Correlation and entanglement measures in trapped few-particle systems

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Abstract. Quantum correlations in few-particle systems are discussed in dependence on the shape of the external confining potential. The energy spectra, as well as the natural orbitals and their occupation numbers, are determined by using the optimized configuration interaction method. Considering the inter-particle interactions of the contact type, the comparison of various entanglement measures is given for the full range of interaction strength from strongly attractive to repulsive values. Entropic correlation measures are also discussed for the case of long-range Coulomb interactions between the particles.

1. Introduction

Interest in theoretical studies of few-particle quantum systems has grown enormously in early 1980s since their experimental realization in the form of semiconductor quantum dots (QDs) [1] or few-ion systems in electromagnetic traps. Other realizations soon became possible due to the rapid development of trapping techniques for ultracold gases [2] and the application of optical lattices to isolate systems containing a few atoms or molecules [3]. The possibility of studying single few-body objects in these experiments represents a remarkable advantage over systems existing in nature, such as atoms or nuclei, that are not directly observable but inferred from experiments on macroscopic bodies containing enormous numbers of individuals. Another advantage of the artificial structures is that their parameters, such as the trapping potential, the number of constituents N, and interaction strength, may be controlled at will [2, 3]. The possibility of fabricating low-dimensional artificial few-body structures gave impetus for their detailed theoretical studies. Two-dimensional systems interacting via Coulomb force are the subject of interest in connection to semiconducting QDs, the perpendicular dimension of which is usually negligible [1]. Studies of one-dimensional systems became increasingly popular after their experimental realization in ultracold gases [4]. The interatomic interaction at low temperatures may be considered as a contact one, $U(\mathbf{r}_1, \mathbf{r}_2) = g_{3D}\delta(\mathbf{r}_1 - \mathbf{r}_2)$ with $g_{3D} = \frac{4\pi\hbar^2 a_{3D}}{m}$ and a_{3D} being the scattering length. Quasi-one dimensional systems are created by using trapping potential with the perpendicular confinement length $a_\perp$ much smaller than the longitudinal one. In this case the effective interaction potential is well approximated by $U(x_1, x_2) = g_{1D}\delta(x_1 - x_2)$, where $g_{1D} \approx \frac{4\hbar^2 a_{3D}}{ma_\perp(a_\perp - 1.46a_{3D})}$ [3], which makes the theoretical description relatively simple.

Artificial few-body systems are under intense research for possible applications in quantum information processing [5]. The parallel theoretical and experimental studies give also hope of better understanding the strongly-coupled many-body physics. In particular, characterizing

states of many-body systems using tools and measures developed in quantum information theory appears useful and inspiring. One of the major conceptual tasks is the quantification of entanglement and analysis of its behavior in many-body states. This work aims to discuss quantum correlations and entanglement measures in the case of two-particle systems confined by different forms of external potentials. For one-dimensional two-particle systems with contact interaction we compare the behavior of various entanglement characteristics in the full range of positive and negative values of the effective interaction strength g_{1D}. For two-dimensional quantum systems with Coulombic interaction the influence of anisotropy of the harmonic confinement on entanglement properties is studied. The numerical approach is based on the Rayleigh-Ritz method in the basis of harmonic oscillator eigenfunctions with nonlinear parameters. We show that the strategy of spectral trace minimization appears effective in determining the energy spectrum and entanglement properties of the two-particle systems.

The plan of our work is as follows. In section 2 various correlation and entanglement measures are presented. A brief description of the numerical approach is given in section 3. In section 4 the efficiency of the spectral trace optimization in solving various two-particle problems is demonstrated. Section 5 is devoted to conclusion.

2. Quantum state characteristics

A quantum state of many-body system is described by N-particle wave function $|\Psi>=: \Psi(\mathbf{r}, \sigma)$ that fulfils the Schrödinger equation

$$\widehat{H}\Psi(\mathbf{r},\sigma) = E\Psi(\mathbf{r},\sigma), \qquad \mathbf{r} = \{\overrightarrow{r_1}, ..., \overrightarrow{r_N}\}, \ \sigma = \{\sigma_1, ..., \sigma_N\}, \tag{1}$$

where σ_i denotes the spin of a particle. We consider the case of spin independent Hamiltonian

$$\widehat{H} = \sum_{i=1}^{N} -\frac{\hbar^2}{2m}\Delta_i + V(\overrightarrow{r_i}) + \sum_{i<j}^{N} U(\overrightarrow{r_i}, \overrightarrow{r_j}), \tag{2}$$

when the $N-$particle wave function factorizes into $\Psi(\mathbf{r}, \sigma) = \chi(\sigma)\phi(\mathbf{r})$. The spin part $\chi(\sigma)$ is a linear combination of the products of single-particle spin states $\chi_{i_1}(\sigma_1)...\chi_{i_N}(\sigma_N)$, whereas the spatial wave function depends on the interaction $U(\overrightarrow{r_i}, \overrightarrow{r_j})$, and the trapping potential $V(\overrightarrow{r})$ through the partial differential equation

$$\sum_{i=1}^{N} [-\frac{\hbar^2}{2m}\Delta_i + V(\overrightarrow{r_i}) + \sum_{i<j}^{N} U(\overrightarrow{r_i}, \overrightarrow{r_j})]\phi(\mathbf{r}) = E\phi(\mathbf{r}) \tag{3}$$

with an appropriate boundary condition. In the case of bound states, which is studied in the present work, the condition is of the form $\phi(\mathbf{r}) = 0$, $\nabla\phi(\mathbf{r}) = 0, |\mathbf{r}| \to \infty$, which means that $\phi(\mathbf{r}) \in \mathcal{L}^2$. The potentials $U(\overrightarrow{r_i}, \overrightarrow{r_j})$ and $V(\overrightarrow{r})$ are assumed to be real, the solution of the Schrödinger equation $\phi(\mathbf{r})$ may be thus chosen as a real function, which is, however, unseparable if $U(\overrightarrow{r_i}, \overrightarrow{r_j}) \neq 0$. In the case of identical particles, the total wave function must be antisymmetric under exchange of any pair of particles if they are fermions (half-odd-integer spin) and symmetric if they are bosons (integer spin).

