

A study and calculation of metallic nanowire properties by density matrix

Abstract

In this paper, the properties of nanowire have been studied under zero of temperature. When the temperature of metal nanowire is so much low, the electrons occupy in the lowest quantum levels. At first for calculation of nanowire properties, we can use analytical method and assume the nanowires as long cylinder and calculate its properties. In continuation, we consider the metal nanowire like interacting electronical gas in the field of positive ions in a cylinder with radius R and length of L , where $R \ll L$. We calculate its energy by density matrix method and then discuss about some metal nanowire properties. Studies show that by increasing of density, some thermodynamic properties of system also increase such as total energy, kinetic energy, pressure and incompressibility also increased.

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1. Introduction

Nanowires are one - dimensional structures, where that their two dimensions are limited from Nano order and its one dimension is unlimited and expands to micrometer. When the temperature of metal nanowire is so much low, the electrons occupy in the lowest quantum levels [1]. By comparing of electrons and ions, we find out that ions are heavier than electrons and so; electrons move very fast than ions, therefor the internal pressure of wire caused by moving of electrons. In fact, the density of electrons is too much and so the conductive electrons are not related to ions and move freely. Therefore free electrical gas with relativity electrons is a good module to find the energy and pressure of nanowire [2]. As before mentioned, we consider the metal nanowire like interacting electronical gas in the field of positive ions in a cylinder with radius R and length of L , where $R \ll L$. In this article we do the calculation regarding to electrical gas at zero temperature and presence of a magnetic field that its direction is parallel to the axis of cylinder. Calculations regarding to multi particles system are in two main parts. First part is regarding to interacting of particles with external field that is completely solvable; but the second part involves the interacting of particles among themselves. View point of technical, calculation of multi particles is unsolvable and difficult. So; we use the approximation method that density matrix is one kind of these methods [3]. Density matrix provides a suitable method to describe quantum multi particles system [4].

2. Analytical solution method for one metal nanowire

Here we consider that the nanowire is similar to long cylinder, now for a particle which is surrounded in a cylinder with length of L and radius of R that its Hamiltonian is as:

$$H = \frac{P^2}{2m} + V(x, y, z)$$

The potential $V(x, y, z) = V(\vec{r})$ then this potential can be written as,

$$V(\vec{r}) = \begin{cases} 0 \rightarrow \rho \leq R \\ \infty \rightarrow \rho > R \end{cases} \quad (1)$$

We have $\rho = \sqrt{x^2 + y^2}$ and also it is suitable to describe in cylindrical coordinates $\vec{r} = (\rho, \theta, z)$. It is the main point to find out the solution of Schrodinger equation in cylindrical coordinates,

$$H\psi = E\psi \quad (2)$$

For solution, substituting Hamiltonian in Schrodinger equation can be written as below equation

$$H = \frac{P^2}{2m} + V(\vec{r}) \Rightarrow H = -\frac{\hbar^2}{2m} \nabla^2$$

Thus in equation (1) $\rho \leq R$ we get $V(\vec{r}) = 0$ and substituting Hamiltonian in equation (2)

$$-\frac{\hbar^2}{2m} \nabla^2 \psi = E\psi \quad (3)$$

For solution of equation of (3) we can write $\nabla^2 \psi$ in cylindrical coordinates

$$\nabla^2 \psi = \frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho \frac{\partial \psi}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2 \psi}{\partial \theta^2} + \frac{\partial^2 \psi}{\partial z^2}$$

By substituting $\nabla^2 \psi$ in equation (3) we get

$$\frac{\partial^2 \psi}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial \psi}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2 \psi}{\partial \theta^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{2m}{\hbar^2} E\psi = 0 \quad (4)$$

To solve equation (4), for separating of variables, we change them

$$\psi = R(\rho) \varphi(\theta) Z(z) \quad (5)$$

By substituting equation (5) in equation (4) we get

$$\frac{\partial^2 R}{R \partial \rho^2} + \frac{1}{R \rho} \frac{\partial R}{\partial \rho} + \frac{1}{\varphi \rho^2} \frac{\partial^2 \varphi}{\partial \theta^2} + \frac{1}{Z} \frac{\partial^2 Z}{\partial z^2} + K^2 = 0$$

For calculation of variables we can write as follow

$$\frac{1}{Z} \frac{\partial^2 Z}{\partial z^2} = -K_z^2$$

$$\frac{\partial^2 Z}{\partial z^2} + K_z^2 Z = 0 \Rightarrow Z(z) = e^{ik_z z} \quad (6)$$

$$\frac{\rho^2}{R} \frac{\partial^2 R}{\partial \rho^2} + \frac{\rho}{R} \frac{\partial R}{\partial \rho} + \frac{1}{\varphi} \frac{\partial^2 \varphi}{\partial \theta^2} + (K^2 - K_z^2) \rho^2 = 0$$

$$\frac{1}{\varphi} \frac{\partial^2 \varphi}{\partial \theta^2} = -l^2 \Rightarrow \frac{\partial^2 \varphi}{\partial \theta^2} + \varphi l^2 = 0 \Rightarrow \varphi = e^{i l \theta} \quad (7)$$

In equation (7) l is quantum number of angular momentum.

$$\frac{\partial^2 R}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial R}{\partial \rho} + \left(\mu^2 - \frac{l^2}{\rho^2} \right) R = 0 \quad (8)$$

In equation (8) $\mu^2 = K^2 - K_z^2$ and $K^2 = \frac{2m}{\hbar^2} E$ are described.

To change the equation (8) in form of standard in Bessel equation, we put $x = \mu\rho$ where the result is Bessel equation.

$$\frac{d^2 R}{dx^2} + \frac{1}{x} \frac{dR}{dx} + \left(1 - \frac{l^2}{x^2} \right) R = 0 \quad (9)$$

Equation (9) is standard form of Bessel equation that its answers are Bessel functions.

$$\alpha = l \Rightarrow J_{+l}(x) = \left(\frac{x}{2} \right)^l \sum_{j=0}^{\infty} \frac{(-1)^j}{j! \Gamma(j+l+1)} \left(\frac{x}{2} \right)^{2j}$$

$$\alpha = -l \Rightarrow J_{-l}(x) = \left(\frac{x}{2} \right)^{-l} \sum_{j=0}^{\infty} \frac{(-1)^j}{j! \Gamma(j-l+1)} \left(\frac{x}{2} \right)^{2j}$$

Also we study the roots of $J_l(x)$ as follow,

$$J_l(x) = 0 \Rightarrow x = x_{ln} \quad , \quad J_l(x_{ln}) = 0 \quad n = 1, 2, \dots$$

x_{ln} is n root of $J_l(x)$. For the first few values of quantum number l , the three first of roots are:

$$l = 0 \Rightarrow J_0(x_{0n}) = 0 \rightarrow x_{01} = 2.405 \quad , \quad x_{02} = 5.52$$

$$l = 1 \Rightarrow J_1(x_{1n}) = 0 \rightarrow x_{11} = 3.832 \quad , \quad x_{12} = 7.016$$

$$l = 2 \Rightarrow J_2(x_{2n}) = 0 \rightarrow x_{21} = 5.136 \quad , \quad x_{22} = 8.417$$

x_{ln} are roots and numbers.

