이학석사 학위논문

Benchmarking multiconfigurational Hartree by the exact wavefunction of two harmonically trapped bosons with contact interaction

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2020 년 8 월

서울대학교 대학원

물리천문학부

곽 영 진

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이 논문을 이학석사 학위논문으로 제출함

2020 년 6 월

서울대학교 대학원

물리천문학부

곽 영 진

곽영진의 이학석사 학위논문을 인준함

2020 년 7월

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Abstract

Benchmarking multiconfigurational Hartree by the exact wavefunction of two harmonically trapped bosons with contact interaction

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We consider two bosons in a one-dimensional harmonic trap, interacting by a contact potential, and compare the exact solution of this problem to a self-consistent numerical solution by using the multiconfigurational time-dependent Hartree (MCTDH) method. We thereby benchmark the predictions of the MCTDH method with a few-body problem that has an analytical solution for the most commonly experimentally realized interaction potential in ultracold quantum gases. It is found that exact ground state energy and first

order correlations are accurately reproduced by MCTDH up to the intermediate dimensionless coupling strengths corresponding to typical background scattering lengths of magnetically trapped ultracold dilute Bose gases. For larger couplings, established for example by (a combination of) Feshbach resonances and optical trapping, the MCTDH approach overestimates the depth of the trap-induced correlation dip of first order correlations in position space, and underestimates the fragmentation, defined as the average relative occupation of orbitals other than the energetically lowest one. We anticipate that qualitatively similar features in the correlation function may arise for larger particle numbers, paving the way for a quantitative assessment of the accuracy of MCTDH by experiments with ultracold atoms.

Keywords : Boson, MCTDH, exact solution, ultracold gas, first order correlations

Student Number : 2015-20317

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Chapter 1. Introduction

1.1 MCTDH

The MCTDH method is a powerful self−consistent numerical approach to the quantum dynamics of many interacting particles, and has been extensively used to predict correlation functions, cf., e.g., Refs. [1−5]. Initially used for the purpose of propagating wavepackets in physical chemistry, where it is by now routinely used [6], in the past decade MCTDH has increasingly been applied to describe the intricate many−body physics of ultracold dilute Bose gases, for example, in Refs. [7−18].

The present study is inspired by the ongoing debate on the convergence of MCTDH, see, e.g., Refs. [19−22]. These convergence issues arise because the MCTDH equations of motion become singular as soon as unoccupied orbitals occur during the real or imaginary time evolution. Hence, some (nonunique) prescription of regularization is needed, see for example [23−26]. Furthermore, it is not clear whether MCTDH is more accurate in comparison to, e.g., the alternative approach of using the truncated Wigner method for either large or small number of particles N [21]. This stems from the fact that neither method, MCTDH nor truncated Wigner (see also,

e.g., Ref. [27]) provides a *control parameter* for its accuracy to be assessed within given numerical resources. This should be compared with (number−conserving) Bogoliubov theory[28, 29], where this control parameter is some power of the inverse of the particle number, $1/N$. Rigorous results on the accuracy of retaining just a single orbital in the field operator expansion are available in the limit of particle number $N \to \infty$, provided the (formal) condition is met that the interaction coupling g decreases as $1/N$, and hence $g = g(N)$ tends to zero in that limit[30, 31]. These rigorous results are, in addition, limited to reproducing the Gross−Pitaevskii energy correctly, while higher−order correlations reveal deviations from mean−field physics even in the large N limit keeping gN fixed cf., e.g., [13, 14].

1.2 Necessity of Benchmarking MCTDH

Importantly, a direct experimental verification of the accuracy of MCTDH in a controllable quantum many−body system is lacking so far. We here aim at benchmarking MCTDH with the exactly solvable model most closely associated with current experiments on ultracold gases: A pair of bosons with repulsive contact interactions trapped in a single harmonic well. Because many−body correlations are strongest in one spatial dimension, we use to this end a one−

dimensional (1D) variant of the originally 3D analytical solution [32–34]: For $N = 2$ in one spatial dimension, one expects deviations from (single–orbital) mean–field physics to be most significant. The present case of strong correlations is therefore an excellent testing ground for the accuracy of MCTDH outside its usual applicability domain of weak correlations. Upon approaching the Tonks–Girardeau "fermionized" limit [35–38], the *self–consistent* determination of the orbitals' shape in a harmonic trap becomes increasingly important, as the usual periodic boundary conditions in a spatially homogeneous system cannot be applied. While it is well known that in 1D, the Lieb–Liniger solution [39] is exact for any N, extracting correlation functions is in general a challenging task [36]. In addition, the Lieb–Liniger solution is not available in harmonic traps.

