International Journal of Scientific Research in Physics and Applied Sciences **Research Paper**
Vol.7, Issue.3, pp.1-5, June (2019) **E-ISSN:** 2348-3423
DOI: https://doi.org/10.26438/ijsrpas/v7i3.15

Static Pair Correlation Functions and Static Structure Factors of Unidirectional Quantum Systems

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Available online at: www.isroset.org

Received: 22/May/2019, Accepted: 12/Jun/2019, Online: 30/Jun/2019

Abstract— Two of the structural functions, static pair correlation function of electrons around positively charged particles and static structure factor, have been theoretically calculated for a one dimensional quantum system with two mobile components occupying same charge density at equal temperatures. The structural functions have been investigated for their density and mass dependence. The reported values of static pair correlation function and structure factors are found to be dependent upon linear density and mass of positive components. Static pair correlation functions for a wide range of temperature, 100K≤T≤ 1500K, has also been generated theoretically. A variation, though diminutive, with temperature has been observed.

Keywords— *Static pair correlation function, Static structure factor, Complex dielectric functions, Plasma frequency , Fabrication techniques*

I. INTRODUCTION

Distinguished quantum systems; quantum dots, quantum wires, quantum wells are dimensionally confined systems whose structural and kinetic properties are quantized in terms of their charge carriers. Such systems, particularly, those restricted to a single dimension were previously supposed not to be ideally realizable. With the advent of advance fabrication techniques[1-9], however, it has become possible to develop such systems in laboratory. Electron beam lithography and wet chemical etching [9,10]are examples of such techniques, used to synthesize CdZnSe/ZnSe or InGaAs/GaAs hetero structures based one and two dimensional quantum systems.

In the present communication, two structural functions, static pair correlation function and static structure factor, of such a one dimensional quantum system has been investigated for their variation and dependence upon various physical parameters, like, temperature, mass and number density of its constituent particles. The mono-dimensional system has been assumed to be a two component system, positive and negative charge carriers, such that they constitute an overall neutral assembly of charged particles. The quantum behaviour of a one dimensional system can be specified by the condition $2r_s<\lambda_{th}$. Here, λ_{th} is de-broglie wavelength($=h/\sqrt{2mk_BT}$; h ,m, k_B & T are planck's constant, mass of charge carrier, boltzman constant & temperature respectively) and $2r_s$ represents the inter-particle separation.

This paper has been organized into four different sections: Introduction, Mathematical formalism, Results and discussion and Conclusion. In Section I a brief review of literature related to current research problem has been made. Section II, mathematical expression for distinct physical quantities has been provided. In section III, detailed computational results as obtained for quantum assembly under consideration has been provided and been thoroughly discussed. Section IV yields the conclusions drawn from the computational results.

II. MATHEMATICAL FORMALISM

Paired correlations of pair of electron and positively charged particles at time, t=0, in any system of moving particles can be expressed through its static pair correlation function, g(r). Expression for $g(r)$ function [11-13] for a one dimensional quantum system can be given as follows:

$$g(r)=1+\frac{1}{2\pi}\int_{-\infty}^{\infty}\left[\begin{array}{l}-\frac{z}{n}\mathrm{Re}\left(\frac{1}{\varepsilon_{\pm}(\kappa,\hbar\kappa^2/2M)}-1\right)\\ +\frac{z}{n}\frac{2}{\pi}\int_0^{\infty}d\omega\,\mathrm{Im}\left(\frac{1}{\varepsilon_{\pm}(\kappa,\omega)}\right)\ \mathrm{x}\ P\left(\frac{\hbar\kappa^2/2M}{\omega^2-(\hbar\kappa^2/2M)}\right)\end{array}\right]e^{i\kappa r}d\kappa \quad (1)$$

In expression (1), M is mass of positively charged particle, z is unit positive integer, $\varepsilon(\kappa,\omega)$ is its complex dielectric function and κ & ω are wave-vector & frequencies of quantum system respectively [14-17].

