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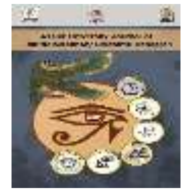

The Quantum Binary and Triplet Distribution Functions for Hydrogen Plasma Model

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ABSTRACT

Binary and triplet distribution functions provide essential insights into the microscopic interactions between particles in hydrogen plasma. These functions describe the probability of finding particles at specific distances and velocities from each other, offering a detailed understanding of the plasma's structure and thermodynamic properties. Hydrogen plasma models are pivotal for advancing our understanding of astrophysical phenomena, such as stellar formation and solar activity, while also playing a key role in the development of fusion energy a promising clean and sustainable energy source. Additionally, these models find applications in diverse fields, including materials processing, semiconductor manufacturing, and plasma medicine. The Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy is a fundamental tool for studying the dynamics of quantum plasmas, providing a rigorous framework for understanding the behaviour of many interacting quantum particles under various conditions. By capturing the correlations and collective interactions among particles, it bridges microscopic dynamics with macroscopic observables. This paper introduces a novel approach to calculating quantum binary and triplet distribution functions for hydrogen plasma models using the BBGKY hierarchy. The findings are analysed and compared with prior studies, shedding light on their implications for both theoretical and practical applications in plasma physics and quantum systems.

INTRODUCTION

The binary and triplet distribution functions are fundamental in understanding the properties of systems in statistical mechanics. In plasma physics, these functions play a crucial role in deriving thermodynamic quantities such as pressure, internal energy, and free energy, among others. Studying the distribution functions in hydrogen plasma is essential for understanding the interactions between charged particles, which aids in improving nuclear fusion models and developing spacecraft propulsion systems, material processing, semiconductor manufacturing, plasma-based lighting and displays, as well as medical and sterilization applications. Junzo Chihara [1] studied radial distribution functions and bound electronic energy levels in hydrogen plasmas. His work examined how radial distribution functions influence bound electronic energy levels, highlighting that particle interactions and plasma effects significantly impact the distribution of electronic energy, thus enhancing our understanding of plasma properties and related technologies. Filinov et al. [2] studied temperature-dependent quantum pair potentials in dense, partially ionized hydrogen plasmas. Their findings contributed to astrophysical models and laboratory experiments, deepening our understanding of plasma properties. Ebeling et al. [3] introduced the method of effective potentials within the quantum-statistical plasma theory framework. This method simplifies complex many-body interactions in plasmas by using effective pair potentials.

Understanding the behavior of hydrogen atoms in plasma jets can help scientists to develop new technologies for fusion energy and plasma-based materials processing. Mazouère et al. [4] investigates the behavior of hydrogen atoms in a plasma jet. The authors use a combination of experimental techniques and theoretical models to analyze the data. Their findings provide valuable insights into the complex dynamics of plasma jets and the behavior of neutral particles within them. Hussein and Ibrahim [5] investigates the behavior of fully ionized plasmas. The study focuses on the quantum mechanical effects on the equation of state of these plasmas. Dharma-Wardana and Perrot [6] used density-functional theory to study a neutral plasma of electrons and protons, calculating pair distribution functions, bound states, and effective charges at various temperatures and electron densities. Their results showed good agreement with machine simulations at high densities and demonstrated the appearance of bound states at high temperatures or low densities. Rogers [7] developed a method to determine effective occupation numbers for bound states in hydrogen plasmas by solving Poisson's equation for pair distribution functions. He separated the electrostatic potential into atomic and plasma parts at low densities, obtaining results consistent with the activity expansion method. In addition, Hussein and Ahmed [8] provided important contributions in calculating the second and third virial coefficients for the square-well potential and deriving expressions for the quantum equation of state for plasmas in thermal equilibrium. Hussein and Ibrahim [9] explored the quantum excess free energy of two-component plasmas and examined how the third virial coefficient plays a significant role at high temperatures.