For the above roots, the asymptotic formula $x_{ln} \approx n\pi + (l - \frac{1}{2})\frac{\pi}{2}$ gives sufficient accuracy.

$$x_{01} = \pi + (0 - \frac{1}{2})\frac{\pi}{2} = \frac{3\pi}{4}$$

$\mu = \frac{x_{ln}}{a} \Rightarrow x_{ln} = a\mu$, in terms of physics a is radius of cylinder but in terms of mathematics a is only a number.

$$J_l(x) = J_l(\rho\mu) = R(\rho) = J_l\left(\frac{x_{ln}}{a}\rho\right) \text{ if } : a = \rho \rightarrow J_l(x_{ln}) = 0$$

According to the above results, we can write general wave function as follow.

$$\varphi_{n,l,k_z} = A_{n,l} e^{il\theta} e^{ik_z z} J_l\left(\frac{x_{ln}}{a}\rho\right) \quad (10)$$

Here $A_{n,l}$ is constant of normalization that for its calculation can use the following equation.

$$A_{n,l} = \frac{2}{a^2 J_{l+1}^2(x_{ln})} \int \rho d\rho f(\rho) J_l\left(\frac{x_{ln}}{a}\rho\right)$$

$f(\rho)$ is an optional function which is considered as follow:

$$f(\rho) = \sum_{n=1}^{\infty} A_n J_l\left(\frac{x_{ln}}{a}\rho\right)$$

By calculation of $A_{n,l}$ the equation of (10) can be written as,

$$\varphi_{n,l,k_z} = \frac{1}{\sqrt{\pi a^2 L J_{l+1}^2(x_{ln})}} e^{il\theta} e^{ik_z z} J_l\left(\frac{x_{ln}}{a}\rho\right) \quad (11)$$

And also according to boundary conditions $R(a) = 0$ spectrum of energy can be obtained by the following equation.

$$E = \frac{\hbar^2}{2m} \left(\left(\frac{x_{ln}}{a}\right)^2 + k_z^2 \right) \quad (12)$$

If the numbers of electrons in nanowire are more than one and two, their energy can be calculated as following.

In state of base system quantum numbers are, $l = 0$, $n = 1$, $m = 0$. As we know from equation (12), the energy of a free electron is,

$$E = \frac{\hbar^2}{2m} \left(\left(\frac{x_{ln}}{a} \right)^2 + k_z^2 \right)$$

If this energy to be generalized for N electrons,

$$E_0 = \sum_{\vec{k}_z, l, n, \bar{s}} \frac{\hbar^2}{2m_e} \left(\left(\frac{x_{ln}}{a} \right)^2 + k_z^2 \right)$$

For calculation of N electrons the sigma sign changes to integral

$$\text{for } \rightarrow l=0, n=1, \sum_{\vec{k}_z, l, n, \bar{s}} \rightarrow \int_0^{k_f} \frac{gL}{2\pi} dk_z, \quad g=2$$

$$E_0 = \frac{2L}{2\pi} \int_0^{k_f} \frac{\hbar^2}{2m_e} \left[\left(\frac{x_{ln}}{a} \right)^2 + k_z^2 \right] dk_z$$

$$E_0 = \frac{\hbar^2}{2m_e} \left[\left(\frac{x_{ln}}{a} \right)^2 \frac{L}{\pi} k_f + \frac{L}{3\pi} k_f^3 \right] \quad (13)$$

To determine number of N electrons by following equation

$$N = \sum_{\vec{k}, \bar{s}} n(\vec{k}) = \int_0^{k_f} \frac{gL}{2\pi} dk_z \Rightarrow N = \frac{2L}{2\pi} k_f \quad (14)$$

$$N = \frac{L}{\pi} k_f \rightarrow \frac{N}{L} = \frac{k_f}{\pi} = \rho$$

To determine average energy at zero temperature

$$\frac{E_0}{N} = \frac{\hbar^2}{2m_e} \left[\left(\frac{x_{ln}}{a} \right)^2 \frac{Lk_f}{\pi} \times \frac{\pi}{Lk_f} + \frac{k_f^3}{3} \frac{L}{\pi} \times \frac{\pi}{Lk_f} \right]$$

$$\frac{E_0}{N} = \frac{\hbar^2}{2m_e} \left[\left(\frac{x_{01}}{a} \right)^2 + \frac{k_f^2}{3} \right] \quad (15)$$

As before we have $x_{01} = \frac{3\pi}{4}$ and by substituting of this equation in equation (15) we can get,

$$\frac{E_0}{N} = \frac{\hbar^2}{2m_e} \left[\left(\frac{\frac{3}{4}\pi}{a} \right)^2 + \frac{\left(\frac{N}{L}\pi \right)^2}{3} \right]$$

$$\frac{E_0}{N} = \frac{\hbar^2}{2m_e} \left[\left(\frac{3\pi}{4a} \right)^2 + \frac{(\rho\pi)^2}{3} \right] \quad (16)$$

3. Calculation of total energy of nanowires by density matrix method

In this part according to interacting of electrons, we can compute the energy of nanowires. For computation of energy of this system, temperature is considered zero. It is necessary to mention that; in calculation we use from zero temperature conditions.

Hamiltonian operator in Schrodinger equation formed from interacting of one and two electrons, it means that the operators only depend of one and two electrons coordinates. For calculation of total energy it is not necessary to know wave function $3N$ dimensions and it is enough to know density of possibility two electrons, one electron at r_1 and another at r_2 .

