

University of Tripoli, Faculty of Science, Department of Physics

Calculation of Ground State Energy of Quantum Dots by Diffusion Monte Carlo (DMC)

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*A dissertation submitted to
the Department of Physics, Faculty of Science, University of Tripoli
in partial fulfillment of the requirements for
the degree of Master of science (M.Sc.)*

Spring, May (2017)

نموذج (17) أ

جامعة طرابلس

إدارة الدراسات العليا والتدريب

قرار لجنة المناقشة والكم

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- بمناقشة الرسالة المقدمة من الطالب / أمنة الصادق خليفة الفقيه لتتيل درجة الإجازة العالية (الماجستير)

في الفيزياء وعنوانها:

((_____ حسابات طاقة الحالة الأرضية للنقاط الكمية باستخدام طريقة DMC _____))

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- عدم إجازة الرسالة ويُمنح الطالب فرصة أخرى لمناقشتها في مدة أقصاها ثلاثة أشهر.
- رفض الرسالة.


التوقيع




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شكر و تقدير

الشكر لله تعالى الذي بنعمه تتم الصالحات أن وفقني بإتمام هذا العمل , أتقدم بجزيل الشكر والامتنان وخالص العرفان والتقدير للأساتذة الأفاضل أ.د محمد عبد العزيز و د. ابراهيم جوان اللذان شرفاني بقبول الإشراف على هذه الرسالة ودعمهما المتواصل وتوجيهاتهما القيمة .

وأتقدم بشكري الجزيل إلى أساتذتي الموقرين في لجنة المناقشة رئاسة وأعضاء لتفضلهم علي بقبول مناقشة هذه الرسالة، وأوجه شكري وخالص احترامي لجميع أعضاء هيئة التدريس بقسم الفيزياء. كما أتقدم بأسمى آيات الشكر لأسرتي وأصدقائي وكل من ساندني و أنار لي درب من دروب المعرفة.

الملخص

طبقت في هذه الرسالة تقنية مونتي كارلو الكمية (QMC) لحساب الحالة الأرضية للنقطة الكمية (helium dot)، وتمت كتابة الخوارزمية بلغة فورتران باستخدام طريقة مونتي كارلو للانتشار (DMC). وقد تم اختبار الخوارزمية المكتوبة أولاً لنظام كمي بسيط كالمتمذب التوافقي في بعد واحد وبعدين ، وقد كانت نتائج هذا الاختبار متوافقة مع النتائج العددية والتحليلية الأخرى.

بعد ذلك طبقت (DMC) للحصول على الحالة الأرضية لكل من (helium dot) وكذلك لذرة الهليوم وكانت النتائج دقيقة جداً مقارنة مع الطرق العددية الأخرى.

Abstract

The quantum Monte Carlo (QMC) technique has been applied to calculate the ground state of quantum dot (Helium dot). An algorithm is written in FORTRAN using Diffusion Monte Carlo (DMC) method.

The written algorithm has been tested first for a simple quantum system, as a Harmonic oscillators in one and two dimensions ,the results from this test correspond with other numerical and analytic results.

Then the ground state of the (Helium dot) and the Helium atom are obtained very accurately compared to other numerical methods.

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Chapter 1

Introduction: Quantum Dots

The quantum size confinement of electrons in semiconductor heterostructures have witnessed a rapid development of new results and ideas in the last few decades[1]. Technological advances in fabrication and precise measurement of various electronic and optical properties have created an exciting field of research in the theoretical and experimental physics of these electronic systems[2]. There have been several interesting developments where theoretical prediction and experimental surprises have resulted in a deeper understanding of the behavior of electrons in semiconductor heterostructures making the field an excellent example of how basic science and technology interact and influence one another[3]. The driving force behind much of the research on mesoscopic systems is the expectation that the miniaturization will lead to new type of electronic and optoelectronic devices much more advanced in their performance than what the existing

devices are specifically being much faster and dissipating less heat. In this thesis we study quantum dots[4].

Quantum dots can be classified according to fabrication methods used to produce them which are of three types: 1) colloidal quantum dots, 2) self assembled quantum dots, 3) electrically coupled single quantum dot[5]. Our interest will concentrate on single quantum dots that can be coupled to external current and voltage probes. These quantum dots can also be subjected to external homogeneous magnetic fields where their magneto-optical and magneto-transport properties can be studied[2]. More precisely, we will study a single two dimensional quantum dot of circular symmetry in which electrons are confined by an external harmonic oscillator potential.

In the rest of this introductory chapter, we will give a brief account of how single quantum dots are made from quantum wells and describe their main characteristic features. Then we give a short description of the quantum monte carlo method to be used for the calculation of the ground state of a many electron quantum dot. Before we conclude this chapter we will give the plan of the rest of the thesis.

1.1 Molecular Beam Epitaxy

The invention of Molecular Beam Epitaxy (MBE) in the late sixties by Arthur and Cho [6] in Bell laboratories has been deriving progress in the area of heterojunction structures and quantum devices. Due to this planar growth technique it has been possible to realize multilayered heterojunction with atomically abrupt interface and precisely controlled composition and doping profiles over distances as short as few nanometers [7]. In MBE apparatus (see Fig 1.1) the substrate is fixed on a heated rotating holder inside a high vacuum chamber. On the opposite side of the chamber effusion cells, containing the

materials to be grown, are sealed by a shutter system. The molecular beams are created by thermally evaporating the materials in the cells.

Abrupt interfaces could be made between semiconductors with different band gaps just by opening and closing shutters to the cells containing the materials. Most of the fundamental research concentrated on III - V group alloys. Such structures include quantum wells (or 2DEG), which are a key building block of band gap engineering and low dimensional electronic systems such as quantum wires (1DEG) and quantum dots (0DEG). Through the use of lithographic patterning and etching techniques quantum wires and quantum dots can be carved out of quantum wells.

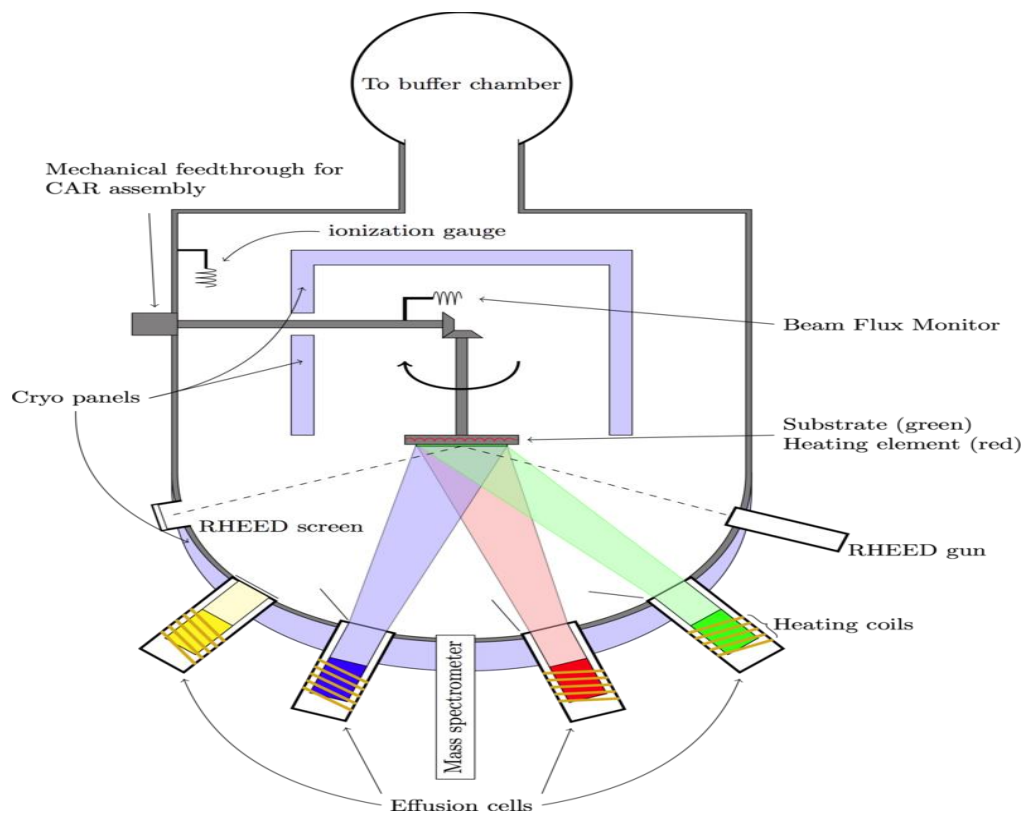


Figure1. 1 Molecular –Beam- Epitaxy (MBE)

1.2 Quantum Wells

Quantum wells are the first and most important semiconductor structures to be produced by MBE. These are electron systems confined to move freely in two dimension thus allowing to study the properties of a clean system of a two dimensional electron gas (2DEG). Quantum wells (see Fig1.2) are very thin, almost flat, semiconductor layers of low band gap material (usually GaAs) sandwiched between two layers of different semiconductor materials of high band gap (AlGaAs). To lower their energy the electrons stay in the quantum well planar region and because their de Broglie wave length is larger than the well width the electronic states become quantized in the direction perpendicular to the interface plane while free to move in the interface plane[7].

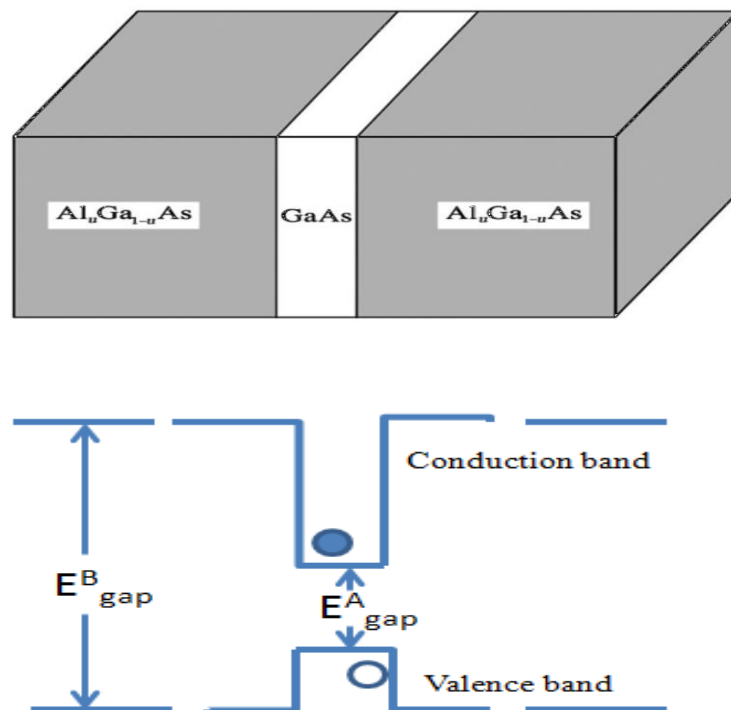


Figure1. 2: Illustration of a quantum well structure and its corresponding energy band diagram.

Magneto transport studies on si/sio₂ system and in selectively doped AlGaAs/GaAs heterojunction culminated in the discovery of two striking quantum phenomena in 2DEG

systems in high magnetic field, the integer and fraction Hall effects [3]. The quantization of the Hall resistance with precision of one part in 10^7 has led to a new resistance standard and to more accurate determination of the fine structure constant which is the coupling strength parameter in electromagnetism. The fractional quantization of the Hall resistance instead has revealed the existence of a new quantum fluid of correlated spin polarized electrons. These discoveries and many others demonstrate that semiconductor devices can be excellent tools for the study of fundamental physics. The transport and optical properties of these heterostructures can be tailored to specific device applications. For instance, quantum well laser are now in common use in optical disk drives of personal computers and in satellite signal receivers.

1.3 Quantum Dots

Further advances in (MBE) and breakthrough in nano lithography has made it possible to confine electrons in more dimensions, thus leading to quasi- one and zero dimensional semiconductor structures. Quasi-zero dimensional structures behave like artificial atoms. Individual atoms are the microscopic limit for small confined electron systems[8]. As a consequence of quantum confinement in all three dimensions the energy levels are discrete. Quantum boxes are so interesting because they are new class of artificially structured materials with atomic like discrete states which is ideal for use in laser structures. Conceptually it all started when a Russian physicist making micro crystals noticed that they exhibit various colors [9]. In trying to understand their physical origins he proposed that the free electrons in the small micro particles are confined in discrete quantum states in the mesoscopic particles and the electronic transition between these states emit the various colors according to their physical size see Fig. (13). This discovery alluded to the possibility of mesoscopic quantum system.

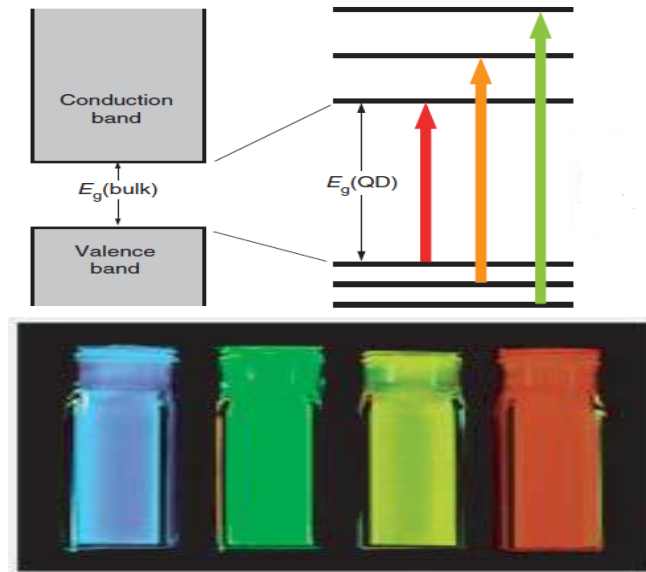


Figure 1.3: Solution of CdSe nanocrystal quantum dots of different sizes emitting different colors illustrating size quantization.

