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The Classical Pair Distribution Function Using Bilal Distribution for One Component Plasma

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This research introduces a novel approach to calculating the binary distribution function of the one-component plasma (OCP) model using the Bilal distribution. The OCP, a fundamental model in plasma physics, is essential for understanding phenomena in fields such as astrophysics, condensed matter physics, and inertial confinement fusion. By employing the Bilal distribution, which offers superior flexibility in fitting non-standard data, we aim to provide a more accurate representation of the pair correlation function in the OCP. Our findings reveal that the Bilal distribution yields result that are in excellent agreement with Monte Carlo simulations and other theoretical predictions. The enhanced flexibility of the Bilal distribution allows for a more accurate description of the short-range and long-range correlations between particles, which are crucial for understanding the thermodynamic properties of the OCP. Additionally, we have investigated the effects of various system parameters, such as the coupling parameter, on the binary distribution function.

1. Introduction

The study of plasmas, the fourth state of matter, is crucial for understanding diverse phenomena across various fields. The One-Component Plasma (OCP) model is a theoretical construct used to study the collective behaviour of charged particles in a plasma. It serves as a simplified yet powerful tool for understanding various plasma phenomena. The binary distribution function is one of the most important functions of statistical mechanics. The importance of the radial distribution function in statistical mechanics since it can calculate all thermodynamic quantities such as pressure, internal energy, free energies, etc. Ott and Bonitz [1] employed first-principal calculations to determine the distribution function DF in strongly coupled OCPs. Desbiens et al.

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[2] developed a parameterization method for calculating DF and static structure factor across coupling regimes in OCPs. In a one-component plasma (OCP), a strongly coupled plasma refers to the state where the Coulomb coupling parameter (Γ) is greater than 5. In this regime, the electrostatic repulsion between the identically charged particles becomes the dominant force compared to their random thermal motion.

When studying non-ideal plasmas, it is necessary to consider collective effects, especially the screening effect: the Coulomb interaction between the two selected particles is reduced by the influence of neighbouring charged particles, i.e. the plasma medium. Many authors present a novel approach for simulating one-component plasma (OCP) with Monte Carlo (MC) methods. Brush et al. [3] pioneered Monte Carlo simulations to study the RDF in OCPs, providing foundational insights. Also, Caillol et al. [4] extended Monte Carlo simulations to two-dimensional OCPs, investigating their structural properties. The OCP consists of a system of identical, point-like particles with the same positive charge (q) immersed in a uniform neutralizing background of negative charge to ensure overall charge neutrality. Interactions between particles occur solely through the long-range Coulomb force, which is attractive for opposite charges and repulsive for like charges. The particles are assumed to be classical (obeying Newtonian mechanics) and have negligible size compared to the average distance between them. Thermal motion of the particles is incorporated through a temperature parameter, leading to a distribution of velocities according to the Maxwell-Boltzmann distribution.

Falkenhagen and Ebeling [5] presented a comprehensive theoretical treatment of electrolytes, including OCPs. Also, Hussein and Osman [6] derived analytical expressions for the DF in OCPs under specific conditions. Classical pair distribution functions can be calculated analytically for simple models (e.g., hard spheres) or obtained from simulations (e.g., molecular dynamics simulations). Experimental techniques like X-ray and neutron scattering provide information related to g(r).

The importance of the classical pair distribution function (g(r)) lies in its ability to bridge the gap between the microscopic and macroscopic world in classical statistical mechanics. Bridging the gap between theoretical models, simulations, and experimental data. Hussein and Osman [7] investigate the second approximation coefficient in the density expansion of the binary distribution function for electrolyte solutions. Hussein et al. [8] investigate the analytical form of the equation of state for dilute relativistic plasmas. It expresses the free energy and pressure as a series expansion related to the thermal parameter.

Several authors have calculated distribution functions, Hussein et al. [**9**] calculated binary and triple quantum distribution functions. Also, Eisa [10] presents analytical expressions for the classical binary and triplet distribution functions for one and two-component plasma in terms of various physical parameters like particle densities and temperatures. Kraft et al. [11] calculated the binary distribution function and the effective potential. Hussein et al. [12] investigated the relationship between these thermodynamic properties and the distribution functions (binary and triplet) for electron gas.