Hussein et al. [10] also investigated the quantum thermodynamic properties of plasmas under weak magnetic fields, noting how pressure decreases at high temperatures and increases at low temperatures with stronger fields. Amemiya [11] conducted experiments to investigate the energy distribution function of electrons in hydrogen plasmas. His research focused on understanding how the energy of electrons in a plasma varies, which is crucial for various applications like plasma processing and fusion energy. The results of his experiments provided valuable insights into the behavior of electrons in hydrogen plasmas and contributed to the advancement of plasma physics research. Hussein et al. [12] investigates the thermodynamic properties of plasma using a quantum mechanical approach. The study utilizes the Green's function technique to calculate the quantum thermodynamic functions, such as free energy and pressure, for both one-component and two-component plasmas. This research provides valuable insights into the behavior of high-density plasmas and has implications for various fields, including astrophysics and plasma physics. Furthermore, Hussein et al. [13] derived binary and triplet distribution functions for plasmas using the Green's function technique, applying the Kirkwood Superposition Approximation and the BBGKY hierarchy in a two-component plasma model. This approach enhanced the understanding of plasma behavior, including quantum effects in electron-ion interactions. Ebeling et al. [14] provides a comprehensive theoretical framework for understanding the behavior of matter in extreme conditions. This seminal work delves into the quantum-statistical properties of dense gases and nonideal plasmas, addressing fundamental questions about their thermodynamic and transport properties. By combining rigorous theoretical analysis with advanced computational techniques, they offer valuable insights into the complex interplay between quantum effects and particle interactions in these systems.

The study of distribution functions in hydrogen plasmas is critical for advancing nuclear fusion research and developing a wide range of industrial and medical plasma technologies. The continued exploration of these functions contributes to the improvement of existing models and the development of new applications in various fields, from space propulsion to medical sterilization. Bonitz et al. [15] discuss how the Kelbg potential, which describes the effective interaction between charged particles in a plasma, plays a pivotal role in improving our understanding of quantum plasmas, particularly in high-density. This effective potential accounts for quantum effects, particularly at finite temperatures, providing a more accurate description of the interactions between charged particles. The Kelbg potential has been instrumental in simulations and theoretical studies of various systems, including plasmas and electrolyte solutions, significantly advancing our knowledge of their behavior and properties. Büchel et al. [16] introduces a novel approach to quantum mechanics, emphasizing the role of the Maxwell-Boltzmann distribution in describing quantum systems.

This research aims to investigate the binary and triplet distribution functions of hydrogen plasma, which provide crucial insights into the microscopic interactions between particles within the plasma. By calculating the position and velocity distribution functions using the BBGKY hierarchy equations. This approach allows for a detailed analysis of the correlations between particles in the plasma, providing valuable information for modeling and simulating plasma behavior

MATERIALS AND METHODS

In statistical mechanics, the BBGKY hierarchy represents a set of coupled equations that describe the dynamics of a system of interacting particles. These equations are essential for understanding the behavior of multi-particle systems in thermodynamic equilibrium.

Ebeling et al. [14] defined the BBGKY hierarchy as

$$\left(\frac{\partial}{\partial t}+\frac{\partial U_{12..s}(r_1,r_2,...,r_s)}{\partial r_s}\frac{\partial}{m_s\partial v_s}-v_s\frac{\partial}{\partial r_s}\right)F_{12....s}$$
$$=-\sum_{c=1,2,..,s+1} n_c m_c\int d^3r_{s+1}d^3v_{s+1}\,\frac{\partial U_{12..s}(r_1,r_2,...,r_{s+1})}{\partial r_1}\frac{\partial}{m_1\partial v_1}\;F_{12..s+1} \qquad (1)$$

Where r_s, v_s, m_s, n_s is the position vector, velocity, mass and density of the particle number s, respectively. Also, the potential energy of the system can be written as:

$$U_{a_1...a_s}=\sum_{a_1<a_2}U_{a_1a_2}+\sum_{a_1<a_2<a_3}U_{a_1a_2a_3}+... \qquad (2)$$

The BBGKY hierarchy consists of a series of distribution functions, each representing the probability density of finding a specific number of particles in a particular configuration.

The equation for an s-particle distribution function includes the (s + 1)-particle distribution function, forming a chain of coupled equations. This hierarchical structure reflects the increasing complexity of describing the interactions between particles as the number of particles considered increases.