The Hamiltonian for an electrical gas which has interacting is as below

$$H = \sum_{i=1}^N U(\vec{r}_i) + \sum_{i<j} V(\vec{r}_i, \vec{r}_j) \quad (17)$$

Here $U(\vec{r}_i)$ the energy of single particle which is included from kinetic energy and energy of between electrons and ions and $V(\vec{r}_i, \vec{r}_j)$ is interacting energy among electrons.

$$U(\vec{r}_i) = \frac{-\hbar^2}{2m} \nabla_i^2 + u(\vec{r}_i) \quad (18)$$

$$\text{While } V(\vec{r}_i, \vec{r}_j) = \frac{1}{4\pi\epsilon_0} \frac{e^2}{|\vec{r}_i - \vec{r}_j|}, \quad u(\vec{r}_i) = \frac{-e^2}{4\pi\epsilon_0} \frac{z_\alpha}{|\vec{r}_i - \vec{R}_\alpha|}$$

Here z_α and \vec{R}_α respectively are atomic number and position vector to every ions.

As before mentioned, to obtain energy we can use density matrix method, because for wave function N particles for interactive particles is $N \sim 10^{23}$ it is like another interesting concepts of physics complicated and not possible to explain the N particles system completely. Here we introduce some quantities which is said density matrix. These quantities, according to wave function of multi particles of φ by integration on additional information is explained.

The first order of density matrix according to wave function of multi particles can be introduced as,

$$\gamma_\sigma(\vec{r}'_1 \vec{\sigma}'_1, \vec{r}_1 \vec{\sigma}_1) = N \sum_{\vec{\sigma}_2, \dots, \vec{\sigma}_N} \int \varphi^*(\vec{r}'_1 \vec{\sigma}'_1, \vec{r}_2 \vec{\sigma}_2, \dots, \vec{r}_N \vec{\sigma}_N) \times \varphi(\vec{r}_1 \vec{\sigma}_1, \vec{r}_2 \vec{\sigma}_2, \dots, \vec{r}_N \vec{\sigma}_N) d\vec{r}_2, \dots, d\vec{r}_N \quad (19)$$

According to equation (19) the form of density matrix of body without spin is written as,

$$\gamma(\vec{r}'_1, \vec{r}_1) = \sum_{\vec{\sigma}_1} \gamma_\sigma(\vec{r}'_1 \vec{\sigma}'_1, \vec{r}_1 \vec{\sigma}_1) \quad (20)$$

If substitute equation (19) in to equation (20),

$$\gamma(\vec{r}'_1, \vec{r}_1) = N \sum_{\vec{\sigma}_1, \vec{\sigma}_2, \dots, \vec{\sigma}_N} \int \varphi^*(\vec{r}'_1 \vec{\sigma}'_1, \vec{r}_2 \vec{\sigma}_2, \dots, \vec{r}_N \vec{\sigma}_N) \times \varphi(\vec{r}_1 \vec{\sigma}_1, \vec{r}_2 \vec{\sigma}_2, \dots, \vec{r}_N \vec{\sigma}_N) d\vec{r}_2, \dots, d\vec{r}_N \quad (21)$$

Also the second order of density matrix is written as,

$$\Gamma_{\sigma}(\vec{r}'_1 \vec{\sigma}'_1, \vec{r}'_2 \vec{\sigma}'_2; \vec{r}_1 \vec{\sigma}_1, \vec{r}_2 \vec{\sigma}_2) = \frac{N(N-1)}{2} \sum_{\vec{\sigma}_3, \dots, \vec{\sigma}_N} \int \varphi^* (\vec{r}'_1 \vec{\sigma}'_1, \vec{r}'_2 \vec{\sigma}'_2, \vec{r}_3 \vec{\sigma}_3, \dots, \vec{r}_N \vec{\sigma}_N) \times \varphi(\vec{r}_1 \vec{\sigma}_1, \vec{r}_2 \vec{\sigma}_2, \dots, \vec{r}_N \vec{\sigma}_N) d\vec{r}_3, \dots, d\vec{r}_N \quad (22)$$

And the form of without spin is as,

$$\Gamma(\vec{r}'_1, \vec{r}'_2; \vec{r}_1, \vec{r}_2) = \sum_{\vec{\sigma}_1, \vec{\sigma}_2} \Gamma_{\sigma}(\vec{r}'_1 \vec{\sigma}'_1, \vec{r}'_2 \vec{\sigma}'_2; \vec{r}_1 \vec{\sigma}_1, \vec{r}_2 \vec{\sigma}_2) \quad (23) \quad \text{Substituting equation (22) in}$$

equation (23)

$$\Gamma(\vec{r}'_1, \vec{r}'_2; \vec{r}_1, \vec{r}_2) = \frac{N(N-1)}{2} \sum_{\vec{\sigma}_1, \vec{\sigma}_2, \vec{\sigma}_3, \dots, \vec{\sigma}_N} \int \varphi^* (\vec{r}'_1 \vec{\sigma}'_1, \vec{r}'_2 \vec{\sigma}'_2, \vec{r}_3 \vec{\sigma}_3, \dots, \vec{r}_N \vec{\sigma}_N) \times \varphi(\vec{r}_1 \vec{\sigma}_1, \vec{r}_2 \vec{\sigma}_2, \dots, \vec{r}_N \vec{\sigma}_N) d\vec{r}_3, \dots, d\vec{r}_N \quad (24)$$

3-1 Total energy of system according to density matrixes

In this part energy of system according to density matrixes which is introduced above, we will explain. Energy state of system according to wave function of total system of φ is as below,

$$E = \langle \varphi | H | \varphi \rangle = \sum_{spin} \int \varphi^* H \varphi d\vec{r}_1 \dots d\vec{r}_N$$

or

$$E = \langle \varphi | H | \varphi \rangle = \int \varphi^* (\vec{r}_1 \vec{\sigma}_1, \dots, \vec{r}_N \vec{\sigma}_N) H \varphi(\vec{r}_1 \vec{\sigma}_1, \dots, \vec{r}_N \vec{\sigma}_N) d\vec{r}_1 \dots d\vec{r}_N \quad (25)$$

From equation of (25) expectation Hamiltonian quantity can be obtained according to density matrixes. To obtain Hamiltonian, substitute equations (17) and (18) in to equation (25).

$$E = \langle \varphi | H | \varphi \rangle = \int \varphi^* (\vec{r}_1 \vec{\sigma}_1, \dots, \vec{r}_N \vec{\sigma}_N) \left[\sum_{i=1}^N \sum_{\vec{\sigma}_1, \dots, \vec{\sigma}_N} \int \varphi^* (\vec{r}_1 \vec{\sigma}_1, \dots, \vec{r}_N \vec{\sigma}_N) \left[\frac{-\hbar^2}{2m} \nabla_i^2 + u_i(\vec{r}_i) \right] \varphi(\vec{r}_1 \vec{\sigma}_1, \dots, \vec{r}_N \vec{\sigma}_N) d\vec{r}_1 \dots d\vec{r}_N \right. \\ \left. + \sum_{i < j} \sum_{\vec{\sigma}_1, \dots, \vec{\sigma}_N} \int \dots \int \varphi^* (\vec{r}_1 \vec{\sigma}_1, \dots, \vec{r}_N \vec{\sigma}_N) V(\vec{r}_i, \vec{r}_j) \varphi(\vec{r}_1 \vec{\sigma}_1, \dots, \vec{r}_N \vec{\sigma}_N) d\vec{r}_1 \dots d\vec{r}_N \right]$$

