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Semiconducting Cylindrical Quantum – wire for Wigner Crystal of Electron Gas System with Density Functional Theory

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ABSTRACT

We have studied the Density Functional Theory (DFT) for Wigner crystal of electron gas in semiconducting cylindrical quantum wire (q-wire). The Wigner crystals are of single & double q-wire electron gas system. The electrons move freely in quasi one dimension as in semiconductor q-wire structure of infinite length in the direction of z-axis of cylinder. For lower density the solid-liquid phase transition is investigated in quasi one dimension and found Wigner transition at zero value temperature in crystalline phase and at critical densities if kinetic energy is lesser than Coulomb potential energy. The DFT of quantum-freezing for quantum-liquid describes the transition properties and the quantum-freezing transition is observed in one dimensional electron gas system that gives the hetero-structures of semiconductor q-wire. We have to calculate the ground state energy and energy difference per particle with electron density function, exchange and correlation energy and approximation of Thomas-Fermi & Weizsäcker and Coulomb potential. The distribution of inhomogeneous electron density in straight line gives Wigner transition in the two-dimension but in this work we have focused on one dimensional structure for quantum freezing density. The calculation of critical density parameter and q-wire width phase transition at zero temperature and Wigner crystal that observed in double layer electron gas system under the highest magnetic field and Wigner transition in quasi one dimension. By DFT as increasing the Wigner transition, decreasing the separation between double electron wire system and if more q-wire is available, the crystal density slightly decreases. This calculation for quasi one dimensional electron gas model with Wigner crystal by DFT is true for other types of models and found the energy of ground state. Our results were found with good agreement comparable to others.

KEYWORDS

Wigner Crystal, Density Functional Theory (DFT), Quantum (q) – wire, Ground State Energy, Electron Gas, Critical Density Parameter.

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INTRODUCTION

The closed-packed electrons form configuration of crystal with zero value of kinetic energy and minimum potential energy [1] at very low density and temperature and termed as Wigner crystal. E. Wigner was calculated the maximum value of correlation energy for the electrons crystal equal to $0.292e^2/r_s$ on neglecting the kinetic energy with the Rayleigh-Schrödinger perturbation theory. The semiconducting q-wire that allows transport of electrons along length of molecule is as electron-waveguide having radius in nanometers with order of deBroglie-wavelength and formed by atomic-chains in one dimension. The carbon nanotubes are also used as q-wires. The q-wire of $GaAs$ substrates is on $(311)A$ surface by molecular beam along $[2^-33]$ $orientation$ [2]. Berggreen and Pepper [3] were presented the transport of electrons in one-dimension with heterostructure of $GaAs-AlGaAs$ and apply the quasi one dimensional method to electron system for investigating electronic properties [4] in the cylindrical q-wires at low temperature. The transmission increases for smaller q-wire from zero. The electrons in Wigner lattice are in confined electric field. The electron localization in the Wigner crystals due to coulomb interaction is presented with heterostructure of semiconductor, grapheme, one dimensional systems etc. [5] with radius of Wigner-Seitz sphere. Coulomb forces for describing Wigner crystal of semiconductor structures with one dimensional electron gas are investigated [6]. Goldoni and Peeters [7] have been found the phases of quantum electron between Wigner crystals consisting first and second order of transition by using DFT. The local field corrections [8,10], short range correlations [9] are described with STLS approximation and short range interaction [10] in one dimensional system of electron gas. The effects of transvers confinements [11] were investigated in ground state of one-dimensional ferro-magnetic q-wire on electron correlation by using dynamical response theory and first order random phase approximation. Bordbar and Taheri [12] were formulated the $Hatree-Fock\ method$ for properties of ground state quasi one dimensional system of electron gas in magnetic field and shown increasing energy with increasing density that depends on correlation and exchange energy approximation [13]. The DFT is the wonderful method to describe the ground state energy. P.F. Loos [14-15] was given the concept of uniform electron gas that is an essential part of DFT with excited states near $Fermi$ level of Fermi $surface$. The ground state energies of quantum liquid are investigated by applying DFT [16-17]. The structure and freezing of ^{4}He is studied under the $Feymman-approximation$ and quantum Monte Carlo approximation. Ghosh [18] was worked on the theoretical density concept that may apply on classical system to mesoscopic model as well as quantum system to microscopic model termed as DFT. Rossi and Elisa [19] are presented the theoretical approach for removing the band edge from absorption-spectra by Coulomb correlation on non-liner optical characteristics of q-wire structure. The two dimensional confinements that may conduct electricity in which transport characteristics dominated by quantum effect so called q-wire. The two dimensional electron gas systems [20-22] are studied theoretically with magnetization or in higher magnetic field associated with wire for Wigner crystal by using concept of $Quantum\ Hall$. The investigation of cyclotron resonance absorption for two dimensional electron gas system is done in higher magnetic field of heterostructure of semiconducting Wigner crystal at $T = 4.2K$ [23]. The electronic-compressibility of carbon nanotube that depends on band-gap in low density crystalline electron lattice was measured by Neda and et.al [24]. And they found carrier number varying band-gap in carbon nanotubes. Rubel [25] was found one dimensional conductive channel in hetero-junction of two materials and predicted the induced electric field macroscopically that may prove by $ab-initio$ calculation. The electronic structure [26] is discussed in