2.1. Correlation and entanglement measures
The concept of entanglement is closely related to quantum correlations. It is commonly accepted that for identical particles the correlations arising purely from their indistinguishable nature should be excluded from the definition of quantum correlations [6, 7]. Therefore, for bosonic (fermionic) particles, the symmetrized (anti-symmetrized) products of one-particle functions are considered as non-entangled and deviations from such states are used to measure the amount

of entanglement. Many ways of measuring the amount of correlation have been developed in quantum chemistry and quantum information science. The most used energetic, statistical and entropic measures will be described in subsections 2.2, 2.3, 2.4, respectively.

2.2. Correlation energy

The energetic correlation measure is usually defined with respect to the mean-field approximation that amounts to including the correlations due to particle statistics, and neglecting those that are due to the inter-particle interaction. The correlation energy is defined as the difference between the approximate and the exact energy of the system. For systems composed of fermionic particles, the mean-field coincides with the Hartree-Fock approximation and so defined measure is used in quantum chemistry since long time [8]. For bosonic systems the mean-field approximation is obtained by representing the many-body state by the product of identical spatial orbitals $\phi(\mathbf{r}) = \varphi(\overrightarrow{r}_1)....\varphi(\overrightarrow{r}_N)$ [2]. The energy functional, defined as the mean-field value of the Hamiltionian (1), reads

$$E[\varphi, \varphi^*] = \int \varphi^*(\overrightarrow{r}) \left[-\frac{\hbar^2}{2m}\Delta + V(\overrightarrow{r}) \right] \varphi(\overrightarrow{r})d^3r + \frac{(N-1)}{2} \int \int U(\overrightarrow{r}, \overrightarrow{r}')|\varphi(\overrightarrow{r})\varphi(\overrightarrow{r}')|^2 d^3r d^3r'$$

(4)

and its minimization under the condition of constancy of the particle number provides the nonlinear Gross-Pitaevskii (GP) equation

$$\left[-\frac{\hbar^2}{2m}\Delta + V(\overrightarrow{r}) + \int U(\overrightarrow{r}, \overrightarrow{r}')|\varphi(\overrightarrow{r}')|^2 d^3r' \right] \varphi(\overrightarrow{r}) = \mu\varphi(\overrightarrow{r}),$$

(5)

where the chemical potential μ has to be determined from the normalization condition $\int |\varphi_{GP}(\overrightarrow{r})|^2 d^3r = 1$. The solution of the GP equation yields the mean-field approximation to the energy $E_{GP} = E[\varphi_{GP}, \varphi_{GP}^*]$, which determines the correlation energy by

$$E_c = E_{GP} - E_{exact}.$$

(6)

2.3. Kutzelnigg coefficient

Among various statistical correlation coefficients discussed by Kutzelnigg et al. [9] the simplest correlation measure is a scalar coefficient that for identical particles is defined as

$$\tau_{ij} = \frac{\langle \overrightarrow{r}_1 \cdot \overrightarrow{r}_2 \rangle_{ij} - \langle \overrightarrow{r} \rangle_i^2}{\langle \overrightarrow{r}^2 \rangle_i - \langle \overrightarrow{r} \rangle_i^2},$$

(7)

where the expectation values are weighted with the probability density $|\phi(\overrightarrow{r}_1, ..., \overrightarrow{r}_N)|^2$ and integrated over the remaining variables. The Kutzelnigg coefficient is bounded by $|\tau_{ij}| \leq 1$.

2.4. Entropic entanglement measures

Entropic correlation measures are based on the Schmidt decomposition [5]. Here we consider the spatial correlations for a pure $N-$particle state $|\phi>$. Upon dividing the full system on two parts 1 and 2, the Schmidt decomposition takes a form

$$|\phi\rangle = \sum_l k_l|v_l\rangle|u_l\rangle,$$

(8)

where $\{v_l\}$ and $\{u_l\}$ are the orthonormal basis sets in the two Hilbert spaces. The spatial wave function $|\phi>$ defines the density matrix

$$\rho = |\phi><\phi|$$

(9)

3

that also contains full information on the state and may be conveniently used to define various quantities describing some of the system properties. For a chosen partition into two subsystems, the reduced density matrices are obtained by taking the trace over the degrees of freedom of the remaining part, namely

$$\rho_1 = Tr_2\rho, \ \rho_2 = Tr_1\rho. \tag{10}$$

The resulting decompositions of the reduced density matrices are given by

$$\rho_1 = \sum_l \lambda_l |v_l\rangle\langle v_l|, \ \rho_2 = \sum_l \lambda_l |u_l\rangle\langle u_l|, \tag{11}$$

where the number of nonzero terms in both sums is the same and is called the Schmidt rank. The common eigenvalues of both matrices, $\lambda_l = k_l^2$, are termed occupancies because $\sum_l \lambda_l = 1$. For distinguishable particles the state is non-entangled if its Schmidt rank equals to 1, otherwise the whole set of occupancies $\{\lambda_l\}$ characterizes the amount of entanglement in the considered state. In order to describe the entanglement by the one quantity, various measures have been constructed from the coefficients k_l, such as

- *von Neumann entropy* [10] $S_{vN} = -Tr\rho Log_2\rho - \sum k_l^2 log_2 k_l^2 = -\sum \lambda_l log_2 \lambda_l$
- *effective number of Schmidt modes* [11] $K = 1/Tr[\rho^2] = 1/\sum \lambda_l^2$
- *linear entropy* [12] $L = 1 - Tr[\rho^2] = 1 - 1/K$
- *robustness* [13] $R = (Tr[\phi])^2 - 1 = (\sum k_l)^2 - 1$

For identical particles the issue is more complicated then for distinguishable ones, since the correlations arising from the particle statistics have to be excluded from the definition of entanglement measures [6, 7]. This will be discussed later when we consider the two-boson and two-fermion systems.

