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TWO-PARTICLE THERMAL DENSITY MATRICES IN ONE DIMENSION USING FINITE DIFFERENCE TIME DOMAIN (FDTD) METHOD

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ABSTRACT

A quantum system in the thermal equilibrium state is a mixed state consisting of statistical ensembles of several different quantum systems can be represented by a thermal density matrix. In this research, the thermal density matrix is calculated for two-particle system case non-interaction in one-dimensional square well and one-dimensional harmonic oscillator using finite difference time domain (FDTD) method. In addition, thermal density matrix calculations are also performed for the case of two particle systems interacting in a one-dimensional harmonic oscillator. We present results of probability densities, partition functions, and internal energies for three cases: two distinguishable particles, two fermions and two bosons. Validation of numerical results of thermal density matrix and probability density is accurate with analytical solutions. Then, the result of partition function and internal energy the system is strongly effect by temperature. At low temperatures, internal energy the system will lead to the lowest energy or ground state.

Introduction

A quantum system can be fully explained by a wave function if the system is in a pure state. A system is said to be in pure state if the N-system is in the same state and there is only one eigen value that has value and the other is zero. One example of the pure state of the atom or molecule is isolated in eigenstate [2]. But in practice, many quantum systems exist not only in pure state but also in mixed states comprising statistical ensembles of several different quantum systems [8], so calculations are required using a statistical operator density matrix. A quantum system in a state of thermal equilibrium is an example of a mixed state that can be represented by a thermal density matrix [4].

Density matrix was calculated using a time dependent Schrodinger equation solution. The analytical solution of the Schrodinger equation can solve only a small number of ideal cases and it is difficult to determine all eigenvalues and wave functions for two or more particles due to complex and long-term mathematical needs [18]. To simplify it requires a simple and fast method in calculating the density matrix even for a single particle system that is by numerical method.

Methods used to calculate numerical density matrix include Path Integral (PI), Monte Carlo (MC), and Finite Difference Time Domain (FDTD) methods. Among all the numerical methods available, the simplest and most appropriate method used to solve numerical solutions of time dependent equations is the FDTD method, because it has better efficiency and higher accuracy than other methods [10]. FDTD method is easy in programming and does not have to use super computer in running program. While Path Integral (PI) and Monte Carlo (MC) method in calculating density matrix requires manipulation of grid count and requires another approach to get wave function.

The FDTD method was successfully developed by Sudiarta and Geldart (2007) to solve a one dimensional, two dimensional, and three dimensional schrodinger equation solution. The solution of Schrodinger equation is done by transforming real time into imaginary time. In 2009, Sudiarta and Geldart used the FDTD method for numerical calculations of the density matrix for a single-particle quantum system with various potentials and explained numerical algorithms to solve single particle system cases in one, two and three dimensions. In addition, numerical equations of the FDTD method can also be used for systems of two or more particles, including bosons and fermions because of their great relevance in physics and quantum chemistry.

So, in this research will be calculated thermal density matrix, density, partition function, and internal energy system two distinguishable particles, two bosons and two fermions in one-dimensional square well and one-dimensional harmonic oscillator using the FDTD method by Sudiarta and Geldart. To get a good numerical method, should be done gradually from low to high dimension. Therefore, in this case study applied two particles in one dimension so that accuracy of thermal density matrix calculation, density, partition function, and internal energy can be easily validated with analytic solution.

Theory and Calculation (if any)

Bloch Density Matrix

The bloch density matrix is formed by summing the product wave function of the Schrodinger equation in imaginary time with the initial conditions selected. The reduction of the time-dependent Schr ¨odinger equation solution for the two-particle system in this study follows the declination techniques that have been done by [18], to obtain a bloch density matrix for a two-particle system,

$$C(\mathbf{R},\mathbf{R}',\beta)=\sum_{k=0}^{\infty}\psi_k(\mathbf{R},\tau=\beta/2)\,\psi_k(\mathbf{R}',\tau=\beta/2)^* \tag{1}$$

Then, the canonical thermal density matrix for a two-particle system is obtained by dividing the bloch density matrix with the system partition function,

$$\rho(\mathbf{R},\mathbf{R}',\beta)=\frac{C(\mathbf{R},\mathbf{R}',\beta)}{Z(\beta)}\,. \tag{2}$$

And for the particle density or diagonal elements the density matrix is obtained by equating the coordinates ie R '= R [1]. Then the obtained density is integrated and used $\int\phi_n(\mathbf{R})\phi_n^*(\mathbf{R}')d\mathbf{R}=1$, it is obtained the partition function for the two particle system shown by the equation below,

$$\int \rho(\mathbf{R},\mathbf{R},\beta)\,d\mathbf{R} = \sum_{n=0}^{\infty} \exp\{-\beta E_n\} = Z(\beta)$$

(3)

While for energy in two particle system can be determined from equation (3) that is [2],

$$U = -\frac{1}{Z(\beta)}\frac{\partial Z(\beta)}{\partial \beta} \tag{4}$$

And the eigen energy value of the two particle system is $E_n = \frac{n_1^2 + n_2^2}{2}$. For two-particle systems have three cases: two distinguishable particles and two indistinguishable particles. Two distinguished particles follow the Maxwell Boltzmann distribution, whereas two indistinguishable particles have two states: the particles have different spins and particles having the same spin. Particles with different spins can occupy the same state according to the Bose Einstein distribution, whereas the particles with the same spin can not be in the same state according to the Fermi Dirac distribution. In the study for particles with different spins used $n_1 = n_2$. As for the same spin particles are used the condition that ($n_1 \neq n_2$).