The predictions about interesting optical properties of quantum boxes are valid for $L < 10$ nm in which coulomb effects (which scale as $1/L$) are a weak perturbation to the quantum confinement effects, which scale as $1/L^2$ [10]. However, significant improvements in micro fabrication capability is still needed to make structures in this size regime with sufficient conformity. For optical properties one usually needs an array of typically more than a million identical quantum boxes. Present day q.boxes are in the $L \sim 1000\text{\AA}$ regime where the coulomb effects between the electrons are still important.

The first quantum dots with electrical contacts were produced by Reed et al [11], using masking and etching techniques common in the semiconductor industry. Using this method quantum dots with diameter in the range of (10-100 nm) were cut out of quantum well structure. Etched dots can have almost any shape or size. The band gap of QD, which defines its charge transport and optical transitions, is increased over the bulk semiconductor value with decreasing size of the dot. An example of the different possibilities is shown in Fig (1.4).

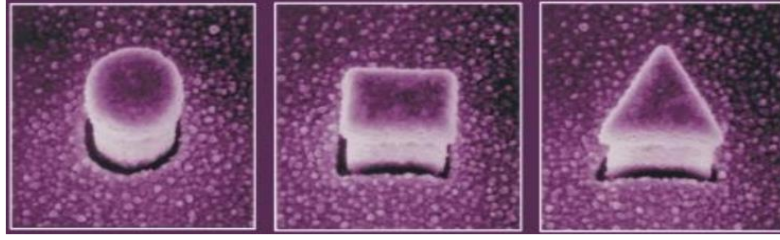


Figure1. 4: circle, rectangle and triangle LKouwemhoven

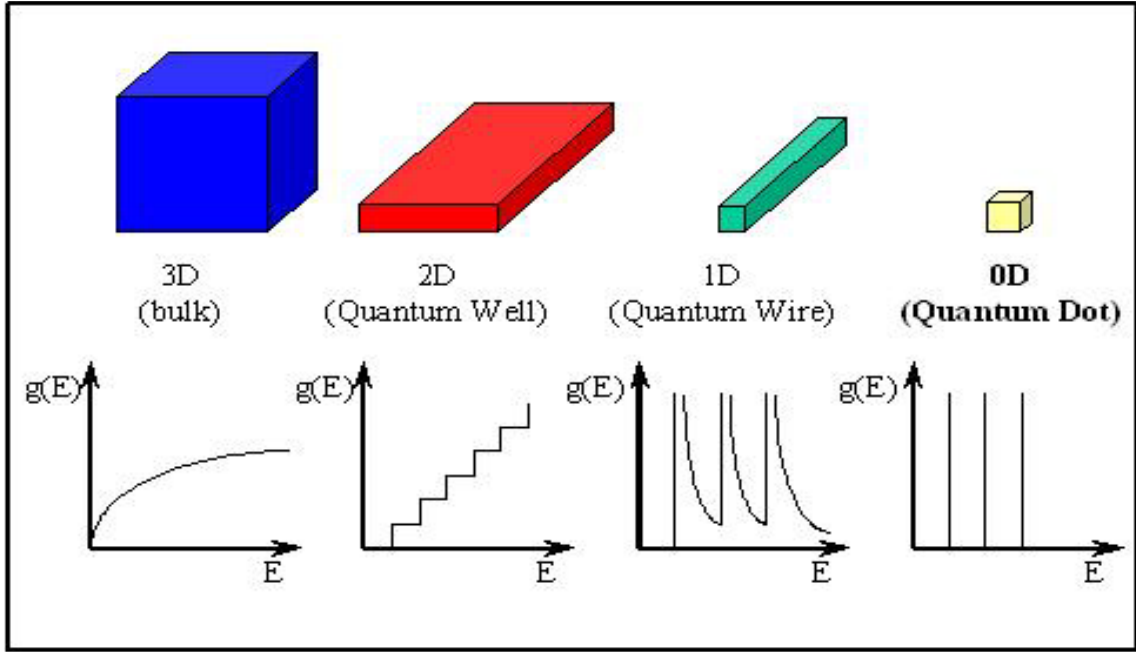
1.4 Density of States

Essential in the physics of these low dimensional structures is their density of state (DOS). The latter is the number of electronic states per unite energy interval. The DOS determines to a large degree the optical and transport properties of these systems and changes dramatically with the degree of confinement. In Fig(1.5), we show schematically how a three dimensional electron system evolves gradually in to a zero-dimensional system [13]. Let us consider a gas of free electrons in different space dimension from basic solid state physics we can calculate the DOS which is depicted in Fig (1.5). In the case of the three dimensional (3D) gas in the bulk with effective mass m^* , we have a free motion of electrons in all three directions with corresponding energy.

$$E = \frac{\hbar^2}{2m^*} (k_x^2 + k_y^2 + k_z^2) , \quad (1.1)$$

Table 1.1: classification of semiconductor structure and their degree of confinement

Structure	Degree of confinement	Dimension of structure
Bulk	0	3D
Quantum well	1	2D
Quantum wire	2	1D
Quantum dot	3	0D



3-D (bulk)	$g(E) = \frac{1}{2\pi^2} \left(\frac{2m^*}{\hbar^2} \right)^{\frac{3}{2}} \sqrt{E_g - E}$	
2-D (slab)	$g(E) = \frac{m^*}{\pi\hbar^2} \sigma(E_g - E)$	
1-D (wire)	$g(E) = \frac{m^*}{\pi\hbar} \sqrt{\frac{m^*}{2(E_g - E)}}$	
0-D (dot)	$g(E) = 2\delta(E_g - E)$	

Figure 1.5: Quantization of density of states

where $k_{x,y,z}$ are the wave vector components in each direction, the energy spectrum is therefore continuous and the corresponding density of states (DOS) is that of a bulk system $D_s \propto \sqrt{E}$ Fig.(1.5). In two-dimensional system on the other hand, the electron motion in the Z-direction is quantized into discrete states (electronic sub bands). The motion is, however, still free in the x-y plane;

$$E = \frac{\hbar^2}{2m^*} (k_x^2 + k_y^2) + E_z^i, \quad (1.2)$$

where $i= 1,2,3,\dots$, and DOS is strongly modified in this case near the quantization energies, showing step-function like behavior Fig (1.5). Additional lateral confinement of the electron motion leads to the one- dimensional system

$$E = \frac{\hbar^2 k_y^2}{2m^*} + E_z^i + E_x^j. \quad (1.3)$$

Where $j= 1,2,3,\dots$. The DOS is highly peaked and its modification from the 2D-DOS takes place at all relevant energies. Finally when the electron motion is confined in all directions one gets a zero dimensional system

$$E = E_x^i + E_y^j + E_z^k, \quad (1.4)$$

$k=1,2,3,\dots$, where the energy spectrum is discrete and DOS is a series of δ -function peaks (Fig1.5) these are quantum dots (QDs) the subject of this thesis ,these manmade object have lateral widths in the range of about ten to a few hundred nm, where the smallest ones are the self assembled system. The thickness of quantum dots created in GaAs/AlGaAs hetrostructures is $\sim 10- 20$ nm. Self-assembled in q- dots are only a few nm high.

In general, system is strictly two-dimensional only if the lowest two-dimensional subband is occupied. This is the same as the condition that the Fermi energy lies far below the second subband, or stated differently, as the condition that the thickness of the electron plane is much less than the average separation of the electrons. Low-dimensional electron system are, therefore low-dimensional only in the dynamical sense. Finally , we add that experimental evidence of the atomic like-delta-functions density of state in nm-scale quantum dots has indeed been reported recently. Similar discrete electronic state were also observed in metal quantum dots, where tunneling transistors containing single nm-scale Aluminum particles were made and discrete spectra of energy levels observed via current-voltage measurements.

1.5 Quantum Monte Carlo

Monte Carlo methods can be loosely described as statistical simulation methods, where statistical simulation is defined in quite general terms to be any method that utilizes sequences of random numbers to perform the simulation. Statistical simulation methods may be contrasted to conventional numerical discretization methods, which typically are applied to ordinary or partial differential equations that describe some underlying physical or mathematical system. In many applications of Monte Carlo, the physical process is simulated directly, and there is no need to even write down the differential equations that describe the behavior of the system. The only requirement is that the physical (or mathematical) system be described by probability distribution functions (PDF's). Once the PDF's are known, the Monte Carlo simulation can proceed by random sampling from the PDF's. Many simulations are then performed (multiple "trials" or "histories") and the desired result is taken as an average over the number of observations (which may be a single observation or perhaps millions of observations). In many practical applications, one can predict the statistical error (the "variance") in this average result, and hence an estimate of the number of Monte Carlo trials that are needed to achieve a given error. If we assume that the physical system can be described by a given probability density function, then the Monte Carlo simulation can proceed by sampling from these PDF's, which necessitates a fast and effective way to generate random numbers uniformly distributed on the interval $[0,1]$. The outcomes of these random samplings, or trials, must be accumulated or tallied in an appropriate manner to produce the desired result, but the essential characteristic of Monte Carlo is the use of random sampling techniques (and perhaps other algebra to manipulate the outcomes) to arrive at a solution of the physical problem. In contrast, a conventional numerical solution approach would start with the mathematical model of the physical system, discretizing the differential equations and then solving a set

of algebraic equations for the unknown state of the system. It should be kept in mind that this general description of Monte Carlo methods may not directly apply to some applications. It is natural to think that Monte Carlo methods are used to simulate random, or stochastic, processes, since these can be described by PDF's. However, this coupling is actually too restrictive because many Monte Carlo applications have no apparent stochastic content, such as the evaluation of a definite integral or the inversion of a system of linear equations. However, in these cases and others, one can pose the desired solution in terms of PDF's, and while this transformation may seem artificial, this step allows the system to be treated as a stochastic process for the purpose of simulation and hence Monte Carlo methods can be applied to simulate the system. There are, at least four ingredients which are crucial in order to understand the basic Monte- Carlo strategy. These are 1) Random variables, 2) probability distribution functions (PDF), 3) moments of a PDF 4) and its pertinent variance.

Chapter 2: This chapter gives general preview on Quantum Monte Carlo methods (QMC) and their types; it will focus on the diffusion quantum Monte Carlo (DMC). Furthermore, numerical logarithm of DMC is introduced.

Chapter 3: This chapter will apply the QMC algorithm to determine the ground state of harmonic oscillator in one and two dimensions. Then discusses the results and comparisons with others. Finally we will calculate the ground state of parabolic confined quantum dots for up to 2 electrons with coulomb repulsion (like helium atom) based on DMC method.

Chapter 2

Quantum Monte Carlo Methods

2.1 Introduction to Many-Body Schrödinger Equation

The Schrödinger equation provides the accepted description for microscopic phenomena at non-relativistic energies. Many molecular and solid state systems are governed by this equation. Unfortunately, the Schrödinger equation can be solved analytically only in a few highly idealized cases; for most realistic systems one needs to resort to numerical solution.

One of the main challenges of condensed-matter physics and quantum chemistry is the accurate solution of the Schrödinger equation. Since the nuclei are about thousand times heavier than the electrons, the most common approach is to decouple the electronic and ionic degrees of freedom that is known as the Born-Oppenheimer approximation. The electronic part of non-relativistic Born-Oppenheimer Hamiltonian for quantum system of

N_e electrons in the presence of N_I nuclei in Hartree atomic units $\hbar = m_e = e = 4\pi\epsilon_0 = 1$ is then given by

$$\mathcal{H} = \frac{1}{2} \sum_i \nabla_i^2 - \sum_i \sum_I \frac{Z_I}{|r_i - R_I|} + \frac{1}{2} \sum_i \sum_{j \neq i} \frac{1}{|r_i - r_j|}, \quad (2.1)$$

where i and j indexes are summed over all electrons and I index is summed over all nuclei.

A spectrum of states $\{\varphi_n\}$ which diagonalizes the stationary Schrödinger equation

$$\mathcal{H}\varphi_n = E\varphi_n, \quad (2.2)$$

with Hamiltonian Eq.(2.1) is the solution of many-body problem.

The first quantitative calculations of multi-electron systems were accomplished by Hartree, and Hylleraas. Fock was initial in using the properly antisymmetric wave function, the Slater determinant, which established the Hartree-Fock (HF) theory. The HF theory replaces the hard problem of many interacting electrons with a system of independent electrons in a self-consistent field (SCF).[12]

In electronic structure of solids, the discoveries of the effective free electron theory together with Pauli exclusion principle and the band theory of Bloch were the first critical steps toward understanding crystals. In 1930s, the foundations for the basic classification of solids into metals, semiconductors and insulators were laid. Soon after, Wigner and Seitz performed the first quantitative calculation of electronic states of sodium metal. Today, the density functional theory (DFT) invented by Hohenberg and Kohn and applied by Kohn and Sham is the principal method for calculations of solids.

2.2 Quantum Monte Carlo Methods

Monte Carlo methods (MC) are a class of powerful stochastic numerical techniques to estimate values of high-dimensions. In this regard the MC methods are often more efficient than Conventional numerical method. Quantum Monte Carlo (QMC) methods are used to solve for the ground state of the Schrödinger equation. There are four methods commonly termed QM :

- 1) The variational quantum Monte Carlo method (VMC) [16,17].
- 2) The diffusion quantum Monte Carlo method (DMC) [18,19,23].
- 3) The Green's function quantum Monte Carlo method (GFMC).[20,21].
- 4) The path integral quantum Monte Carlo method (PIMC) [22].

These methods are by their nature strongly related and each has its own peculiar advantages and disadvantages relative to the others. To reveal this relation we will discuss two of the above mentioned methods employed in our computation, namely the Diffusion MC and the path integral MC methods. Here we follow closely Ref.14 for DMC and Ref.15 for PIMC.

2.3 Diffusion Quantum Monte Carlo

Diffusion Monte Carlo (DMC) method is a relatively recent numerical method to solve the Schrödinger equation for the ground state of many particle quantum systems.

The DMC method can be formulated in two different ways. These will be outlined first, followed by an overview of the computational algorithm [13].