3. Optimized Configuration Interaction Method
3.1. Configuration Interaction Method
One of most efficient ways to solve differential equations is the spectral approach which in quantum mechanics is known under the name of the *Rayleigh-Ritz* (RR) method [14]. The approach consists in approximating the solution of the Schrödinger equation as a finite linear combination

$$\phi(\mathbf{r}) \approx \phi^{(M)}(\mathbf{r}) = \sum_{\alpha=0}^{M-1} c_\alpha \psi_\alpha(\mathbf{r}), \tag{12}$$

where the trial functions $\psi_\alpha(\overrightarrow{r})$ are taken from some Hilbert space basis that may be assumed orthonormal for convenience. Treating the coefficients c_α as variational parameters, one obtains a set of linear equations

$$\sum_{\beta=0}^{M-1} (H_{\alpha\beta} - \varepsilon\delta_{\alpha\beta})c_\beta = 0, \ \alpha = 0, 1, ..., M-1, \tag{13}$$

where $H_{\alpha\beta} = \langle\alpha|\widehat{H}|\beta\rangle$ denotes the matrix elements of the Hamiltonian between the states of the basis, $|\alpha\rangle = \psi_\alpha$. The eigenvectors of the above equations $\{c_\beta\}_\alpha$ determine Mth order approximations to wave functions $\phi_\alpha^{(M)}(\overrightarrow{r})$. The corresponding eigenvalues $\varepsilon_\alpha^{(M)}$ are the variational upper bounds to the exact bound-state energies of $\alpha = 0, ..., M-1$ states. The accuracy of the method can be systematically improved by increasing the number M of included basis functions, which yields successive approximations to the larger and larger number of states. In this way a desired part of the spectrum may be determined with the approximate eigenvalues

monotonically converging to the exact bound-state energies [14]. Considering the few-particle case it is convenient to use basis sets of a proper symmetry under exchange of particle, i.e., taking the basis functions in the bosonic (fermionic) case as permanents (determinants) constructed from the one-particle basis functions. In quantum chemistry such an approach is termed configuration interaction (CI) method. In condensed matter physics the method is known under the name of "exact diagonalization", although the results become exact only in the limit $M \to \infty$.

3.2. Nonlinear Parameters

The convergence properties of the RR method depend strongly on the choice of the expansion basis. The more similar are the trial functions to the exact eigenfunctions of the considered problem, the quicker is the convergence. Fortunately, flexibility of the method can be increased by introducing a set of adjustable parameters $\Omega = \{\Omega_1, ..., \Omega_K\}$ into the functions of the basis $|\alpha\rangle_\Omega$ and exploiting the freedom in choosing their values so as to improve the convergence of the scheme [15]. Optimization strategies may be divided into two classes: those where nonlinear parameters are fixed so as to obtain the quickest convergence to the minimum energy value, and those where they are fixed before performing RR diagonalization. The former approach applies to a particular level, the approximate energy of which is determined only after diagonalization of the RR matrix. Establishing the quickest convergence, requires thus repeating diagonalization many times for different values of nonlinear parameters, which leads to computationally expensive algorithms of iterative optimization [16]. Another problem is that the energy as a function of nonlinear parameters exhibits numerous local minima and deterministic optimization algorithms do not guarantee achieving a global minimum. This may be overcome by the stochastic variational approach where the search of the best values of nonlinear parameters is performed starting from randomly chosen sets of initial values. In this approach good convergence for small atoms, molecules and few-nucleon systems is obtained [17], but the approximate wave functions are not orthogonal, since calculation are performed for each of energy levels independently. Therefore, the strategy of fixing nonlinear parameters by optimization of the convergence rate is mainly used when only the ground state of the system is of interest and high accuracy is required.

Whenever a larger part of the spectrum is to be determined, fixing the values of nonlinear parameters before diagonalization of the RR matrix is more advantageous, since numerical calculations are much simpler and approximate eigenstates are automatically orthonormal. Various strategies of fixing nonlinear parameters are possible and their convergence properties have to be checked a posteriori for a given system. Fixing nonlinear parameters so as to ensure the proper asymptotic behavior of trial functions, has proven effective for simple systems [18], but an extension of this approach to other systems and other basis sets is problematic, since asymptotic expansions which are uniformly valid in the nonlinear parameters are difficult to construct. Therefore, ad hoc methods are more popular, e.g. with nonlinear parameters fixed so as to minimize the expectation value of the Hamiltonian in a chosen state of the trial basis, or so as to vanish some nondiagonal elements of the RR matrix. Depending on the considered system, one or the other gives a better convergence rate, but none of the method can be regarded as justified by any principle.

3.3. Spectral Trace Optimization

We observed [19] that the choice of nonlinear parameters might be based on the principle of minimal sensitivity [20] which states that nonphysical parameters introduced into calculation should be fixed so as to make the given order approximation to the physical quantity as less sensitive as possible to the variations of them. The only physical quantity which may be calculated before diagonalization of the RR matrix is its trace $Tr_M H = \sum_{\alpha=1}^{M} {}_\Omega < \alpha |\widehat{H}| \alpha >_\Omega$, which represents the Mth order approximation to the sum of energies of the M lowest bound-

states. Therefore, in the optimized RR method [19] we require the values of nonlinear parameters in Mth order calculation to be chosen so as to render the trace of the truncated matrix $Tr_M H$ stationary

$$\frac{\delta}{\delta\Omega_i} Tr_M H = 0, \quad i = 1, ..., K. \tag{14}$$

The effectiveness of the optimized RR scheme may be demonstrated for one-dimensional oscillators with various powers of anharmonicity k, described by the Hamiltonians

$$\widehat{H} = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{\omega^2 x^2}{2} + \lambda x^k, \tag{15}$$

using the basis of the eigenfunctions of the harmonic oscillator $\widehat{H} = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{\Omega^2 x^2}{2}$ of an arbitrary frequency Ω, that are given by

$$\langle x|n\rangle_\Omega = \psi_n^\Omega(x) = \left(\frac{\Omega}{\sqrt{\pi}2^n n!}\right)^{\frac{1}{2}} H_n(\Omega x)e^{-\frac{\Omega^2 x^2}{2}}. \tag{16}$$