Reduce Two Particles to One Particle

The reduction of one particle (1-RDM) is essentially the square of a wave function that has all the coordinates of a particle, be it a particle one or a second particle. It can be seen in (5) below that the RDM of a single particle has only been $|\psi|^2$ integrated into all the coordinates except, with the coordinates of the particle one. The equation for reducing two particles to a single particle is

$$\rho(x_1, x_1') = \frac{\int \rho(x_1, x_2; x_1', x_2)\,dx_2}{Tr[\rho]} \tag{5}$$

with $\rho(x_1, x_1')$ is a particle density submatrix and Tr [ρ] is worth one if it is normalized [1].

Experimental Method

Numerical Method

Following the technique [17] the numerical solution of the time-dependent Schrodinger equation for two 1D particles with potential $V(x_1, x_2)$ is,

$$i\hbar\frac{\partial \psi(x_1,x_2,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x_1,x_2,t)}{\partial x^2} + V(x_1,x_2)\psi(x_1,x_2,t) \tag{6}$$

By using the atomic unit conversion ħ = m = 1 and the real time transformation into the imaginary time τ = it equation (6) will be

$$\frac{\partial \psi(x_1,x_2,\tau)}{\partial \tau} = \frac{1}{2}\frac{\partial^2 \psi(x_1,x_2,\tau)}{\partial x^2} - V(x_1,x_2)\psi(x_1,x_2,\tau) \tag{7}$$

The process of numericalization of equation (7) is to discretize using a finite difference scheme. By applying $\psi^n(i_1, i2) = \psi((i_1 + i_2)\Delta x,\ n\Delta\tau)$ with Δx and Δτ are space and time. For time derivatives it is a forward finite difference and a space derivative is twice a central finite difference.

$$\frac{\partial\psi(x_1,x_2,\tau)}{\partial\tau}=\frac{\psi^{n+1}(i_1,i_2)-\psi^{n}(i_1,i_2)}{\Delta\tau} \tag{8}$$

$$\begin{aligned}\frac{\partial^2\psi(x_1,x_2,\tau)}{\partial x^2}=&\frac{\psi^{n}(i_1+1,i_2)-2\psi^{n}(i_1,i_2)+\psi^{n}(i_1-1,i_2)}{\Delta x^2}+\\&\frac{\psi^{n}(i_1,i_2+1)-2\psi^{n}(i_1,i_2)+\psi^{n}(i_1,i_2-1)}{\Delta x^2}\end{aligned} \tag{9}$$

$$\psi^{n+1}(i_1,i_2)=\alpha\psi^{n}(i_1,i_2)+\beta\begin{bmatrix}\psi^{n}(i_1+1,i_2)-2\psi^{n}(i_1,i_2)+\psi^{n}(i_1-1,i_2)+\\\psi^{n}(i_1,i_2+1)-2\psi^{n}(i_1,i_2)+\psi^{n}(i_1,i_2-1)\end{bmatrix} \tag{10}$$

with constant $\alpha=\left[\dfrac{1-\frac{\Delta\tau}{2}V(i_1,i_2)}{1+\frac{\Delta\tau}{2}V(i_1,i_2)}\right]$ dan $\beta=\left[\dfrac{\Delta\tau}{2(\Delta x^2)\left(1+\frac{\Delta\tau}{2}V(i_1,i_2)\right)}\right]$

For a stable simulation, the value of Δτ must be stable and given by the relationship

$$\Delta\tau\le\left[\frac{1}{2\Delta x^2}\right]^{-1} \tag{11}$$

To get all the conditions (eigenstate) in the simulation used the initial wave function is a random function. Each simulation process is completed marked by the convergence of energy and randomized functions. Equation (7) is used iteratively to develop wave functions for the initial function. Then the numerical equation bloch density matrix is determined by using (1).

Result and Discussion

One-dimensional Square Well

Numerical equations of two-particle systems with dimensional widths a = π with V (x1, x2) = 0 for 0 < x1, x2 < π and V (x1, x2) = for x1, x2 > π and x1, x2 < 0. Wave functions for potential wells for the three cases of distinguishable particles, bosons (symmetry) and fermions (antisymmetry) is,

$$\psi_{Distinguishable}(x_1,x_2)=\begin{cases}\sqrt{\dfrac{2}{\pi}}[\sin(n_1x_1)\sin(n_2x_2)] & \text{For } 0<x_{12}<\pi\\ 0 & \text{For } x_{12}>\pi \text{ and } x_{12}<0\end{cases} \tag{12}$$

$$\psi_{Boson}(x_1,x_2)=\begin{cases}\sqrt{\dfrac{2}{\pi}}[\sin(n_1x_1)\sin(n_2x_2)+\sin(n_1x_2)\sin(n_2x_1)] & \text{For } 0<x_{12}<\pi\\ 0 & \text{For } x_{12}>\pi \text{ and } x_{12}<0\end{cases} \tag{13}$$

$$\psi_{Fermion}(x_1,x_2)=\begin{cases}\sqrt{\dfrac{2}{\pi}}[\sin(n_1x_1)\sin(n_2x_2)-\sin(n_1x_2)\sin(n_2x_1)] & \text{For } 0<x_{12}<\pi\\ 0 & \text{For } x_{12}>\pi \text{ and } x_{12}<0\end{cases} \tag{14}$$

Bloch density matrix is obtained from wave function using equation (1) for the three cases of two distinguishable particles (15), boson and fermion (16) is

$$C(x_1,x_1',x_2,x_2',\beta)=\begin{cases}\dfrac{2}{\pi^2}\displaystyle\sum_{n1=0}^{\infty}\sum_{n2=0}^{\infty}\begin{matrix}exp(-(n_1^2+n_2^2)\beta/2)\ x\\ [sin(n_1x_1)sin(n_2x_2)]\ x\\ [sin(n_1x_1')sin(n_2x_2')]\end{matrix} & For\,0<\mathrm{x}_{12}<\pi\ and\ 0<\mathrm{x}_{12}'<\pi\\ 0 & otherwise\end{cases}\tag{15}$$

and

$$C(x_1,x_1',x_2,x_2',\beta)=\begin{cases}\dfrac{2}{\pi^2}\displaystyle\sum_{n_1}\sum_{n_2}\begin{matrix}exp(-(n_1^2+n_2^2)\beta/2)\ x\\ [sin(n_1x_1)sin(n_2x_2)-sin(n_1x_2)sin(n_2x_1)]\ x\\ [sin(n_1x_1')sin(n_2x_2')-sin(n_1x_2')sin(n_2x_1')]\end{matrix} & For\,0<\mathrm{x}_{12}<\pi\ \text{and}\ 0<\mathrm{x}_{12}'<\pi\\ 0 & otherwise\end{cases}\tag{16}$$