The first formulation is based on the similarity between the imaginary time Schrödinger equation and a generalized diffusion equation. The kinetic (potential) energy term of the Schrödinger equation corresponds to the diffusion (source/sink or reaction) term in the generalized diffusion equation. The diffusion–reaction equation arising can be solved by

employing stochastic methods. Indeed, the imaginary time Schrödinger equation can be solved by simulating random walks of particles which are subject to birth/death processes imposed by the source/sink term. The probability distribution of the random walks is identical to the wave function. This is possible only for wave functions which are positive everywhere, a feature, which limits the range of applicability of the DMC method. Such a formulation of the DMC method was given for the first time by Anderson who used this method to calculate the ground state energy of small molecules ion such as H_3^+ [14].

A second formulation of the DMC method arises from the Feynman path integral solution of the time-dependent Schrödinger equation. By means of path integrals the wave function can be expressed as a multidimensional integral which can be evaluated by employing the Monte Carlo method. Algorithms to solve the diffusion-reaction equation obeyed by the wave function and algorithms to evaluate the path integral representation of the wave function yield essentially one and the same formulation of the DMC method.[15]

i) Diffusion Equation Formulation

Consider the time-dependent Schrödinger equation for a free particle moving in one dimension:

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 \psi(x, t)}{\partial x^2}, \quad (2.3)$$

where m is the mass of the particle. Eq (2.3) can be written as

$$\frac{\partial \psi(x, t)}{\partial t} = D \frac{\partial^2 \psi(x, t)}{\partial x^2} \quad (2.4)$$

where $D = \frac{i\hbar}{2m}$ is imaginary diffusion constant. We can write this equation with a real diffusion constant by replacing the time t to imaginary values as $t \rightarrow -i\tau$, then Eq (2.4) reads

$$\frac{\partial \psi(x, \tau)}{\partial \tau} = \frac{\hbar}{2m} \frac{\partial^2 \psi(x, \tau)}{\partial x^2}, \quad (2.5)$$

The initial wave function of the system can be written as:

$$\psi(x, 0) = \sum_{n=0}^{\infty} c_n \psi_n(x) \quad (2.6)$$

The solution of the real time Schrödinger equation is giving by:

$$\psi(x, t) = \sum_{n=0}^{\infty} c_n e^{\frac{-iE_n t}{\hbar}} \psi_n(x) \quad (2.7)$$

The solution of the imaginary time equation can be written as:

$$\psi(x, \tau) = \sum_{n=0}^{\infty} c_n e^{\frac{-E_n \tau}{\hbar}} \psi_n(x) \quad (2.8)$$

if $\tau \rightarrow \infty$, this equation is exponentially damped, with higher energies damped faster than lower energies. The ground state wave function in this case is written as:

$$\lim_{\tau \rightarrow \infty} \psi(x, \tau) = c_0 e^{\frac{-E_0 \tau}{\hbar}} \psi_0(x) \quad (2.9)$$

This behavior of the wave function provides the basis of the DMC method.

ii) Path Integral Formalism

The solution of the imaginary time Schrödinger Eq. (2.3) can be written as

$$\psi(x, \tau) = \int_{-\infty}^{\infty} dx_0 K(x, \tau | x_0, 0) \psi(x, 0) \quad (2.10)$$

where the propagator $K(x, \tau | x_0, 0)$ is expressed in terms of the well-known path integral, modified by the replacement t to be $t \rightarrow -i\tau$

$$\begin{aligned} K(x, \tau | x_0, 0) = & \lim_{N \rightarrow \infty} \int_{-\infty}^{\infty} dx_1 \dots \int_{-\infty}^{\infty} dx_{N-1} \left(\frac{m}{2\pi\hbar\Delta\tau} \right)^{\frac{N}{2}} \\ & \times \exp \left\{ -\frac{\Delta\tau}{\hbar} \sum_{j=1}^N \left[\frac{m}{2\Delta\tau^2} (x_j - x_{j-1})^2 + V(x_j) - E_R \right] \right\} \end{aligned} \quad (2.11)$$

Here $\Delta\tau = \tau/N$ is a small time step. set $x_N \equiv x$. The wave function $\psi(x, \tau)$ can be written in the form

$$\psi(x, \tau) = \lim_{N \rightarrow \infty} \int_{-\infty}^{\infty} \left(\prod_{j=0}^{N-1} dx_j \right) \prod_{n=1}^N W(x_n) \times P(x_n, x_{n-1}) \psi(x, 0), \quad (2.12)$$

where $P(x_n, x_{n-1})$ is defined as:

$$P(x_n, x_{n-1}) = \left(\frac{m}{2\pi\hbar\Delta\tau} \right)^{\frac{1}{2}} \exp \left[-\frac{m(x_n - x_{n-1})^2}{2\hbar\Delta\tau} \right], \quad (2.13)$$

and $W(x_n)$ is defined as:

$$W(x_n) = \exp \left[-\frac{[V(x_j) - E_R]\Delta\tau}{\hbar} \right]. \quad (2.14)$$

The function $P(x_n, x_{n-1})$ is related to the kinetic energy term in Eq.(2.11). This function can be thought of as a Gaussian probability density for the random variable x_n with mean equal to x_{n-1} and variance σ is giving by:

$$\sigma = \sqrt{\hbar\Delta\tau/m}. \quad (2.15)$$

The so-called weight function $W(x_n)$ depends on both the potential energy in Eq.(2.11) and the reference energy E_R . The main difference between the functions P and W is that the former can be interpreted as a probability density since

$$\int_{-\infty}^{\infty} dy P(x, y) = 1, \quad (2.16)$$

while the latter cannot.

The path integral Eq.(2.12) can be evaluated analytically only for particular forms of the potential energy $V(x)$. Fortunately, by choosing N sufficiently large, one can evaluate Eq.(2.12) numerically to any desired accuracy. However, since a suitable N is necessarily a large number, the standard algorithms of numerical integration cannot be employed directly, instead, one uses the so-called Monte Carlo method. According to this method any (convergent) N -dimensional integral of the form

$$I = \int_{-\infty}^{\infty} \left(\prod_{j=0}^{N-1} dx_j \right) f(x_0, \dots, x_{N-1}) P(x_0, \dots, x_{N-1}), \quad (2.17)$$

where P is a probability density, i.e., $P(x_0, \dots, x_{N-1}) \geq 0$, and

$$\int_{-\infty}^{\infty} \left(\prod_{j=0}^{N-1} dx_j \right) P(x_0, \dots, x_{N-1}) = 1, \quad (2.18)$$

integration of Eq.(2.18) can be approximated by the expression

$$II = \frac{1}{N} \sum_{i=0}^N f(x_0^i, \dots, x_{N-1}^i). \quad (2.19)$$

Where $x_j^i \in P$, i can take the value from one to N i.e. $i = 1, 2, \dots, N$; and $j = 0, \dots, N - 1$, are selected randomly with the probability density P . The larger N , the better is the approximation $I \approx II$. In fact, according to the central limit theorem [15], the values of I obtained as a result of different simulations are distributed normally, i.e., according to a Gaussian distribution, around the exact value I , the standard deviation being proportional to $1/\sqrt{N}$.

In order to evaluate $\psi(x, \tau)$ in Eq.(2.12), for given x, τ and N , one defines

$$P(x_0, \dots, x_{N-1}) = \prod_{n=0}^N P(x_n, x_{n-1}), \quad (2.20)$$

and

$$f(x_0, \dots, x_{N-1}) = \psi(x, 0) \prod_{n=1}^N W(x_n), \quad (2.21)$$

such that one can apply eq.(2.17) and Eq.(2.19). For this purpose we note that due to

$$\int_{-\infty}^{\infty} dy P(x, y) P(x, z) = P(x, z), \quad (2.22)$$

and Eq.(2.16) the probability distribution Eq.(2.20) does indeed obey the property

Eq.(2.18). The expression Eq.(2.19) can now be invoked to evaluate $\psi(x, \tau)$ by means the

path integral Eq.(2.16). This requires the generation of sets of coordinate vectors $x^{(i)} \in$

$$P, x^{(i)} = (x_0^{(i)}, x_1^{(i)}, \dots, x_N^{(i)}) \text{ for } i=1,2,\dots,N \text{ where } x_N^{(i)} = x.$$

In order to obtain vectors $x^{(i)}$ which sample the probability density P one proceeds as follows:

In a first step one generates, for a fixed $x = x_N^{(i)}$, a Gaussian random number with $x_{N-1}^{(i)}$ mean value $x_N^{(i)}$ (i.e., a Gaussian random number distributed about $x_N^{(i)}$) and variance σ , according to the probability density $P(x_N^{(i)}, x_{N-1}^{(i)})$ given by Eq.(2.13).

In a second step, a Gaussian random number $x_{N-2}^{(i)}$, with mean $x_{N-1}^{(i)}$ and variance σ , is generated according to $P(x_{N-1}^{(i)}, x_{N-2}^{(i)})$.

The steps are continued to produce random numbers $x_n^{(i)}$ until one reaches $x_0^{(i)}$.

Two consecutive random numbers $x_n^{(i)}$ and $x_{n-1}^{(i)}$ are related through the equation

$$x_n^{(i)} = x_{n-1}^{(i)} + \sigma \rho_n^{(i)}, \quad (2.23)$$

where σ is given by Eq.(2.15) and $\rho_n^{(i)}$ is a Gaussian random number with zero mean and a variance equal to one. The $\rho_n^{(i)}$'s can be generated numerically by means of algorithms referred to as random number generators. One can check, using Eq. (2.23) and Eq. (2.13), that the mean and the variance of $x_n^{(i)}(x_{n-1}^{(i)})$ are equal to $x_{n-1}^{(i)}(x_n^{(i)})$ and σ , respectively.

Therefore, the coordinate vectors $\{x_{N-1}^{(i)}, \dots, x_0^{(i)}\}$, obtained through equation Eq. (2.18) for $i = 1, 2, \dots, N$, are distributed according to the probability density Eq. (2.20). We note in passing that the sequence of positions x_n given by Eq. (2.23) defines a stochastic process, namely the well known Brownian diffusion process.

Repeating N times the sampling of P the wave function $\psi(x, \tau)$ can be determined according to Eq. (2.19) and Eq. (2.17). Unfortunately, the algorithm outlined is impractical since it provides only a route to calculate $\psi(x, \tau)$ for a chosen time τ , but no systematic

method to obtain the ground state energy and wave function, which requires a description for $\tau \rightarrow \infty$.

2.4 The components of DMC algorithm

The above Monte Carlo method can be used to determine simultaneously both E_0 and φ_0 . The basic idea is to consider the wave function itself as a probability density. This implies that the wave function should be a positive definite function, a constraint which limits the applicability of the suggested method. By sampling the initial wave function $\psi(x, 0)$ at N_0 points one generates as many Gaussian random walks which evolve in time according to Eq. (2.15) or, equivalently according to Eq. (2.18), instead of tracing the motion of each random walk separately, one follows the motion of a whole ensemble of random walks simultaneously. The advantage of this procedure is that one can sample the wave function of the system, through the actual position of the random walks and the products of the weights W along the corresponding trajectories, after each time step $\Delta\tau$. This procedure, as we explain below, also provides the possibility to readjust the value of E_R after each time step and to follow the time evolution of the system for as many time steps as are needed to converge to the ground state wave function and energy.

The DMC method, interprets the integrand in Eq. (2.17), i.e.,

$$W(x_N)P(x_N, x_{N-1}) \dots W(x_2)P(x_2, x_1)W(x_1)P(x_1, x_0)\psi(x_0, 0) \quad (2.24)$$

as a product of probabilities and weights to be modeled by a series of sequential stochastic processes $0, 1, 2, \dots, N$. We will explain now how these processes are described numerically.

Initial State

$\psi(x_0, 0)$: The 0-th process describes particles distributed according to the initial wave function, which is typically chosen as a Dirac δ – function

$$\psi(x_0, 0) = \delta(x - x_0), \quad (2.25)$$

where x_0 is located in an area where the ground state of the quantum system is expected to be large. The initial distribution Eq. (2.25) is obtained by simply placing all particles initially at position x_0 .

Diffusive Displacement

$P(x_n, x_{n-1})$: As we explained earlier, the successive positions $x_{n-1}x_n$, in Eq. (2.24) can be generated through Eq. (2.23). The Monte Carlo algorithm produces the positions $x_1 = x_0 + \sigma\rho_1, x_2 = x_1 + \sigma\rho_2$, etc by generating a series of random numbers with normal distribution $\rho_n, n = 1, 2, \dots$

Birth–Death Process

Instead of accumulating the product of the weight factors $W(x_n)$ for each particle, it is more efficient numerically to replicate the particles after each time step with a probability proportional to $W(x_n)$. In this way, after each time step $\Delta\tau$, the (un normalized) wave function is given by a histogram of the spatial distribution of the particles. The calculation of the wave function $\psi(x, \tau)$ can be regarded as a simulated diffusion–reaction process of some imaginary particles. In the replication process each particle is replaced by the number

$$m_n = \min[\text{int}[W(x_n) + u], 3], \quad (2.26)$$

where $\text{int}(x)$ denotes the integer part of x and u represents a random number uniformly distributed in the interval $[0, 1]$. In case $m_n = 0$ the particle is deleted and one stops the diffusion process; this is referred to as a “death” of a particle. In case $m_n = 1$ the particle is unaffected and one continues with the next diffusion step. In case $m_n = 2$, one continues with the next diffusion step, but begins also a new series. In case of $m_n = 3$, two new

series of diffusive displacements starting at the present location x_n . This latter case is referred to as the “birth” of a particle (of two particles for $m_n = 3$). From Eq. (2.21) one can see that at most two new particles can be generated whereas one would expect that for $\text{int}(W(x_n) + u) \geq 4$ three or more new series would be started. This limitation on the birth rate of the particles is necessary in order to avoid numerical instabilities, especially at the beginning of the Monte Carlo simulation, when E_R may differ significantly from E_0 . The error resulting from the limitation $m_n \leq 3$ is expected to be small since for sufficiently small $\Delta\tau$ we have

$$W(x) \approx 1 - \frac{V(x) - E_R}{\hbar} \Delta\tau, \quad (2.27)$$

which, evidently, assumes values around unity.

2.5 The DMC algorithm

The DMC algorithm used to obtain the ground state energy is as follows:-

1- Initialization:-

- i- N_0 initial walkers are distributed randomly in space.
- ii- E_R the reference energy is set to be the average potential energy of the walkers.
- iii- A step size $\Delta\tau$ (the time is advanced by a small $\Delta\tau$) is carried out.