The static structure factor represents the coupled motion of electrons around positively charged impurity in Fourier-space. Expression for static structure factor is given as follows:

$$S(\kappa) = f_-\left(1+\frac{\kappa_+^{2} f_+}{\kappa^2}\right) \Big/ \left(1+\frac{\kappa_+^{2} f_+}{\kappa^2}+\frac{\kappa_-^{2} f_-}{\kappa^2}\right) \tag{2}$$

Here, $\kappa_+^{2} = \kappa_-^{2} = \frac{\omega_{p\pm}^{2}}{v_\pm^{2}}$ (3)

And,

$$f_\pm = e^{-h^2\kappa^2/8m_\pm^2 v_\pm^2}\left\{1+\frac{1}{3}\left(\frac{h\kappa}{2\sqrt{2}\,m_\pm v_\pm}\right)^2+\frac{1}{10}\left(\frac{h\kappa}{2\sqrt{2}\,m_\pm v_\pm}\right)^4+\dots\dots\right\} \tag{4}$$

In expression (3), $v_\pm = \sqrt{k_B T_\pm / m_\pm}$, are thermal velocities of positive and negative components and $\omega_{p\pm} = \sqrt{\pi n_\pm e^2\kappa^2(\ln\kappa)/m_\pm}$, are plasma frequencies [18-21] of positively and negatively charged mobile particles.

III. RESULTS AND DISCUSSION

Static pair correlation function of a weakly bound one dimensional quantum system is given by the expression (1). The system is constituted by neutral assembly of negatively (electrons) and positively charged particles having some finite mass. The same expression is used to calculate the static pair correlation function, $g(r)$, of a one dimensional quantum system having number density of 0.95x10^{-2} particles per Å. Such a dense system correspond to, 2r_s =1.05263 x 10^{-6} cm, where, 2r_s indicates the mean inter-particle distance. One can notice that to retain charge neutrality, number of positively charged particles are assumed to be equal to number of negatively charged particles. Further, the system is considered to be at a temperature, T=100K. Thermal de-Broglie wavelength, λ_{th}, of the plasma system under investigation turns to be λ_{th} =131.7Å and therefore, 2r_s< λ_{th}, which indicates the system is mildly quantum mechanical wherein the particles are weakly coupled.

Computed results for $g(r)$ function of such a quantum mechanical assembly of paired particles are plotted in Figure1, as their variation with r/r_s, for different masses of positively charged particles(i.e. m_+ = 1.0m_e(——), 2.5m_e(——), 5.0m_e(——), 7.5m_e (——)and 10.0m_e(——)).

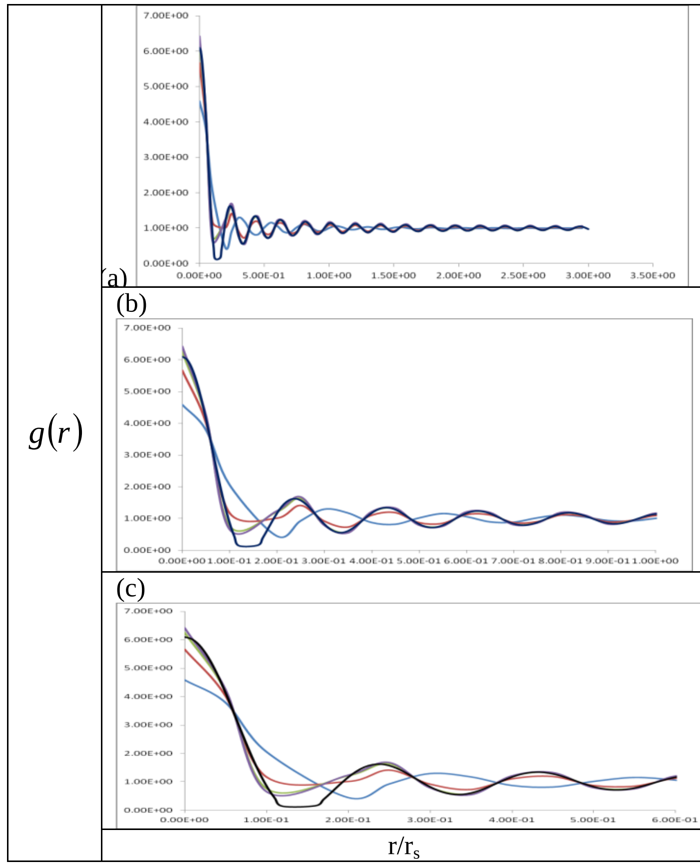

Figure 1: Variation of static pair correlation function with r/r_s for different masses of positively charged particles:1.0m_e(——), 2.5m_e(——), 5.0m_e(——), 7.5m_e (——)and 10.0m_e(——)