Bloch density matrix for the case of two distinguishable particles, two boson and two fermion are then reduced to a single particle density matrix equation so that the above equation,

$$C(x_1,x_1',\beta)=\begin{cases}\dfrac{1}{\pi}\displaystyle\sum_{n1=0}^{\infty}\begin{matrix}exp(-(n_1^2+n_2^2)\beta/2)\ x\\ [sin(n_1x_1)sin(n_1x_1')]\end{matrix} & For\,0<\mathrm{x}_{12}<\pi\ \text{and}\ 0<\mathrm{x}_{12}'<\pi\\ 0 & otherwise\end{cases}\tag{17}$$

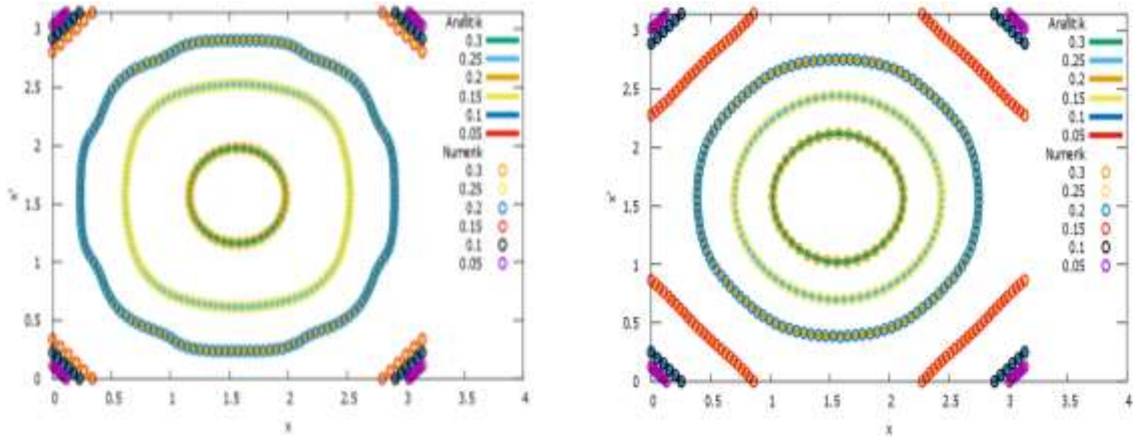
and

$$C(x_1,x_1',\beta)=\begin{cases}\dfrac{1}{\pi}\displaystyle\sum_{n1}^{\infty}\sum_{n2}^{\infty}\begin{matrix}exp(-(n_1^2+n_2^2)\beta/2)\ x\\ [sin(n_1x_1)sin(n_1x_1')+\\ sin(n_2x_1)sin(n_2x_1')]\end{matrix} & For\,0<\mathrm{x}_{12}<\pi\ \text{and}\ 0<\mathrm{x}_{12}'<\pi\\ 0 & otherwise\end{cases}\tag{18}$$

To calculate the analytical solution of probability density, partition function, and internal energy are obtained by deriving equations (17) and (18) using equations (2), (3), (4) and (5).

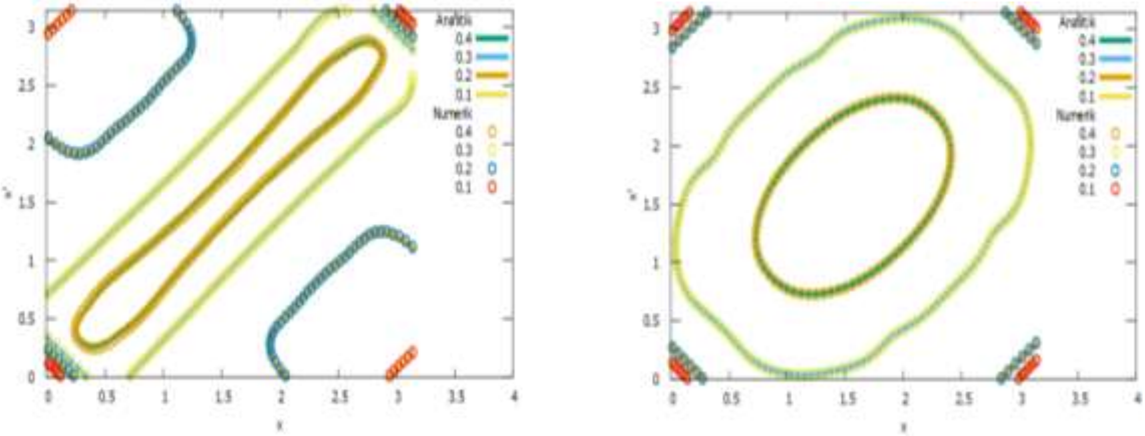
The density matrix analytical solution used as a comparison is the Bloch Density Matrix equation disclosed by [12] by taking temperature T = 1 for low temperatures and T = 10 for high temperature (with T in one unit temperature) for two distinguishable particles, two bosons and two fermions. Comparison of density matrix results using FDTD method with reference can be seen in Figure 5.1, Figure 5.2 and Figure 5.3.