After simplification, we can get,

$$E = \int d\vec{r}_1 \left\{ \left[\frac{-\hbar^2}{2m} \nabla_1^2 + u_1(\vec{r}_1) \right] N \sum_{\vec{\sigma}_1, \dots, \vec{\sigma}_N} \int \dots \int \varphi^* (\vec{r}'_1 \vec{\sigma}'_1, \dots, \vec{r}_N \vec{\sigma}_N) \varphi(\vec{r}_1 \vec{\sigma}_1, \dots, \vec{r}_N \vec{\sigma}_N) d\vec{r}_2 \dots d\vec{r}_N \right\} \Big|_{\vec{r}'_1 = \vec{r}_1} \\ + \int \int d\vec{r}_1 d\vec{r}_2 \left\{ V(\vec{r}_1, \vec{r}_2) \frac{N(N-1)}{N} \sum_{\vec{\sigma}_1, \vec{\sigma}_2, \vec{\sigma}_3, \dots, \vec{\sigma}_N} \int \dots \int \varphi^* (\vec{r}'_1 \vec{\sigma}'_1, \vec{r}'_2 \vec{\sigma}'_2, \vec{r}_3 \vec{\sigma}_3, \dots, \vec{r}_N \vec{\sigma}_N) \right. \\ \left. \times \varphi(\vec{r}_1 \vec{\sigma}_1, \vec{r}_2 \vec{\sigma}_2, \vec{r}_3 \vec{\sigma}_3, \dots, \vec{r}_N \vec{\sigma}_N) d\vec{r}_1 \dots d\vec{r}_N \right\} \Big|_{\substack{\vec{r}'_1 = \vec{r}_1 \\ \vec{r}'_2 = \vec{r}_2}} \quad (26)$$

If substitute integrals from equations (21) and (24) that respectively density matrixes not related on spin first and second orders, in equation (26), we get below equation.

$$E = \int d\vec{r}_1 \left[\frac{-\hbar^2}{2m} \nabla_1^2 + u_1(\vec{r}_1) \right] \gamma(\vec{r}_1, \vec{r}'_1) \Big|_{\vec{r}'_1 = \vec{r}_1} \\ + \int \int d\vec{r}_1 d\vec{r}_2 V(\vec{r}_1, \vec{r}_2) \Gamma(\vec{r}'_1, \vec{r}'_2; \vec{r}_1, \vec{r}_2) \Big|_{\substack{\vec{r}'_1 = \vec{r}_1 \\ \vec{r}'_2 = \vec{r}_2}} \quad (27)$$

The expression of two particles $\sum_{i < j} V(\vec{r}_i, \vec{r}_j)$ only related to density matrix of diametric element of two bodies, so we can write the equation (27) as follow;

$$E = \int d\vec{r}_1 \left[\frac{-\hbar^2}{2m} \nabla_1^2 + u(\vec{r}_1) \right] \gamma(\vec{r}_1, \vec{r}_1) \Big|_{\vec{r}_1 = \vec{r}_1} + \iint d\vec{r}_1 d\vec{r}_2 V(\vec{r}_1, \vec{r}_2) \Gamma(\vec{r}_1, \vec{r}_2) \quad (28)$$

At first, for calculation of this integral, must calculate the density matrixes of $\gamma(\vec{r}_1, \vec{r}_1')$, and $\Gamma(\vec{r}_1, \vec{r}_2)$. These matrixes are accurately countable by wave functions multi particles.

We form, the wave functions in the shape of states of single particle determinant that density matrixes takes simple shape. This matter at first time accepted by Dirac.

$$\varphi(\vec{r}_1 \vec{\sigma}_1, \dots, \vec{r}_N \vec{\sigma}_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_1(\vec{r}_1 \vec{\sigma}_1) & \dots & \varphi_1(\vec{r}_N \vec{\sigma}_N) \\ \varphi_2(\vec{r}_1 \vec{\sigma}_1) & \dots & \varphi_2(\vec{r}_N \vec{\sigma}_N) \\ \vdots & \vdots & \vdots \\ \varphi_N(\vec{r}_1 \vec{\sigma}_1) & \dots & \varphi_N(\vec{r}_N \vec{\sigma}_N) \end{vmatrix} \quad (29)$$

We use equation (19),

$$\gamma_\sigma(\vec{r}'_1 \vec{\sigma}'_1, \vec{r}_1 \vec{\sigma}_1) = N \sum_{\vec{\sigma}_2, \dots, \vec{\sigma}_N} \int \varphi^*(\vec{r}'_1 \vec{\sigma}'_1, \vec{r}_2 \vec{\sigma}_2, \dots, \vec{r}_N \vec{\sigma}_N) \times \varphi(\vec{r}_1 \vec{\sigma}_1, \vec{r}_2 \vec{\sigma}_2, \dots, \vec{r}_N \vec{\sigma}_N) d\vec{r}_2, \dots, d\vec{r}_N \quad (30)$$

Now, we

substitute equation (29) in equation (30)

$$\gamma_\sigma(\vec{r}'_1 \vec{\sigma}'_1, \vec{r}_1 \vec{\sigma}_1) = \frac{N}{N!} \sum_{\vec{\sigma}_2, \dots, \vec{\sigma}_N} \int \dots \int d\vec{r}_2, \dots, d\vec{r}_N \sum_{i, j, k, l, \dots} \varepsilon_{ijkl\dots} \varphi_i^*(\vec{r}'_1 \vec{\sigma}'_1) \varphi_j^*(\vec{r}_2 \vec{\sigma}_2) \times \sum_{i', j', k', l', \dots} \varepsilon_{i'j'k'l'\dots} \varphi_{i'}(\vec{r}_1 \vec{\sigma}_1) \varphi_{j'}(\vec{r}_2 \vec{\sigma}_2) \quad (31)$$

Also we have that,

$$\sum_{\vec{\sigma}} \int d\vec{r} \varphi_i^*(\vec{r}_1 \vec{\sigma}_1) \varphi_j(\vec{r}_1 \vec{\sigma}_1) = \delta_{ij} \quad (32)$$