molecular or ionic crystals and shown the formation of solids in which $Coulomb-interactions$ and cohesion are responsible. The equilibrium density of the two dimensional system is obtained by developing density function on the basis of $Thomas-Fermi\ von\ Weizsäcker\ approximation$ for Fermi gas [27]. They also explain the kinetic energy functional,$Hartree-Fock\ approximation$, total interaction with two dimensional geometry. The Thomas-Fermi model is solved right way for ground state electron gas by developing exchange and correlation energies [28]. The induced magnetic field in two dimensional electron gases is for semiconducting hetro-junction GaAs [29-30] q-wire of Wigner crystal. The calculation of mobility is done by using exchange-correlation effects [30]. Vinod and et.al, [31] were studied the q-wire correlation energy in limits $b \to 0$ & $r_s \to 0$ for $r_s < 1$ and found structure factor by single loop approximation. The exchange and correlation energies are found numerically in low density [32] for $0 < r_s < 20$, and evaluated the local field of quasi one dimensional electron gas by many body technics in the cylindrical q-wires. Lin [32] was explained about ground state of electron-hydrogen system and obtained the potential curve by using close coupling method that works better with correlation effects. The triangular lattice of Wigner crystal electron-fluid phase transition is predicted for two dimensional electron systems with DFT [33]. The correlation effects are calculated by quantum Monte Carlo process for two dimensional electron gas system in $z = 0$ plane at metallic-densities [33] that more commendatory for $r_s < 5$ [34] and proposed the excitonic crystal [35] for bilayer of electron-hole. The two dimensional electron system of Wigner cluster [36] is obtained at zero temperature in potential-wall. The quasi two dimensional electron gas system and two electrons quantum dot are used for investigating the three dimensional character of exchange and correlation energy of DFT that gives solicitation of graphite, and quantum structure of semiconductor [37]. The double walls of GaAs are enhanced by exchange sub-stantially with applying quantum kinetic theory computing $Hartree-Fock$-Wigner equation for the two dimensional electron gas systems [38].

METHODS

Let us consider the cylindrical q-wire [4, 32] is of infinite length with radius (b) in which the movement of electrons along z – direction in one dimension at the lowest sub-band that becomes true for $r_s \geq \frac{b}{4a_B^*}$ where, r_s is the Wigner – Seitz radius in one dimension and a_B^* represents the effective Bohr's radius approximately equal to 103Å that is larger with compare to standard value as 0.529Å for hydrogen atom and 0.265Å for helium atom. a_B^* is manifested with $\epsilon\ and\ m^*$ which is dielectric constant of semiconductor and effective mass of electron respectively of the materials. The distribution of inhomogeneous electron density $\{\rho(z)\}$ with homogeneous electron density $\{\rho_o\}$ and written as