The numerical results obtained by the FDTD method for density matrix are accurate with analytic results. The result of density matrix in two dimensional form has been converted into one dimension by assuming x '= x, so that the density of particle or diagonal element of density matrix n(x) = ρ (x, x, β) with T = 1, T = 10, and T = 100. The results obtained by using FDTD method are very suitable with the analytic result. The comparison of the results is shown in **Figure 5.4**.



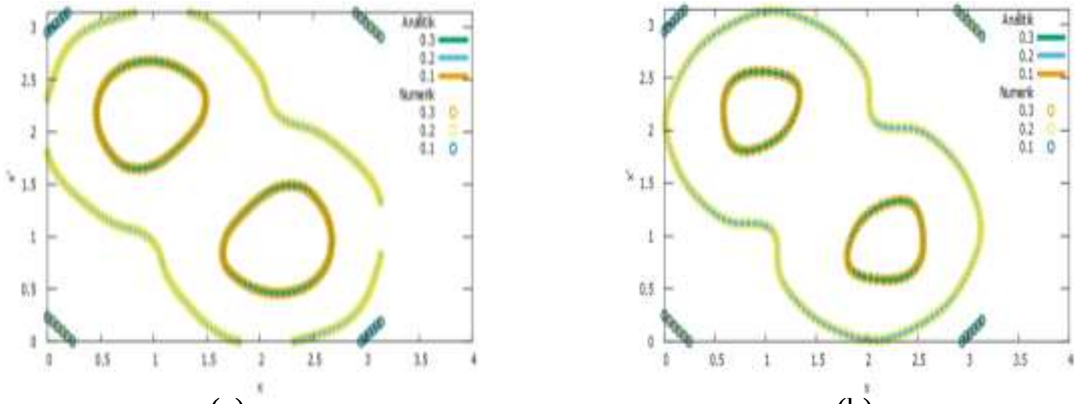
(a) (b)

Figure 5.1. Comparison of the numerical results of the thermal density matrix (circle) with the analytical solution (line) for two distingusable particles systems reduced to 1 particle (1-RDM) in one-dimensional square well at (a) β = 0.1 (T = 10) and (b) β = 1 (T = 1)



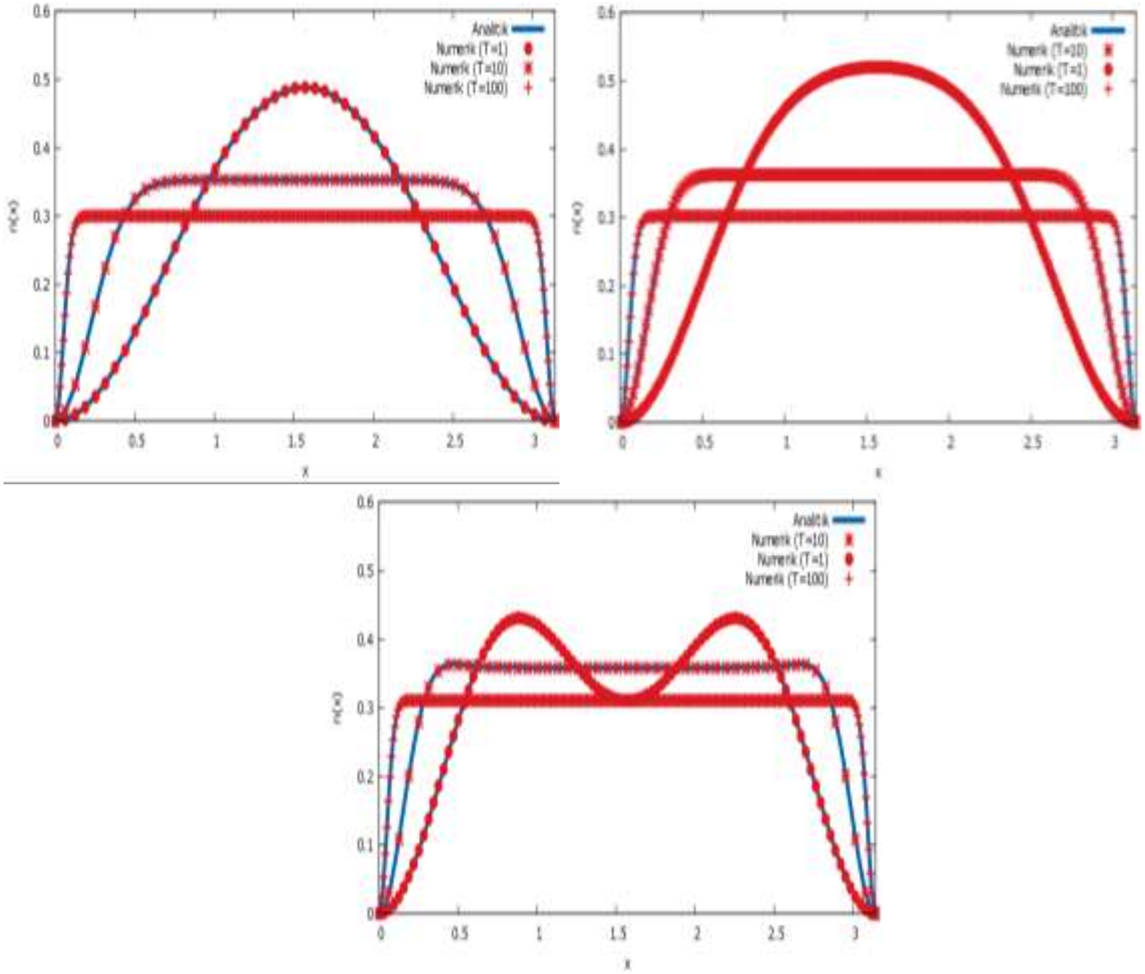
(a) (b)

Figure 5.2. Comparison of the numerical results of the thermal density matrix (circle) with the analytical solution (line) for two boson systems reduced to 1 particle (1-RDM) in one-dimensional square well at (a) β = 0.1 (T = 10) and (b) β = 1 (T = 1)