Ebeling [13] investigated three expressions for the classical total entropy for several model systems such as one-component plasma (OCP) using the multiparticle correlation function. (OCP) is a spatially homogeneous collection of classical non-relativistic point particles with uniform charge and mass. The OCP model also describes the correlation effects of an idealized plasma model. One-component plasma (OCP) serves as a simplified model of plasma, aiding the analysis of particle behaviour in space environments like solar winds. Additionally, OCPs play a vital role in developing advanced materials, electronic devices, and nuclear fusion technologies [14-16].

Recently, many authors were interested in introducing new lifetime distributions for fitting real lifetime data. The Bilal distribution, introduced by Abd-Elrahman [17**-18**], has emerged as a valuable tool for statistical modelling due to its unique properties and versatility. While traditional distributions like the exponential and Lindley have limitations, the Bilal distribution offers advantages in various contexts. Abd al-Rahman and Niazi [1**9**] develop methods for estimating the parameters of the Bilal distribution based on Type II censored data, where only a subset of the data is observed due to censoring. The Bilal Distribution Function is a probability distribution that is used in various fields, such as finance and risk analysis. It is characterized by its unique and versatile properties, making it a valuable tool in statistical modelling [**20**]. Abd-Elrahman [20] proposes a new model that potentially offers a better alternative to the generalized Bilal distribution for reliability analysis. It might also discuss applications of this new model.

Many authors explore the applications of the generalized Bilal distribution in various sectors, including hydrology, economics, and engineering. Shi et al. [21] estimated specific parameters of the generalized Bilal distribution under a specific data collection scheme (adaptive type II progressive hybrid censoring) used in reliability studies. They might also address the concept of entropy in relation to the Bilal distribution. Akhter et al. [22] introduce a generalized Bilal distribution with additional parameters to enhance its flexibility and provide a better fit for a wider range of data sets.

Bilal Distribution provides flexibility in modelling diverse and complex real-world scenarios. Classical and Bayesian methods for finding an estimate value of the parameter μ of the Bilal distribution based on a type 2 integer censored sample are presented by Abd al-Rahman and Niazi [19].

Therefore, the BD model can be used in many practical data analyses. Classical distributions are essential in calculating the physical behaviour of matter such as solids, liquids, and plasma. This research investigates the application of the Bilal distribution function, known for its flexibility in modelling complex scenarios, to analyse the behaviour of particles in a one-component plasma (OCP). Also, It focuses on the binary distribution function (g(r)), a key tool in statistical mechanics that bridges the gap between microscopic and macroscopic properties. It provides information about the spatial arrangement of particles within the system, enabling the calculation of various physical properties. While classical pair distribution functions can be determined analytically for simple models or through simulations, this research aims to investigate the potential of the Bilal distribution as an alternative approach for modelling g(r) in OCPs.

The statistical thermodynamics of charged particle systems is the theoretical basis for the study of plasmas. Of particular interest are the pair distribution functions, which provide information about the molecular structure of these systems and further enable the calculation of the macroscopic properties of the system.

The Bilal distribution offers several distinct advantages over existing methods for modeling the classical pair-distribution function (f(r)) of One-Component Plasmas (OCPs). Traditional methods like analytical solutions might be limited to simple OCP models. In contrast, the Bilal distribution's inherent flexibility allows it to potentially capture complex features of real-world OCPs, including non-idealities and long-range Coulomb interactions. Castello and Tolias [23] investigated the structural and thermodynamic properties of dense Yukawa one-component plasma liquids using advanced integral equation theory approaches. Unlike simulations that require significant computational resources, the Bilal distribution can be fitted to experimental data or simulation results. This data-driven approach can be particularly valuable when dealing with complex OCP systems where analytical solutions are intractable. The Bilal distribution has a well-defined probability density function with a manageable number of parameters. These parameters can be estimated using established techniques like maximum likelihood estimation, making the Bilal distribution a user-friendly and computationally efficient approach. Fernando and DeWitt [24] calculated pair distribution function of charged particles and thier results expected that quantitative agreement with Monte Carlo results can be improved considerably and the value of parameters improved. Brush et al. [25] studying the equilibrium states of a single-component plasma of ions moving in the background of a uniform equation, using the Monte Carlo (MC) method.