As is evident from the figure, $g(r)$ function shows the characteristic trend of variation with r/r_s, $g(r=0)$ is maximum and decreases to a minimum for lower values of r. With further increase in r/r_s, it increases and thereafter fluctuates about $g(r)$=1. However, with increase in mass of positive charge, the maximum value of $g(r)$i.e. $g(r=0)$ increases, is numerically lowest for m_+ = m_e and is the highest for m_+ =10.0 m_e. Also the decrease with increase in r/r_s is, sharper for heavier positive charge particles as compared to lighter positive charge particles and is least when mass of positively charged particle is equal to negatively charged particle i.e. mass of electron. This comparative trend is same for further increase in r/r_s, as can be seen from the figure, the height of secondary maxima is most sharp for m_+ =10.0 m_e and is least sharp for m_+ = m_e. This can also be noted from the figure 1(a), that the secondary and thereafter maxima are shifted towards higher values of r/r_s with decrease in mass, for m_+ =1.0 m_e, the secondary maxima value is at r/r_s~0.31, whereas for m_+ =10.0 m_e this lies at r/r_s~2.3. The overall trend, however, remains the same for all values of masses of positive component, characterizing the short range order of the system. In Figure 1(b) and Figure 1(c), same variation is shown up to r/r_s =1.0 and r/r_s =0.6 As compared to classical system with similar number densities[13], the oscillations in $g(r)$ about one in present system seems to be less damped.

In Figure2, variation of function of system of particles with same number density and r_s value is plotted for different temperatures ranging from100K≤T≤ 1500K, mass of the positive component is assumed to be five times the mass of the negative component. Here also, the static pair correlation function retains its peculiar behaviour even at higher temperatures (i.e. T= 1000K &1500K). Variation at T=100K is shown with(—); T=500K(—); T=1000K(—); and T=1500K with(—).

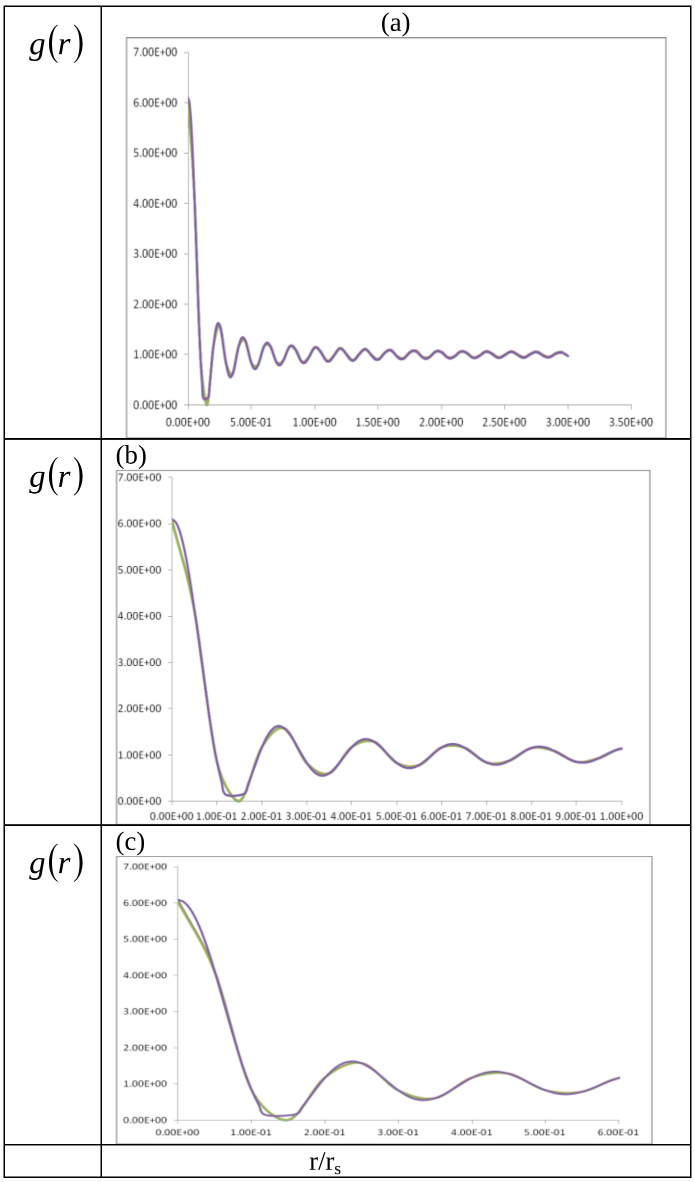

Figure 2: Variation of static pair correlation function with r/r_s at different temperatures: (—) 100K,(—) 500K, (—) 1000K and (—) 1500K.