The analytically solvable $N = 2$ problem supplies an exact statement on the shape of the orbitals and level occupation statistics. It can thus assess the accuracy of MCTDH, which determines these quantities, for a large but finite number M of field operator modes. We provide below, with an *experimentally realizable* interaction potential, an accurate quantitative statement to which extent MCTDH is "numerically exact" [40], i.e., controllably reproduces for $M \to \infty$

an exact solution of the Schrödinger equation[①]. The coupling strength can be changed over a large range via Feshbach resonances [41], facilitating experimental access to the validity domain of MCTDH. We demonstrate that for large couplings, MCTDH increasingly overestimates a trap-induced dip in nonlocal first-order correlations, which can be used as a sensitive measure of the accuracy of MCTDH.

① An exactly solvable model (which is readily integrable for any N) and the convergence of MCTDH towards its solutions was studied with a harmonic interaction potential in Ref. [7], with the obvious limitation that this interaction is not realized in ultracold atomic gases.

Chapter 2. Two harmonically trapped bosons in 1D

2.1 Analytical solution

The Hamiltonian is

$$H = -\frac{\hbar^2}{2m}\Delta_{\vec{x}} + \frac{1}{2}m\omega^2\vec{x}^2 + g\delta(x_1 - x_2) \quad (1)$$

where $\vec{x} = (x_1, x_2)$ is the position vector of the atoms, m their mass, ω the frequency of the trapping potential, and g is the 1D interaction coupling constant. Below, we use $\hbar\omega$ as unit of energy, and $l = \sqrt{\hbar/m\omega}$ as length scale. The solution of the Schrödinger equation can be found by the separation ansatz [32, 34]

$$\Psi(R, r) = \Psi_{\mathrm{COM}}(R)\,\psi_{\mathrm{rel}}(r), \quad (2)$$

where we introduced relative, $r = \frac{1}{\sqrt{2}}(x_1 - x_2)$ and center-of-mass (COM) $R = \frac{1}{\sqrt{2}}(x_1 + x_2)$ coordinates. Relative and COM wavefunctions are then given by

$$\Psi_{\mathrm{COM}}(R) \propto e^{-R^2/2}H_n(R),$$
$$\psi_{\mathrm{rel}}(r) \propto e^{-r^2/2}\,U(-\nu, \frac{1}{2};\, r^2), \quad (3)$$

where H_n is the Hermite polynomial of order n and $U(-a, b; x)$ is a confluent hypergeometricfunction [42]; we omitted the

normalization constants. A new quantum number ν parametrizes the total energy of the system

$$E = 2\nu + n + 1, \tag{4}$$

where the g dependence of ν is found by solving [34]

$$\frac{\Gamma\left(-\nu+\frac{1}{2}\right)}{\Gamma(-\nu)} = -\frac{g}{2\sqrt{2}} \tag{5}$$

Clearly, the wavefunction in Eq. (2) describes the system we consider exactly. In the following, we compare ground state energy, single−particle density matrix (SPDM) and the shape of the orbitals, obtained by employing this exact solution with the results from MCTDH calculations, varying the coupling g and the number of orbitals M. We note here that the $N = 2$ harmonic trap wavefunction has previously been used to compare to MCTDH results [22], however for only up to intermediate values of *negative* $g \sim O(-1)$, for maximally $M = 10$ orbitals, and without the crucial comparison of *nonlocal* first−order correlations we present below, which encapsulate MCTDH self−consistency in particular for strong correlations.

Using Eqs. (2) and (3), the SPDM $\rho^{(1)}(x,x') = \int \Psi^*(x,x_1)\Psi(x_1,x')\mathrm{d}\,x_1$ of the ground state, which is obtained from $n = 0$ and $\nu = \nu_0$ with ν_0 being the minimal value of ν from solving

Eq. (5), is given by

$$\rho^{(1)}(x,x') \propto e^{-(x^2+x'^2)/2} \times \int \mathrm{d}x_1 e^{-x_1^2} U\left(-\nu_0, \frac{1}{2}; \frac{(x-x_1)^2}{2}\right) U\left(-\nu_0, \frac{1}{2}; \frac{(x_1-x')^2}{2}\right) \quad (6)$$

where the integral may be calculated numerically to in principle arbitrary accuracy.