If we use equation (32) in equation (31), we get;

$$\gamma_\sigma(\vec{r}'_1 \vec{\sigma}'_1, \vec{r}_1 \vec{\sigma}_1) = \frac{N}{N!} \sum_{i, j, k} \sum_{i', j', k'} \varepsilon_{ijk} \varepsilon_{i'j'k'} \varphi_i^*(\vec{r}'_1 \vec{\sigma}'_1) \varphi_{i'}(\vec{r}_1 \vec{\sigma}_1) \delta_{ij} \delta_{kk} \delta_{ll}$$

After simplification,

$$\gamma_{\sigma}(\vec{r}'_1 \vec{\sigma}'_1, \vec{r}_1 \vec{\sigma}_1) = \sum_i \varphi_i^*(\vec{r}'_1 \vec{\sigma}'_1) \varphi_i(\vec{r}_1 \vec{\sigma}_1) \quad (33)$$

Equation (33) shows the relation between density matrix of first order and wave function of single particle.

If there is no relation on spin, we can proof by summation of spin,

$$\begin{aligned} \gamma_{\sigma}(\vec{r}'_1 \vec{\sigma}'_1, \vec{r}_1 \vec{\sigma}_1) &= \sum_i \varphi_i^*(\vec{r}'_1 \vec{\sigma}'_1) \varphi_i(\vec{r}_1 \vec{\sigma}_1) \\ \sum_{\vec{\sigma}'_1} \gamma_{\sigma}(\vec{r}'_1 \vec{\sigma}'_1, \vec{r}_1 \vec{\sigma}_1) &= \sum_{\vec{\sigma}'_1} \sum_i \varphi_i^*(\vec{r}'_1 \vec{\sigma}'_1) \varphi_i(\vec{r}_1 \vec{\sigma}_1) \\ \gamma(\vec{r}'_1, \vec{r}_1) &= \sum_{\vec{\sigma}'_1} \sum_i \varphi_i^*(\vec{r}'_1) \varphi_i(\vec{r}_1) \eta_{\vec{\sigma}'_1}^{\dagger} \eta_{\vec{\sigma}_1} \\ \gamma(\vec{r}'_1, \vec{r}_1) &= \sum_i \varphi_i^*(\vec{r}'_1) \varphi_i(\vec{r}_1) \quad (34) \end{aligned}$$

Also for calculation of density matrix of second order which is appeared in integration of equation (28), we calculate by substitution of equation (29) in equation (22).

$$\begin{aligned} \Gamma_{\sigma}(\vec{r}'_1 \vec{\sigma}'_1, \vec{r}'_2 \vec{\sigma}'_2; \vec{r}_1 \vec{\sigma}_1, \vec{r}_2 \vec{\sigma}_2) &= \frac{N(N-1)}{2} \sum_{\vec{\sigma}_3, \dots, \vec{\sigma}_N} \int \varphi^*(\vec{r}'_1 \vec{\sigma}'_1, \vec{r}'_2 \vec{\sigma}'_2, \vec{r}_3 \vec{\sigma}_3, \dots, \vec{r}_N \vec{\sigma}_N) \\ &\quad \times \varphi(\vec{r}_1 \vec{\sigma}_1, \vec{r}_2 \vec{\sigma}_2, \dots, \vec{r}_N \vec{\sigma}_N) d\vec{r}_3, \dots, d\vec{r}_N \\ \Gamma_{\sigma}(\vec{r}'_1 \vec{\sigma}'_1, \vec{r}'_2 \vec{\sigma}'_2; \vec{r}_1 \vec{\sigma}_1, \vec{r}_2 \vec{\sigma}_2) &= \frac{N(N-1)}{2} \sum_{\vec{\sigma}_3, \dots, \vec{\sigma}_N} \int \dots \int d\vec{r}_3, \dots, d\vec{r}_N \psi^*(\vec{r}'_1 \vec{\sigma}'_1, \vec{r}'_2 \vec{\sigma}'_2, \vec{r}_3 \vec{\sigma}_3, \dots, \vec{r}_N \vec{\sigma}_N) \\ &\quad \times \psi(\vec{r}_1 \vec{\sigma}_1, \vec{r}_2 \vec{\sigma}_2, \dots, \vec{r}_N \vec{\sigma}_N) \\ \Gamma_{\sigma}(\vec{r}'_1 \vec{\sigma}'_1, \vec{r}'_2 \vec{\sigma}'_2; \vec{r}_1 \vec{\sigma}_1, \vec{r}_2 \vec{\sigma}_2) &= \frac{1}{2} \left\{ \left[\sum_i \varphi_i^*(\vec{r}'_1 \vec{\sigma}'_1) \varphi_i(\vec{r}_1 \vec{\sigma}_1) \right] \left[\sum_j \varphi_j^*(\vec{r}'_2 \vec{\sigma}'_2) \varphi_j(\vec{r}_2 \vec{\sigma}_2) \right] \right. \\ &\quad \left. - \left[\sum_i \varphi_i^*(\vec{r}'_1 \vec{\sigma}'_1) \varphi_i(\vec{r}_2 \vec{\sigma}_2) \right] \left[\sum_j \varphi_j^*(\vec{r}'_2 \vec{\sigma}'_2) \varphi_j(\vec{r}_1 \vec{\sigma}_1) \right] \right\} \quad (35) \end{aligned}$$

We add $\vec{\sigma}'_1$ and $\vec{\sigma}'_2$ on both side of equation (35);

$$\begin{aligned} \sum_{\vec{\sigma}'_1, \vec{\sigma}'_2} \Gamma_{\sigma}(\vec{r}'_1 \vec{\sigma}'_1, \vec{r}'_2 \vec{\sigma}'_2; \vec{r}_1 \vec{\sigma}_1, \vec{r}_2 \vec{\sigma}_2) &= \left\{ \left[\sum_{\vec{\sigma}'_1} \sum_i \varphi_i^*(\vec{r}'_1) \varphi_i(\vec{r}_1) \eta_{\vec{\sigma}'_1}^{\dagger} \eta_{\vec{\sigma}_1} \right] \left[\sum_{\vec{\sigma}'_2} \sum_j \varphi_j^*(\vec{r}'_2) \varphi_j(\vec{r}_2) \eta_{\vec{\sigma}'_2}^{\dagger} \eta_{\vec{\sigma}_2} \right] \right. \\ &\quad \left. - \frac{1}{V} \left[\sum_{\vec{\sigma}'_1, \vec{\sigma}'_2} \sum_i \varphi_i^*(\vec{r}'_1) \varphi_i(\vec{r}_2) \eta_{\vec{\sigma}'_1}^{\dagger} \eta_{\vec{\sigma}_2} \right] \left[\sum_{\vec{\sigma}_1, \vec{\sigma}_2} \sum_j \varphi_j^*(\vec{r}'_2) \varphi_j(\vec{r}_1) \eta_{\vec{\sigma}_2}^{\dagger} \eta_{\vec{\sigma}_1} \right] \right\} \end{aligned}$$