The first equation for s = 1 in the BBGKY is

$$\left(\frac{\partial}{\partial t}+v_1\frac{\partial}{\partial r_1}\right)F_1(r_1,v_1,t)=\int m_2 d^3r_2d^3v_2\;\frac{\partial U(r_{12})}{\partial r_1}\frac{\partial}{m_1\partial v_1}\;F_{12}(r_1,r_2,v_1,v_2,t) \qquad (3)$$

The Kelbg potential has proven to be a valuable tool in understanding the behavior of hydrgen plasma. It provides a way to approximate the interaction between charged particles at finite temperatures, taking into account quantum effects. Bonitz et al. [15] define the Kelbg potential as:

$$U_{12} = q_1 q_2 \frac{1}{r_{12}} [1 - \exp(\frac{-r_{12}^2}{\lambda_{12}^2}) + \sqrt{\pi}\, \frac{r_{12}}{\lambda_{12}} (1 - erf(\frac{r_{12}}{\lambda_{12}})] \tag{4}$$

such that λ_{12} is the thermal wavelength and erf(x) is the standard error function.

The second equation for s = 2 in the BBGKY is

$$\begin{aligned}
&(\frac{\partial}{\partial t} + \frac{\partial U_{12}(r_{12})}{\partial r_1} \frac{\partial}{m_\alpha \partial v_1} + \frac{\partial U_{12}(r_{12})}{\partial r_2} \frac{\partial}{m_\alpha \partial v_2} - v_1 \frac{\partial}{\partial r_1} - v_2 \frac{\partial}{\partial r_2}) F_{12}(r_{12}, v_1, v_2, t) \\
&= -\sum_c n_c m_c \int d^3 r_3 d^3 v_3 \; \frac{\partial U_{13}(r_{13})}{\partial r_1} \frac{\partial}{m_\alpha \partial v_1} \quad F_{123}(r_1, r_2, r_3, v_1, v_2, v_3, t) \\
&- \sum_c n_c m_c \int d^3 r_3 d^3 v_3 \; \frac{\partial U_{23}(r_{23})}{\partial r_2} \frac{\partial}{m_\alpha \partial v_2} \quad F_{123}(r_1, r_2, r_3, v_1, v_2, v_3, t)
\end{aligned} \tag{5}$$

Where

$$F_{12}(r_{12}, v_1, v_2) = \; F_1(v_1) F_2(v_2) \, [1 + g_{12}(r_{12})], \tag{6}$$

$g_{12}(r_{12})$ is the two particle correlation function

Also,

$$\begin{aligned}
F_{123}(r_1, r_2, r_3, v_1, v_2, v_3) = \; & F_1(v_1) F_2(v_2) \; F_3(v_3) [1 + g_{12}(r_{12}) + g_{13}(r_{13}) \\
& + g_{23}(r_{23}) + g_{123}(r_1, r_2, r_3)]
\end{aligned} \tag{7}$$

Where $g_{123}(r_1, r_2, r_3)$ is the three particle correlation function.

The Maxwell-Boltzmann distribution is a fundamental concept in statistical mechanics and has many applications in various fields of physics. It is used to describe the behavior of gases, plasmas, and other systems in thermal equilibrium. In a hydrogen plasma, which is a gas of ionized hydrogen atoms, the Maxwell-Boltzmann distribution describes the statistical distribution of the velocities of electrons and protons [16] as:

$$F_i(v_i) = \alpha \exp(\frac{-\beta_i m_i v_i^2}{2}) \quad (8)$$

Where $\alpha = \left(\frac{\beta_i}{2\pi m_i}\right)^{3/2}$

The Binary Correlation Function BCF, denoted by $g_{12}(r_{12})$, describes the probability of finding two particles, one at position r_1 and the other at position r_2, relative to the probability of finding them at random positions. In a hydrogen plasma, the BCF is influenced by the Coulomb interaction between the electrons and protons, as well as quantum effects at high densities.

$$g_{12}(r_{12}) = \exp(-\beta U_{12}) \quad (9)$$

The Triplet Correlation Function TCF, denoted by $g_{123}(r_1, r_2, r_3)$ describes the probability of finding three particles at positions r_1, r_2, and r_3, relative to the probability of finding them at random positions. TCFs are more complex than BCFs and are often approximated using closure relations, such as the Kirkwood superposition approximation.