We have shown [19] that with Ω fixed in Mth order calculation so as to fulfil the stationarity condition (14), well converged results for the spectrum of the quartic oscillator ($k = 4$) in both the single- and double-well cases are obtained automatically. A particularly good test is provided by quasi-solvable example of the sextic oscillator $\widehat{H} = -\frac{1}{2}\frac{d^2}{dx^2} - \frac{35}{\sqrt{2}}x^2 + x^6$, for which nine states of even parity ($n = 0, 2, ..., 16$) are known exactly. The exponential convergence of the optimized RR scheme is evidenced in Fig.1(a) adapted from Ref. [21], where the relative errors $\delta E_n^{(N)}(\Omega_{opt})$ for the ground-state ($n = 0$) and the highest of the analytically known excited states ($n = 16$), are plotted in function of M. The quick convergence of various moments of the position operator $x_n^{k(M)}(\Omega_{opt}) = \langle n|x^k|n\rangle$, shown in Fig.1 (b) and (c) for $n = 0$ and $n = 16$ states, indicates that approximations to wave functions are also accurate. The optimized RR method works also well for oscillators with higher anharmonicities which present a more stringent test for effectiveness of nonlinear parameters optimization. Even in the difficult cases of multi-well oscillators with $k = 10$, the 50-digits accuracy is easily achieved with RR matrices of order $M < 100$ [21].
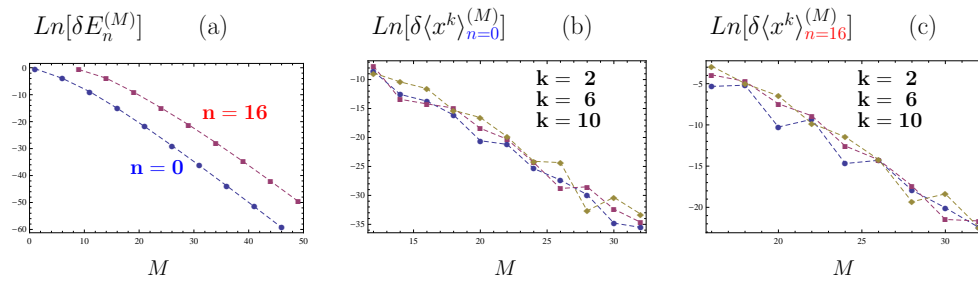

Figure 1. Relative errors, for energy $\delta E_n^{(M)}(\Omega_{opt})$ and various moments for n=0 and n=16 state of the sextic oscillator in function of the dimension M of the optimized RR matrix.

In the case of a central potential $V(r)$ at fixed angular momentum l, the Schrödinger equation for the radial function $\frac{u(r)}{r}$ reduces to the one-variable eigenequation for the radial Hamiltonian

$$\widehat{H}^{(l)} = -\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} + V(r). \tag{17}$$

An appropriate two-parameter basis for the RR method may be constructed from the set of eigenfunctions of the pseudo-harmonic oscillator Hamiltonian $\widehat{H} = -\frac{1}{2}\frac{d^2}{dr^2} + \frac{\Omega^2 r^2}{2} + \frac{(\gamma^2 - 2\gamma + 3/4)}{2r^2}$ that are given by [22]

$$\langle r|n\rangle_{\gamma,\Omega} = u_n^{\gamma,\Omega}(r) = (-1)^n \frac{1}{\Gamma(\gamma)} \sqrt{\frac{2\Omega^\gamma \Gamma(\gamma+n)}{n!}} r^{\gamma-\frac{1}{2}} e^{-\frac{1}{2}r^2\Omega}{}_1F_1(-n;\gamma;\Omega r^2). \tag{18}$$

The strategy of fixing the parameters Ω and γ through the stationarity of the trace condition (14) has been tested [21] for the anharmonic oscillator Hamiltonian

$$\widehat{H}^{(l)} = -\frac{1}{2r}\frac{d^2}{dr^2}r + \frac{l(l+1)}{2r^2} + \frac{\omega^2 r^2}{2} + \lambda r^s. \tag{19}$$

The RR calculation are well defined if $\gamma > -s/2$, since only in this case the matrix elements ${}_{\Omega,\gamma}\langle m|r^k|n\rangle_{\Omega,\gamma}$ appear finite for $k = 1, 2, ...$ [23]. The method proved effective in determining the lower part of the spectrum even in the case of spiked oscillators with $s < -2$ which are most difficult to tackle numerically. The energy estimates in function of the truncation order M are shown in Fig.2 (adapted from Ref. [21]) on two quasi-solvable examples of the "antisextic" oscillator ($s = -6$) with $l = 0$, where ground-states energies are analytically known. The convergence is exponential, albeit its rate is generally slower than in the case of positive power oscillators. In contradistinction to the positive power case, where optimization of the Ω parameter was only important, for spiked oscillators the value of the parameter γ plays a crucial role. The optimum value of γ depends strongly on λ and grows with M. The condition $\gamma_{opt} > 3$ is fulfilled, although the smaller is λ, the closer γ_{opt} is to the value 3, where the matrix elements become singular, which explains the worsening of convergence with decreasing λ.
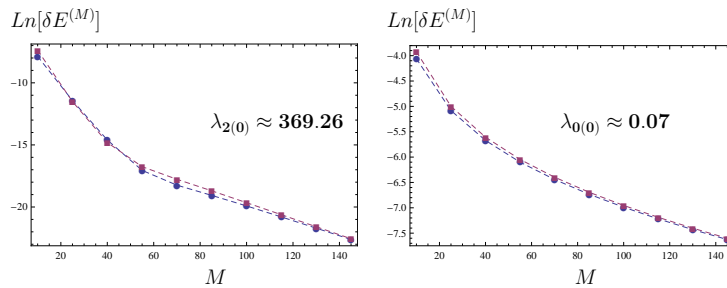

Figure 2. Relative energy errors for the ground-state of the radial "antisextic" oscillator in function of the dimension M of the optimized RR matrix for various interaction strength λ.