2.2 The MCTDH method

The notion of self−consistency embodied by MCTDH is that it determines the shape and time dependence of the *orbitals* $\varphi_i(x,t)$ *self−consistently* together with their occupation distribution $C_{\vec{N}}(t)$ in Fock space, where $\vec{N} = (N_0, N_1, \dots, N_{M-1})$ $(\sum_0^{M-1} N_i = N)$ is the occupation vector. The coupled MCDTH equations of motion are [34]

$$i\hbar \frac{\partial \boldsymbol{C}(t)}{\partial t} = \boldsymbol{H}(t)\boldsymbol{C}(t),$$

$$i\hbar \frac{\partial |\varphi_j\rangle}{\partial t} = \hat{P}\left[\hat{h}|\varphi_j\rangle + \sum_{k,s,q,l=1}^{M} \rho_{jk}^{-1}\rho_{ksql}\widehat{W}_{sl}|\varphi_q\rangle\right]. \quad (7)$$

Here, $\boldsymbol{C}(t)$ is the column vector that consists of all possible expansion coefficients $C_{\vec{N}}(t)$, $\boldsymbol{H}(t)$ corresponds to the time−dependent Hamiltonian matrix in the basis $|\vec{N};\, t\rangle$, $\hat{h}$ is the single−particle Hamiltonian, $\widehat{W}_{sl} = g \int\int \mathrm{d}\, x\, \varphi_s^*(x)\varphi_l(x)$, and $\hat{P} = 1 - \sum_{k'=1}^{M} |\varphi_{k'}\rangle\langle\varphi_{k'}|$ is an orthogonal subspace projection operator. Finally,

ρ_{ksql} is the matrix element of the two-particle density matrix. To find the self-consistent solution of the above equations, we use MCTDH-X software package, provided by [4] and first implemented in [43, 44].

Chapter 3. Benchmarking MCTDH

3.1 Convergence of MCTDH to exact ground energy

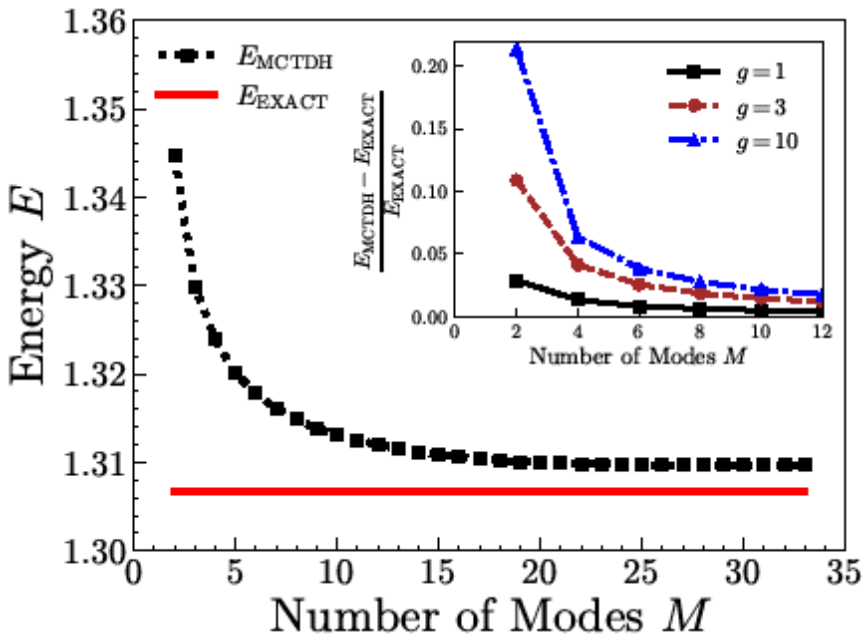

Fig 1. Convergence of the ground state energy, calculated via MCTDH-X with increasing number of orbitals (black squares), $M = 2, \ldots, 33$ towards the exact value from Eq. (4) (red solid); the coupling $g = 1$. Inset: The relative error for the ground state energy for $g = 1$ (black solid), $g = 3$ (brown dashed) and $g = 10$ (blue dash-dotted).