Improving results based on considering the binary distribution function alone is generally very difficult, and any optimization must include triangular and quaternary distribution functions. Although there are many experimental and theoretical methods for determining the binary distribution function, they do not give a complete description of the structure found in fluids at equilibrium. Mazhit [26] explored correlation functions in OCPs, highlighting the influence of coupling strength. Jancovici [27] obtained exact analytical results for the DF in two-dimensional OCPs.

The Bilal distribution is a relatively new probability distribution introduced in the field of statistics. It has gained attention due to its flexibility in modelling various real-world phenomena. Distribution functions describe placement and energies plasma populations in space. The statistical origin of these distributions is associated with the framework of classical statistical mechanics. The particle distribution and correlation function within a one-component plasma are influenced by the Coulomb coupling parameter (Γ), which quantifies the strength of particle interactions relative to thermal energy.

The paper is organized into four main sections. Section 2 introduces the concept of n-particle reduced distribution functions, which are essential for describing the statistical properties of many-particle systems. Section 3 focuses on the one-component plasma (OCP) model and derives its distribution function. Section 4 addresses the challenge of estimating parameters for the strongly coupled OCP model.

2. Definition of n-particle reduced distribution functions in Statistical Mechanics

The states of particle n in the phase space in classical statistical mechanics are described by the probability distribution function f (r_i), where r_i , i= 1,2,3,…,n is the position of particle number i.

The classical system (OCP) is an ideal system of ions immersed in a uniform sea of electrons such that the entire system is electrically neutral [8-9].

The continuous Bilal distribution introduced by Abd-Elrahman [17] has a probability density function (pdf) given by

$$(1) f_{BD}(r_i) = \frac{6}{\mu} e^{-\frac{2r_i}{\mu}} \left(1 - e^{-\frac{r_i}{\mu}}\right), \quad r_i \geq 0$$

Where μ is a shape parameter for our distribution ($\mu > 0$)

For a system containing N particles we can define the n-particle reduced distribution functions of order s< N,

$$f^{(s)}(r) = \int f^N \prod_{i=s+1}^{N} d^3 r, \qquad (2)$$

For physical system with phase space, the distribution will be $f(r_1, r_2 \ldots, r_N)$ for N point particles in R^3 with positions. The binary distribution function for r_1, r_2 is given by

$$f^{(2)}(r_1, r_2) = F^{(1)}(r_1) F^{(1)}(r_2)[1 + G(r_1, r_2)] \qquad (3)$$

Where $G(r_1, r_2)$ is the correlation function between two particles.

In the pseudopotential theory the binary correlation function can be defined by pseudopotential [26]. The correlation function g(r) determines particle distribution in the system. i.e. radial distribution functions, are applied for evaluation of plasmas thermodynamic characteristics such as pressure, free energy etc.

$$G(r_1, r_2) = 1 - \frac{v(r_{12})}{KT} \qquad (4)$$

Where $v(r_{12})$ is the Coulomb potential, T is the plasma temperature and K is the Boltzmann constant.

3. Distribution function for one-component plasma (OCP) Model

The one-component plasma (OCP) in d dimensions is a system of identical point particles carrying a charge e and interacting through the d dimensional Coulomb potential; to ensure charge neutrality the particles are immersed in a uniform background of opposite charge. The Coulomb potential v(r) in d dimensions is the solution of Poisson's equation [16]:

$$\Delta v(r) = -2\pi^{\frac{d}{2}}\left[\Gamma\left(\frac{d}{2}\right)\right]^{-1} e^2\delta(r) \qquad (5)$$

where Δ denotes the d-dimensional Laplace operator. The OCP is the simplest possible model of a continuous Coulomb fluid and is hence of considerable theoretical importance.

In two dimensions, the Coulomb interaction potential between two particles at a distance r from one another is[17]

$$v(r) = \frac{e^2}{r} l^{-\frac{r}{r_D}} \qquad (6)$$

where $r_D = \sqrt{\frac{KT}{4\pi e^2 n}}$, e is a charge of electron, n stands for particles concentration.