In Fig. 3 (adapted from Ref. [21]) the accuracy of our method of fixing nonlinear parameters is compared with that obtained with nonlinear parameters being optimum for convergence of the ground state energy of the "antisextic" oscillator [24] for the RR matrix of dimension $M = 80$. The later strategy gives very good approximation for the ground state, but the accuracy rapidly decreases for higher levels, while the trace optimization strategy provides a uniformly good approximation for all the lowest levels. This makes our strategy particularly appropriate when determination of a larger part of the quantum spectrum is required. This part of spectrum might be successfully utilized to obtain accurate results for the free energy [19], or the time evolution in anharmonic potentials [25]. With a modern software environment the optimized RR scheme may be implemented in a way allowing an arbitrary precision calculation by taking advantage of the present computer algebra abilities to deal with exact numbers. This is especially important for determining the tiny energy splitting in the case of multi-well potentials with nearly degenerate levels [21].
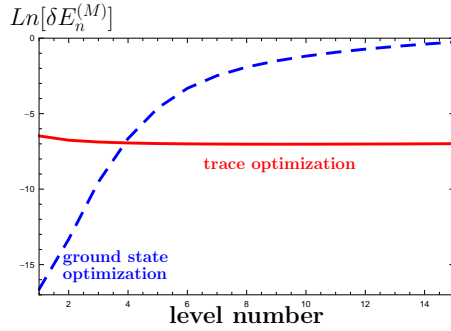
Figure 3. Relative errors of bound state energies of the spiked oscillator of $\lambda = 0.1$ in function of the level number, determined with nonlinear parameters chosen so as to optimize the ground-state energy (blue) and the trace of the RR matrix (red).

4. Two-particle systems

In the following we will study two-particle confined systems with the Hamiltonian given by

$$\widehat{H} = -\frac{\hbar^2}{2m}\Delta_1 + V(\overrightarrow{r_1}) - \frac{\hbar^2}{2m}\Delta_2 + V(\overrightarrow{r_2}) + U(\overrightarrow{r_1}, \overrightarrow{r_2}). \tag{20}$$

In this case, the only possible partition is into two one-particle systems with identical reduced density matrices of a simple one-particle form $\rho(\overrightarrow{r}, \overrightarrow{r}') = \int \phi(\overrightarrow{r}, \overrightarrow{r}'')\phi(\overrightarrow{r}'', \overrightarrow{r}')d^3r''$, the eigenfunctions of which are just the natural orbitals (NOs), well known in quantum chemistry. The Schmidt decomposition of the two-particle function is unambiguous

$$\phi(\overrightarrow{r_1}, \overrightarrow{r_2}) = \sum k_l v_l(\overrightarrow{r_1}) v_l(\overrightarrow{r_2}), \tag{21}$$

with the coefficients k_l being real but not necessarily positive, which enables determination of occupancies $\lambda_l = k_l^2$ without necessity of calculating the density matrix. The coefficients k_l may be directly calculated using the optimized CI approach by representing the spatial wave function as

$$\phi(\overrightarrow{r_1}, \overrightarrow{r_2}) = \sum_{j \geq i} c_{ij}\psi_{ij}(\overrightarrow{r_1}, \overrightarrow{r_2}), \tag{22}$$

where $\psi_{ij}(\overrightarrow{r_1}, \overrightarrow{r_2}) = b_{ij}[\varphi_i^\Omega(\overrightarrow{r_1})\varphi_j^\Omega(\overrightarrow{r_2}) \pm \varphi_j^\Omega(\overrightarrow{r_1})\varphi_i^\Omega(\overrightarrow{r_2})]$ with $b_{ii} = 1/2$ and $b_{ij} = 1/\sqrt{2}$ for $i \neq j$, and the upper (lower) sign corresponds to bosons (fermions). Using the same basis of an arbitrary frequency Ω (16) to expand the natural orbitals as

$$v(\overrightarrow{r}) = \sum p_n \varphi_n^\Omega(\overrightarrow{r}), \tag{23}$$

turns the eigenproblem (21) into an algebraic equation

$$\sum (A_{mn} - k_n \delta_{mn})p_n = 0, \tag{24}$$

where $A_{nn} = c_{nn}$ and $A_{mn} = 2^{-1/2}c_{mn}$ for $m \neq n$ with c_{nm} determined from diagonalization of $[H]_{M \times M}$. By diagonalization of the matrix $[A]_{M \times M}$, the approximate coefficients k_n and the corresponding occupancies $\lambda_n = k_n^2$ may be determined. Due to the fact that $\sum A_{nm}^2 = 1$, their numerical values satisfy $\sum k_n^2 = \sum \lambda_n = 1$. The application of the method for determining two-particle wave functions has been tested in the doctor's thesis of P.Kościk [26].

We will show the efficacy of optimization of the CI method through the stationarity of the trace condition in determining spectra and NOs of trapped two-particle systems on two examples. First is a one-dimensional system in anharmonic confinement of single- and double-well shape with the interparticle interactions of the contact type. The second is a two-dimensional system of Coulombically interacting particles confined in an anisotropic harmonic potential.

4.1. Two-boson system

The state of two identical bosons is non-entangled only if its Schmidt rank equals 1 or 2 [6, 7]. In the first case, $\lambda_0 = 1$ and the state is the product of the same natural orbital

$$\phi(\mathbf{r}_1, \mathbf{r}_2) = v_0(\mathbf{r}_1)v_0(\mathbf{r}_2). \tag{25}$$

We will call such a state "condensed", as representing a two-particle analogue of the Bose-Einstein condensate, according to the Penrose-Onsager criterion [27]. In the second case, $\lambda_0 = \lambda_1 = \frac{1}{2}$, and the Schmidt decomposition of wave function comprises two cases

$$\phi(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}} \left(v_0(\mathbf{r}_1)v_0(\mathbf{r}_2) \pm v_1(\mathbf{r}_1)v_1(\mathbf{r}_2) \right). \tag{26}$$

In both cases the two natural orbitals are equally populated and wave function can be written as a permanent of two orthogonal orbitals, $\phi(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}} \left(\eta(\mathbf{r}_1)\chi(\mathbf{r}_2) + \chi(\mathbf{r}_1)\eta(\mathbf{r}_2) \right)$, where $\eta = \frac{1}{\sqrt{2}}(v_0 - iv_1)$, $\chi = \frac{1}{\sqrt{2}}(v_0 + iv_1)$ for the plus sign, and $\eta = \frac{1}{\sqrt{2}}(v_0 - v_1)$, $\chi = \frac{1}{\sqrt{2}}(v_0 + v_1)$ for the minus sign in (26). We will call the states of this kind "fragmented", as being two-particle examples of the many-body fragmentation phenomenon [28].