$$g_{123}(r_1, r_2, r_3) = \exp(-\beta[U_{12} + U_{13} + U_{23}]) \quad (10)$$

For calculating BDF and TDF For Hydrogen plasma. Substituting from equations (8) and (9) into equation (6) we get:

$$F_{12}(r_{12}, v_1, v_2) = \left(\frac{\beta_1\beta_2}{4\pi^2 m_1 m_2}\right)^{3/2} \exp(\frac{-\beta_1 m_1 v_1^2 - \beta_2 m_2 v_2^2}{2} + q_1 q_2 \frac{1}{r_{12}}[1 - \exp(\frac{-r_{12}^2}{\lambda_{12}^2})$$

$$+ \sqrt{\pi}\,\frac{r_{12}}{\lambda_{12}}(1 - erf(\frac{r_{12}}{\lambda_{12}})] \quad (11)$$

Also, substituting from equations (8) ,(9)and (10) into equation (7) we get:

$$F_{123}(r_1,r_2,r_3,v_1,v_2,v_3)=\left(\frac{\beta_1\beta_2\beta_3}{8\pi^3 m_1 m_2 m_3}\right)^{3/2}\exp\left(\frac{-\beta_1 m_1 v_1^2-\beta_2 m_2 v_2^2-\beta_3 m_3 v_3^2}{2}\right)[1+$$
$$\exp[\frac{-\beta q_1 q_2}{r_{12}}[1-\exp(\frac{-r_{12}^2}{\lambda_{12}^2})+\sqrt{\pi}\frac{r_{12}}{\lambda_{12}}(1-\mathrm{erf}(\frac{r_{12}}{\lambda_{12}})]]]+\exp[\frac{-\beta q_1 q_3}{r_{13}}[1-\exp(\frac{-r_{13}^2}{\lambda_{13}^2})+$$
$$\sqrt{\pi}\frac{r_{13}}{\lambda_{13}}(1-\mathrm{erf}(\frac{r_{13}}{\lambda_{13}})]]]+\exp[\frac{-\beta q_2 q_3}{r_{23}}[1-\exp(\frac{-r_{23}^2}{\lambda_{23}^2}+\sqrt{\pi}\frac{r_{23}}{\lambda_{23}}(1-\mathrm{erf}(\frac{r_{23}}{\lambda_{23}})]]]$$
$$+\exp[-\beta[\frac{q_1 q_2}{r_{12}}[1-\exp(\frac{-r_{12}^2}{\lambda_{12}^2})+\sqrt{\pi}\frac{r_{12}}{\lambda_{12}}(1-\mathrm{erf}(\frac{r_{12}}{\lambda_{12}}))]\,]+\frac{q_1 q_3}{r_{13}}[1-\exp(\frac{-r_{13}^2}{\lambda_{13}^2})+$$
$$\sqrt{\pi}\frac{r_{13}}{\lambda_{13}}(1-\mathrm{erf}(\frac{r_{13}}{\lambda_{13}}))]]+\frac{q_2 q_3}{r_{23}}[1-\exp(\frac{-r_{23}^2}{\lambda_{23}^2})+\sqrt{\pi}\frac{r_{23}}{\lambda_{23}}(1-\mathrm{erf}(\frac{r_{23}}{\lambda_{23}}))]]]] \quad (12)$$

DISCUSSION

The present study investigates the behavior of hydrogen plasma through the analysis of various distribution functions. **Figure 1** illustrates the Maxwell-Boltzmann velocity distribution for hydrogen plasma at different temperatures. As expected, the distribution shifts towards higher velocities with increasing temperature. This indicates that higher temperatures lead to increased particle kinetic energy, resulting in a broader range of velocities.

Figure 2 compares various pair potentials, including the Coulomb, Debye-Hückel, and Kelbg potentials. The Kelbg potential, which accounts for quantum effects, exhibits a more realistic behavior at short distances compared to the classical potentials. This suggests that quantum effects play a significant role in determining the interaction between particles at small separations.