Substituting from the equations (6),(4) and (1) into equation (3) we get

$$f_{BD}^{12} = \frac{36}{\mu^2 r_{12}} e^{-\frac{3(r_1+r_2)}{\mu}} l^{-\frac{r_{12}}{r_D}}\left(1 - e^{-\frac{r_1}{\mu}} - e^{-\frac{r_2}{\mu}} + e^{-\frac{(r_1+r_2)}{\mu}}\right)$$

$$\times\left[2r_{12} l^{-\frac{r_{12}}{r_D}} - e^2\right], \quad r_1 \geq 0, r_2 \geq 0, \mu > 0\,. \qquad (7)$$

4. Estimation of parameters for strongly coupled (OCP) Model

The distribution of particles and correlation function g(r) depending on the strength of their electrical interactions (Coulomb coupling parameter, Γ)[2]. The value of Γ for OCPs is calculated using the following equation:

$$\Gamma = \frac{q^2}{4\pi\varepsilon_0 KT}\frac{a}{\lambda_D} \qquad (8)$$

Where q is the charge of each particle, ε_0 is the vacuum permittivity k is the Boltzmann constant, T is the temperature of the plasma, a is the average inter-particle distance and λ_D is the Debye length (a measure of screening in a plasma).

For weak interactions ($\Gamma < 5$), a correlation function considers the Debye-Hückel effect, where particles arrange to weaken the overall electric field. Also, for strong interactions ($\Gamma \geq 5$), there are another correlation function accounts for the oscillations and their decay observed in g(r) after its first peak.

In a one-component plasma (OCP), a strongly coupled plasma refers to the state where the Coulomb coupling parameter (Γ) is greater than 5. In this regime, the electrostatic repulsion between the identically charged particles becomes the dominant force compared to their random thermal motion. Desbiens et. al [2] presents a comprehensive parametrization for the pair correlation function and static structure factor of the one-component plasma mode as:

$$g(r) = 1 + (\sigma - 1)\frac{\cos\left(\alpha\frac{r}{\xi} - 1 + \beta\sqrt{(\frac{r}{\xi} - 1}\right)}{\cosh((\frac{r}{\xi} - 1)\left((\sigma - \epsilon)e^{-\sqrt{(\frac{r}{\xi}-1)}/\gamma} + \epsilon\right)} \quad (9)$$

In the latter equations, and in the following, the distance r is in units of the Wigner-Seitz radius a. A least square fit method has been used to calculate the parameters for strongly coupled (OCP) Model $\xi = 1.63 + 7.93 \times 10^{-3}\sqrt{\Gamma} + \frac{2.56}{\Gamma^2}$, $\sigma = 1 + 1.09 \times 10^{-2}(ln\Gamma)^3$, $\alpha = 6.9 + \sqrt[3]{\frac{0.86}{\Gamma}}$,

$\beta = 0.23 - 1.78e^{-\frac{\Gamma}{60.2}}$ and $\epsilon = 0.99 + \frac{0.66}{\Gamma^{2/3}}$

Substituting from the equations (1) and (9) into equation (3) we get

$$f_{BD}^{12} = \frac{36}{\mu^2}e^{-\frac{2(r_1+r_2)}{\mu}}\left(1 + e^{-\frac{(r_1+r_2)}{\mu}}\right) - e^{-\frac{r_1}{\mu}}\frac{\sigma\cos\left(\alpha\frac{r_1}{\xi}-1+\beta\sqrt{(\frac{r_1}{\xi}-1}\right)}{\cosh((\frac{r_1}{\xi}-1)\left((\sigma-\epsilon)e^{-\sqrt{(\frac{r_1}{\xi}-1)}/\gamma}+\epsilon\right)} - 1.09 \times$$

$$10^{-2}(ln\Gamma)^3e^{-\frac{r_2}{\mu}}\frac{\cos\left(\alpha\frac{r_2}{\xi}-1+\beta\sqrt{(\frac{r_2}{\xi}-1}\right)}{\cosh((\frac{r_2}{\xi}-1)\left((\sigma-\epsilon)e^{-\sqrt{(\frac{r_2}{\xi}-1)}/\gamma}+\epsilon\right)} + \cdots \quad r_1 \geq 0, r_2 \geq 0, \mu > 0\,.$$

(10)

To estimate the parameter μ in the Bilal distribution, we employ a maximum likelihood estimation (MLE) approach. MLE involves finding the value of μ that maximizes the likelihood function, which is the product of the probability density function evaluated at each data point.