In order to verify convergence of the ground state energy to the exact result, we performed extensive MCTDH calculations for a wide range of the number of orbitals, $M = 2, \ldots, 33$. In Fig. 1, we present the

comparison between the exact and numerical values of the ground state energy for the interaction coupling $g = 1$. We conclude that the numerical value converges rapidly for a large number of orbitals. The relative error between the exact and converged numerical values becomes less than 3 ‰ when $M > 15$. We however also notice that upon further increase of M, the error does not decrease significantly further. Specifically, for $M = 20$ the error is 2.48‰, and for $M = 33$ it is still 2.26 ‰.

From Fig. 1 we see that for large M the energy converges exponentially with a small relative error, corresponding to results of similar calculations that employed interaction rescaling, for a smaller number of orbitals, see [45]. To illustrate the dependence of the convergence on g, the relative error for the energy, $(E_{\mathrm{MCTDH}} - E_{\mathrm{exact}})/E_{\mathrm{exact}}$, is shown in the inset of Fig. 1 for $M = 2, \ldots, 12$ and $g = 1,\ 3,$ and 10. The MCTDH calculations still converge reasonably well for sufficiently large M to the exact energy. However, the computational cost (the M needed for convergence) is, as expected, seen to increase for larger values of g.

3.2 Density matrix

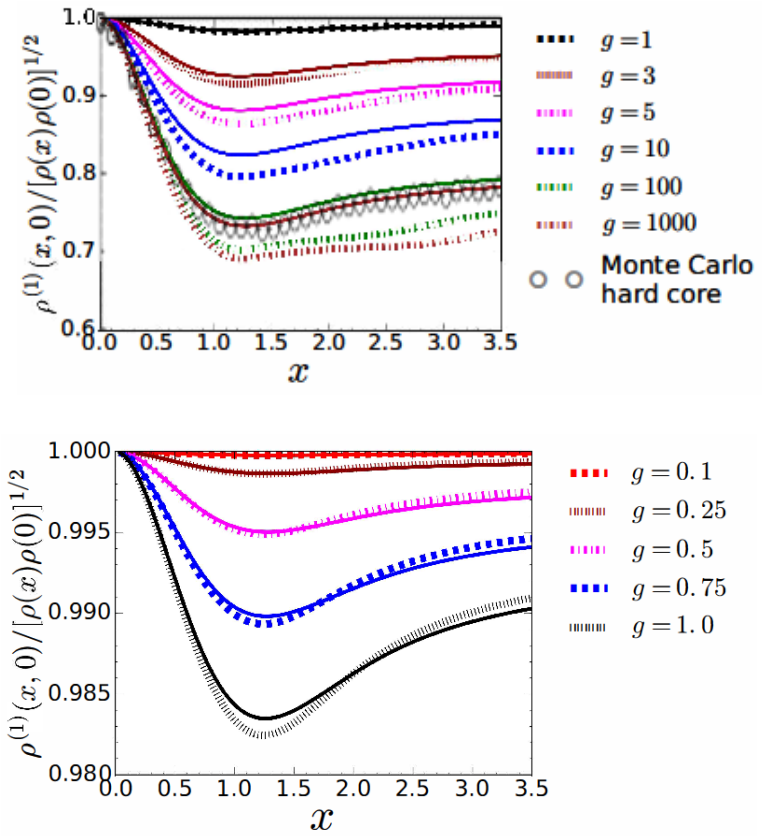

Fig 2. Top: SPDM $\rho^{(1)}(x,x')/\sqrt{\rho(x)\rho(x')}$ as a function of x and $x'=0$ for $N=2$ interacting bosons in a harmonic trap, in the strong coupling regime. The gray circles are the Monte Carlo results of Minguzzi et al. [35] for hard−core bosons $(g\to\infty)$, with the size of the circles representing the error bars in the Monte Carlo data. The lines are MCTDH results for various g and $M=10$. The solid lines show the analytical result. Bottom: Comparison of MCDTH results $(M=10)$ with the 1D analytical solution in the range of intermediate

interaction couplings.

Generally, correlation functions are more sensitive to the accuracy of MCTDH predictions than the ground state energy is, cf. [13, 14, 47]. Therefore, we now concentrate on a comparison of the analytics to numerics in the form of the first−order correlations, as encapsulated by the SPDM. We compare the results of our MCTDH calculations, in addition, with the Monte Carlo calculations performed by Minguzzi *et al.* in Ref. [35] for the SPDM of a pair of hard−core bosons in a 1D harmonic trap. The emphasis for this part of the paper is to assess the accuracy of MCTDH when g in the Hamiltonian Eq. (1) is varied from weak over intermediate to strong coupling, so that we here fix $M = 10$.