Figures 3 and 4 illustrate the dependence of the BDF and TDF on distance and velocity for different temperatures (β values). As the distance between particles increases, the BDF generally decreases, indicating a reduced probability of finding particles close together. Additionally, as temperature increases (lower β), the BDF tends to spread out over a wider range of velocities, reflecting increased thermal motion. As the parameter β increases, thermal fluctuations decrease, and both binary and triplet distribution functions decrease.

Figures 5 and 6 compare the BDF and TDF calculated using different theoretical approaches (Fillinov et al. [2], Ebeling et al. [3], and our model). These comparisons highlight the impact of different approximations and assumptions on the predicted distribution functions. While the overall trends are similar, there are noticeable differences, particularly at short distances and high temperatures. The comparison demonstrates the influence of the β parameter and confirms the convergence of our results with previous studies at distances approaching r~1.

These findings provide valuable information for understanding the behavior of dense plasmas, where quantum effects play a crucial role. Further analysis of these distribution functions can help refine theoretical models and improve the accuracy of simulations.

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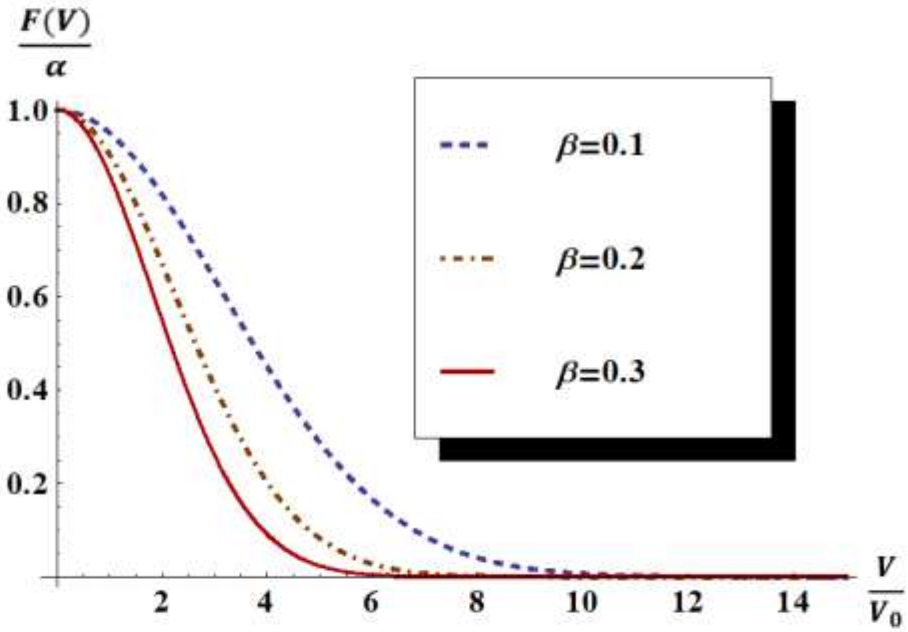

Figure 1: Maxwell-Boltzmann distribution for Hydrogen Plasma in the velocity of particle interval (0,15) in different values for β=1/KT (different temperature) ,V_0 initial velocity.