5. Conclusion

This research investigated the applicability of the Bilal distribution function, known for its flexibility in modelling complex scenarios, to analyse the behaviour of particles in a one-component plasma (OCP). The focus was on the binary distribution function (f(r)), a key tool in statistical mechanics that bridges the gap between microscopic and macroscopic properties. It provides information about the spatial arrangement of particles within the system, enabling the calculation of various physical properties. We notice from figure 1 that the values of the distribution functions converge with the increase of r for the different values of the μ parameter. Binary distribution functions converge faster with increasing values of r. See Figure 2. The behaviour of the distribution function shown in Figure 3 varies with increasing values of r and μ.

Comparison Bilal distribution with Existing Methods such as Analytical Solutions and Simulations, Bilal distribution offers a data-driven alternative to limited analytical solutions for complex OCP models. While simulations provide detailed information, the Bilal distribution can be a more computationally efficient approach, especially when a general understanding of g(r) is desired. Figure 4 show the Comparison between the binary distribution function from our result and Monte Carlo simulation, Eisa [10] and Jancovici [27] for r =(0,1) for OCP Plasma with μ =0.8

By leveraging these unique strengths, the Bilal distribution emerges as a promising tool for modelling g(r) in OCPs, complementing existing methods and potentially offering new insights into the behaviour of these fascinating systems. Three Dimensional modelling for the Classical binary distribution function with r_1,r_2 =(0,1) for OCP Plasma and μ =0.8 was given in figure 5.

Finally, The Bilal distribution, a flexible and computationally efficient model, offers several advantages over existing methods for modelling the binary distribution function (g(r)) in one-component plasmas (OCPs). Its ability to capture complex interactions and its data-driven approach make it valuable for analysing non-ideal plasmas. However, parameter estimation can be challenging, and the accuracy of the model may depend on specific OCP properties. In conclusion, the Bilal distribution emerges as a promising tool for modelling g(r) in OCPs, complementing existing methods and potentially offering new insights into the behaviour of these fascinating systems.

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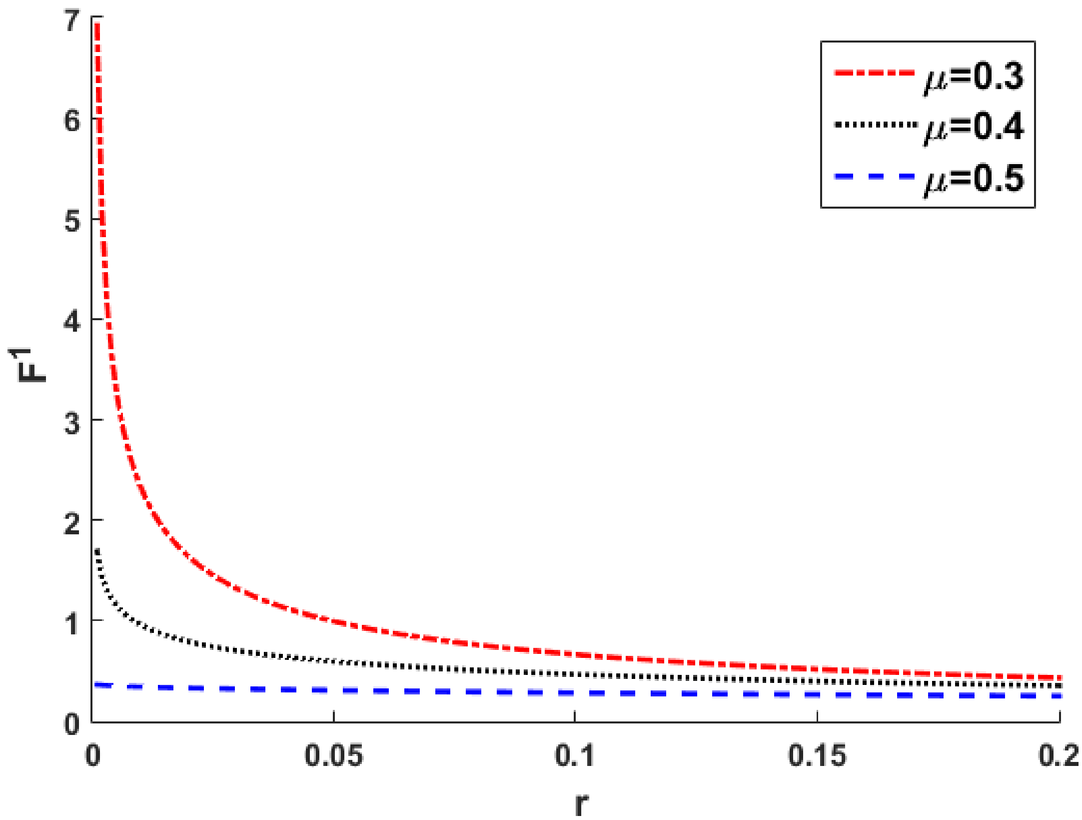

Figure 1 : The Classical one particle distribution function for r =(0,0.2) for OCP Plasma with different values of μ parameter .