(a) (b)

Figure 5.3. Comparison of the numerical results of the thermal density matrix (circle) with the analytical solution (line) for two fermion reduced to 1 particle (1-RDM) in one-dimensional square well at (a) β = 0.1 (T = 10) and (b) β = 1 (T = 1)



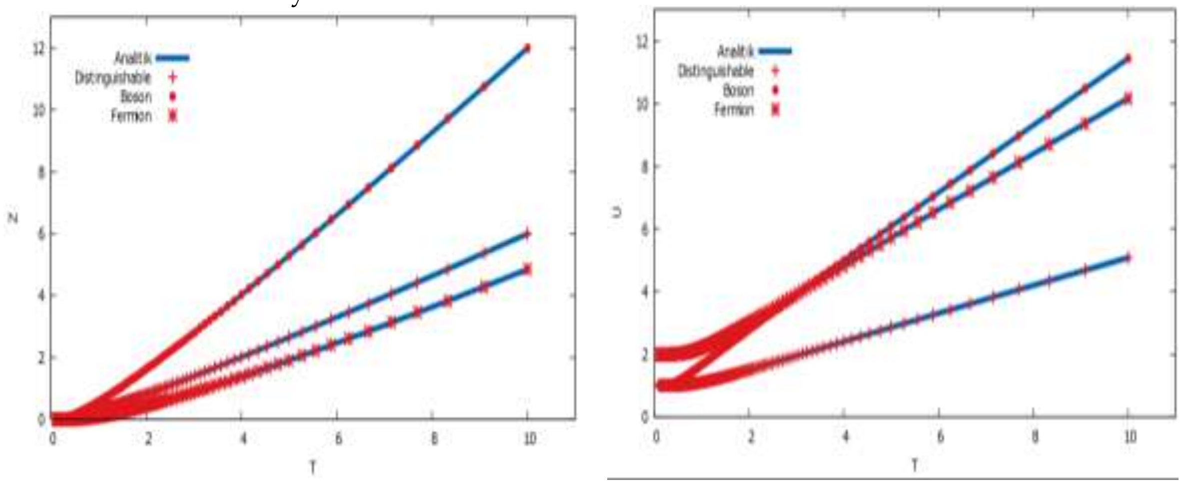
(c)

Figure 5.4. Comparison of numerical results of density with analytical solutions (Lines) for two particle systems reduced to 1 particles n (x) = ρ (x1, x1, β) in potential wells 1D at β = 0.01 (T = 100) (Plus), β = 0.1 (T = 10) (Croses), and β = 1 (T = 1) (Circle) for all three cases (a) distinguishable, (b) bosons and (c) fermions.

Figure 5.1, **5.2**, **5.3** and **5.4** describe particle distribution or particle probability for three cases: two distinguishable particles, boson ($n_1 = n_2$) and fermion ($n_1 \neq n_2$). The energy of a particle can not be known, but what can be done is to know the probability that a particle has a certain energy. In this study used closed systems or canonical systems that have contact with heat or environmental sources. Because the system is in an equilibrium state with a heat source, the system temperature must be equal to the heat source. Although the temperature is constant, the system energy will fluctuate due to the flow of energy going out and entering the system. Since energy is not constant, we can statistically say that any given energy has a certain probability.

For symetris or boson states, the particles described by the wave function are able to occupy the same position in space and do not violate Pauli rules so that the resulting graphic results show that both particles occupy the same peak. If the particles are exchanged, since the particles are indistinguishable, the distribution/probability of particles must be the same. On the other hand, for antisymetris or fermionic conditions, the particles have negligible probabilities that are found close to each other because the particles should not be in the same space so that the results obtained show that both particles do not occupy the same peak. So the difference between the boson and the fermion is only on the phases only.

As the preceding explanation, that the density of the particle represents the distribution or probability of the particle. By knowing the probability of a micro state or the probability of a particle system, then with that result can be determined the partition function and internal energy the system. The numerical results for the partition function and internal energy shown in **Figure 5.5** are validated by analytical solutions obtained from the density matrix of (3) and (4) with the temperature range from T = 0.1 to T = 10. The resulting obtained already in accordance with analytical solutions.



(a) (b)

Figure 5.5. Comparison of the numerical results of the partition function (a) and the internal energy (b) as a function of temperature with analytical solutions (Lines) for two particle systems in a potential well 1D for two distingusable particles (Square), two bosons (Circle) and two fermions (Triangle).

Partition function and internal energyis a function that explains the statistical properties of a system in equilibrium state. These two functions are interconnected with energy in the system can be expressed in the form of partition function or its derivative and both depend on temperature and other parameters such as gas volume and pressure. In this study, it is reviewed only the effect of temperature on a canonical ensemble system. Partition functions and internal energy are proportional to the temperature corresponding to (3) and (4). At low temperatures the energy in the system will lead to the lowest energy.

One-dimensional Harmonic Oscillator

The next case study to be discussed is a two particle system in one-dimensional harmonic oscillator with potential $V(x_1,x_2) = \frac{x_1^2+x_2^2}{2}$. By following the form of equation (1) then obtained thermal density matrix for two-particle system non-interacting is [5],