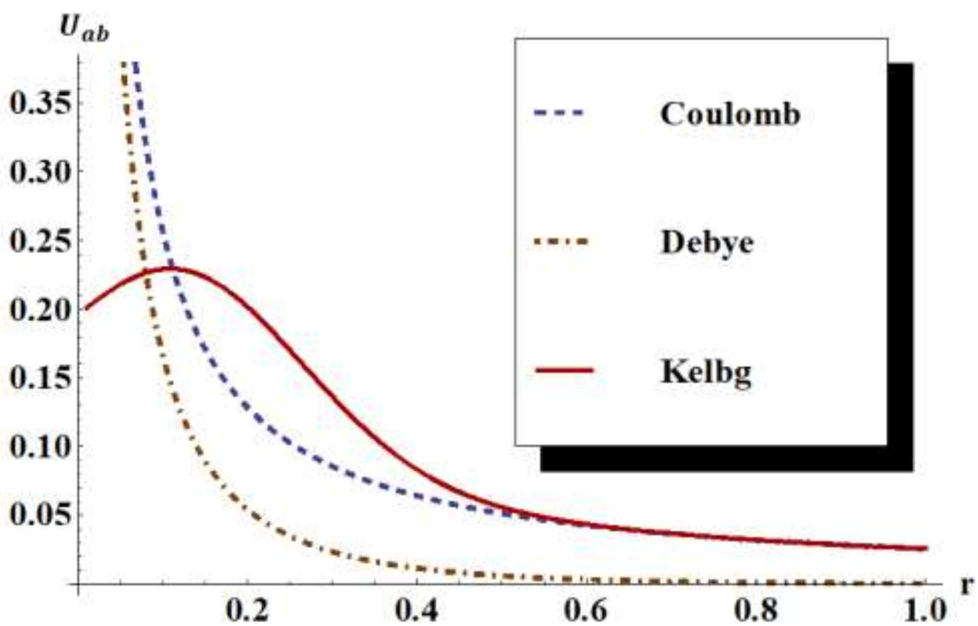

Figure 2: Comparison between the Kelbg-potential with various other potentials in the distance interval (0.01,1) at T=10^4.

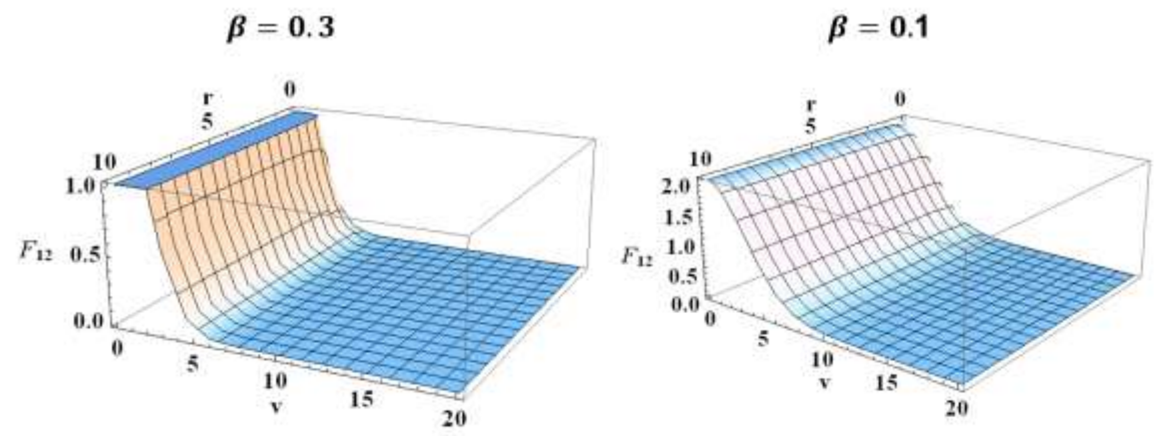

Figure 3: Relation between the quantum binary distribution function (BDF) for Hydrogen Plasma , distance in the interval (0.001,10) and velocity of particle interval (0,20) at β=0.1 , 0.3.

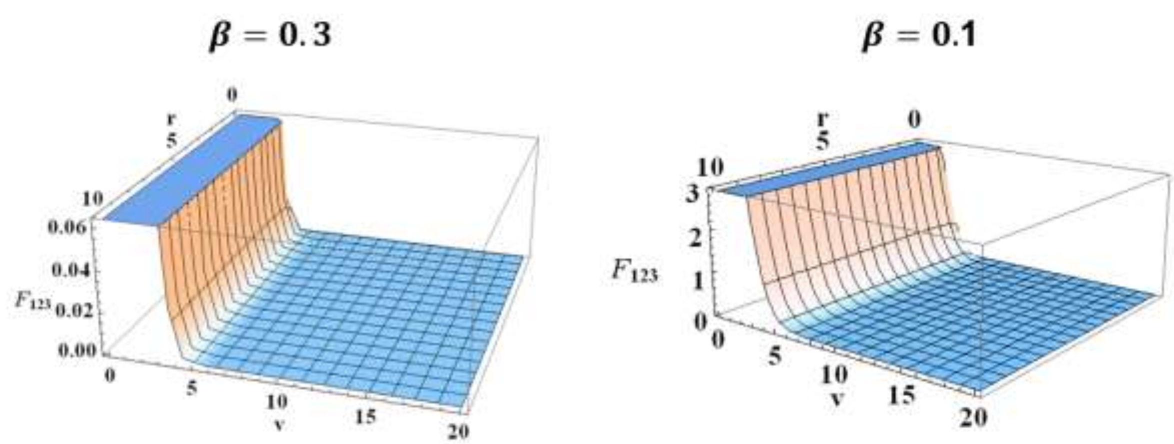

Figure 4: Relation between the quantum triplet distribution function (TDF) for Hydrogen Plasma , distance in the interval (0.001,10) and velocity of particle interval (0,20) at β=0.1,0.3.