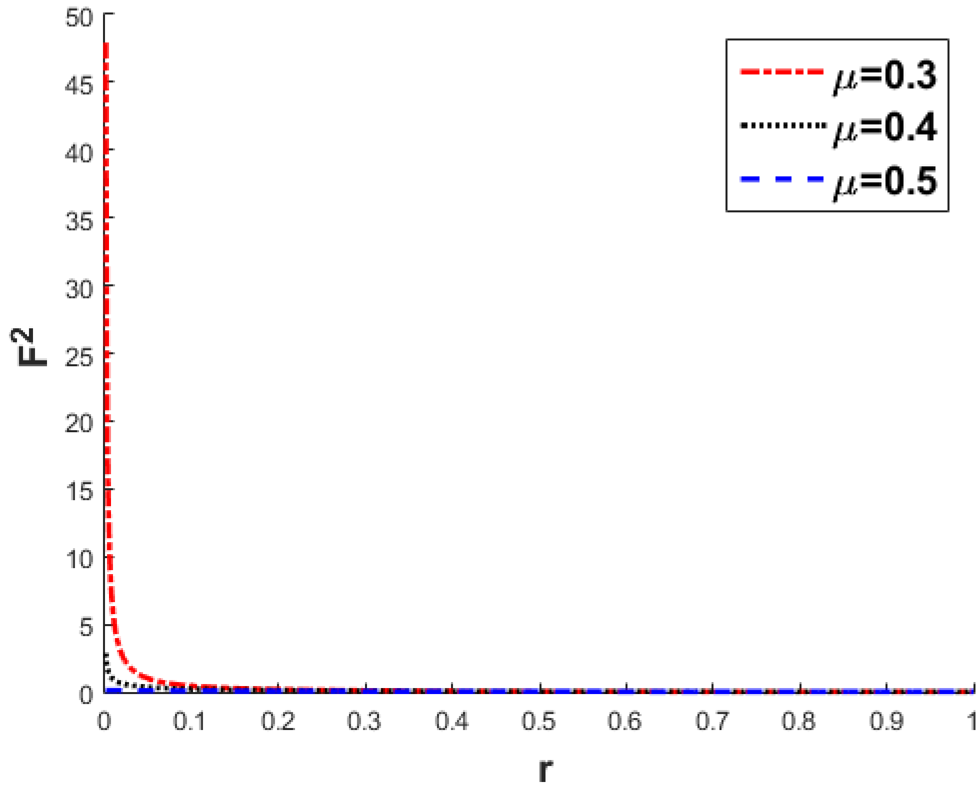

Figure 2 : The Classical binary distribution function for r =(0,1) for OCP Plasma with different values of μ parameter .