As is clearly indicated by the figure, there is no evident change in the variation in $g(r)$ function at different temperatures and the plots at different temperatures are hardly distinguishable. For all temperature values, there is a sharp decrease in $g(r)$ for r/r_s≤0.2 and thereafter a periodic variation about 1.0, with constant decrease in amplitude, is seen with increase in r/r_s values. Moreover, for all values of temperature, $g(r)$ function saturates to a numerical value of one for r/r_s>2.75, as is shown in Figure 2(b). In Figure 2(c), the same variation is shown for r/r_s<0.1. There is a little decrease in $g(r=0)$values with increase in temperature. This variation of $g(r)$function with increase in temperature is in contrast to that of one component [13] system which shows makeable difference in variation of $g(r)$ function at different temperatures.

Variation of $g(r)$ function with r/r_s for two component quantum system at T=100K is plotted in Figure3 at four different densities of electrons: n=0.56x10^{-2} Å^{-1} with (—); n=0.95x10^{-2}Å^{-1} (—); n=2.8x10^{-2}Å^{-1}(—); n=5.6x10^{-2}Å^{-1}(—). The respective $2r_s$ values are 1.78x10^{-6} *cm*; 1.05x10^{-6} *cm*; 0.357x10^{-6} *cm*; 0.1786x10^{-6} *cm*. Hence, effect of density variation up to one order are being investigated.

As is clearly evident from the plot, with increase in density of particles, amplitude of $g(r)$ at r=0, decreases remarkably. Also, the $g(r)$ function for largest number of particles occupying a unit length, shows the least damping, at n=0.56x10^{-2}*Å*$^{-1}$ $g(r=0)\cong$ 10 whereas at n=5.6x10^{-2}Å^{-1}, $g(r=0)\cong$1.9. Moreover, quantum systems with greater inter-particle separations show much sharper decrease in $g(r)$ function value as compared to least denser systems for $2r_s$=1.786x10^{-6} *cm* & 1.056x10^{-6} *cm*, it decreases to minimum for r/r_s<0.15 whereas for $2r_s$=0.356x10^{-6} & 0.1786x10^{-6} *cm*, it attains the minimum for r/r_s=0.4 & 0.7 respectively. For larger values of r/r_s, trend of variation is same for all values of number density, the function shows oscillatory behaviour about one with decreasing amplitude and for further increase in r/r_s attains the constant value (i.e. one). Variation for larger values of r/r_s at all densities is shown in figure 3(b), and it can be observed from the figure that $g(r)$ remains constant (=1.0) for r/r_s ≥2.5, at all number densities.