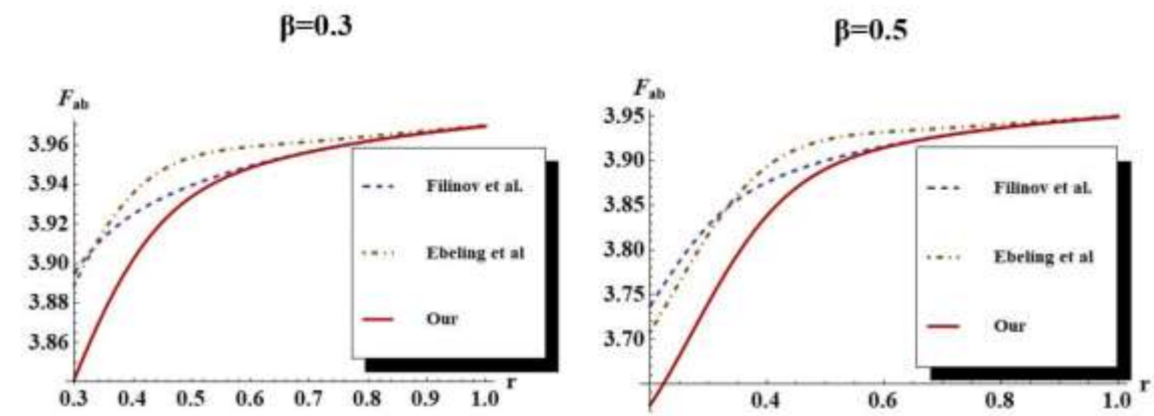

Figure 5: Comparison between the quantum binary distribution functions for both Fillinov et al. [2], Ebeling et al. [3] and Our for Hydrogen plasma , distance in the interval (0.001,10) and β=0.3 , 0.5.

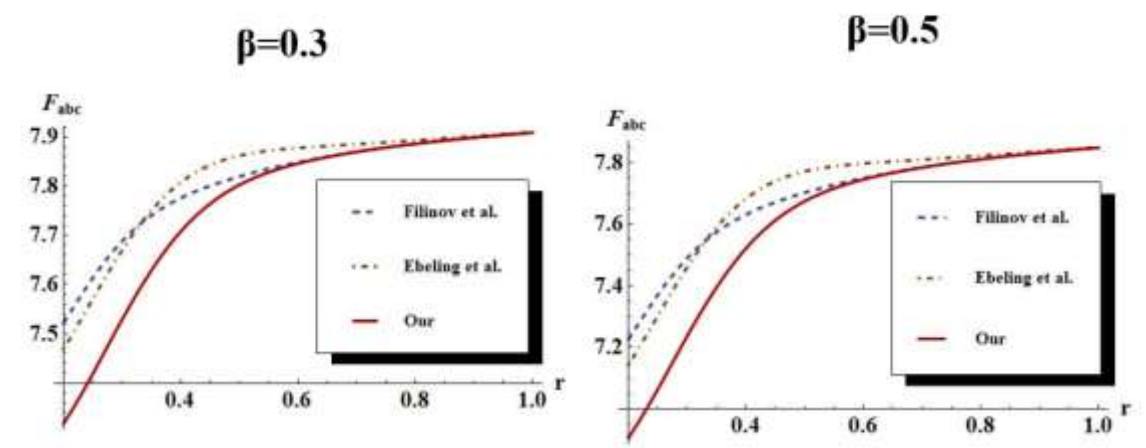

Figure 6: Comparison between the quantum triplet distribution functions for both Fillinov et al. [2], Ebeling et al. [3] and Our for Hydrogen plasma, distance in the interval (0.001,10) and β=0.3 , 0.5.