In Fig. 2, we plot the normalized SPDM $\rho^{(1)}(x,x')/\sqrt{\rho(x)\rho(x')}$ as function of x, and at fixed $x' = 0$, for relatively large values of g. The gray circles in the top panel are taken from the Monte Carlo data of Ref. [35], while the solid lines show the comparison of MCTDH results with the 1D variant of the 3D analytical solution for $N = 2$ bosons in a harmonic trap [32, 33]. We observe that the qualitative behavior of the MCTDH results is in accord with the analytical result as well as with the hard−core Monte Carlo calculations − the dip in the first−order correlations located at approximately $x = l$ is

consistently visible. Note that this dip in the correlation function $\rho^{(1)}(x,x')$ corresponds to a peak in *phase fluctuations*, defined according to [47] $\langle\hat{\psi}^{\dagger}(x)\hat{\psi}(x')\rangle = \sqrt{\rho(x)\rho(x')}\exp\left[-\frac{1}{2}\langle\delta\hat{\phi}_{xx'}^{2}\rangle\right]$, where $\delta\hat{\phi}_{xx'} = \hat{\phi}(x) - \hat{\phi}(x')$ is the phase difference operator and $\rho(x) = \langle\hat{\psi}^{\dagger}(x)\hat{\psi}(x)\rangle$ is the mean local density.

The correlation dip is due to the presence and geometry of the trap and, consequently, related to the shape of the occupied orbitals and exists even for relatively small interaction couplings. The built-in self-consistency of the MCTDH method is crucial in order to correctly describe the correlation phenomena in trapped quantum many-body systems, because the depth and location of the correlation dip sensitively depends on the self-consistently determined orbital shape.

We note in the top panel of Fig. 2 a sizable quantitative difference to the analytical solutions already for interaction strengths that are far below the hard-core limit of $g \to \infty$. However, for couplings commonly realized in experiments with magnetic traps (see for concrete estimates below), the agreement between the analytical results and MCTDH is very satisfactory, see the lower panel of Fig. 2, even for the relatively modest number of orbitals $M = 10$ used in these calculations. The characteristic dip in the correlation function appears for any interaction strength and is correctly reproduced by

the MCTDH method to good accuracy in its location, while the depth of the dip is somewhat exaggerated by MCTDH in particular for larger than intermediate couplings, $g \gg 1$.

3.3 Fragmentation

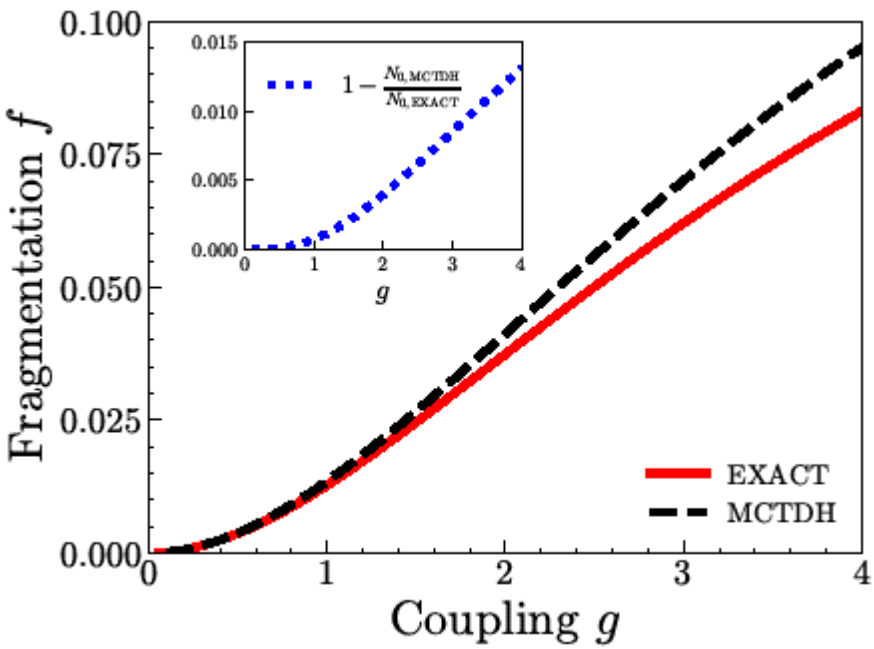

Fig 3. Fragmentation $\boldsymbol{f}$ as defined in Eq. (9), obtained from the diagonalization of the analytical SPDM (red solid) and from MCTDH (black dashed) with $\boldsymbol{M = 10}$ orbitals, for the range $\boldsymbol{g = 0.1, \ldots, 4}$. The inset shows the relative numerical error in the occupation number of the energetically lowest orbital.

