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Lily Masyari Angraini; I. Wayan Sudiarta; I. G. N. Yudi Handayana; Marzuki

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Application of Diffusion Monte Carlo Method to Obtain The Ground State of A Particle in A Double Well Potential

Lily Masyari Angraini[1], I Wayan Sudiarta[1, a)], I G. N. Yudi Handayana[1], and Marzuki [1]

[1]Department of Physics, Faculty of Mathematics and Natural Sciences, University of Mataram, West Nusa Tenggara, Indonesia 83125.

[a)]Corresponding author: wayan.sudiarta@unram.ac.id

Abstract. In this paper, a diffusion Monte Carlo (DMC) method to determine the ground state of a particle in a double well potential is presented. The DMC method uses displacements, creations and deletions of diffusers or walkers. The effects of double well parameters on the ground state are studied. For validation of our DMC method, a harmonic oscillator potential is used and the DMC method gives accurate results. In the double well potential, the DMC results has shown that the ground state energy increases as the depth of the double well increases.

INTRODUCTION

The double-well potential is important for many applications in physics and chemistry. Many applications have been developed using the potential, especially for Bose-Einstein condensates phenomena [1,2,3]. For Bose-Einstein condensates, the application of the double-well potential has been successful to present of phase coherence [4], matter-wave implies that the appearing of quantum effects of an atomic Bose-Einstein condensate when it is interacting with a single-mode quantum traveling-wave laser field [2]. The other way to use the double-well potential in Bose-Einstein condensates problem is providing a natural generalization of atom interferometry [5,6]. Yuan Et all [2] used the double-well potential to trap the Bose-Einstein condensates for investigating the symmetry breaking phenomena and phase transition.

Common methods to solve the double-well potential are WKB approximation [7], canonical approach [8], and FDTD method [9]. Unfortunately, these methods can be described the ground state only in a few particles of boson and in few dimensions. In this paper, we apply the diffusion Monte Carlo (DMC) method to determine ground states of a double well potential.

The outline of this paper is as follows: the overview of the diffusion Monte Carlo method theory, numerical results of energies for one particle in an oscillator harmonic potential and a double-well potential, and in the last section is concluded.

METHOD

The DMC formulation for a particle in 2D double-well potential is established by the Schrodinger equation given by [10]

$$i\frac{\partial\Psi}{\partial t} = -\frac{1}{2}\left[\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2}\right] + \frac{1}{2}k\left((x^2 - a^2)^2 + y^2\right)\Psi \tag{1}$$

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where k and a are the double well parameters and we have used units such that $\hbar = m = 1$.

By replacing $V(x) \to V(x) - E_R$ and $E_n \to E_n - E_R$, and then we transform the real time to imaginary time by using a new variable $\tau = it$. This leads to a diffusion equation

$$\frac{\partial\Psi}{\partial\tau} = \frac{1}{2}\left[\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2}\right] - \left[\frac{1}{2}k\left((x^2 - a^2)^2 + y^2\right) - E_R\right]\Psi \tag{2}$$

In Eq. 3, there are two terms that can cause the wave function to vary with time: (1) a diffusion term which is represented by $\frac{1}{2}\left[\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2}\right]$ and (2) a birth-death process which is described by $\left[\frac{1}{2}k\left((x^2 - a^2)^2 + y^2\right) - E_R\right]\Psi$.

The solution of Eq. 2 can be expanded in eigen functions $\{\phi_n(x,y)\}$ as

$$\Psi(x,y,\tau) = \sum_{n=0}^{\infty} c_n \phi_n(x,y) e^{-(E_n - E_R)\tau} \tag{3}$$

It is noted from Eq. (3) that asymptotic behavior of the wave function for $\tau \to \infty$ (see Kosztin et al [10] for more detail) is

(i) diverging exponentially, $\lim_{\tau\to\infty} \Psi(x,y,\tau) = \infty$, for $E_R > E_0$;

(ii) vanishing exponentially, $\lim_{\tau\to\infty} \Psi(x,y,\tau) = 0$, for $E_R < E_0$;

(iii) approaching the ground state, $\lim_{\tau\to\infty} \Psi(x,y,\tau) = c_0\phi_0(x,y)$, for $E_R = E_0$ with a constant factor c_0.

A numerical procedure for the DMC method in this paper is following Kosztin et al [10]. First step is the setting of initial state at $\tau = 0$. Walkers are set to be distributed randomly as an initial wave function $\Psi(x_0, y_{0,} 0)$. The location of initial walkers is positioned in an area where the ground state is expected to be large. The next step is diffusive displacement where random walks produce new position by Gaussian random number generators. The last step is birth-death process of replication of walkers with weight factors $W(x_n, y_n)$ given by

$$W(x_n, y_n) \equiv \exp\left[-\frac{[V(x_n, y_n) - E_R]\Delta\tau}{\hbar}\right] \tag{4}$$

Efficient numerically to replicate each particle is described by [10]

$$w_n = min[int\,[W(x_{n.}y_n) + u], 3] \tag{5}$$

where u is a random number in an interval [0, 1]. "death " is a condition of a particle that caused by $w_n = 0$. In this case, the walker is eliminated. If $w_n = 2, 3$, it means new walkers are added and begin a new series of diffusive displacement and commonly it is referred to as "birth" of walker. The last condition is $w_n = 1$ where the walker is unaffected and continues with the next diffusion step.