2- Iteration:

- i- The walkers' positions are changed by random variate from a Gaussian distribution with mean 0 and standard deviation $\sqrt{\Delta\tau}$
- ii- For each walker the number m is calculated by $m = \text{integer} [w + u]$

where u is a random number uniformly distributed from 0 to 1, and $w(x)$ is the weight of the walker with position x defined as $w(x) = \exp [(E_R - V(x)) \Delta\tau]$

There are three cases to consider:-

if $m = 0$ the walker is destroyed

if $m = 1$ nothing is done

if $m > 1$, $m-1$ copies of the walker are made.

iii-To prevent uncontrolled growth, a maximum of two copies of any given walker are made at each iteration.

3- The update reference energy is calculated by the function:

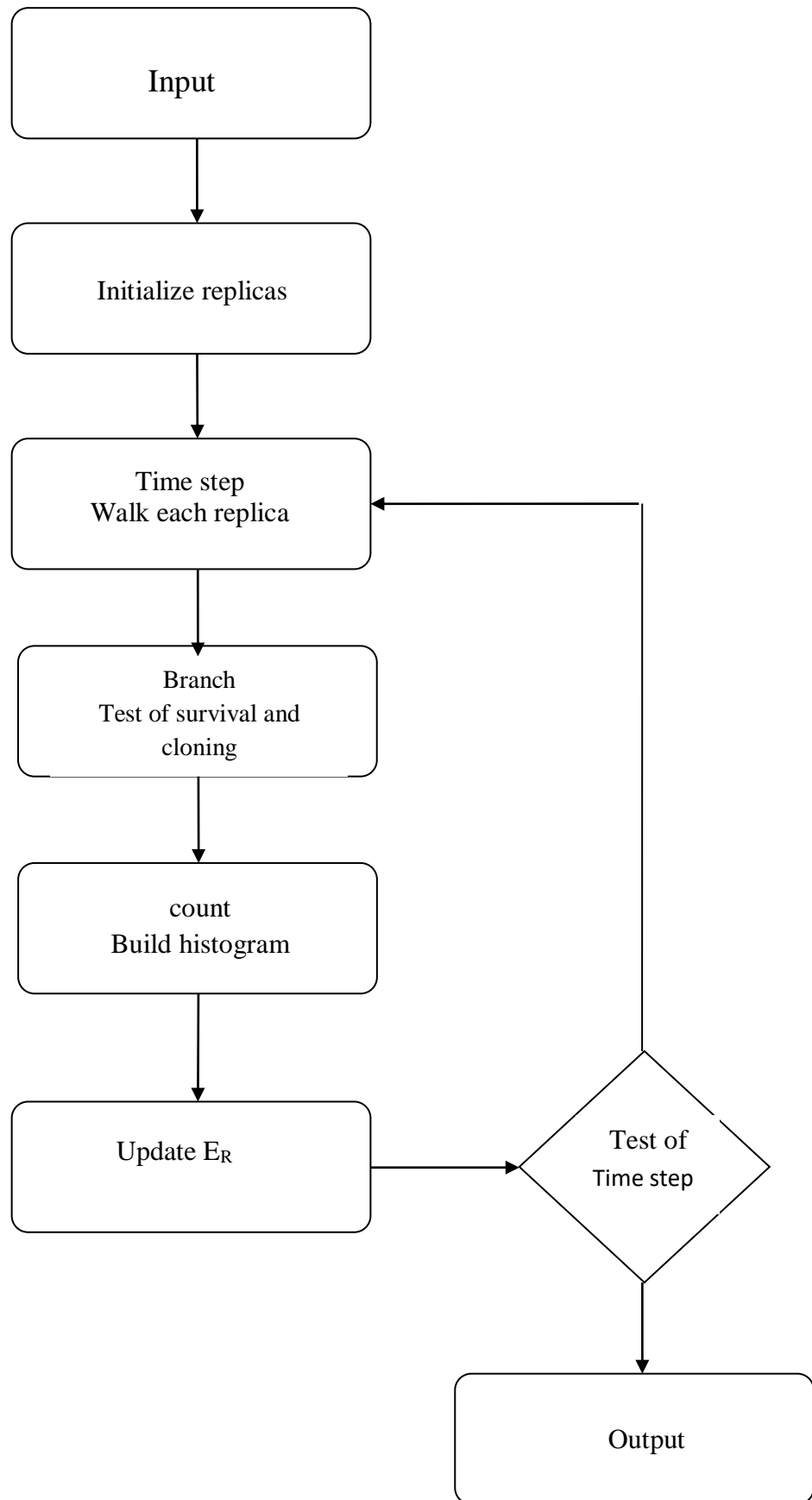
$$E_R = E_R + \alpha \left(1 - \frac{N}{N_0}\right), \quad (2.28)$$

where α is a control parameter to improve convergence, and N is the current number of walkers or replicas.

4- To estimate the ground state energy, the reference energies of successive iterations are averaged.

5- To estimate the ground state wave function, the special distribution (histogram) of the walkers of successive iterations is recorded and normalized.

2.6 DMC algorithm flow chart



Chapter 3

The ground state for two electron q.dot and Helium atom

3.1 Introduction

In this chapter we implement an algorithm for the DMC method presented in the previous chapter and apply this algorithm to obtain the ground state energy and the wave function for sample of quantum systems. One of the examples chosen below is the harmonic oscillator, have an analytical solution and, therefore, allow one to test the diffusion Monte Carlo method. Another example the Helium atom, cannot be solved exactly and, hence, the DMC method provides a convenient way of solving the problem. The obtained results for these cases turn out to be in good agreement with the results

obtained by means of other numerical methods. We also apply this algorithm to obtain the ground state energy and wave function for a quantum dot in two dimension.

We will present results obtained by means of the DMC program for the ground state energy and wave function of few quantum mechanical systems. The program was coded in Fortran. In each case we specify the units used and present numerical results ,and we will show that the agreement between the diffusion Monte Carlo result and the analytical expressions is very good. The numerical work in this chapter includes the following:

- 1- The 1-D (Harmonic oscillator one particle)
- 2- The 2-D (Harmonic oscillator one particle)
- 3- The 2-D (Harmonic oscillator two particles (non-interacting))
- 4- The 2- D (Two particles interacting in parabolic confinement (QDs))
- 5- The 3-D (Helium atom)

3.2 Test of algorithm

a) The Ground state of the Harmonic Oscillator in one dimension (single particle)

The potential of the simple Harmonic oscillator (SHO) is given as

$$V(x) = \frac{1}{2}m\omega^2 x^2 \quad (3.1)$$

The problem has a ground state energy of

$$E_0 = \frac{1}{2} \hbar\omega \quad (3.2)$$

And the ground state wave function is

$$\varphi_0 = \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}} \exp - \left(\frac{m\omega x^2}{2\hbar}\right) \quad (3.3)$$

In dimensionless units where $m\omega/\hbar = 1$, the potential is given by $V(x) = 1/2 x^2$ and the energy in units of $\hbar\omega$ is $E_0 = 1/2$ and the wave function is

$$\varphi_0 = (\pi)^{-\frac{1}{4}} \exp - \left(\frac{x^2}{2}\right) \quad (3.4)$$

We have applied the DMC algorithm with input parameters as follows (see Appendix D#1) for an initial number of replicas ($N_0 = 500$), the maximum number of replicas ($N_{\max}=1500$), the seed value for the random number generators (gasdev), the number of time steps =10000 , the value of the time step ($\Delta\tau = 0.01$). The obtained value of the energy with these parameters is $E_0 = 0.5$,

where the calculated history of E_0 is shown in Fig. (3.1) .

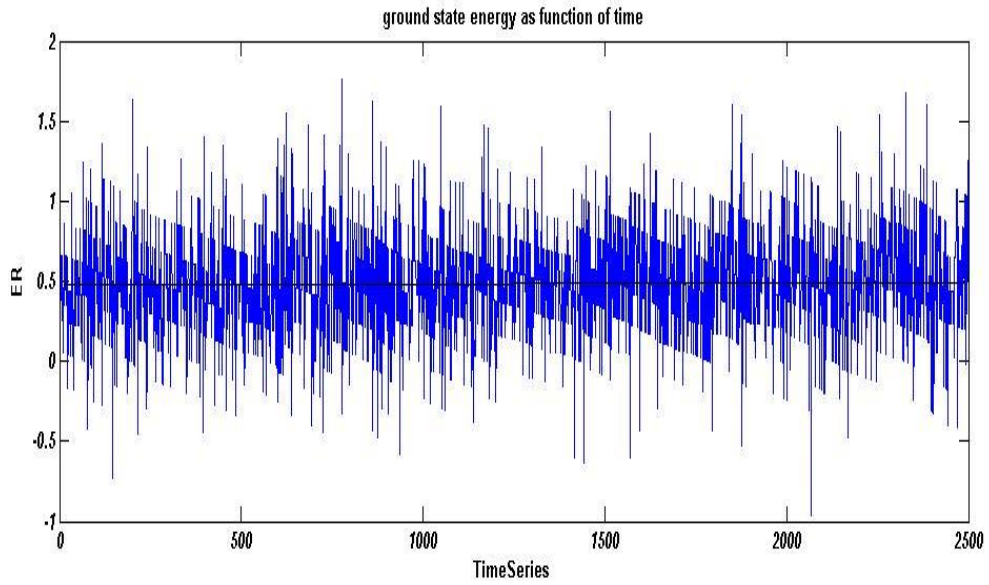


Fig3.1: Fluctuations of Reference energy E_R about its average value $E_R = 0.5$

In Fig (3.1) shows that fluctuations of E_R about its average value $E_R = 0.5$ after the distribution of replicas has reached its stationary form. The relatively large fluctuations are due to the birth–death processes which persist even if the replicas are distributed according to the exact ground state wave function $\varphi_0(x)$ and the reference energy E_R has been adapted to the exact ground state energy. The probability distribution for ground state is shown in Fig.(3.2).These results are in agreement with the analytical solution.

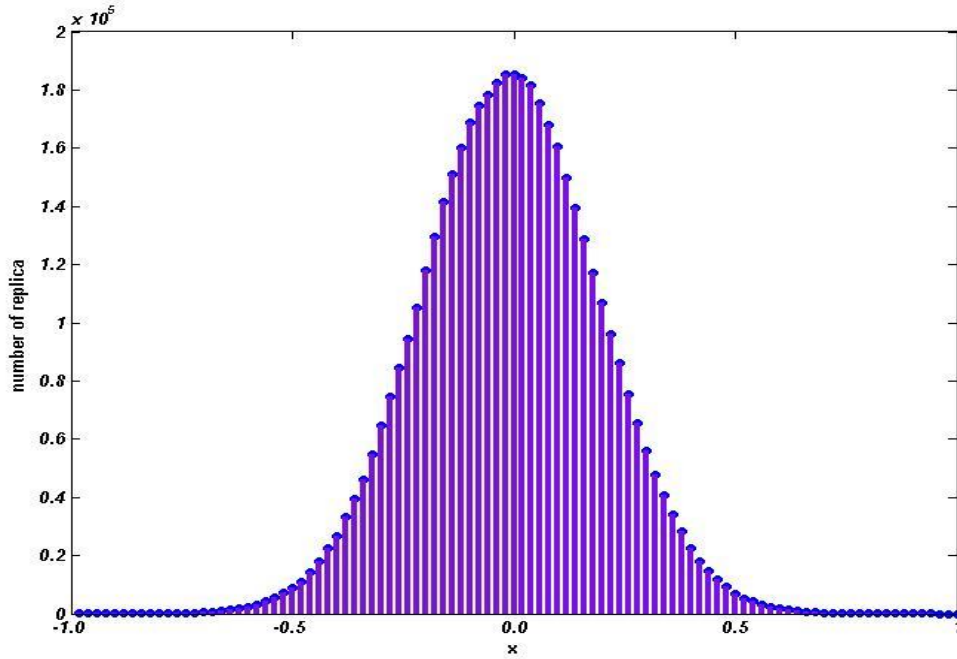


Fig. 3.2: histogram particle number distribution for replicas (DMC wave function for 1-D Harmonic Oscillator)

b) The Ground state of the Harmonic Oscillator in two dimension (single particle)

The potential in 2-D for a single particle (In dimensionless units where $m\omega/\hbar = 1$) is defined through

$$V(x, y) = \frac{1}{2}(x^2 + y^2) \quad (3.5)$$

The exact ground state energy is $E_0 = 1$ See Fig (3.3) for DMC results.

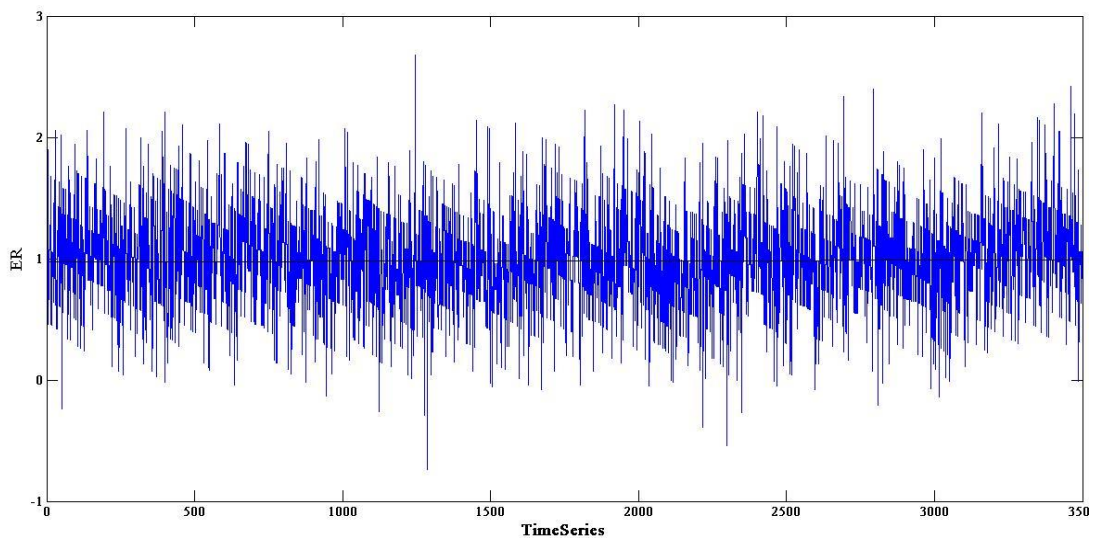


Fig3.3: Fluctuations of Reference energy E_R about its average value $E_R \approx 1$

and the probability distribution for the ground state is showing in Fig 3.4 , this figure shows the probability as function of coordinates resulting from running DMC program (see Appendix D #2), where we used number of initial clones $N_0 = 500$ for 10,000 time steps and as expected the ground state energy resulted from this calculation.