$$\rho_o = \rho(z) - \rho_o \boldsymbol{\lambda} \cos(kz) \quad (1)$$

Where, k is wave vector in the one dimension and small parameter is $\boldsymbol{\lambda}\ (\ll 1)$. The electron density depending on the unity degeneracy of valley (g_v) is expressed as $\rho_o = \frac{2}{\pi} g_v k_f$ where, k_f is Fermi-wavenumber in one-dimension and $k = \frac{2\pi}{r_s}$, where, $r_s = \frac{\pi}{4 g_v k_f a_B^*}$, for equidistant electrons in straight line for solid phase. So, we may equation 1 be written as

$$\rho(z) = \frac{2}{\pi} g_v k_f \{1 + \boldsymbol{\lambda} \cos(8 a_B^*\ g_v k_f\ z)\} \quad (2)$$

The movement of electrons freely in quasi one dimension electronic system of electrons predicted in semi-conducting hetero-structure of q-wire and observed transition of quantum-freezing in one dimension. The excitonic-crystal [37] of quasi one dimensional q-wire semiconductor is found for range of density $1 < r_s \leq 5.5$. The DFT describes the transition of freezing of quantum liquid and all the theoretical approach are explained with DFT of freezing with charge density, explained above with equation (1) and (2), of energy function for inhomogeneous phase and homogeneous phase of electrons for single q-wire and double q-wire of Wigner crystal. In this work, to calculate the ground-state energy and energy difference, we discus about the correlation energy (ε_c) and the exchange energy (ε_x) of quasi one dimension

electron gas system over electron density function as

$$\varepsilon_c(\rho) = -\frac{c_0}{\pi} g_v k_f \int\{1 + \lambda \cos(8a_B^* g_v k_f z)\}\left\{\frac{-1+c_1 r_s+c_2 r_s^2}{1+c_3 r_s+c_4 r_s^2+c_5 r_s^3}\right\} dz \quad (3)$$

And

$$\varepsilon_x(\rho) = -\frac{x_0}{\pi} g_v k_f \int\{1 + \lambda \cos(8a_B^* g_v k_f z)\}\left\{\frac{-1+x_1 r_s+x_2 r_s^2}{1+x_3 r_s+x_4 r_s^2+x_5 r_s^3}\right\} dz \quad (4)$$

Where, the parameters c_i *and* x_i depend on the radius of q-wire and Wigner-Seitz radius. For calculating Wigner crystal of ground-state energy, here, we use the Thomas-Fermi and Weizsäcker- approximation for functional kinetic energy (T) and potential energy (U) of Coulomb interaction over density function in one dimension for inhomogeneous and homogeneous respectively manifested as

$$T(\rho) = C_k \rho_o^3\{1 + \boldsymbol{\lambda} \cos(kz)\}^3 + \frac{1}{8}\frac{\nabla\rho(z)\,\nabla\rho(z)}{\rho(z)} \quad (5)$$

$$U(\rho) = \frac{1}{2}\int \frac{\{\rho(z')-\rho_o\}\{\rho(z')-\rho_o\}}{\sqrt{b^2+(z-z')^2}}\, dz' \quad (6)$$

The exchange energy, ε_x, the correlation energy, ε_c, the kinetic energy, T, and the potential energy, U, all are the function of ρ. For zero value of applied potential, the energy of ground-state, ε_o, of electrons over the electron density function, $\rho(\boldsymbol{r})$, is manifested as

$$\varepsilon_o(\rho) = \int[\,\varepsilon_c\{\rho(\boldsymbol{r})\} + \varepsilon_x\{\rho(\boldsymbol{r}) + T\{\rho(\boldsymbol{r}) + U\{\rho(\boldsymbol{r})\}]\, d\boldsymbol{r} \quad (7)$$

The above equation (7) is for calculation of Wigner crystal in the higher dimension and identifies the inhomogeneous phase and homogeneous phase for energy at ground-state of charge density function. This describes phase-transition of liquid-solid in quasi one dimension electron gas system and found hetro-structure of semiconducting q-wire. For inhomogeneous phases and homogeneous phases, the energy difference, $\Delta\varepsilon = \varepsilon_i - \varepsilon_h$, per particle to the second-order of $\boldsymbol{\lambda}$ in atomic unit is

$$\frac{\varepsilon_i-\varepsilon_h}{\lambda^2} = \frac{4}{\pi^2} g_v^2 k_f^2 C_k + \frac{\pi^2}{4r_s^2} + \frac{g_v k_f}{\pi} K_o(k\,b) - \frac{1}{8}\frac{\pi x_o}{g_v k_f} - \frac{1}{8}\frac{\pi c_o}{g_v k_f} \quad (8)$$

Where, $K_o(k\,b)$ represent the modified Bessel's function.