Using the SPDM, one may formally define an important figure of

merit, the fragmentation. By diagonalizing the SPDM, one obtains its eigenfunctions, ϕ_i, and eigenvalues, N_i, which are in the many−body context referred to as *natural orbitals* and *occupation numbers*, respectively,

$$\rho^{(1)}(x,x') = \sum_{i=0}^{M-1} N_i \phi_i^*(x') \phi_i(x). \tag{8}$$

Here, the sum for MCTDH runs over the finite set $i = \{0, \ldots, M-1\}$ and for the exact solution over an infinite set $i = \{0, \ldots, \infty\}$. While a "macroscopic" orbital occupation defining fragmented condensates [48, 49] obviously cannot be obtained when $N = 2$, the average relative occupation of orbitals other than the energetically lowest is still well defined. We thus *define* the

$$\text{Fragmentation} \qquad f \coloneqq \frac{N - N_0}{N} \tag{9}$$

as the relative occupation number of all orbitals excluding the most populated one (which has $i := 0$), sorting occupation numbers N_i from largest to smallest.

In Fig. 3, we display the exact fragmentation f calculated using the exact density matrix in Eq. (6). We obtain the exact occupation numbers by first expressing $\rho^{(1)}(x,x')$ in a harmonic oscillator eigenfunctions basis of dimension $M_{ho} = 50$ (which proved sufficiently large) and by then diagonalizing it, evaluating the

integrals via the Gauss–Hermite approximation. The sizable difference when $g \gg 1$, is further illustrated in the inset, which shows the error in the occupation of the lowest orbital, $1 - N_{0,\mathrm{MCTDH}}/N_{0,\mathrm{exact}}$. Note that the fragmentation f obtained via MCTDH is always *larger* than the exact value, which is in agreement with the observation that the former approach overestimates the correlation dip in the first-order correlations (and hence also overestimates phase fluctuations), cf. Fig. 2.

3.4 Natural orbital

In Fig. 4, we plot the first six natural orbitals contained in the diagonalized SPDM Eq. (8). We conclude that sizable deviations between exact and MCTDH natural orbitals start to occur for $i = 4$ and above; within the resolution of the figure, we detected no discernible deviation in the first four, that is energetically lowest, natural orbitals, $i = 0, \ldots, 3$, the exact and MCTDH curves lying precisely on top of each other in this range. We also note in this context that the occupation numbers N_i for $i > 2$ are very small. For example, N_3 is about an order of magnitude less than N_2, for