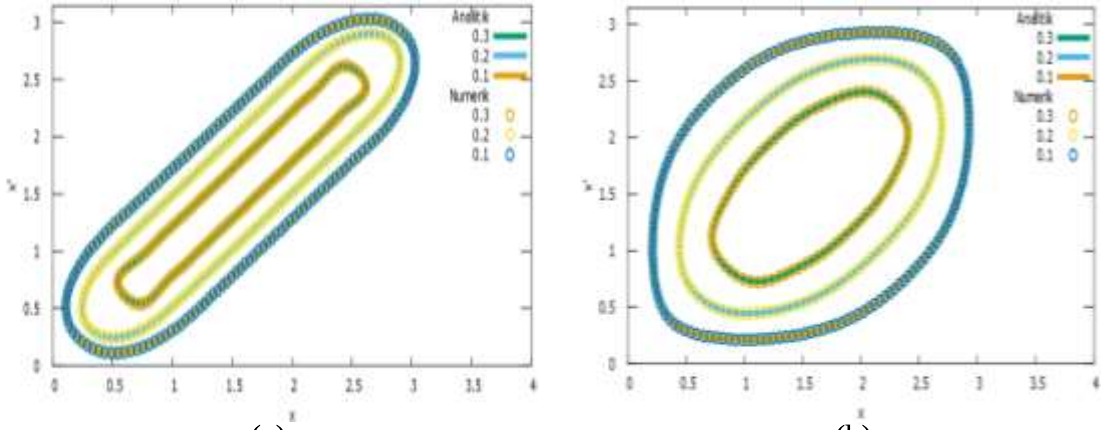
$$\rho(x_1,x_1',\beta)=\sqrt{\frac{1}{2\pi\sinh(\beta)}}\exp\left\{-\frac{1}{2\sinh(\beta)}\left[(x_1^2+x_1'^2)\cosh(\beta)-2x_1x_1'\right]\right\} \tag{19}$$

By following steps such as equations (2), (3), and (4) we can obtain probaility density, partition function and internal energy for two particle systems in harmonic oscillators.

To test the results of the accuracy of the research results for a two-particle system in a 1D harmonic oscillator potential, validation is required with analytic results. Two interacting particle systems such as two distinguishable particles, bosons and fermions have no analytical solution, then the numerical solution for a two-particle system in a harmonic oscillator potential is validated using a two-part system non-interacting because it has an analytical solution. In this study only calculate the density matrix for two identical two particles system is boson.

Two Particle non-interacting

Comparison of density matrix results using FDTD method with analytical solution for two-part system without interaction can be seen in **Figure 5.6**,



(a) (b)

Figure 5.6. Comparison of numerical results of thermal density matrix (Circle) with an analytical solution (Line) for 2 particles system without interaction reduced to 1 particle in 1D harmonic oscillator potential at (a) β = 0.1 (T = 10) and (b) β = 1 (T = 1)

The numerical results of the density matrix by the FDTD method obtained for the two-particle system non-interacting very well with the analytical solution of equation (20). Then from density matrix can be determined density of particle or diagonal element of density matrix n (x) = ρ (x, x, β) for system of two particles non-interaction in harmonic oscillator potential at temperature T = 1, T = 10, and T = 100. The result obtained by using FDTD method is very suitable with analytic result. The comparison of the results is shown in **Figure 5.7**.

By subtracting the density matrix from equation (20) it can be determined the partition function and the internal energy using (3) and (4). As the previous explanation on the two-particle system in the 1D potential well that partition function and internal energy is effected by temperature. With the partition function and internal energy proportional to the temperature change of the system and it also applies to the two-particle system in the harmonic oscillator potential. The numerical results for partition function and internal energy shown in **Figure 5.8** are validated by analytical solutions obtained from the density matrix with the temperature range from T = 0.1 to T = 10. The results obtained correspond to the analytical solution.

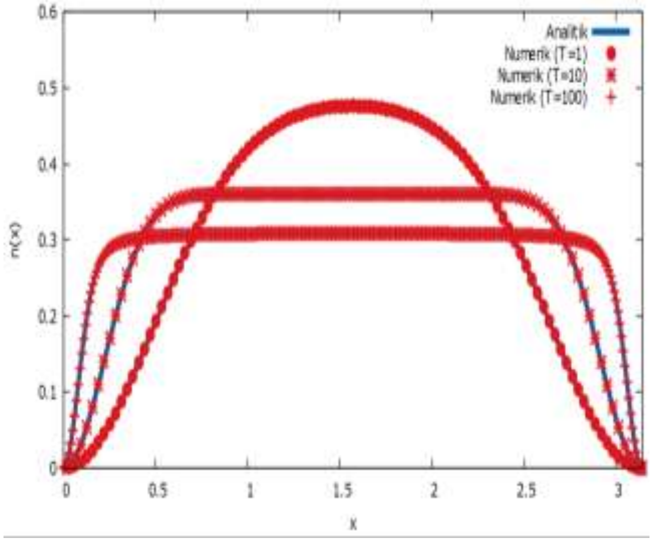
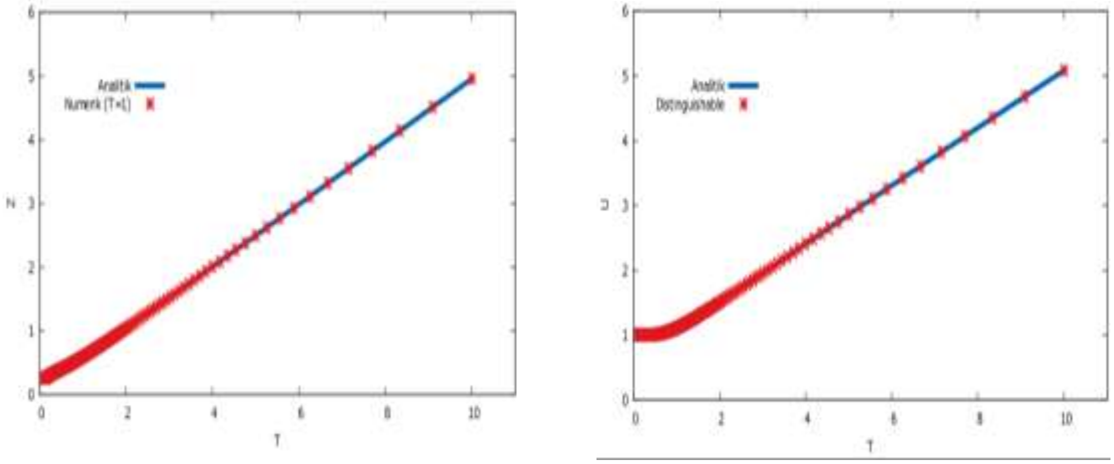


Figure 5.7. Comparison of numerical results of density or diagonal elements of density matrix with analytical solutions (Lines) for 2 particles system non-interacting reduced to 1 particles n (x) = ρ (x1, x1, β) in 1D harmonic oscillator potential at β = 0.01 (T = 100) (Plus), β = 0.1 (T = 10) (Crosses), and β = 1 (T = 1) (Circles).