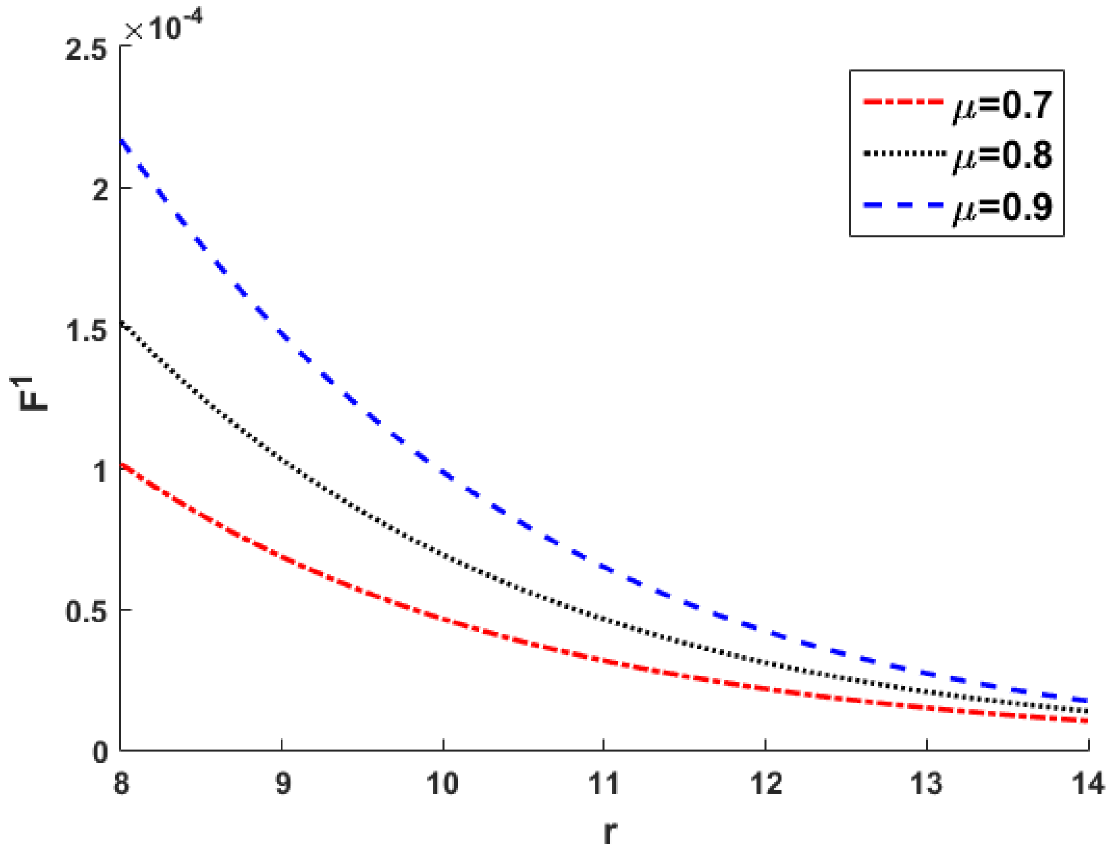

Figure 3 : The Classical distribution function for r =(8,14) for OCP Plasma with different values of μ parameter .

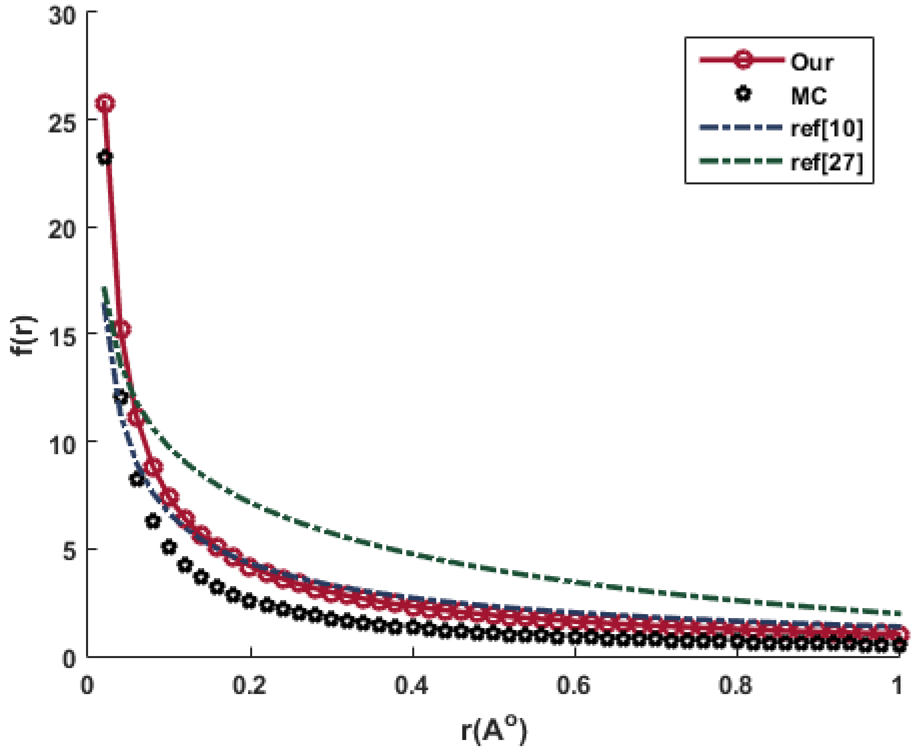

Figure 4 : Comparison between the binary distribution function from our result and monte carlo simulation , Eisa **[10] and** Jancovici **[27] for r =(0,1) for OCP Plasma with** μ **=0.8 .**

