by the dipolar particles are more entangled than those formed by the charged ones. Moreover, in the case \( d = 1 \), we carried out a comprehensive study of the effect of changing both \( N \) and \( g \) on the behavior of the von Neumann entropy. Our
results showed that the von Neumann entropy grows monotonically with $N$. Among other things, it was found that the range of values of $g$ in which the von Neumann entropy makes its most rapid variations tends to increase with $N$.

V. APPENDIX

We found that for a countably infinite set of $g$ values, the wavefunctions of the relative motion Schrödinger equation

$$\left[-\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} x^2 + \frac{g}{\sqrt{2}|x|}\right] \phi(x) = E_{rel}\phi(x),$$  \hfill (32)  

can be derived in closed form. The solutions of the above equation, in the even-parity case, which is all that we are interested in here, may be represented by

$$\phi^{(+)}(x) = |x|e^{-\frac{2}{x^2}} \sum_{k=0}^{\infty} a_k |x|^k,$$  \hfill (33)  

where the coefficients of $a_k$ satisfy the recurrence relation

$$(-1 - 2E_{rel} + 2k)a_{k-2} + \sqrt{2}ga_{k-1} - k(k + 1)a_k = 0,$$  \hfill (34)  

where $a_0 \neq 0$ and $a_k = 0$, for $k < 0$. The series (33) terminates after the $n$th term if, and only if, $E_{rel} = (3 + 2n)/2$ and $a_{n+1} = 0$, which for a given $n$ determines the values of $E_{rel}$ and $g$ at which closed form solutions of (32) can be found. For example for $n = 1$ we find $g = \sqrt{2}$, which corresponds to $\phi^{(+)} = e^{-\frac{x^2}{2}}(|x| + x^2)$ and $E_{rel} = 2.5$.

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