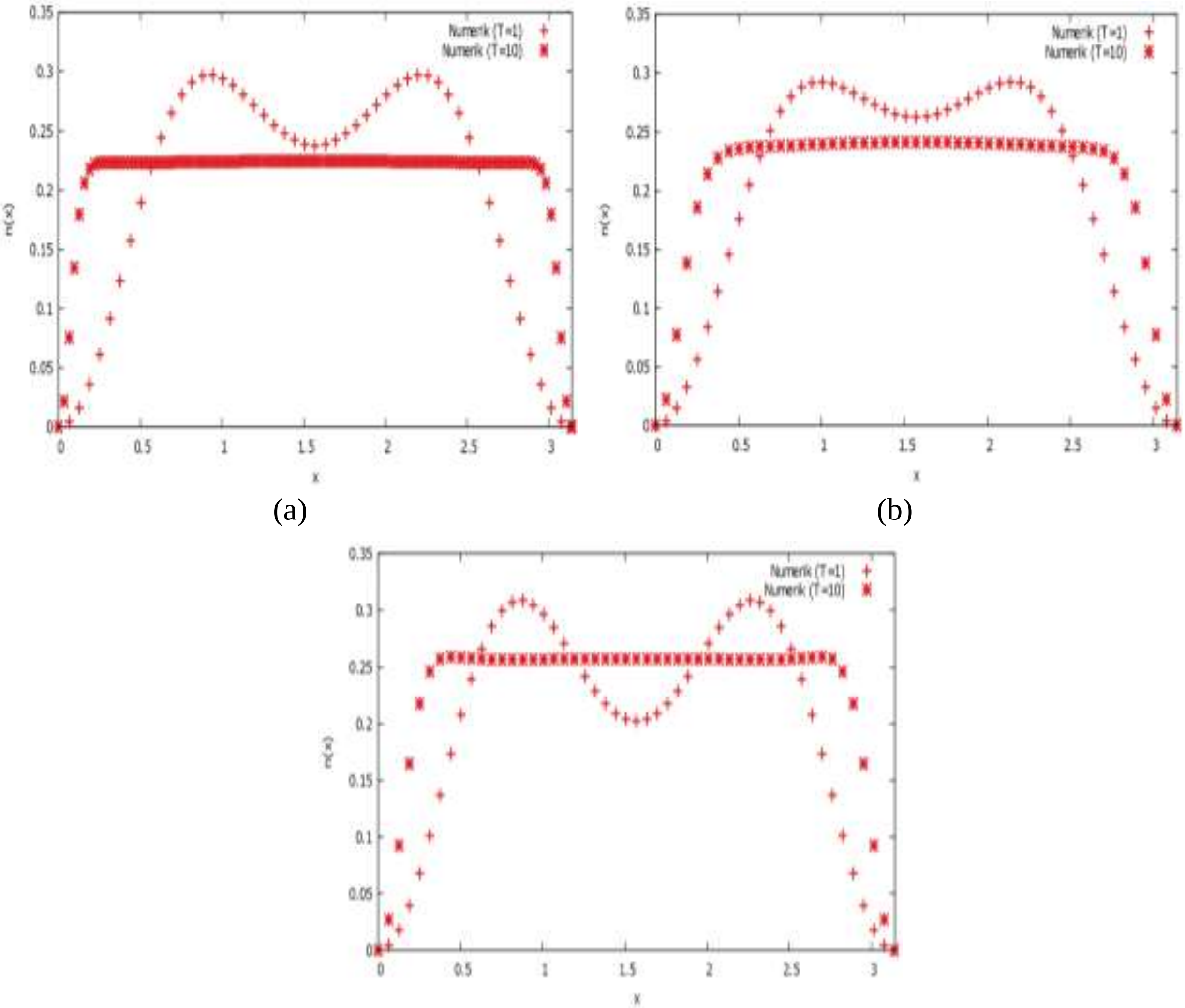


(a) (b)

Figure 5.8. Comparison of the numerical results of the partition function (a) and internal energy (b) as a function of temperature for the two-particle system non-interaction with the analytical solution (Line) in the 1D harmonic oscillator potential

Two Particle interacting

After validation of the numerical solution using a two-particle system non-interacting. The results obtained are accurate and in accordance with analytical solutions for density matrix, probability density, partition function and internal energy. From the validation results can be determined the results of numerical density matrix, probability density, partition function, and internal energy for two-particles system interacting with each other. Comparison of density results using the FDTD method with analytical solution for a two-particle system non-interaction can be seen in **Figure 5.9**,