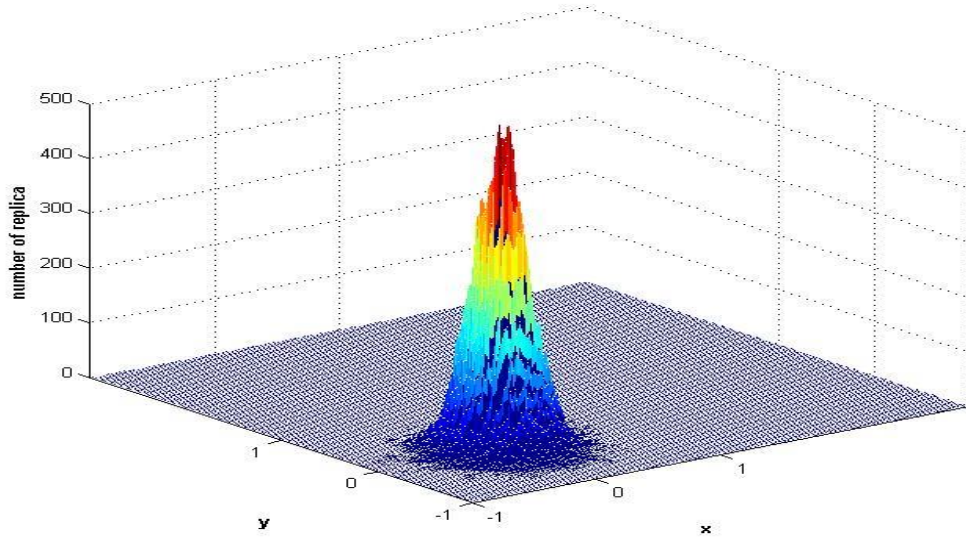


Fig. 3.4: probability distribution (in dimensionless units) as a function of the coordinate displacements obtained by the DMC method for single particle in 2-D harmonic oscillator.

c) The Ground state of the Harmonic Oscillator in two dimension (Two non-interacting particles)

In this case the potential becomes a harmonic potential in x and a harmonic potential in y (so that in dimensionless units), where the Coulomb interaction between the two particles is turned off resulting in a potential of the form

$$V(x, y) = \frac{1}{2} [(x_1^2 + y_1^2) + (x_2^2 + y_2^2)] \quad (3.6)$$

The appropriate DMC program is #3 (see Appendix D) and running it results in the ground state energy of value $E_0 = 2.0$ matching the exact result. Fig (3.5) shows the probability distribution of one of these non interacting particles.

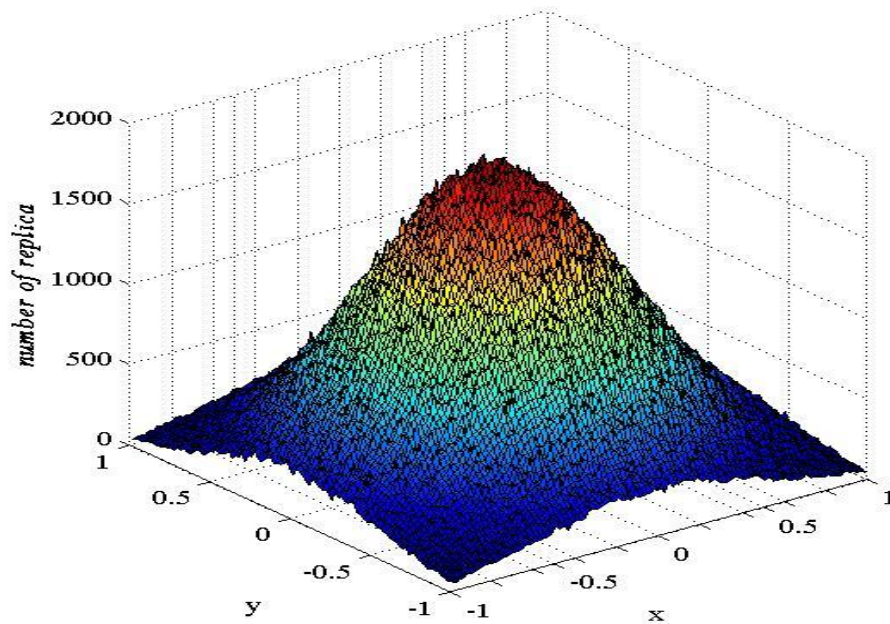


Fig. 3.5: probability distribution (in dimensionless units) as a function of the coordinate displacements obtained by the DMC method for one of the 2-D harmonic oscillator.

3.3 The Ground state of the quantum dot

(Harmonic Oscillator in two dimension (Two interacting electrons in parabolic confinement))

Long before the advent of quantum dots the problem of two electrons interacting via coulomb potential confined in 3D Harmonic potential was considered by Kestner and Sinanoglu for the first time in 1962 [24]. The problem was introduced in their study of electron correlation in the hope of establishing an exact solution at least in terms of power series. Later in 1989 S. Kais et al [25] have realized that the exact ground state wave function could be written in closed form in the special case of $k = \frac{1}{4}$. In 1993 M.Tout [26], found that one could solve for countably infinite set of the eigenvalues but not the complete spectrum analytically. The model, subsequently, attracted attention in

the context of 2- electron quantum dot with harmonic confinement in two dimensions [27].

It is well known that the Schrödinger equation for two unconfined interacting particle may always be reduced to a system of two one-particle equations : one for the center of mass (C.M.) and one for the relative coordinate. In general this separation is not possible if the interacting particles are confined by external potential [e.g, two interacting electrons confined by external coulomb potential modeling helium like atoms]. However, a harmonic confinement does not obstruct separability. Restricting the number of particle N to N=2 electrons and confining them in the 2D x-y plane by an external parabolic confinement constitutes the simplest realistic many particle quantum system for which exact ground state wave function could be written in closed form for particular values of the force constant.

The Hamiltonian of two interacting electrons in a harmonic dot in two-dimensional(2D) plane is

$$H(\vec{r}_1, \vec{r}_2) = -\frac{1}{2}\nabla_{r_1}^2 - \frac{1}{2}\nabla_{r_2}^2 + \frac{1}{2}\omega^2(r_1^2 + r_2^2) + \frac{1}{|\vec{r}_1 - \vec{r}_2|} \quad (3.7)$$

Where \vec{r}_1, \vec{r}_2 are the coordinate of the two electrons in the x-y plane using units in the appendix A. Introducing the center of mass (CM) and relative coordinates $\vec{r} = \vec{r}_1 - \vec{r}_2$ for the relative, and $\vec{R} = \frac{1}{2}(\vec{r}_1 + \vec{r}_2)$, for CM coordinates, the above Hamiltonian Eq.(3.7) separates in two parts

$$H(\vec{R}, \vec{r}) = H_{cm}(\vec{R}) + H_{rel}(\vec{r}) \quad (3.8)$$

In this case the total wave function for the system can be written as a product

$$\psi(\bar{r}, \bar{R}) = \varphi(\bar{r})\chi(\bar{R}) \quad (3.9)$$

and the Schrödinger equation separates in to two one particle Eq. (3.7) for the center of mass coordinate with total mass $M=2$ and Eq.(3.8) for the relative coordinate with reduced mass $\mu = 1/2$

$$H(\bar{R})\chi(\bar{R}) = E_R\chi(\bar{R}) \quad (3.10)$$

$$H(\bar{r})\varphi(\bar{r}) = E_r\varphi(\bar{r}) \quad (3.11)$$

The solution of Eq.(3.7) is a well known exactly solvable problem and we will worry about it no further. Eq. (3.8) will be written in plane polar coordinate to separate the angular from radial parts due to conservation of angular momentum and it will contain the coulomb interaction of the two electrons

$$H(\bar{r}) = -\bar{\nabla}^2 + \frac{1}{4}r^2 + \frac{\alpha}{r} \quad (3.12)$$

$$H(\rho, \varphi) = -\frac{1}{\rho^2} \left(\rho \frac{\partial}{\partial \rho} \rho \frac{\partial}{\partial \rho} + \frac{\partial^2}{\partial \varphi^2} \right) + \frac{1}{4} \rho^2 + \frac{\alpha}{\rho} \quad , \quad (3.13)$$

where α is a coulomb coupling constant (see Appendix B).

Fig(3.6) show the results of DMC for a range of values of the coulomb coupling constant $\alpha \in (0.01 - 40)$. To explain the trends of these curves we propose the following two partitions of the original total Hamiltonian:

I- In the strong coupling Limit $\alpha \gg 1$ (e.g. $\alpha = 40$) the coulomb interaction dominates over the kinetic energy and as a zeroth approximation (which gives a lower bound on the exact quantum ground state energy) we neglect the kinetic energy part of the Hamiltonian and we are left with

$$H_T = H_{conf} + H_{int} \quad (3.14)$$

This is a solvable classical problem[31], which is also known as the low density limit, the strong correlation limit and the Wigner crystal limit.

II- In the weak coupling limit $\alpha \ll 1$ (e.g. $\alpha = 0.01$) the kinetic energy dominate, and the interaction can be considered as a perturbation on the single particle state of the non-interacting particle confined in the harmonic potential thus the total Hamiltonian can be written as

$$H = H_1(\bar{r}_1) + H_2(\bar{r}_2) + V_{int}(|\bar{r}_1 - \bar{r}_2|) \quad (3.15)$$

neglecting V_{int} in the zeroth order and including it as first order perturbation[28]

For $\alpha \ll 1$ the system is essentially perturbed by coulomb coupling. Consequently it is amenable to description within perturbation theory which yield [28].

$$E = E^{(0)} + E^{(1)} \quad (3.16)$$

$$E \cong 2 + \sqrt{\frac{\pi}{2}} \alpha, \quad (3.17)$$

for the ground state energy.

For $\alpha \gg 1$ the system has the character of the coulomb crystal (wegnier crystal) perturbed by quantum effects due to the kinetic energy [29].

$$E \cong \frac{3}{4}(2\alpha)^{2/3} + 1.5. \quad (3.18)$$

Note that $\alpha \rightarrow 0$ $E \rightarrow 2$, which is the exact result for the non interacting electrons

$\alpha \rightarrow \infty$ $E \rightarrow \frac{3}{4}(2\alpha)^{2/3}$, which is the exact result for the classical wigner crystal[30].

Table3.1: The ground state energy of confined QD for various values of coulomb coupling constant(α)

α	E (DMC result)	E (approximation result)
0	2.00	2.00
0.01	2.021	2.0125
0.5	2.531	2.627
1	3.01	!!!
4	4.850	4.5
10	7.356	7.026
40	15.712	15.425

We used DMC program #4 (see Appendix D) to calculate the ground state energy for an initial number of replicas ($N_0 = 500$), the maximum number of replicas ($N_{max}=1000$), the seed value for the random number generators (gasdev), the number of time steps =20000 , the value of the time step ($\Delta\tau = 0.01$), for different values of coupling constant α as shown in table (3.1). The free space Coulomb interaction constant in these dimensionless unite is $\alpha \cong 1.9$.In Fig. (3.7) we show the probability distribution of the separation distance between the two interacting particles \mathbf{r} for different interaction constant α . The figure shows that as the interaction increases the most probable of separation distance \mathbf{r} is also increased.

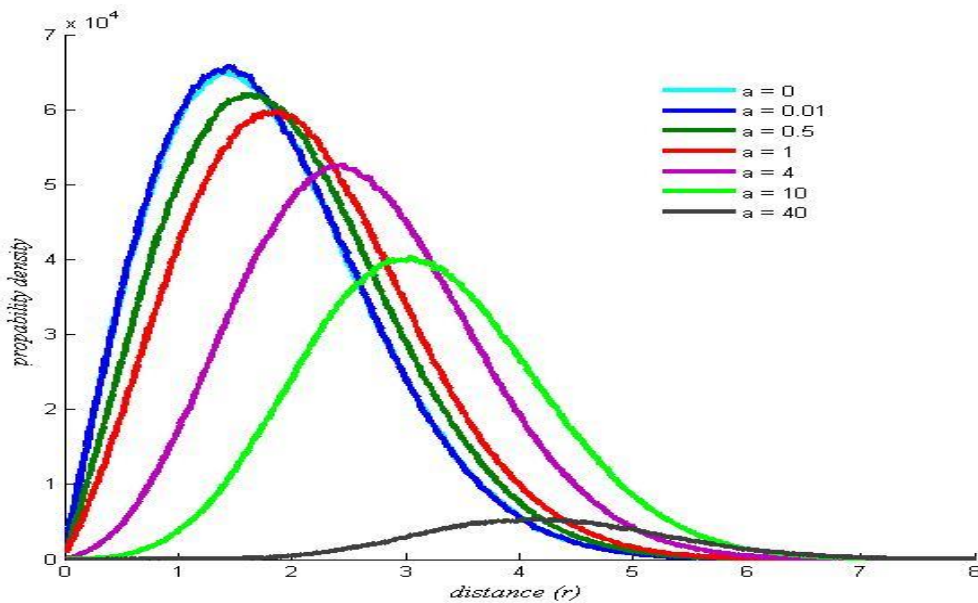


Fig 3.6: probability density of distance between the two particles

3.4 The Ground state of the Helium Atom

In this part of the third chapter we will implement DMC method for calculating the ground state of the helium atom. If we use dimensionless units with $\hbar = m_e = e = 1$, the Hamiltonian for the motion of the two electrons can be written as

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}}, \quad (3.19)$$

where $r_{12} = |\mathbf{r}_{12}| = |\mathbf{r}_1 - \mathbf{r}_2|$.