After simplification, we get:

$$\Gamma(\vec{r}'_1, \vec{r}'_2; \vec{r}_1, \vec{r}_2) = \frac{1}{2} \left\{ \sum_i \varphi_i^*(\vec{r}'_1) \varphi_i(\vec{r}_1) \sum_j \varphi_j^*(\vec{r}'_2) \varphi_j(\vec{r}_2) - \frac{1}{V} \sum_i \varphi_i^*(\vec{r}'_1) \varphi_i(\vec{r}_2) \sum_j \varphi_j^*(\vec{r}'_2) \varphi_j(\vec{r}_1) \right\}$$

$$\Gamma(\vec{r}'_1, \vec{r}'_2; \vec{r}_1, \vec{r}_2) = \frac{1}{2} \left\{ \gamma(\vec{r}'_1, \vec{r}_1) \gamma(\vec{r}'_2, \vec{r}_2) - \frac{1}{v} [\gamma(\vec{r}'_1, \vec{r}_2)]^2 \right\} \quad (36)$$

Density matrix of second order is related to diametric element and equation (36) can be written as;

$$\Gamma(\vec{r}_1, \vec{r}_2) = \frac{1}{2} \left\{ \gamma(\vec{r}_1, \vec{r}_1) \gamma(\vec{r}_2, \vec{r}_2) - \frac{1}{v} [\gamma(\vec{r}_1, \vec{r}_2)]^2 \right\} \quad (37)$$

Also, density of particles $\rho_0(\vec{r})$ is:

$$\rho_0(\vec{r}_1) = N \sum_{\vec{\sigma}_1, \dots, \vec{\sigma}_N} \int \dots \int d\vec{r}_2, \dots, d\vec{r}_N |\varphi(\vec{r}_1 \vec{\sigma}_1, \dots, \vec{r}_N \vec{\sigma}_N)|^2 \quad (38)$$

If equation (38) with diametric state is compared with equation (21), we will obtain;

$$\gamma(\vec{r}_1, \vec{r}_1) = \rho_0(\vec{r}_1) \ \& \ \gamma(\vec{r}_2, \vec{r}_2) = \rho_0(\vec{r}_2)$$

By this result, equation (37) can be written as:

$$\Gamma(\vec{r}_1, \vec{r}_2) = \frac{1}{2} \left\{ \rho_0(\vec{r}_1) \rho_0(\vec{r}_2) - \frac{1}{v} [\gamma(\vec{r}_1, \vec{r}_2)]^2 \right\} \quad (39)$$

As before mentioned, for calculation of integral equation (28) must density of matrixes $\gamma(\vec{r}_1, \vec{r}'_1)$ and $\Gamma(\vec{r}_1, \vec{r}_2)$ are calculated, as equation (34) is seen, we must use the wave function of single particle in cylindrical coordinates as before in part of calculation of nanowire without interacting, equation (11) was obtained.

$$\varphi_{n,l,k_z}(\rho, \theta, z) = \frac{1}{\sqrt{\pi a^2 L J_{l+1}(x_{ln})}} e^{il\theta} e^{ik_z z} J_l\left(\frac{x_{ln}}{a} \rho\right)$$

$$\gamma(\vec{r}'_1, \vec{r}_1) = \sum_i \varphi_i^*(\vec{r}'_1) \varphi_i(\vec{r}_1)$$

$$\gamma(\vec{r}'_1, \vec{r}_1) = \sum_{n,l,k_z} \frac{1}{\pi a^2 L [J_{l+1}(x_{ln})]^2} e^{-il\theta'_1} e^{-ik_z z'_1} J_l\left(\frac{x_{ln}}{a} \rho'_1\right) e^{il\theta_1} e^{ik_z z_1} J_l\left(\frac{x_{ln}}{a} \rho_1\right) \quad (40)$$

in equation (40) If we change, the summation to integral

$$\sum_{n,l,k_z} \rightarrow \int_0^{k_f} \frac{L}{2\pi} dk_z$$

$$\gamma(\vec{r}'_1, \vec{r}_1) = \int_0^{k_f} \frac{L}{2\pi} dk_z \frac{1}{\pi a^2 L [J_{l+1}(x_{ln})]^2} e^{-il\theta'_1} e^{-ik_z z'_1} J_l\left(\frac{x_{ln}}{a} \rho'_1\right) e^{il\theta_1} e^{ik_z z_1} J_l\left(\frac{x_{ln}}{a} \rho_1\right)$$

$$\gamma(\vec{r}'_1, \vec{r}_1) = \frac{1}{2\pi^2 a^2} \sum_{n,l} \frac{1}{[J_{l+1}(x_{ln})]^2} \int_0^{k_f} dk_z e^{-il\theta'_1} e^{-ik_z z'_1} J_l\left(\frac{x_{ln}}{a} \rho'_1\right) e^{il\theta_1} e^{ik_z z_1} J_l\left(\frac{x_{ln}}{a} \rho_1\right)$$

$$\gamma(\vec{r}'_1, \vec{r}_1) = \frac{1}{2\pi^2 a^2} \sum_{n,l} \frac{1}{[J_{l+1}(x_{ln})]^2} J_l\left(\frac{x_{ln}}{a} \rho'_1\right) J_l\left(\frac{x_{ln}}{a} \rho_1\right) e^{-il\theta'_1} e^{il\theta_1} \int_0^{k_f} dk_z e^{-ik_z z'_1} e^{ik_z z_1} \quad (41)$$