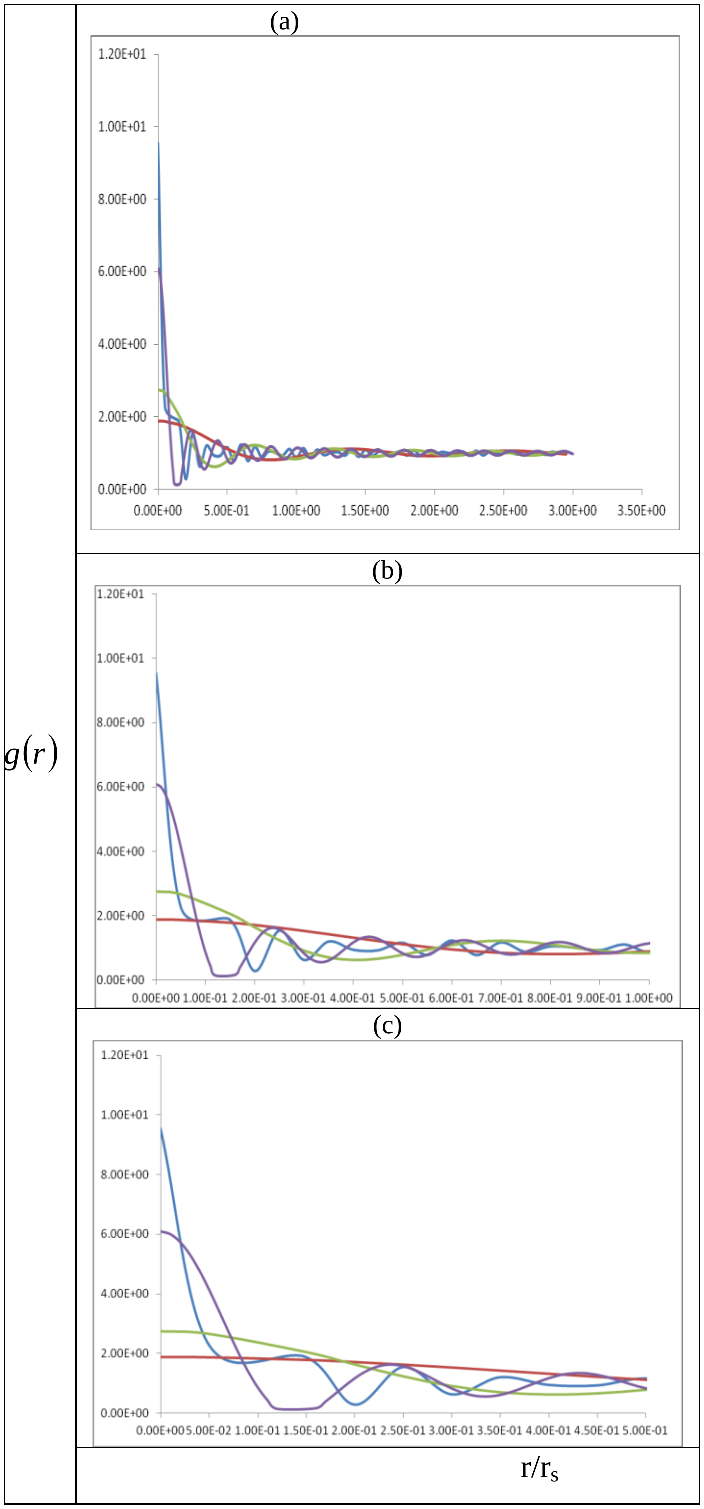

Figure 3: Variation of static pair correlation function with r/r_s for different number densities: n=0.56x10^{-2} Å^{-1} with (——); n=0.95x10^{-2}Å^{-1} (——); n=2.8x10^{-2}Å^{-1}(——); n=5.6x10^{-2}Å^{-1}(——).

Static structure factor expresses the correlated movement between pair of positive and negative charge particles in

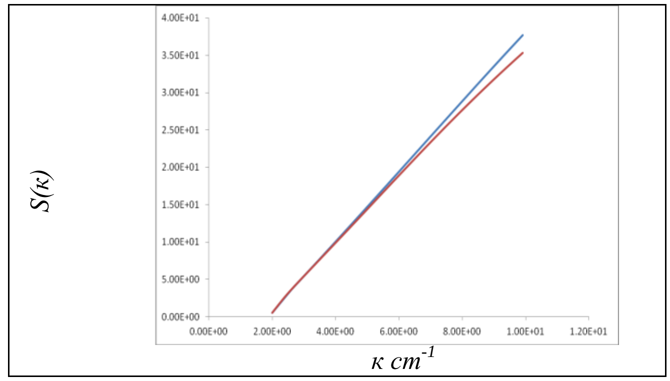

Figure 4: Variation of static structure factor *S(κ)* with wave-vector *κ:* 100K(——) and 500K(——).

Fourier space. Such a function has been computed by expression (2) and its variation versus wave-vector is shown in Figure4. Here, number density has been considered to be 0.95x10^{-2} cm^{-1} which corresponds to $2r_s$ value 1.056x10^{-6} *cm*. It can be observed that structure factor, *S(κ)* shows a proportional increase for increase in wave-vector. It can further be noticed that values for *S(κ)* function increases with increase in temperature at 100K(——) and 500K(——). For lower values of wave-vector, κ (κ≤5 cm^{-1}), there is a little variation with increase in temperature. With further increase in κ values, however, the two plots become distinguishable and for κ≥7.5 cm-1, the structure factor for system at higher temperature (500K) is quite high in comparison to that at lower temperature (100K).

IV. CONCLUSION

Static pair correlation function for one dimensional quantum system is found to be dependent upon number density of particles. The function shows a little variation with change in temperature but changes drastically for increase in mass of the positive component. Static structure factor is also found to be temperature dependant. The trend for variation is peculiar and remained unchanged for change in physical parameters.

The preferred spelling of the word “acknowledgment” in America is without an “e” after the “g”. Avoid the stilted expression, “One of us (R. B. G.) thanks . . .” Instead, try “R. B. G. thanks”. Put sponsor acknowledgments in the unnumbered footnote on the first page.

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