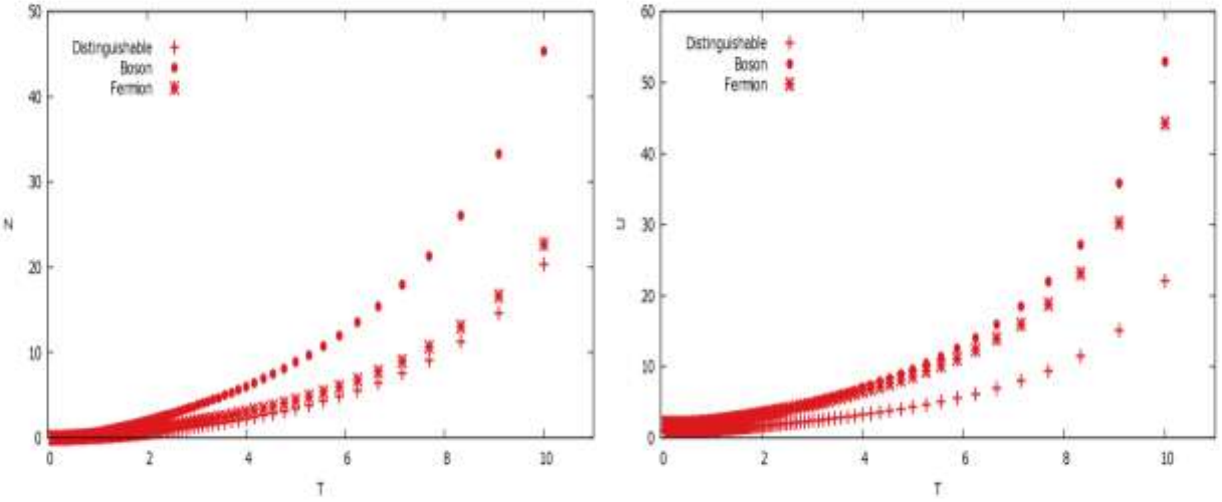


(a) (b)

(c)

Figure 5.9. The numerical results of the density or diagonal elements of the density matrix for the two particle interacting systems are reduced to 1 particles n (x) = ρ (x1, x1, β) in 1D harmonic oscillator potential at β = 0.1 (T = 10) (Crosses) and β = 1 (T = 1) (Plus) for all three cases (a) distinguishable, (b) bosons and (c) fermions.

The numerical results for partition functions and internal energy shown in **Figure 5.10** for the two-particle system interacting in 1D harmonic oscillator potential obtained from the density matrix with a constant temperature range of T = 0.1 to T = 10 for all three cases. Although the temperature is constant, the system energy will fluctuate due to the flow of energy out and enter the system. Since energy is not constant, it can be statistically said that any given energy has a certain probability. In addition, the energy in when at low temperatures will lead to the lowest energy.



(a) (b)

Figure 5.10. The numerical results of the partition function (a) and internal energy (b) as a function of temperature for the two particle systems interacting in 1D harmonic oscillator potential for (distingusable) particles (Plus), for bosons (Circles) and for fermions (Crosses).

Conclusion

Validation of numerical results of density matrix and density using FDTD method with analytical solution is highly accurate for two distinguishable particles, two bosons and two fermions non-interacting in one-dimensional potential wells and two interaction bosons in a harmonic oscillator potential. Numerical results for partition functions and internal energy that are validated with analytical solutions are appropriate and from these results it is seen that the partition function and internal energy is strongly effect by temperature changes.

References

Books with an author:

[1] Feynmann R P. 1972. Statistical Mechanics. Reading, MA : *Benjamin*.

[2] Greiner W, dkk. 1995. Thermodynamics and Statistical Mechanics. New York : *Springer*.

[3] Karl Blum. 2012. *Density Matrix Theory and Applications 3rd Edition*. Germany : *Springer-Verlag Berlin Heidelberg.*

[4] Landau L. D. and Lifshitz E. M. 1958. Statistical Physics. London-Paris: Pergamon Press.

[5] Neumann J V. 1955. Mathematical Foundations of Quantum Mechanics. Princeton : Princeton University Press.

Journal articles:

[6] Bransden B. H. *dan* Charles J. J. *1989*. Introduction to quantum mechanics. *Longman Scientific & Technical.*

[7] Borrmann P. 1994. Path Integral Density Functional Theory. Oldenburg: Carl von Ossietzky Universit at Oldenburg.

[8] D Ter Haar. 1961. Theory and Applications of the Density Matrix. Oxport : The Clarendon Laboratory. Online at http://iopscience.iop.org/0034-4885/24/1/307.

[9] Fano U. 1957. Description of States in Quantum Mechanics by Density Matrix and Operator Techniques. Washington : *National Bureau of Standards. Volume 29, Number 1*.

[10] Klem A. D. dan Storer R. G. 1973. The Structure of Quantum Fluids: Helium and Neon. Geelong : Mathematics Department, Gordon Institute of Technology. .*Aust. J. Phys.,* 1973, 26, 43-59.

[11] Kunz, K. S., & Luebbers, R. J. 1993. The Finite Difference Time Domain Method for Electromagneticcs. Boca Raton: CRC press.

[12] March N H, dkk. 1967. The Many-Body Problem in Quantum Mechanics. New York : Dover.

[13] Malone F. D, dkk. 2015. Interaction Picture Density Matrix Quantum Monte Carlo. London: Imperial College London. *The Journal of Chemical Physics 143, 044116 (2015).*

[14] McWeeny R. 1960. Some Recent Advances in Density Matrix Theory. Keele : Unverstiy College of North Staffordshire. *Volume 32, Number 2.*

[15] Novac I. 2001. Two Particles in a Box. Singapure : National University of Singapure.

[16] Storer R G. 1968. Path-integral Calculation of The Quantum Statistical Density Matrix for Attractive Coulomb Forces. *J. Math. Phys.* **9** 964.

[17] Sudiarta I W and Geldart D J W. 2007. Solving the Schr¨odinger Equation using The Finite Difference Time Domain Method. *J. Phys. A: Math. Theor.* **40** 1885 http://doi:10.1088/1751–8113/40/8/013.

[18] Sudiarta I W and Geldart D J. 2009. The Finite Difference Time Domain Method for Computing the Single-Particle Density Matrix. *J. Phys. A: Math. Theor.* 42 (2009) 285002 (20pp). http://doi:10.1088/1751-8113/42/28/285002.