As before mentioned, our goal is to gain the energy of base state at zero temperature. So $n = 1$ and $l = 0$, and equation (41) is written as;

$$\gamma(\vec{r}'_1, \vec{r}_1) = \frac{1}{2\pi^2 a^2} \frac{1}{[J_1(x_{01})]^2} J_0\left(\frac{x_{01}}{a} \rho'_1\right) J_0\left(\frac{x_{01}}{a} \rho_1\right) \int_0^{k_f} dk_z e^{i(z_1 - z'_1)k_z}$$

$$\gamma(\vec{r}'_1, \vec{r}_1) = \frac{1}{2\pi^2 a^2} \frac{1}{[J_1(x_{01})]^2} J_0\left(\frac{x_{01}}{a} \rho'_1\right) J_0\left(\frac{x_{01}}{a} \rho_1\right) \frac{1}{i(z_1 - z'_1)} \left[e^{i(z_1 - z'_1)k_f} - 1 \right]$$

$$\gamma(\vec{r}'_1, \vec{r}_1) = \frac{1.7835}{\pi^2 a^2} \left(1 - \frac{9\pi^2}{64} \frac{\rho_1^2}{a^2} + \frac{81\pi^4}{16384} \frac{\rho_1^4}{a^4} - \dots \right)$$

$$\times \left(1 - \frac{9\pi^2}{64} \frac{\rho_1'^2}{a^2} + \frac{81\pi^4}{16384} \frac{\rho_1'^4}{a^4} - \dots \right) \frac{1}{i(z_1 - z'_1)} \left[e^{i(z_1 - z'_1)k_f} - 1 \right] \quad (42)$$

If in equation (42), $\vec{r}'_1 = \vec{r}_1$ is placed,

$$\gamma(\vec{r}_1, \vec{r}_1) = \rho_0(\vec{r}_1) = \rho_0$$

On the other hand, for density matrix of two particles is obtained.

$$\Gamma(\vec{r}_1, \vec{r}_2) = \frac{1}{2} \left\{ \rho_0(\vec{r}_1) \rho_0(\vec{r}_2) - \frac{1}{V} [\gamma(\vec{r}_1, \vec{r}_2)]^2 \right\} \Rightarrow \Gamma(\vec{r}_1, \vec{r}_2) = \frac{1}{2} \left\{ \rho_0^2 - \frac{1}{2} [\gamma(\vec{r}_1, \vec{r}_2)]^2 \right\}$$

$$2\Gamma(\vec{r}_1, \vec{r}_2) = \rho_0^2 - \frac{1}{2} \left[\frac{1.7835}{\pi^2 a^2} \left(1 - \frac{9\pi^2}{64} \frac{\rho_1^2}{a^2} + \frac{81\pi^4}{16384} \frac{\rho_1^4}{a^4} - \dots \right) \right. \\ \left. \times \left(1 - \frac{9\pi^2}{64} \frac{\rho_1'^2}{a^2} + \frac{81\pi^4}{16384} \frac{\rho_1'^4}{a^4} - \dots \right) \frac{1}{i(z_1 - z'_1)} \left[e^{i(z_1 - z'_1)k_f} - 1 \right] \right]^2 \quad (43)$$

As before mentioned, by calculation of $\gamma(\vec{r}'_1, \vec{r}_1)$ and $\Gamma(\vec{r}_1, \vec{r}_2)$, can find integral relation of equation (28), as from equations of (42) and (43) these two matrixes are calculated. Now, we refer to equation (28) means before obtained total energy of system.

$$E = \int d\vec{r}_1 \left[\frac{-\hbar^2}{2m} \nabla_1^2 + u(\vec{r}_1) \right] \gamma(\vec{r}_1, \vec{r}_1) \Big|_{\vec{r}'_1 = \vec{r}_1} + \iint d\vec{r}_1 d\vec{r}_2 V(\vec{r}_1, \vec{r}_2) \Gamma(\vec{r}_1, \vec{r}_2) \quad (44)$$

We replace the equations (42) and (43) in integral relation (44) and the numerical solution has done this integral and the results has described as graphic.

4. Discussion and conclusion

Here, we discuss about the thermodynamic properties of metallic nanowires and the integral relation of (44) is calculated in form of numerical that use for all properties. In all calculations, the radius of wire is considered $10nm$. In figs of (1), (2) and (3) the amount of kinetic energy per particle, amount of interacting energy electron-ion and amount of interacting energy electron-electron per particle according to different densities is drawn. As it is observed, the amount of kinetic energy per particle increases by increasing density; but the amount of interacting energy electron-ion and amount of interacting energy electron-electron per particle decrease by increasing density. In following figs observed that the curves of energy have not minimum point. It means that the system is not bound. The result which come out form these three figs; the total energy are made from these three energies.