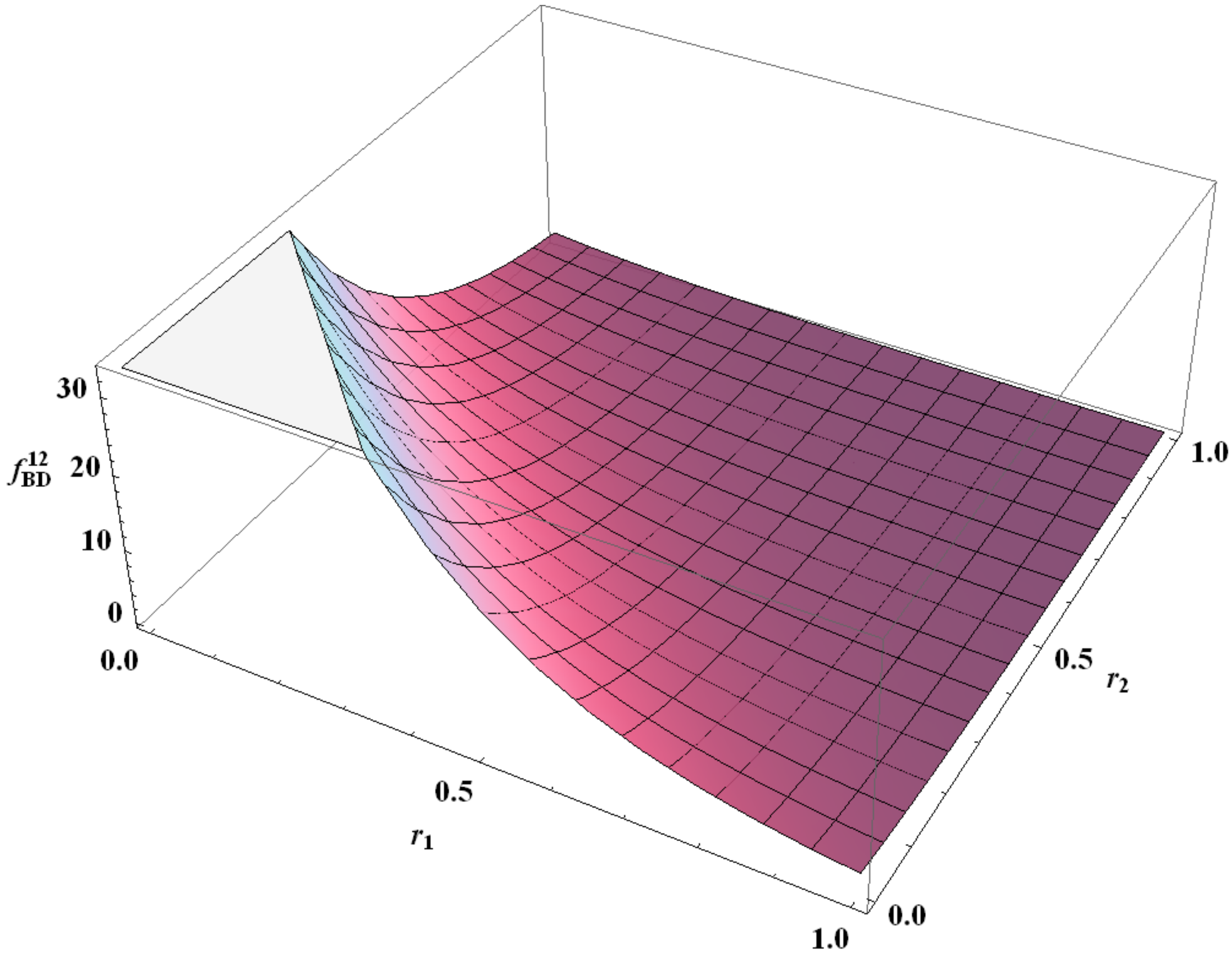

Figure 5 : The Classical binary distribution function for r_1,r_2 =(0,1) for OCP Plasma with μ =0.8 .