Here we consider a one-dimensional system of two bosons in an anharmonic trapping potential

$$V(x) = wx^2 + x^4. \tag{27}$$

For $w < 0$ the potential has two wells, the depth of which decreases with increasing w, undergoing a transition to single-well behavior at $w = 0$. For $w \geq 0$ the potential shape changes from purely quartic to a harmonic one in the limit $w \to \infty$. A pleasant feature of one-dimensional bosonic systems is their solvability for arbitrary trapping potential in the strong repulsion limit. At $g_{1D} \to \infty$, the N−boson wave-function may be represented via Bose-Fermi mapping as the modulus of the wave function of N noninteracting fermions [29], which is known as the Tonks-Girardeau gas and provides useful asymptotic results for verifying numerical calculations performed at large g_{1D}. In the case of a two-particle system, the $g_{1D} \to \infty$ limit of the ground state wave function is given by $\psi_{2,Bose}^{TG}(x_1, x_2) = \frac{1}{\sqrt{2}}|\psi_0(x_1)\psi_1(x_2) - \psi_1(x_1)\psi_0(x_2)|$, where ψ_0 and ψ_1 are the two lowest one-particle states.

The harmonic limit of the trapping potential (27) is the easiest to discuss, since in this case the two-particle eigenfunctions $\phi(\mathbf{r}_1, \mathbf{r}_2)$ are known exactly in an implicit form [30] and the NO's occupancies may be determined by performing their diagonalization numerically. The three largest occupancies, $\lambda_0, \lambda_1, \lambda_2$ for the ground state are plotted in Fig.4 in function of the interaction strength. At $g_{1D} = 0$, the value of λ_0 equals 1, and only in this case all other occupancies do vanish, which means that the state of two harmonically confined bosons is non-entangled only if the bosons do not interact. The weakly entangled "condensed state", where only one NO is significantly occupied, is realized only in the case of very weak interaction, $|g_{1D}| < 0.1$. With increasing $|g_{1D}|$ the entanglement grows, which shows up in the smooth increase of λ_1 and λ_2 at the cost of λ_0, for both repulsive and attractive interactions. In the repulsive case, the occupancies monotonically approach their Tonks-Girardeau limits $\lambda_0^{TG} \approx 0.7745$, $\lambda_1^{TG} \approx 0.1765$ and $\lambda_2^{TG} \approx 0.0414$. In this limit all the remaining NOs are also occupied, however the sum of their occupancies is only about 0.0076. In the case of strongly attractive interaction, the situation is different, since the ground state does not tend to the fermion-like state. In fact, the fermionized state exists but there are infinitely many states of energy lower than this. As can be seen in Fig.4, at $g_{1D} \to -\infty$ the occupancies of NO's become uniformly small, which means that in this limit the ground state is maximally entangled.

Having obtained a sufficient amount of the coefficients k_l, we determined the accurate approximations to the correlation measures discussed in Sect.2.1. The results are presented
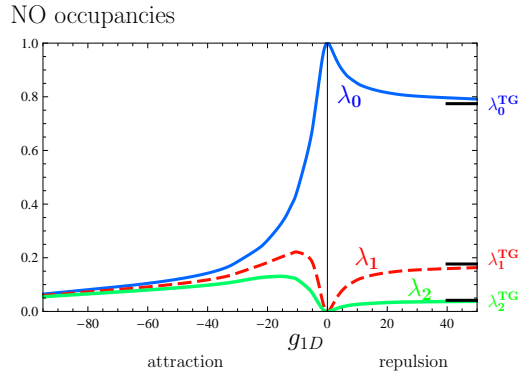
NO occupancies

Figure 4. The largest occupancies λ_0, λ_1 and λ_2 for the harmonically confined two-boson system in function of g_{1D}, their Tonks-Girardeau limits λ_0^{TG}, λ_1^{TG} and λ_2^{TG} are marked by horizontal lines.

in Fig. 5 in comparison with the correlation energy and the Kutzelnigg coefficient. All the correlation measures grow monotonically with increasing interaction strength $|g_{1D}|$, and all but the correlation energy remain bounded in the limit $g_{1D} \to \infty$.

correlation measures
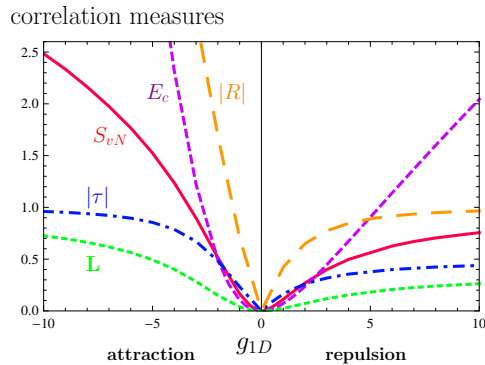
Figure 5. Comparison of the correlation energy E_c, robustness R, von Neumann entropy S_{vN}, linear entropy L, and the Kutzelning coefficient τ, in function of the interaction strength g_{1D}, for the two-boson system confined in the harmonic oscillator potential.

The role played by correlations can be examined further by testing the number of NOs that are needed for accurate determination of the two-particle wave function by the expansion (21) truncated at the nth term, $\psi^{nNO}(x_1, x_2)$. The successive approximation to the ground state energy $E^{nNO} = \langle\psi^{nNO}|H|\psi^{nNO}\rangle/||\psi^{nNO}||^2$ obtained by including up to four most occupied orbitals are shown in Fig.6 in function of the interaction strength and compared with the exact result and the GP approximation. As $|g_{1D}|$ increases, more and more orbitals in the sum (21) are necessary to obtain a satisfactory approximation to the energy. The one-orbital approximation and the GP energy E_{GP} are very close up to $|g_{1D}| \approx 5$, only for larger values of $|g_{1D}|$ the GP approximation performs slightly better than E^{1NO}. However, the difference between the exact energy and the GP approximation (correlation energy) starts to be noticeable already at $|g_{1D}| > 0.1$ and grows monotonically for increasing interaction strength. This shows that the correlation effects may be neglected in determining the ground state energy only in the case of very weak interactions.