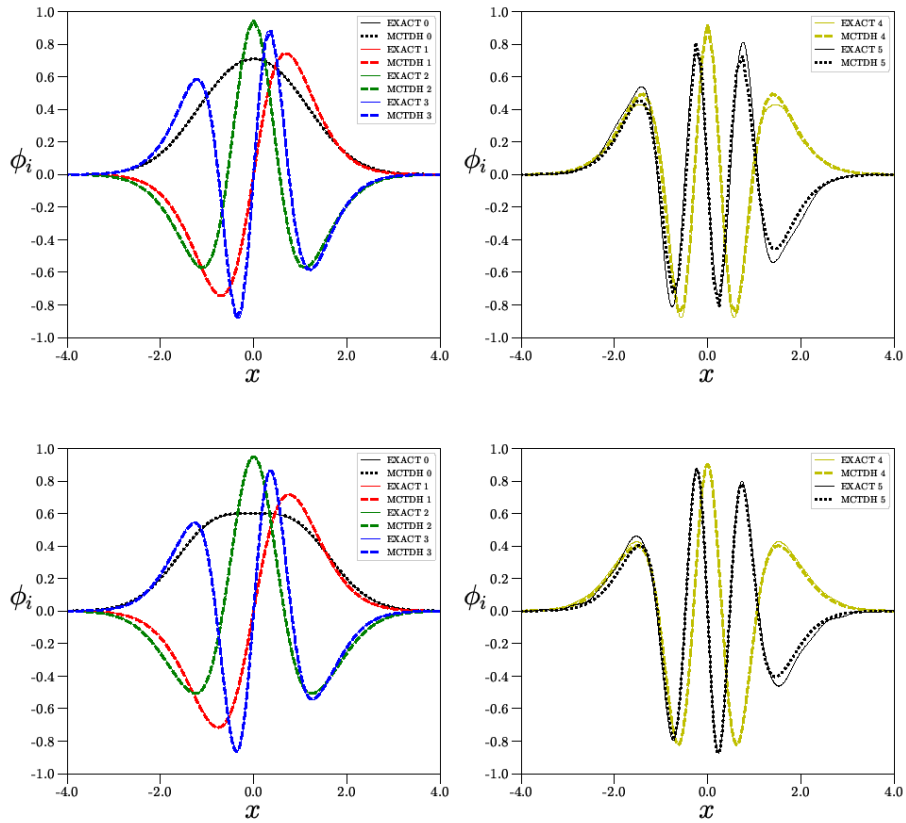

Fig 4. The first six natural orbitals $\boldsymbol{\phi_i(x)}$, $\boldsymbol{i = 0, \ldots, 5}$, in Eq. (8), obtained via MCTDH (dashed, $\boldsymbol{M = 10}$) and the exact results (solid), from diagonalizing the SPDM in Eq. (6) (solid). Left: $\boldsymbol{i = 0, \ldots, 3}$, right: $\boldsymbol{i = 4, 5}$. Top row: $\boldsymbol{g = 1}$, bottom row $\boldsymbol{g = 10}$.

both $g = 1$ and $g = 10$ and for both MCTDH and exact occupation numbers[②]. Therefore, it is indeed the occupation number difference

[②] Specifically, for $\mathrm{g} = 1$, $\mathrm{N}_2 \simeq 2.09 \times 10^{-3}$ (exact), $\mathrm{N}_2 \simeq 2.20 \times 10^{-4}$ (MCTDH, $\mathrm{M} = 10$), $\mathrm{N}_2 \simeq 2.14 \times 10^{-3}$ (MCTDH, $\mathrm{M} = 33$), while $\mathrm{N}_3 \simeq 4.12 \times 10^{-4}$ (exact), $\mathrm{N}_3 \simeq 4.34 \times 10^{-4}$ (MCTDH, $\mathrm{M} = 10$), $\mathrm{N}_3 \simeq 4.27 \times 10^{-3}$ (MCTDH, $\mathrm{M} = 33$).

of the lower natural orbitals (rather than their precise shape) which explains the different fragmentation obtained by MCTDH and exact solution. As a corollary, going to much larger M does not significantly decrease the $f-$difference further.

Chapter 4. Conclusion

We now illustrate the above general considerations by concrete numbers for an experimentally realizable system. In a *quasi−1D* Bose gas, and far away from geometric resonances [50], we have $g = 4a_{sc}\,l/l_{\perp}^{2}$ where $l_{\perp}$ is the transverse trapping length. For $^{87}\mathrm{Rb}$, this implies $g = 1.96 \times a_{\mathrm{sc}}[a_{\mathrm{Rb}}]\nu_{\perp}[\mathrm{kHz}]/\sqrt{\nu[\mathrm{Hz}]}$, where the background scattering length $a_{\mathrm{Rb}} = 5.29\mathrm{nm}$, $\omega_{\perp,\nu} = 2\pi\nu_{\perp,\nu}$, and the frequencies are scaled with typical experimental values see, e.g., [51, 52]. With the background scattering length of $^{87}\mathrm{Rb}$ and $g \sim O(1)$, the MCTDH results are in satisfactory accord with the analytical result for quasi−1D setups accessible by magnetic trapping.

Limits of the MCTDH approach can be explored, e.g., in optical lattices when one increases g towards the Tonks−Girardeau regime [37, 38]. While only at a filling of two per one−dimensional tube our results can strictly be applied, we anticipate that also for larger N qualitatively similar features as those in Fig. 2, and in particular the trap−induced correlation dip, should persist and be observable for example with (a combination of) Feshbach resonances [41] and higher aspect ratios. Variation of g and N and measurement of, e.g., the first−order correlations which have been investigated here paves

the way for a quantitative experimental assessment of the accuracy of MCTDH.

The detailed analysis of higher-order correlations [53] will then reveal further precise information on the applicability of the MCTDH method to strongly correlated systems.