The terms $-\frac{2}{r_i}$ represent the negative (attractive) potential energy between each electron with charge -1 and the Helium nucleus with charge +2, and the term $+\frac{1}{r_{12}}$ represents the positive (repulsive) potential energy between the two electrons.

If the repulsive term $\frac{1}{r_{12}}$ were not present, then the Hamiltonian would be that of two independent Hydrogen-like atoms. It can be shown that the energy and ground state wave function of a Hydrogen-like atom whose nucleus has charge Z are given by

$$E_0 = -\frac{Z^2}{2} \quad (3.20)$$

$$\psi_0 \sim e^{-Zr} \quad (3.21)$$

The wave function of the combined atom with two non-interacting electrons would be the product of two such wave functions:

$$\psi(r_1, r_2) \sim e^{-2r_1} e^{-2r_2}, \quad (3.22)$$

the DMC algorithm can be speeded up with the use of a suitable trial wave function which is called a guide function or trial wave function given by the Pade-Jastrow form:

$$\psi_T(r_1, r_2) = e^{-2r_1} e^{-2r_2} e^{\frac{r_{12}}{2(1+\alpha r_{12})}}, \quad (3.23)$$

with $\alpha \sim 0.15$ as a variational parameter, the last term increases the probability of the two electrons being far away from each other.

The local energy of the trial wave function is given by

$$E_L(\mathbf{R}) = \frac{1}{\psi_T} \left[-\frac{1}{2} \nabla_1^2 - \frac{1}{2} \nabla_2^2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}} \right] \psi_T. \quad (3.24)$$

The final form for the local energy of the trail wave function (see Appendix C)

$$E_L(\mathbf{R}) = -4 + \frac{\alpha}{(1+\alpha r_{12})} + \frac{\alpha}{(1+\alpha r_{12})^2} + \frac{\alpha}{(1+\alpha r_{12})^3} - \frac{\alpha}{4(1+\alpha r_{12})^4} + \frac{\hat{r}_{12} \cdot (\hat{r}_1 - \hat{r}_2)}{(1+\alpha r_{12})^2}. \quad (3.25)$$

The diffusion equation has the form

$$\frac{\partial \psi(\mathbf{R}, \tau)}{\partial \tau} = \frac{1}{2} \nabla_R^2 \psi(\mathbf{R}, \tau) - V(\mathbf{R}) \psi(\mathbf{R}, \tau), \quad (3.26)$$

where $\mathbf{R} \equiv \mathbf{R}(\mathbf{r}_1, \mathbf{r}_2)$ is the coordinate phase space.

We solve the following wave function $\rho(\mathbf{R}, \tau) = \psi(\mathbf{R}, \tau) \psi_T(\mathbf{R})$ instead of $\psi(\mathbf{R}, \tau)$ which obeys the equation

$$\frac{\partial \rho(\mathbf{R}, \tau)}{\partial \tau} = \frac{1}{2} \nabla_R \cdot [\nabla_R - \mathbf{F}(\mathbf{R})] \rho(\mathbf{R}, \tau) - [E_L(\mathbf{R}) - E_T(\mathbf{R})] \rho(\mathbf{R}, \tau), \quad (3.27)$$

where E_L the local energy, E_T trail energy and $\mathbf{F}(\mathbf{R})$ Fokker-blank force function given by

$$\mathbf{F}(\mathbf{R}) = \frac{2}{\psi_T(\mathbf{R})} \nabla_R \psi_T(\mathbf{R}). \quad (3.28)$$

We start with N pairs of electrons (walkers) with positions \mathbf{R} for each pair (six dimension) and a trail energy $E_T(\mathbf{R})$, Then try to move each walker position \mathbf{R} to new position \mathbf{R}' by moving them randomly using normal distribution with six random number $\boldsymbol{\eta}$ given by

$$\mathbf{R}' = \mathbf{R} + \Delta\tau \mathbf{F}(\mathbf{R}) + \boldsymbol{\eta} \sqrt{\Delta\tau}. \quad (3.29)$$

For each new position \mathbf{R}' we assign a weight function ω given by

$$\omega = \frac{G(\mathbf{R}, \mathbf{R}'; \Delta\tau) \psi_T^2(\mathbf{R}')}{G(\mathbf{R}', \mathbf{R}; \Delta\tau) \psi_T^2(\mathbf{R})}, \quad (3.30)$$

where $G(\mathbf{R}', \mathbf{R}; \Delta\tau)$ is an approximate Green's function giving by

$$G(\mathbf{R}', \mathbf{R}; \Delta\tau) = \frac{1}{\sqrt{2\pi\Delta\tau}} \exp \left[-\frac{(\mathbf{R}' - \mathbf{R} - \frac{1}{2} \mathbf{F}(\mathbf{R}) \Delta\tau)^2}{2\Delta\tau} \right]. \quad (3.31)$$

If $\omega \geq 1.0$ we accept the new position \mathbf{R}' and try to determine the number of new clones of this position (walker) by

$$q = \exp[-\Delta\tau[E_L(\mathbf{R}') - E_T(\mathbf{R})]], \quad (3.32)$$

if $q < r$, where r is a uniform random number then the walker is dead and cannot be counted or cloned.

If q is larger than 1.0 then there will be an increase in the number of this particular walker but if q is small then the new position is not favored and the walker is killed and removed from stored positions.

Then going over all possible walkers (representing one time step), we count the number of new alive walkers N_{new} if this number is greater than the old number of walkers N_{old} then the trial energy E_T should be decreased so to keep the number of walkers constant in future time steps and this is done by relation

$$E_T = E_T + 0.1 \ln \frac{N_{old}}{N_{new}} \quad (3.33)$$

After many iterations the expected value of E_T will reach some constant average then the ground state energy of the helium atom is equal to this average. [32]

A DMC program is written for treating the helium atom (see Appendix D #5) with initial input $N_0 = 2000$ walkers, with initial random number positions and initial guess of trial energy $E_T = -2.85$ and time step $\Delta\tau = 0.3$, the program is run for about 100000 time steps and the average energy was calculated resulting in a value of $\langle E_T \rangle = -2.8804$

We can be compared this result with other results in the table (3.2) [33], [34].

Table3.2: Comparison with other theoretical predictions and experime

Method	Ground state energy
Our work DMC	-2.8804
$e^{-2r_1-2r_2}$	-2.75
$e^{-\alpha r_1-\alpha r_2}$ with $\alpha = 27/16$	-2.84765
Hartree-Fock	-2.8617
Pad_e-Jastrow vmc-he.cpp	-2.878
Hylleraas (1929) 10 variational parameters	-2.90363
Pekeris (1959) 1,078 variational parameters	-2.90372
Experiment	-2.90372

3.5 Conclusion

In conclusion we have applied DMC technique to calculate the ground state of several quantum systems . We first tested the Algorithm on simple quantum systems where exact results are known analytically, such as single electron harmonic oscillator and two non-interacting electrons parabolic dot. Next we used the DMC algorithm to find the ground state of two more challenging problems which no known exact analytical solution in a parabolic dot (helium dot) and elemental helium atom we compared our result with known numerical results where possible and found our results to compare very well.

We hope to continue the application of the algorithm to more complicated realistic systems and improve its performance and include many particle effects, spin effects and magnetic field.

Appendix A: The two particle problem(coordinates relative to the center of mass)

consider the two particle Hamiltonian in dimensionless unite

$$H = -\frac{1}{2}V_1^2 - \frac{1}{2}V_2^2 + \frac{1}{2}(x_1^2 + x_2^2 + y_1^2 + y_2^2) + \frac{\alpha}{r}$$

$$H = -\frac{1}{2}\frac{d^2}{dx_1^2} - \frac{1}{2}\frac{d^2}{dx_2^2} - \frac{1}{2}\frac{d^2}{dy_1^2} - \frac{1}{2}\frac{d^2}{dy_2^2} + \frac{1}{2}(x_1^2 + x_2^2 + y_1^2 + y_2^2) + \frac{\alpha}{r} \quad (a.1)$$

where we have written r for the distance between particles, \vec{r} . Such potentials which are only functions of the scalar distance r , are called central potentials.

$$r = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2} = \sqrt{x^2 + y^2} \quad (a.2)$$

where $\vec{r} = (x_1 - x_2)\hat{i} + (y_1 - y_2)\hat{j}$

we might want to treat separately the Center-of-mass and relative motion:

let relative coordinate

$$x_{rel} \rightarrow x = x_1 - x_2 \quad y_{rel} \rightarrow y = y_1 - y_2 \quad (a.3)$$

and center-of-mass coordinate where $m_1 = m_2$

$$x_{cm} \rightarrow X = \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2} = \frac{x_1 + x_2}{2} \quad (a.4)$$

$$y_{cm} \rightarrow Y = \frac{m_1 y_1 + m_2 y_2}{m_1 + m_2} = \frac{y_1 + y_2}{2} \quad (a.5)$$

with utilize chain rule

$$\left. \begin{aligned} \frac{d}{dx_1} &= \frac{dx}{dx_1} \cdot \frac{d}{dx} + \frac{dX}{dx_1} \cdot \frac{d}{dX} \\ \frac{d}{dx_1} &= \frac{d}{dx} + \frac{1}{2} \frac{d}{dX} \\ \frac{d^2}{dx_1^2} &= \frac{d^2}{dx^2} + \frac{d}{dx} \cdot \frac{d}{dX} + \frac{1}{4} \frac{d^2}{dX^2} \end{aligned} \right) \quad (a.6)$$

and

$$\left. \begin{aligned} \frac{d}{dx_2} &= \frac{dx}{dx_2} \cdot \frac{d}{dx} + \frac{dX}{dx_2} \cdot \frac{d}{dX} \\ \frac{d}{dx_2} &= -\frac{d}{dx} + \frac{1}{2} \frac{d}{dX} \\ \frac{d^2}{dx_2^2} &= \frac{d^2}{dx^2} - \frac{d}{dx} \cdot \frac{d}{dX} + \frac{1}{4} \frac{d^2}{dX^2} \end{aligned} \right) \quad (a.7)$$

where $\frac{dx}{dx_1} = 1$, $\frac{dX}{dx_1} = \frac{1}{2}$, $\frac{dx}{dx_2} = -1$, $\frac{dX}{dx_2} = \frac{1}{2}$

$$\frac{d^2}{dx_1^2} + \frac{d^2}{dx_2^2} = 2 \frac{d^2}{dx^2} + \frac{1}{2} \frac{d^2}{dX^2} \quad (a.8)$$

as same as $\frac{d^2}{dy_1^2} + \frac{d^2}{dy_2^2} = 2 \frac{d^2}{dy^2} + \frac{1}{2} \frac{d^2}{dY^2}$ (a.9)

Using Eq. (a.3) and Eq.(a.4) we find

$$\left. \begin{aligned} x + 2X &= 2x_1 \xrightarrow{\text{yields}} x_1 = \frac{x}{2} + X \\ x_1^2 &= \left(\frac{x}{2} + X\right)^2 = \frac{x^2}{4} + xX + X^2 \end{aligned} \right) \quad (a.10)$$

$$\left. \begin{aligned} 2X - x &= 2x_2 \xrightarrow{\text{yields}} x_2 = -\frac{x}{2} + X \\ x_2^2 &= \left(-\frac{x}{2} + X\right)^2 = \frac{x^2}{4} - xX + X^2 \end{aligned} \right) \quad (a.11)$$

where $x_1^2 + x_2^2 = 2X^2 + \frac{1}{2}x^2$ (a.12)

as same as $y_1^2 + y_2^2 = 2Y^2 + \frac{1}{2}y^2$ (a.13)

Compensation Eq.(a.8), Eq.(a.9), Eq.(a.12) and Eq.(a.13) in equation (a.1) we find

$$H = -\frac{1}{2} \left(2 \frac{d^2}{dx^2} + \frac{1}{2} \frac{d^2}{dX^2} + 2 \frac{d^2}{dy^2} - \frac{1}{2} \frac{d^2}{dY^2} \right) + \frac{1}{2} \left(2X^2 + \frac{1}{2}x^2 + 2Y^2 + \frac{1}{2}y^2 \right) + \frac{\alpha}{r}$$

$$H = -\frac{d^2}{dx^2} - \frac{d^2}{dy^2} + \frac{1}{4}(x^2 + y^2) - \frac{d^2}{4dX^2} - \frac{d^2}{4dY^2} + X^2 + Y^2 + \frac{\alpha}{r} \quad (a.14)$$

where $R^2 = X^2 + Y^2$ and $r^2 = x^2 + y^2$

$$H = -\nabla_{rel}^2 + \frac{r^2}{4} + \frac{\alpha}{r} - \frac{\nabla_c^2}{4} + R^2$$

$$H = \left(-\nabla_{rel}^2 + \frac{r^2}{4} + \frac{\alpha}{r} \right) + \left(-\frac{\nabla_c^2}{4} + R^2 \right) = \hat{H}_{rel} + \hat{H}_c \quad (a.15)$$

$$\hat{H}_{rel} = -\nabla_{rel}^2 + \frac{r^2}{4} + \frac{\alpha}{r} \quad (a.16)$$

as a harmonic oscillator where $\omega = \sqrt{\frac{k}{\mu}}$ $k = \frac{1}{2}$ $\mu = \frac{1}{2}$ $\omega_r = 1$

and $\hat{H}_c = -\frac{\nabla_c^2}{4} + R^2$ as a harmonic oscillator where $k = 2$ $M = 2$ $\omega_c = 1$

we find $\omega_c = \omega_r$.

Appendix B: A coulomb coupling constant

The coulomb coupling constant is a tool for measuring the interaction. This constant can be calculated as following, where the coulomb potential is giving by:

$$V_q = \frac{1}{4\pi\epsilon_0} \frac{q_1 q_2}{\rho} \quad (\text{b.1})$$

Where ϵ_0 is the permittivity and q is the electron charge.