The average kinetic energy approximation at temperature = 0, is $\langle K\rangle = \frac{\pi^2 n^2}{24m}$ and the average potential energy approximation of q-wire is $\langle V\rangle = \frac{e^2}{\sqrt{a_B^{*2} r_s^2 + b^2}}$. If the two q-wires of same radius are parallel to each other at d separation, the ground-state energy-function of electron gas system is $\varepsilon\{\rho^{(1)}, \rho^{(2)}\}$ on neglecting tunneling-effect between q-wires for $\frac{d}{b} \geq 1$. The additional approximation of the potential energy for single q-wire is $\langle V\rangle = \frac{e^2}{\sqrt{a_B^{*2} r_s^2 + d^2}}$.

RESULTS AND DISCUSSION

The semiconducting Wigner crystal q-wire in quasi one-dimension is hetro-structure in the electron gas system that formed by transition of quantum freezing and described the ground-state energy and energy differences per particle by DFT. In quasi one-dimension semi-conducting q-wire, the excitonic-crystal was found for densities as $1 < r_s \leq 5.5$ [37] but in recent the densities of $r_s \approx 1$ and its calculation with the values in Table 1 of excitonic Wigner crystal. The freezing point was found at critical density (r_{sc}) for q-wire radius $(b) < 2a_B^*$. The properties of solid-liquid transition using thermodynamical parameters have been described with DFT of quantum freezing. The energy of ground state over density function of electron is expressed with the single as well as double q-wire Wigner crystal with application of Thomas-Fermi von Weizsäcker approximation, Coulomb potential, correlation and exchange energies. We have plot density function parameter (r_s) with average energy difference per particle $(\Delta\varepsilon/\lambda^2)$ with equation (8) shown in Figure 1 for radius $0.5a_B^*$ represented by dashed line and a_B^* represented by solid line. This helps us for calculating Wigner crystal in inhomogeneous phase and homogeneous phase and explains the phase transition of solid-liquid in quasi one-dimensional system of electron gas and obtains the quantum freezing transition of heterostructure semiconducting q-wire. The quantum freezing transition located at critical-densities (r_{sc}) for the separation $(d = nb)$ between double q-wire system of radius b = a_B^* of both in Table 2 where, $n = 1, 2, 4, \ldots$ The DFT

gives result using correlation energy of critical density and obtain Wigner crystallization in one dimension and on extending the calculation for two dimension in the double q-wire system with neglecting the tunneling effect for $d/b \geq 1$. The average energy difference per particle ($\Delta\varepsilon/\lambda^2$) is shown in figure 2 in phases of inhomogeneous and homogeneous. On decreasing the separation (d), increasing the critical density (r_{sc}) at the Wigner-transition.

Table 1: q-wire radius and density parameter for calculation of Wigner crystal

q-wire radius (b)	Critical Density Parameter (r_{sc})
$0.5a_B^*$	5.35
$1.0a_B^*$	5.71

Table 2: Separation between q-wires and density parameter for calculation of Wigner crystal