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Appendix

MCTDH-X

MCTDH-X is one of the mostly used software to implement multi-configurational time dependent Hartree method numerically. It is mainly written with C and Fortran which is referred to have fast performance to proceed same code ran by other programming languages like python, and java and etc. This comes from the fact that C and Fortran are the programming language similar with assembly which have one-to-one correspondence machine code, so we can reduce unnecessary part of the code to optimize the performance. The author of MCTDH-X program has developed the code as common research purpose and suggested other to participate the development so the update for the software is relatively frequent. There exist simple scripts which enable scientist to implement the software without knowing detailed programming knowledge to run this program. However, as there are a few researchers on ultracold gas, reliability of the software is not clearly solved. Our research opened the way to relieve concerns about the software.

Set-up for Computation

One of the fascinating issues for our research is that we ran the program by using common desktop. We used intel i7-7700k and 64GB RAM for this research. It is not common to use 64 GB RAM for usual purpose, but 16 GB RAM was enough for most part of our research. The requirement for RAM becomes exponentially larger as $m+n$ becomes larger (m is the number of orbital and n is the number of particle), 64 GB is necessary when we try to calculate numerical solution when $n=2$ and $m=33$.

I used Ubuntu Desktop 16.04 LTS for our PC. It is because Windows OS is not suitable to use long-term calculation because performance becomes slower as uptime becomes higher. Recently Windows OS reduced this problem but most of libraries are available on Linux OS, and still Windows OS consumes some resource to operator.

For the computation machine, it is important to reduce bottleneck caused by Human. Running several programs at that time cannot utilize the full memory and computing power. Most of researchers working on science field are not familiar with job scheduling system which could be easily implemented. Job scheduling is a method in which computer runs another work just after currently working job is done. Therefore, when we try to utilize computational resource

without wasting IDLE time of computational machine, it is not an option to use job scheduler. On Ubuntu machine, Torque/PBS is easily available by using simple commands and it takes little resource for computing machine. Pushbullet is one of the best options to alarm research that the work is done. By using basic shell scripting knowledge, Pushbullet can let the researcher know the time queued job is done.

Trial and Error

On MCTDH-X, we can change the parameters to implement various situation in physics. This parameter can control the number of point of data in coordinate space and coordinate space region. Using narrow coordinate space increases the numbers of data point representing orbital data per unit distance, but it could bother physical validity of the configuration. Increasing number of points takes much more time to get the result. Therefore, it is important to calibrate appropriate number to get the results in a reasonable time period.

Further Consideration

There becomes more necessity to incorporate computational

approach to achieve new discovery. Using supercomputing cluster is one of the best option people takes for their result. But using supercomputer requires expensive funds and supercomputing system in SNU is not stable. As my experience to study computational skill which earns the grand prize on supercomputing competition, constructing supercomputing infrastructure on Physics department can produce way-breaking result for research process. Cloud computing service allows us to construct simple maintenance system.

요 약

우리는 접촉 퍼텐셜에 의해 상호작용하는 1차원 조화 덫에 있는 두 개의 보손을 고려하며, 이 문제의 완전 해를 다중 짜임새 시간 의존 하트리 (MCTDH) 방법으로 얻은 자체 모순없는 수치 해와 비교한다. 따라서 우리는 초저온 양자 기체에서 가장 흔히 실험적으로 구현되고 있으며 해석적 해를 가진 소수체 문제와 MCTDH 방법으로 예측된 결과를 벤치마킹한다. 자기적으로 갇힌 초저온 희석 보스 기체의 전형적인 배경 산란길이에 해당하는 중간정도의 무차원 결합세기까지 MCTDH 방법을 통해 정확한 접지 상태 에너지와 1차 상관 관계를 정확하게 재현하는 것으로 확인되었다. 예를 들어 페쉬바흐 공명 및 광학 덫치기의 조합에 의해 구성되는 더 강한 결합세기의 경우, MCTDH 접근방식은 위치 공간에서 1차 상관관계의 덫-유도 상관관계 오목함의 깊이를 과대평가하고 에너지가 가장 낮은 것을 제외한 궤도의 평균적인 상대적 점유로 정의되는 토막내기를 과소평가한다. 우리는 상관 함수의 정성적으로 유사한 특성이 더 큰 입자 수에 대해 발생할 수 있다고 예상하며, 초저온 원자에 대한 실험을 통해 MCTDH의 정확도를 정량적으로 평가할 수 있는 길을 열어준다.

주요어 : 보손, MCTDH, 완전해, 초저온 기체, 1차 상관 관계

학 번 : 2015-20317