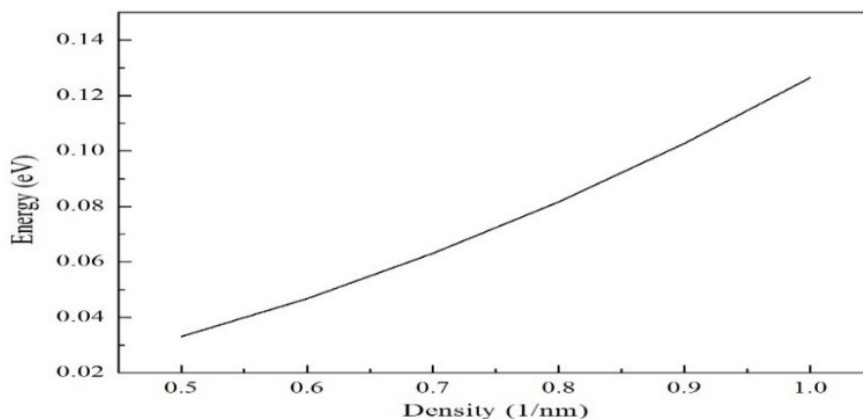


Fig. (1): amount of kinetic energy per particle

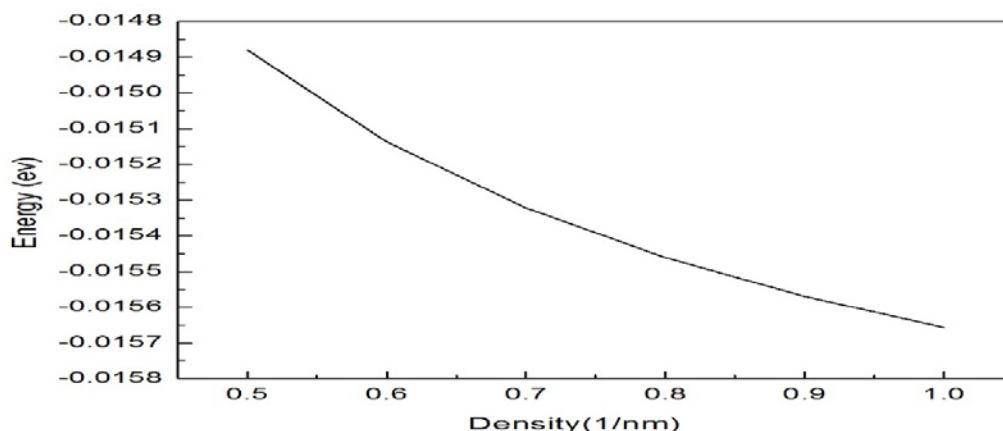


Fig. (2): amount of interacting energy electron-ion per particle

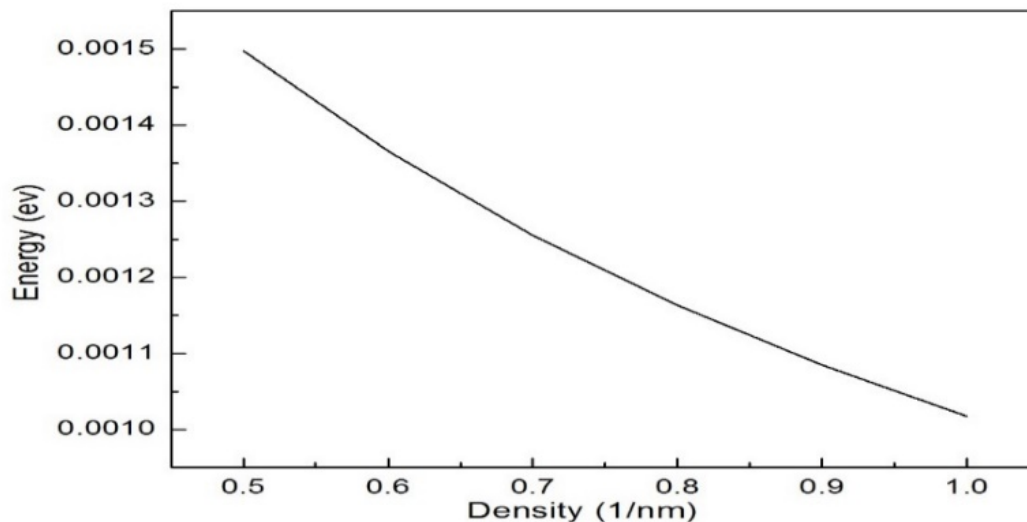


Fig. (3): amount of interacting energy electron-electron per particle

But; the basic difference between two interacting energy observed as; the amount of interacting energy electron-ion is per negative particle and the amount of interaction energy electron-electron is per positive particle.

Right now, we have to study the behavior of total energy of system per particle and draw its diagram. In fig (4) the total energy per particle according to different densities is drawn and the result is as: this energy increases by increasing density and also its curve has not the minimum point, it means that the system is not bound. If to see the behavior of total energy per particle, it is similar to kinetic energy per particle. But; there is difference between these two energies, the total energy per particle is smaller than the kinetic energy per particle. Its reason is completely clear, the amount of interacting energy electron-ion and electron-electron is a small part of kinetic energy.

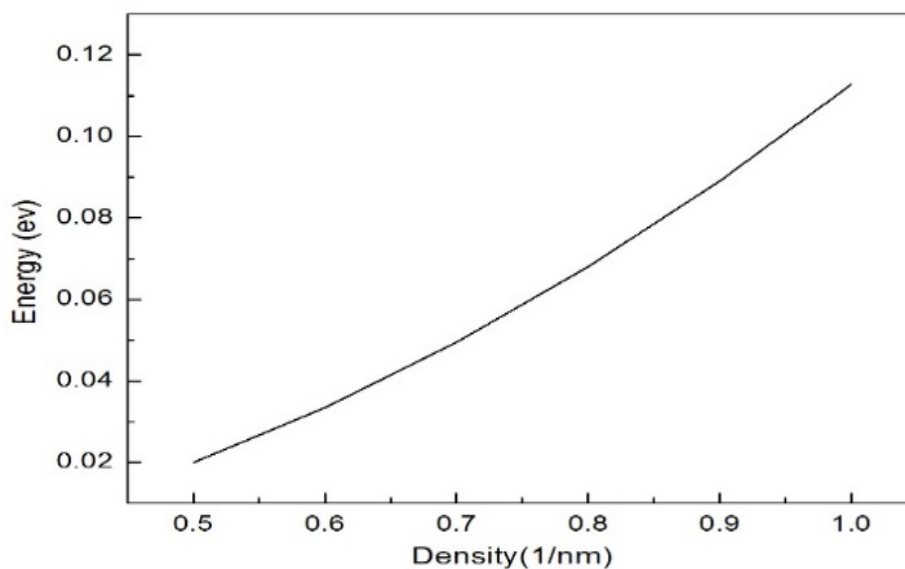


Fig. (4): total energy per particle

The pressure of system can be calculated from the following equation:

$$P(\rho) = \frac{\rho^2}{\pi a^2} \frac{\partial(E(\rho) / N)}{\partial \rho} \quad (45)$$

In fig (5) the pressure according different density is drawn. It is clear on the fig that the pressure increases by increasing density.

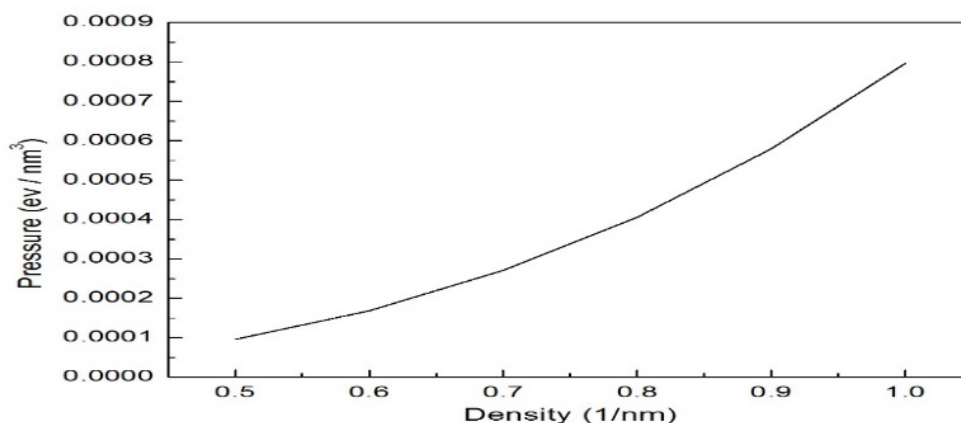


Fig. (5): pressure according to density (equation state)

Incompressibility of system can be found as follow;

$$k = \rho \frac{\partial P(\rho)}{\partial \rho} \quad (46)$$

In fig (6) incompressibility is drawn according to different density and it observed that the amount of incompressibility increase by increasing density.

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