Separation (d)	Critical Density Parameter (r_{sc})
b	5.47
$2b$	5.65
$4b$	5.71

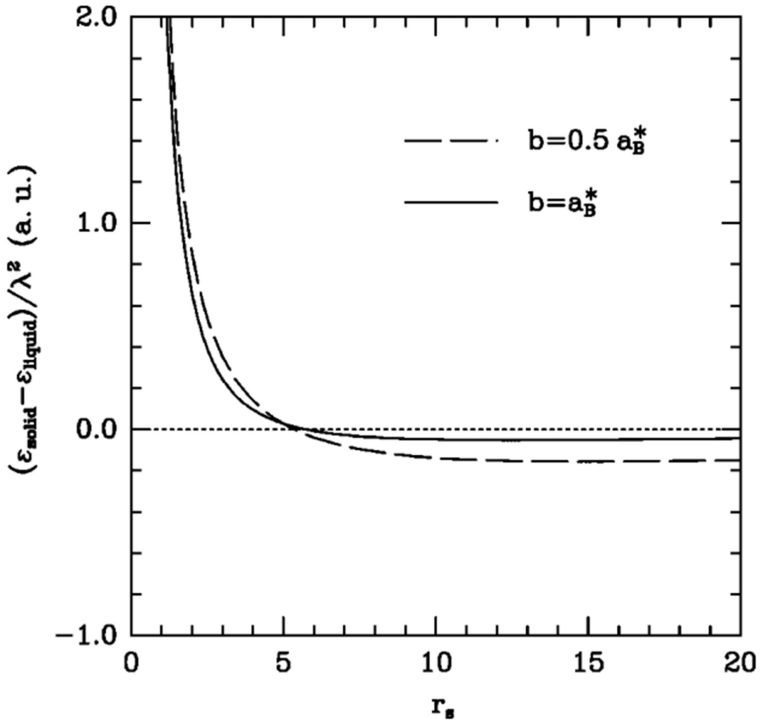

Figure 1: Plot density function parameter (r_s) with average energy difference per particle ($\Delta\varepsilon/\lambda^2$) for single q-wire

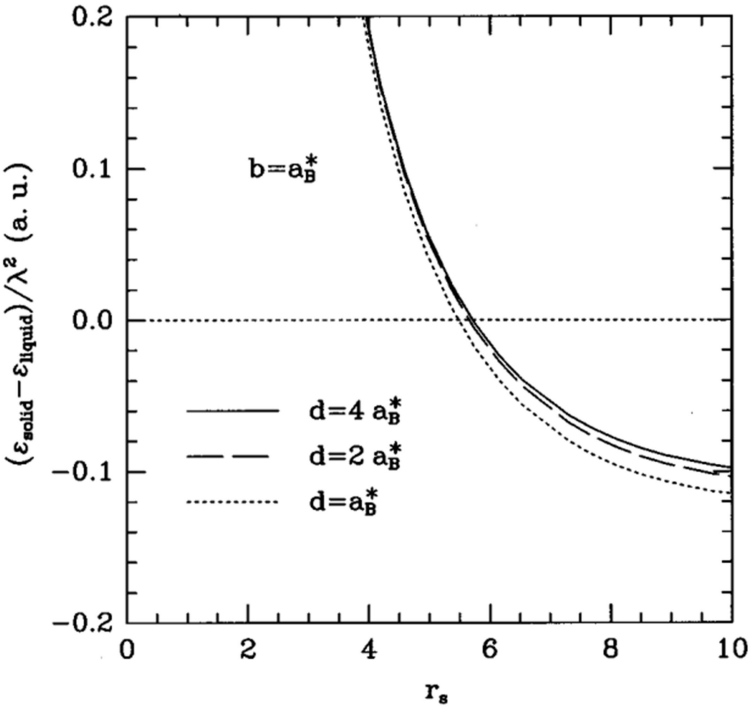

Figure 2: Plot density function parameter (r_s) with average energy difference per particle ($\Delta\varepsilon/\lambda^2$) for double q-wire

CONCLUSIONS

We have scrutinized the semiconducting cylindrical single and double q-wires for Wigner crystal of one and two dimensional electron gas systems with DFT. For it, we have used the correlation energy and the exchange energy and found the quasi one dimensional electron model for Wigner crystal that comparable with others. The calculation of ground state energy is done by DFT and calculation of exchange energy, correlation energy, Thomas-Fermi von Weizsäcker approximation kinetic energy and potential energy of Coulomb interaction over density in one dimensional electron systems. The inhomogeneous phase and homogeneous phase are identified for charge density of energy and described the phase transition of liquid-solid by DFT of quantum freezing. By neglecting the tunneling effects between two parallel q-wires having same radius, the ground state energies have been found. In results, the critical density of single and double q-wire electron systems at which increasing the Wigner transition, decreasing the separation that is good agreement with others.

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