The Hamiltonian for the Harmonic oscillator is written as:

$$\hat{H} = -\frac{\hbar^2}{m} \frac{d^2}{dx^2} + \frac{1}{4} m\omega^2 x^2 + V_q \quad (\text{b.2})$$

where \hbar is Planck's constant, m is the electron mass and ω is the angular frequency.

Eq(b.2) can be put in dimensionless unite as following:

first divided Eq(b.2) by $\hbar\omega$ so Eq(b.2) reads as :

$$\frac{\hat{H}}{\hbar\omega} = -\frac{\hbar}{m\omega} \frac{d^2}{dx^2} + \frac{1}{4} \frac{m\omega}{\hbar} x^2 + \frac{V_q}{\hbar\omega} \quad (\text{b.3})$$

Second let x be dimensionless quantity by as:

$$x = \beta \rho \quad (\text{b.4})$$

from Eq(b.4) we get:

$$\frac{d}{dx} = \frac{1}{\beta} \frac{d}{d\rho} \quad \text{and} \quad \frac{d^2}{dx^2} = \frac{1}{\beta^2} \frac{d^2}{d\rho^2} \quad (\text{b.5})$$

Plug Eq(b.5) into Eq(b.3) we get:

$$\frac{\hat{H}}{\hbar\omega} = -\frac{\hbar}{m\omega} \frac{1}{\beta^2} \frac{d^2}{d\rho^2} + \frac{1}{4} \frac{m\omega}{\hbar} \beta^2 \rho^2 + \frac{1}{4\pi\epsilon_0} \frac{e^2}{\hbar\omega\beta\rho} \quad (\text{b.6})$$

Eq(b.6) to be dimensionless the term $\frac{m\omega\beta^2}{\hbar}$ must be equal one:

$$\beta = \sqrt{\frac{\hbar}{m\omega}} \quad (\text{b.7})$$

The Eq(b.6) reads as:

$$\frac{\hat{H}}{\hbar\omega} = -\frac{d^2}{d\rho^2} + \frac{1}{4}\rho^2 + \left(\frac{1}{4\pi\epsilon_0} \frac{e^2}{\sqrt{\frac{\hbar^3\omega}{m}}} \right) \frac{1}{\rho} \quad (\text{b.8})$$

Then the coulomb coupling constant α is giving by:

$$\alpha = \frac{1}{4\pi\epsilon_0} \frac{e^2}{\sqrt{\frac{\hbar^3\omega}{m}}} \quad (\text{b.9})$$

for $\omega = 1.154 \times 10^{16} \text{HZ}$ then α is calculated to be $\alpha = 1.9$

Appendix C: The local energy of the trail wave function

We can write

$$\psi = f(r_1)f(r_2)g(r_{12}) \quad (\text{c.1})$$

Where $f(r) = e^{-2r}$ and $g(r) = e^{\frac{r}{2(1+\alpha r)}}$ then

$$\nabla_1^2 f(r_1)g(r_{12}) = (\nabla_1^2 f(r_1))g(r_{12}) + f(r_1)(\nabla_1^2 g(r_{12})) + 2(\vec{\nabla}_1 f(r_1)) \cdot (\vec{\nabla}_1 g(r_{12})) \quad (\text{c.2})$$

The Laplacian of a scalar function can be computed as follows:

$$\nabla_1^2 f(r_1) = \vec{\nabla} \cdot (\vec{\nabla} f(r_1)) = (\vec{\nabla} f(r_1)) \cdot \hat{r}_1 + f(r_1) \vec{\nabla} \cdot \hat{r}_1 = f''(r_1) + \frac{2}{r_1} f'(r_1) \quad (\text{c.3})$$

Where $\hat{r} = \vec{r}_1/r_1$ is a unit vector. Similarly

$$\nabla_1^2 g(r_{12}) = g''(r_{12}) + \frac{2}{r_{12}} g'(r_{12}) \quad (\text{c.4})$$

$$(\vec{\nabla}_1 f(r_1)) \cdot (\vec{\nabla}_1 g(r_{12})) = \hat{r}_1 \cdot \hat{r}_{12} f'(r_1) g'(r_{12}) \quad (\text{c.5})$$

and $(\vec{\nabla}_2 f(r_2)) \cdot (\vec{\nabla}_2 g(r_{12})) = \hat{r}_2 \cdot \hat{r}_{21} f'(r_2) g'(r_{12}) \quad (\text{c.6})$

Note that $r_{12} = r_{21}$, but $\hat{r}_{12} = -\hat{r}_{21}$.

The derivatives of the scalar functions are easily computed:

$$\frac{f'(r)}{f(r)} = -2, \quad \frac{f''(r)}{f(r)} = 4 \quad (\text{c.7})$$

$$\frac{g'(r)}{g(r)} = \frac{1}{2(1+\alpha r)^2}, \quad \frac{g''(r)}{g(r)} = \frac{1}{4(1+\alpha r)^4} - \frac{\alpha}{(1+\alpha r)^3} \quad (\text{c.8})$$

the local energy is given by

$$E_L = -\frac{f''(r_1)}{2f(r_1)} - \frac{f''(r_2)}{2f(r_2)} - \frac{g''(r_{12})}{2g(r_{12})} - \frac{f'(r_1)}{r_1 f(r_1)} - \frac{f'(r_2)}{r_2 f(r_2)} - \frac{g'(r_{12})}{2g(r_{12})} - \frac{\hat{r}_1 \cdot \hat{r}_{12} f'(r_1) g'(r_{12})}{f(r_1) g(r_{12})} \\ - \frac{\hat{r}_2 \cdot \hat{r}_{21} f'(r_2) g'(r_{12})}{f(r_2) g(r_{12})} - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}} \quad (\text{c.9})$$

gives the final form for the local energy of the trail wave function

$$E_L = -4 + \frac{\alpha}{(1+\alpha r_{12})} + \frac{\alpha}{(1+\alpha r_{12})^2} + \frac{\alpha}{(1+\alpha r_{12})^3} - \frac{\alpha}{4(1+\alpha r_{12})^4} + \frac{\hat{r}_{12} \cdot (\hat{r}_1 - \hat{r}_2)}{(1+\alpha r_{12})^2}$$

*Appendix D: DMC programs***1- DMC program for Harmonic oscillator in one dimension**

```

DIMENSION X1(5000),X2(5000), KM(2000),M(5000)
OPEN (8,file='amna1.dat',status='new')
WRITE (*,*) 'ENTER N1,Nmax, dt'
READ (*,*) N1,Nmax, dt
DO 1 i = 1,4000
  X1(i) = 0.0
  X2(i) = 0.0
  IF (i .lt. 2001) KM(i)=0
1  CONTINUE
  ER =1.0
  ERA=0.0
  ER2=0.0
  KC=0
  DO 2 j = 1,10000
    k = 0
    DO 3 i = 1,N1
X2(i) = X1(i) + (SQRT(dt) * gasdev(0))
      V = (X2(i))**2/2.0
      W = EXP(-dt*(V-ER))
      Call RANDOM_NUMBER(ranval)
      wm = int(W + ranval)
      IF(wm .GT. 2) Then
        wm=2
      ENDIF
      M(i) = wm
3  CONTINUE
    DO 4 i=1,N1
      IF (M(i).GT.0) THEN
        DO 5 kk = 1,M(i)
          k = k+1
          X1(k) = X2(i)
5      CONTINUE
        ENDIF
4  CONTINUE
    N2 = k
    xn1=N1
    xn2=N2
    ss= (1.0 / dt) * ( 1 - (xn2/xn1))
    ERN = ER + ss
    term = ABS(ERN - ER)
    N1 = N2
    IF(N1 .GT. Nmax) Then
      N1=Nmax
    ENDIF
    ER = ERN
c  WRITE (*,*) ' ERN = ',ERN
  WRITE (8,15) ER
15  FORMAT(6X,F4.2)

```

```

        IF ( j .GT. 200) Then
        KC=KC+1
        ERA=ERA+ER
        ER2=ER2+ER*ER
        DO 7 i1=1,N2
            ii=int(X2(i1)*10+50)
            IF ( ii .GT. 0) then
                KM(ii)=KM(ii)+1
            ENDIF
7      CONTINUE
        ENDIF
2      CONTINUE
        ERA=ERA/KC
        ER2=ER2/KC
        WRITE (8,10) ERA,ER2,j
10     FORMAT(6X,F4.2,6X,F20.15,6X,I6)
        DO 8 i2=1,200
            WRITE (8,20) KM(i2)
20     FORMAT(I6)
8      CONTINUE
        STOP
        END

```

2- DMC program for Harmonic Oscillator in 2-D one particle

```

DIMENSION X1(5000),X2(5000), Y1(5000),Y2(5000),KM(200,200), M(5000)
OPEN (8,file='amna21.dat',status='new')
WRITE (*,*) 'ENTER N1,Nmax, dt'
READ (*,*) N1,Nmax, dt
DO 1 i = 1,5000
    X1(i) = 0.0
    X2(i) = 0.0
    Y1(i) = 0.0
    Y2(i) = 0.0
1  CONTINUE
DO 2 i= 1,200
DO 3 j= 1,200
    KM(i,j) = 0
3  CONTINUE
2  CONTINUE
    ER =0.0
    ERA=0.0
    ER2=0.0
    KC=0
DO 4 j = 1,4000
    k = 0
DO 5 i = 1,N1
X2(i) = X1(i) + (SQRT(dt) * gasdev(0))
Y2(i) = Y1(i) + (SQRT(dt) * gasdev(0))
    V = ((X2(i)**2 + (Y2(i)**2)/2.0
        W = EXP(-dt*(V-ER))
    CALL RANDOM_NUMBER(ranval)

```

```

    wm = int(W + ranval)
    IF (wm .GT. 2) THEN
        wm=2
    ENDIF
    M ( i ) = wm
5 CONTINUE
    DO 6 i=1,N1
        IF (M(i).GT.0) THEN
            DO 7 kk = 1,M(i)
                k = k+1
                X1(k) = X2(i)
                Y1(k) = Y2(i)
7 CONTINUE
            ENDIF
6 CONTINUE
    N2 = k
    xn1=N1
    xn2=N2
    ss= ( 1.0/dt ) * ( 1 - (xn2/xn1))
    ERN = ER + ss
    term = ABS(ERN - ER)
    N1 = N2
    IF(N1 .GT. Nmax) THEN
        N1=Nmax
    ENDIF
    ER = ERN
    WRITE (8,36) ERN
36 FORMAT(6X,F4.2)
    IF( j .GT. 20) Then
        KC=KC+1
        ERA=ERA+ER
        ER2=ER2+ER*ER
        DO 8 i1=1,N2
            ii=int(X2(i1)*10+50)
            jj=int(Y2(i1)*10+50)
            if ( ii .and. jj.GT. 0) then
                KM(ii,jj)= KM(ii,jj)+1
            ENDIF
8 CONTINUE
        ENDIF
        ERA=ERA/KC
        ER2=ER2/KC
4 CONTINUE
c ERA=ERA/KC
c ER2=ER2/KC
c WRITE (8,30) ERA,ER2,KC
c30FORMAT(6X,F4.2,6X,F20.15,6X,I6)
c DO 9 ii=1,200
c 9 WRITE (8,35) ( KM(ii,jj),jj=1,200)
c 35 FORMAT(200(6X,I15))

```

STOP
END

3- ***DMC program for Harmonic Oscillator in 2-D two particle***

```

DIMENSION X11(500),X12(500),
Y11(500),Y12(500),X21(500),X22(500),Y21(500),Y22(500),KM1(200,200),KM2(200,
200),M(5000)
OPEN(9,file='amna222.dat',status=' new')
WRITE (*,*) 'ENTER N1,Nmax, dt'
READ (*,*) N1,Nmax, dt
DO 1 i = 1,100
  X11(i) = 0.0
  X12(i) = 0.0
  Y11(i) = 0.0
  Y12(i) = 0.0
  X21(i) = 0.0
  X22(i) = 0.0
  Y21(i) = 0.0
  Y22(i) = 0.0
1 CONTINUE
  DO 2 i= 1,100
    DO 3 j= 1,100
      KM1(i,j) = 0
3 CONTINUE
2 CONTINUE
  DO 4 k= 1,100
    DO 5 l= 1,100
      KM2(k,l) = 0
5 CONTINUE
4 CONTINUE
  ER =1.0
  ERA=0.0
  ER2=0.0
  KC=0
  DO 6 j = 1,20000
    k = 0
    DO 7 i = 1,N1
      X12(i) =X11(i) +(SQRT(dt)*gasdev(0))
      Y12(i)=Y11(i)+(SQRT(dt)* gasdev(0))
      X22(i)=X21(i)+(SQRT(dt) gasdev(0))
      Y22(i)=Y21(i)+(SQRT(dt)*gasdev(0))
      V=((X12(i)**2+(Y12(i))**2+ (X22(i))**2 + (Y22(i))**2)/2.0
      W = EXP(-dt*(V-ER))
      Call RANDOM_NUMBER(ranval)
      wm = int(W + ranval)
      IF(wm .GT. 2) THEN
        wm=2
      ENDIF
      M(i) = wm
7 CONTINUE
    DO 8 i=1,N1

```

```

      IF (M(i).GT.0) THEN
        DO 9 kk = 1,M(i)
          k = k+1
          X11(k) = X12(i)
          Y11(k) = Y12(i)
          X21(k) = X22(i)
          Y21(k) = Y22(i)
9      CONTINUE
      ENDIF
8      CONTINUE
      N2 = k
      xn1=N1
      xn2=N2
      ss= (1.0 / dt * ( 1 - (xn2/xn1)))
      ERN = ER + ss
      term = ABS(ERN - ER)
      N1 = N2
      IF(N1 .GT. Nmax) THEN
        N1=Nmax
        ENDIF
      ER = ERN
      IF( j .GT. 200) THEN
        KC=KC+1
        ERA=ERA+ER
        ER2=ER2+ER*ER
        Do 10 i1=1,N2
          ii=int(X12(i1)*25+50)
          jj=int(Y12(i1)*25+50)
          kk=int(X22(i1)*25+50)
          ll=int(Y22(i1)*25+50)
          IF ( ii.GT.0 .and. jj.GT. 0) THEN
            IF (kk .GT.0.and. ll.GT. 0) THEN
              KM1(ii,jj)= KM1(ii,jj)+1
              KM2(kk,ll)= KM2(kk,ll)+1
            ENDIF
          ENDIF
10      CONTINUE
        ENDIF
6      CONTINUE
      ERA=ERA/KC
      ER2=ER2/KC
      WRITE (9,30) ERA,ER2,KC
30FORMAT(6X,F4.2,6X,F20.15,6X,I6)
      WRITE(9,35) ( (KM1(ii,jj),ii=1,100),jj=1,100)
35  FORMAT (100(10X,I15))
      C WRITE(9,36) ((KM2(kk,ll),kk=1,100), ll=1,100)
c 36  FORMAT (100(3X,I10))
      STOP
      END