The correlations effects are best visible in the two-boson probability density. In Fig.7 the approximate GP two-particle density is compared with the approximations obtained by taking into account one, two, and three NOs, and the exact density for strongly correlated case $(g_{1D} = 5)$. In this case the bosons are located with great probability on diametrical positions with respect to the center of the trap, which shows up in the exact two-particle density. The GP distribution does not capture this behavior. The one-orbital approximation differs from the GP approximation but also fails. Only after taking three NOs into account the approximate two-particle distribution properly describes the exact behavior.
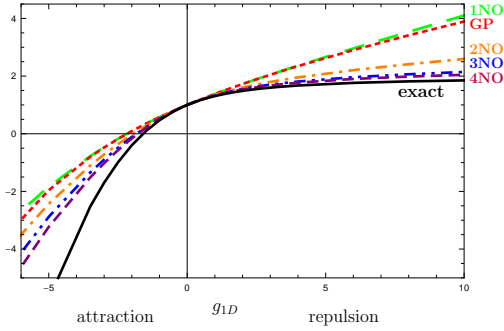
Figure 6. Ground-state energy of the harmonically confined two-boson system in the approximation including n natural orbitals (nNO) for $n = 1, 2, 3, 4$ compared with the GP approximation and the exact result.

approximations to the two-particle density   exact result
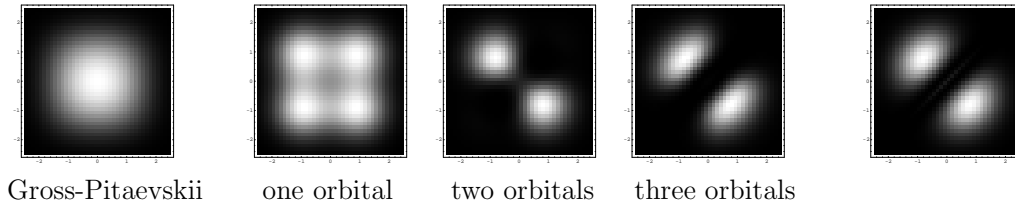
Gross-Pitaevskii   one orbital   two orbitals   three orbitals

Figure 7. The GP density $|\psi_{GP}(x_1, x_2)|^2$ (left column) compared with approximations $|\psi^{nNO}(x_1, x_2)|^2$ for $n = 1, 2$ and 3 orbitals (three middle columns) and the exact result $|\psi(x_1, x_2)|^2$ (right column) for two harmonically confined boson interacting with the strength $g_{1D} = 5$.

In the case of anharmonic confinement (27) we applied the optimized CI method with the harmonic oscillator one-particle basis (16) to solve the two-boson problem. With Ω fixed through the stationarity of the trace condition (14) a sufficiently large set of NOs may be obtained so as to determine the von Neumann entropy to a desired accuracy. In Fig.8 the results are plotted in function of $g1D$ for several values of the parameter w. For $w > 0$, when the trapping potential is single-well shaped, the dependence of von Neumann on g_{1D} is similar as in the harmonic confinement case. For decreasing w, the increase of the von Neumann entropy becomes more rapid and around $w \approx -3$ the character of the dependence changes markedly. The deeper is the double-well potential the smaller is the value of g_{1D} for which the Tonks-Girardeau behavior $S_{vN}^{TG} = 1$ is approximately achieved. This tendency has been observed before for the δ-split [31] and double-well potential [32].
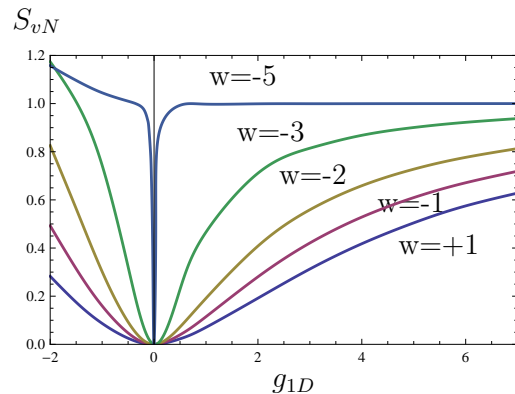

Figure 8. The von Neumann entropy for anharmonic confining potential $V(x) = wx^2 + x^4$ for $w = 1, -1, -2, -3, -5$ as a function of $g1D$.

The analysis of the Tonks-Girardeau limit, $g_{1D} \to \infty$, is presented in function of the parameter w in Fig.9. The two largest occupancies, shown on the left side of the figure, approach the Tonks-Girardeau values of the harmonically confined system in the limit of $w \to \infty$. For finite values of w, the anharmonic term in the potential (27) plays a role, being the more important the smaller is the value of w. Below $w \approx -3$, when the confinement potential becomes deeply double-well shaped, the occupancy of the orbital v_1 increases more rapidly and for $w < -5$ becomes practically equal to the occupancy of the lowest orbital ($\lambda_0 \approx \lambda_1 \approx 0.5$), so the state is almost perfectly fragmented and non-entangled. The Tonks-Girardeau limit of the von Neumann entropy in function of w is shown in the right part of Fig.9. In the limit of $w \to -\infty$ the state becomes non-entangled as $S_{vN} \to 1$ and the Schmidt rank tends to 2 with $\lambda_0 \approx \lambda_1 \to 1/2$. However, the dependence on w is not monotonous and S_{vN} takes also the value 1 at a finite w, but the corresponding ground state is entangled, since the values of two lowest occupancies (marked by crosses on the figure) do not sum up to one and the remaining Schmidt eigenvalues do not vanish. For identical bosons the value of entropy alone is not sufficient to assert whether the state is entangled or not, which was also observed in the case of delta-split potential [32].
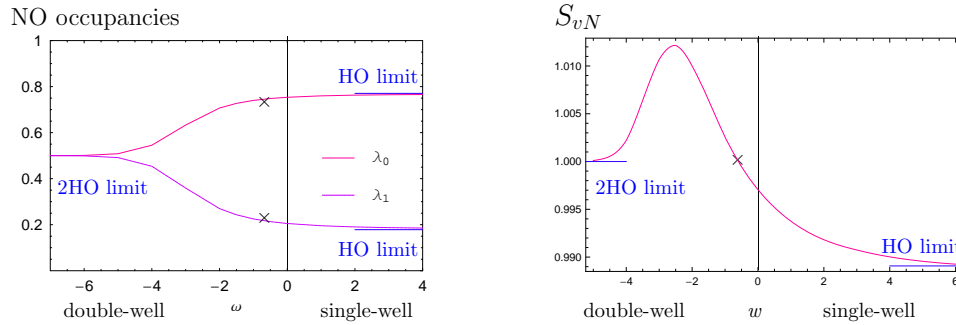