RESULT AND DISCUSSION

Oscillator harmonic potential

To validate the DMC method, we perform DMC simulation for a particle in a harmonic oscillator potential in n dimensions. The potential is given by $V(x) = \frac{1}{2}\sum_{i=1}^{n} x_i^2$. The ground energies are $E_n = (n - \frac{1}{2})$. The wave functions are products of $\exp(-x_i^2/2)$. The numerical results of ground energies for one dimension to five dimensions are given in Tab. 1. It is noted that the numerical energies are in a good agreement with the exact energies.

An example of comparison between numerical and analytical ground state wave functions is shown in Fig. 1. The numerical wave function is also in a good agreement with the analytical wave function.

TABLE1. Numerical ground state-energies for a particle in oscillator harmonic potential in n dimensions computed by the DMC method are compared with exact energies.

Dimension	Exact	E	$\|\Delta E\|$
1	0.5	0.508819	0.008819
2	1.0	1.009488	0.009488
3	1.5	1.517112	0.017112
4	2.0	2.016395	0.016395
5	2.5	2.520226	0.020226

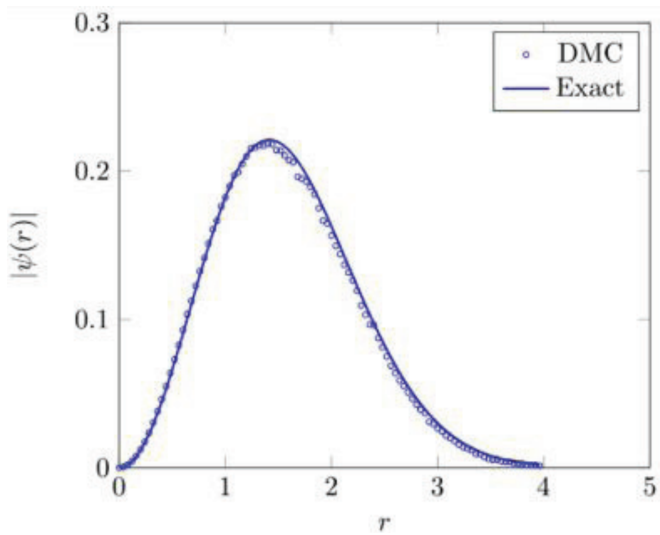


FIGURE 1. Numerical ground state wave function (symbol: circles) and analytical wave function (line) for a particle in two dimensional oscillator harmonic potential.

Double-Well Potential

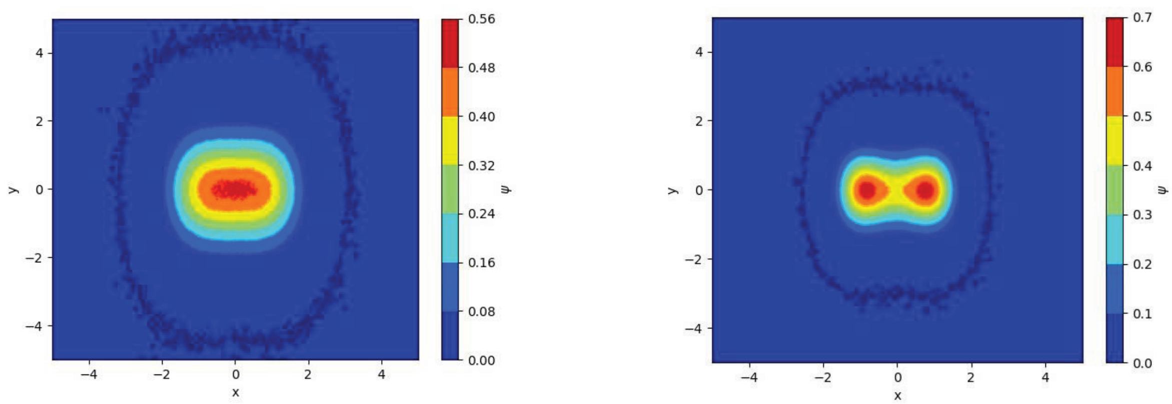
To demonstrate further application of the DMC method to obtain the ground state of a particle in a double well potential, we consider a particle in one dimension and two dimensional double well potential. Numerical ground state energies for one dimensional double well potential and two dimensional double well potential can be found in Tab. 2 and 3 respectively. A variation of the numerical wave function of two dimension double well potential for $k = 1$ and $k = 5$ with $a = 1$ is given in Fig. 2. It is shown in Tab. 2 and 3 that the ground state energies are dependent on the value of parameter k which is proportional to the depth of the double well. The ground state energies increase as the value of k increases.

TABLE 2. Ground state energies for a particle in 1D double well potential with parameter a = 1.

k	Number of Final Walkers (N)	E
1	1,569	0.574373
2	1,162	0.875431
3	2,681	1.168308
4	3,288	1.418263
5	3,448	1.664104

TABLE 3. Ground state energies for a particle in 2D double well potential with parameter a = 1.

k	Number of Final Walkers (N)	E
1	2,147	1.067650
2	4,272	1.581590
3	2,473	2.009591
4	2,826	2.404963
5	1,857	2.758406



(a) **(b)**

FIGURE 2. A variation of wave functions of two dimensional double well potential with *a = 1,* **(a)** *k =1* and **(b)** *k = 5*

CONCLUSION

A numerical method known as diffusion Monte Carlo (DMC) to obtain the ground state of a particle in a double well potential has been presented. The DMC method is validated using a harmonic oscillator potential. It has been shown that the DMC results are accurate compared to analytical results. The ground state energies for the double potential well potential are dependent on the depth of the well.

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