```

4- DMC program for Harmonic Oscillator in 2-D/ Two particles interacting in parabolic confinement (quantum dot)

```

DIMENSION X11(500),X12(500), Y11(500),Y12(500),X21(500),
X22(500),Y21(500),Y22(500) , KM1(200,200),KM2(200,200), KM3(1000),M(5000)
OPEN(9,file='amna2dot.dat',status=' new')
WRITE (*,*) 'ENTER N1,Nmax, dt, a'
READ (*,*) N1,Nmax, dt, a
DO 1 i = 1,100
  X11(i) = 0.0
  X12(i) = 0.0
  Y11(i) = 0.0
  Y12(i) = 0.0
  X21(i) = 0.0
  X22(i) = 0.0
  Y21(i) = 0.0
  Y22(i) = 0.0
1 CONTINUE
DO 2 i= 1,100
  DO 3 j= 1,100
    KM1(i,j) = 0
3 CONTINUE
2 CONTINUE
DO 4 k= 1,100
  DO 5 l= 1,100
    KM2(k,l) = 0
5 CONTINUE
4 CONTINUE
DO 33 j= 1,10000
  KM3(j) = 0
33 CONTINUE
ER =1.0
ERA =0.0
ER2 =0.0
KC =0
seg = 0.000001
DO 6 j = 1,10000
  k = 0
DO 7 i = 1,N1
X12(i)=X11(i)+(SQRT(dt)* gasdev(0))
Y12(i)=Y11(i)+(SQRT(dt)* gasdev(0))
X22(i)=X21(i)+(SQRT(dt)* gasdev(0))
Y22(i)=Y21(i)+(SQRT(dt)* gasdev(0))
r=seg+SQRT((Y22(i)-Y12(i))**2 + (X22(i)- X12(i))**2)
V=((X12(i))**2+(Y12(i))**2+ (X22(i))**2 + (Y22(i))**2)/2.0)+( a/r)
W = EXP(-dt*(V-ER))
Call RANDOM_NUMBER(ranval)
wm = int(W + ranval)
IF(wm .GT. 2) THEN
  wm=2
ENDIF

```

```

      M(i) = wm
7  CONTINUE
      DO 8 i=1,N1
        IF (M(i).GT.0) THEN
          DO 9 kk = 1,M(i)
            k = k+1
            X11(k) = X12(i)
            Y11(k) = Y12(i)
            X21(k) = X22(i)
            Y21(k) = Y22(i)
9          CONTINUE
        ENDIF
8      CONTINUE
      N2 = k
      xn1=N1
      xn2=N2
      ss= ( 1.0/dt ) * ( 1 - (xn2/xn1))
      ERN = ER + ss
      term = ABS(ERN - ER)
      N1 = N2
      IF(N1 .GT. Nmax) THEN
        N1=Nmax
      ENDIF
      ER = ERN
      IF( j .GT. 200) THEN
        KC=KC+1
        ERA=ERA+ER
        ER2=ER2+ER*ER
        DO 10 i1=1,N2
          ii=int(X12(i1)*50+50)
          jj=int(Y12(i1)*50+50)
          kk=int(X22(i1)*50+50)
          ll=int(Y22(i1)*50+50)
          IF(ii.GT.0.and. jj.GT. 0) THEN
            IF(kk.GT.0.and.ll.GT. 0) THEN
              KM1(ii,jj)= KM1(ii,jj)+1
              KM2(kk,ll)= KM2(kk,ll)+1
            ENDIF
          ENDIF
        ENDIF
        r=seg+SQRT((Y22(i1)- Y12(i1))**2 + (X22(i1)- X12(i1))**2)
        qq=int(r*50)
        KM3(qq)=KM3(qq)+1
10     CONTINUE
      ENDIF
6  CONTINUE
      ERA=ERA/KC
      ER2=ER2/KC
      WRITE (9,30) a, ERA,ER2,KC
30FORMAT(6X,F4.2,6X,F4.2,6X, F20.15,6X,I6)
cWRITE(9,35)((KM2(kk,ll),kk=1,100), ll=1,100)

```

```

    Do 11 qq=1,500
      WRITE (9,55) KM3(qq)
55  FORMAT(3X,10I6)
11  CONTINUE
    STOP
    END

```

5- *DMC program in three dimension for the Helium Atom*

C DMC Program for Helium atome ***** Main Program *******

```

C %% Initialization%% *****
  DIMENSION R(2500,6),N(2500)
  INTEGER nA, nT ,NN
  OPEN (8,file='helium.dat',status='new')
  WRITE (*,*) 'ENTER N_T,M,dt'
  READ (*,*) N_T,M,dt
  DO 1 i = 1,2500
    DO 2 j = 1,6
      CALL RANDOM_NUMBER(ranval)
      R(i,j) = (ranval - 0.5)
2  CONTINUE
    N(i)= 0.0
    CALL RANDOM_NUMBER(rs)
    IF (rs.ge.0.5) THEN
      N(i)= 1.0
    ENDIF
1  CONTINUE
    Esum = 0
    Esum2 = 0
    E_T = -2.85
    NN = N_T
    nT = 0
    nA = 0
    MT = 0.4* M
    Do 4 i = 1,MT
  CALL onetimestep(NN,R,N,dt,Esum, Esum2,E_T,N_T)
4  CONTINUE
    nA = 0
    nT = 0
    Esum = 0
    Esum2 = 0
    NN= N_T
    E_T = -2.85
    DO 5 mm = 1,M
  CALLonetimestep(NN,R,N,dt,Esum, Esum2,E_T,N_T)
5  CONTINUE
C*****COMPUTE AVERAGE*****
  Eave = Esum / M
  Eave2 = Esum2 / M
  WRITE (8,35) Eave,Eave2,E_T
35 FORMAT(6X,F20.8,6X,F20.15, 6X,I15)
  STOP

```

END

```

C***** findseparations*****
SUBROUTINE findseparations(Q,r1, r2,r12)
  DIMENSION Q(6)
  REAL r1,r2,r12
  r1 = 0
  r2 = 0
  r12= 0
  del = 10**-20
  DO 10 i1 = 1,3
    i2 = i1 + 3
    r1 = r1+ Q(i1)**2
    r2 = r2+ Q(i2)**2
    r12 = r12+(Q(i1)-Q(i2))**2
10  CONTINUE
    r1=sqrt(r1) + del
    r2=sqrt(r2) + del
    r12=sqrt(r12) + del
  RETURN
END

```

```

c ***pade-Jastrow wave function parameter psi_T ***
SUBROUTINE guidefunction(Q1, psi_T)
  DIMENSION Q1(6)
  alpha1 = 0.15
  CALL findseparations(Q1,r1,r2,r12)
  psi_T = exp ( -2*r1-2*r2 +(r12/ (2*(1+alpha1*r12))))
c  WRITE (8,35) psi_T
c 35  FORMAT(6X,F4.2)
  RETURN
END

```

```

c*****Local energy*****
SUBROUTINE Localenergy(Q2,E_L)
  DIMENSION Q2(6)
  alpha2 = 0.15
  CALL findseparations(Q2,r1,r2,r12)
  ss = 1/ (1+ alpha2*r12)
  dp = 0
  DO 11 i1=1,3
    i2= i1+3
    dp = dp +((Q2(i1)-Q2(i2))/r12 )* ((Q2(i1)/r1)-(Q2(i2)/r2))
11  CONTINUE
  E_L = -4 + alpha2*( ss + ss**2 + ss**3)-(ss**4 /4)+(dp * ss**2)
  RETURN
END

```

```

c***** The Fokker-Planck force*****
SUBROUTINE findForce (QQ,FF)
  DIMENSION QQ(6),FF(6)
  integer d

```

```

    alpha2 = 0.15
    CALL findseparations(QQ,r1,r2,r12)
      DO 12 d= 1,6
        FF(d) = 0
12    CONTINUE
        ss = 1/ (1+ alpha2*r12)**2
        DO 13 i1= 1,3
          i2= i1+3
          FF(i1) = FF(i1) + (-4*(QQ(i1)/r1)) + ss *((QQ(i1)-QQ(i2))/r12)
          FF(i2) = FF(i2) + (-4*(QQ(i2)/r2)) + ss *((QQ(i2)-QQ(i1))/r12)
13    CONTINUE
        RETURN
      END

```

```

c** The Fokker-PlanckGreen'sfunction** SUBROUTINE GreensFunction(R2, R1,dt,gg)
  DIMENSION R2(6),R1(6),F(6)
  CALL findForce (R1,F)
    gg=0
  DO 14 i = 1,6
    dR = R2(i) - R1(i) - F(i)*dt/2
    gg = gg + dR**2
14  CONTINUE
    gg = -gg/ (2*dt)
    RETURN
  END

```

```

c***** onetime step*****
SUBROUTINE onestimestep (NN,R,N,dt, Esum,Esum2,E_T,N_T)
  DIMENSION R(2500,6),N(2500)
  N1 = NN
  DO 15 jj = 1,N1
    CALLoneMonteCarlostep (jj,R,N,dt, nT,nA,NN,E_T)
15  CONTINUE
    CALL stack(N,R,NN)
    fnt=1.0*N_T
    fnn=1.0*NN +1.0
    E_T = E_T + 0.1*log(fnt/fnn)
    Esum = Esum + E_T
    Esum2 = Esum2 + E_T **2
    RETURN
  END

```

```

c***** stack *****
SUBROUTINE stack(N,R,NN)
  DIMENSION R(2500,6),N(2500)
  k=1
  DO 32 i= 1,NN
    IF (N(i) .eq. 1.0 ) THEN
      DO 33 j= 1,6
        R(k,j) = R(i,j)
33  CONTINUE
      N(i) = 1.0

```

```

        k = k+1
    ENDIF
32  CONTINUE
    DO 34 i= k,NN
    DO 36 j =1,6
        R(i,j)=0.0
36  CONTINUE
        N(i)= 0.0
34  CONTINUE
    NN = k-1
    RETURN
    END

```

```

c***** oneMonteCarlostep *****

```

```

SUBROUTINEoneMonteCarlostep(nr,R,N, dt,nT,nA,NN,E_T)

```

```

c **define position variables for this walker R(d)

```

```

        DIMENSIONR(2500,6),R1(6), R2(6),F1(6),N(2500)

```

```

        integer d,NN,nr

```

```

    DO 18 d = 1,6

```

```

        R1(d) = R(nr,d)

```

```

18  CONTINUE

```

```

        CALL findForce (R1,F1)

```

```

    DO 19 d = 1,6

```

```

        R2(d) = R1(d)+ (F1(d)*dt)/2 +(gasdev(0)* sqrt(dt))

```

```

19  CONTINUE

```

```

c ***The Metropolis acceptance test***

```

```

    CALL GreensFunction (R1,R2,dt,g2)

```

```

    CALL guidefunction(R2,t2)

```

```

    CALL GreensFunction (R2,R1,dt,g1)

```

```

    CALL guidefunction(R1,t1)

```

```

    W = exp(g2-g1)*((t2**2)/(t1**2))

```

```

        nT = nT +1

```

```

    CALL random_number (rs)

```

```

        IF (W.GT.rs) THEN

```

```

            DO 20 d= 1,6

```

```

                R(nr,d) = R2(d)

```

```

20  CONTINUE

```

```

            nA = nA + 1

```

```

        ELSE

```

```

            RETURN

```

```

        ENDIF

```

```

C***** branching step*****

```

```

    CALL Localenergy(R2,E_L)

```

```

        q = exp (-dt*(E_L - E_T))

```

```

        s = int(10*q)

```

```

    CALL random_number (rs)

```

```

    IF ((q-s).GT.rs) THEN

```

```

        s = s+1

```

```

    ENDIF

```

```

    IF ( s .ge. 11) THEN

```

```

        s=11

```

```

    ENDIF
    if ( s .gt. 9 ) THEN
DO 30   i= 1,s
    IF (s.GT.9.And.NN.LT.2495) THEN
        NN = NN +1
DO 35 d= 1,6
    R(NN,d) = R2(d)
35   CONTINUE
    N(NN) = 1
    ENDIF
30   CONTINUE
    ENDIF
    IF (s .lt. 9) THEN
        N(nr) = 0
    ENDIF
    RETURN
    END

```

```

C ****function// Random number ****   FUNCTION gasdev(idum)
    INTEGER idum
    REAL gasdev
C   USES ran Returns a normally distributed deviate with zero mean and unit variance,
    using ran(idum) as the source of uniform deviates.
    INTEGER iset
    REAL fac,gset,rsq,v1,v2,ran
    SAVE iset,gset
    DATA iset/0/
    if (idum.lt.0) iset=0
    if (iset.eq.0) then
1     v1=2.*ran(idum)-1
        v2=2.*ran(idum)-1
c   from -1 to +1 in each direction,
        rsq=v1**2+v2**2
c   see if they are in the unit circle,
        if(rsq.ge.1..or.rsq.eq.0.)goto 1
        fac=sqrt(-2.*log(rsq)/rsq)
c   Now make the Box-Muller transformation to get two normal deviates. Return one and
    save the other for next time.
        gset=v1*fac
        gasdev=v2*fac
        iset=1
c   Set flag.
        else
c   We have an extra deviate handy,
        gasdev=gset
c   so return it,
        iset=0
c   and unset the flag.
        endif
    return
    END

```

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