Figure 9. The two largest NO occupancies (left) and the von Neumann entropy (right) in the anharmonic confining potential $V(x) = wx^2 + x^4$ in the Tonks-Girardeau limit. The limits of a harmonic confinement $w \to \infty$ (HO limit) and of two independent harmonic wells $w \to -\infty$ (2HO limit) are marked.

4.2. Two fermions

A two-dimensional system of charged particles in an anisotropic harmonic potential is commonly used as a model of a semiconductor QD [1]. The Hamiltonian of a two-electron QD is given by

$$\hat{H} = \sum_{i=1}^{2}[\frac{\mathbf{p}_i^2}{2} + \frac{1}{2}(\omega_x^2 x_i^2 + \omega_y^2 y_i^2)] + \frac{e^2}{|\mathbf{r}_2 - \mathbf{r}_1|}. \tag{28}$$

After rescaling $E \to e^4 E$ and $\omega_{x,y} \to 2e^4\omega_{x,y}$, the Schrödinger equation takes the form

$$\left[\sum_{i=1}^{2}[-\frac{1}{2}\nabla_{r_i}^2 + 2\omega_x^2 x_i^2 + 2\omega_y^2 y_i^2] + \frac{1}{|\mathbf{r}_2 - \mathbf{r}_1|}\right]\phi(\mathbf{r}_1, \mathbf{r}_2) = E\phi(\mathbf{r}_1, \mathbf{r}_2), \tag{29}$$

where the dimensionless parameters $\omega_{x,y}$ denote the ratio of confinement to Coulombic interaction energies. The center of mass motion may be separated out and solved exactly. The relative motion equation

$$[-\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + \omega_x^2 x^2 + \omega_y^2 y^2 + \frac{1}{\sqrt{x^2 + y^2}}]\phi^r = E^{\mathbf{r}}\phi^r \tag{30}$$

is separable in only two particular cases: $\omega_x = \omega_y = \omega_\rho$ (in polar coordinates) and $\omega_y : \omega_x = 2$ (in parabolic coordinates). Both cases are quasi-solvable. The closed-form solutions exist at particular values ω_ρ of the isotropic confinement [33] and at particular values $\omega_y = 2\omega_x$ of the anisotropic confinement [34]. The values of frequencies at which the exact solutions are known correspond to the weak confinement case ($\omega_{x,y} \ll 1$), where the correlations between the electrons are the strongest and tend to create the so-called Wigner molecules. This regime is especially interesting, as the numerical calculations are rather demanding. The exact solutions will thus serve us to check the results of calculation performed by the optimized RR method.

We aim to discuss how the anisotropy of confinement influences the entanglement properties of the system. Considering the two-fermion ground-state with symmetric spatial wave function, which corresponds to the singlet spin structure, we determined the coefficients k_l of the Schmidt decomposition of the two-particle function at different aspect ratios of the confinement frequencies. The resulting von Neumann entropy is presented in Fig.10 in function of the dimensionless parameter $\sqrt{\omega_x^{-1}}$ that represents the ratio of interaction to confinement energies. It can be seen that for weak interactions the entanglement properties do not depend on the shape of the trap. For stronger interactions the dependence on the aspect ratio of harmonic frequencies grows, the von Neumann entropy being smaller at stronger anisotropies.
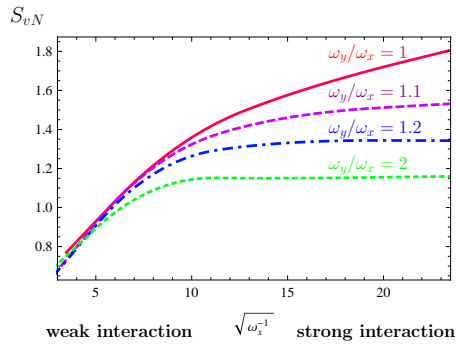

Figure 10. Von Neumann spatial entropy as a function of $\sqrt{\omega_x^{-1}}$ for anisotropy ratios $\omega_x/\omega_y = 1,\ 1.1,\ 1.2,$ and 2.

5. Conclusion

We applied the optimized CI method to calculate spectra of two-particle confined systems. Optimization of the scheme has been done by introducing nonlinear parameters into the functions of the one-particle basis and fixing their values by minimization of the trace of the truncated Hamiltonian matrix. Such optimization strategy proved efficient in solving one-particle problems to arbitrary precision with the computational cost much lower than that of iterative optimization of nonlinear parameters. In our scheme the desired part of energy spectrum is determined to a desired accuracy in one run and the approximate eigenvectors are mutually orthogonal, which enables effective determination of various system properties.

In the two-particle case the optimized CI method enables a direct derivation of the natural orbital occupancies and determination of entropic entanglement measures. Comparison of various entanglement measures has been performed for the ground state of two bosons in a one-dimensional trap. The dependence of the von Neumann entropy on the interaction strength has been discussed on the example of anharmonic confinement potential when its shape changes from a harmonic to a deep double-well. Influence of anisotropy on spatial entanglement properties has been discussed for a singlet ground-state of the two-dimensional QD consisting of two Coulombically interacting electrons confined in an anisotropic harmonic potential. The increase of correlations with increasing anisotropy has been demonstrated.

Acknowledgments

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