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Calculation of Quasi-one-dimensional Interacting Electron Gas Using the Hartree-Fock Method

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In this paper, the Hartree-Fock method has been formulated to investigate some of the ground state properties of quasi-one-dimensional interacting electron gas in the presence of the magnetic field. The bare coulomb interaction between electrons has been assumed. For this system, we have also computed some of its thermodynamic and magnetic properties such as the energy, pressure, incompressibility, spin-polarization and magnetic susceptibility for different values of the magnetic field. Based on the results, the total energy increases by increasing the density for all relevant magnetic fields. The system becomes more stable by increasing the magnetic field. The system also shows a phase transition at high magnetic fields.

Keywords: Quasi-one-dimensional interacting electron gas, Hartree-Fock method, Magnetic field

INTRODUCTION

In recent years, some researchers have been interested to the one-dimensional and quasi-one-dimensional fermionic systems [1-6]. One of these systems is the quasi-one-dimensional electron gas which is a simple model for studying the metallic nanowires [7-9]. Many efforts have been made to understand the physics of quasi-one-dimensional systems, experimentally [10,11] and theoretically [12-14]. Many-body effects of quasi-one-dimensional electron gas with oscillator confinement have been described by local-field correction formulated by the self-consistent theory of Singwi, Tcsi, Land, and Sjolander. The exchange energy and correlation energy of system have been obtained with numerical methods [15]. Compressibility, chemical potential, screening properties, and bound-state energy of positively and negatively charged impurities have been derived analytically and numerically [16]. For quasi-one-dimensional electron gas with long-

range coulomb interaction, spin-susceptibility and correction energy have been calculated by static-structure factor. Using the ground state energy calculations, the density and width dependence of the spin-susceptibility and compressibility have been investigated for the one-dimensional electron gas with the long-range coulomb interaction [8]. Spin-resolved corrections have been studied at the ground state of a quasi-one-dimensional electron gas for an arbitrary spin-polarization with the method mentioned [17]. The ground-state properties of a one dimensional spin-1/2 fermionic system with an attractive δ-function potential have been investigated by Bethe ansatz method [18]. Using the electron transport in the quasi-one-dimensional electron gas, the dependence of energy level variation of one-dimensional quantum wires on the spatial confinement and electron concentration have been shown[19]. The second quantization method has been also used to investigate some thermodynamic properties of pin-polarized metallic nanowire in the presence of magnetic field by considering the interacting electron gas model for this system [9].

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The Hartree- Fock method is a varitional method which is used for calculation of many-body interacting systems. The self-consistent field approach was developed by Roothan to solve the Hartree-Fock theory [20]. Ciftja *et al.* used this method for a finite two-dimensional electron gas with a coulomb potential, and obtained the analytical expression for the energy of this system [21]. Inter-Landau-level collective excitation spectrum of quasi-one-dimensional electron gases cannot be explained by some techniques such as Kohn's theorem, so Yang and Aers utilized the Hartree-Fock method for this system [22]. The ground state energies of the non-magnetic and magnetic electron gases in one-dimension have been computed with the Hartree-Fock method in which the bare coulomb interaction between electrons has been assumed [23]. In this paper, we intend to formulate the Hartree-Fock method for calculating some properties of a quasi-one-dimensional interacting electron gas in the presence of a uniform magnetic field. We obtain an expression for the energy of system, and compute some thermodynamic and magnetic characteristics of this system as a function of magnetic field.

HARTEE FOCK METHOD

Hamiltonian of a system is written as the following relation,

$$H = \sum_{i=1}^{N} U(r_i) + \frac{1}{2}\sum_{i \neq j} V(r_i, r_j)$$ (1)

Where $U(r_i)$ is the single-particle hamiltonian and $V(r_i, r_j)$ is the interaction potential between particles. The energy of system is obtained by calculating the expectation value of Hamiltonian,

$$E = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle}$$ (2)

where

$$\Psi(r_1 s_1, r_2 s_2, ..., r_N s_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_1(r_1 s_1) & \psi_1(r_2 s_2) & \cdots & \psi_1(r_N s_N) \\ \psi_2(r_1 s_1) & \psi_2(r_2 s_2) & \vdots & \psi_2(r_N s_N) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_N(r_1 s_1) & \psi_N(r_2 s_2) & \cdots & \psi_N(r_N s_N) \end{vmatrix}$$ (3)

$\psi_i(r_i, s_i)$ is the single-particle wave function. The single particle wave function is normalized,

$$\sum_s \int dr \psi_i^*(rs)\psi_j(rs) = \delta_{ij}$$ (4)

By inserting Eq. (3) in Eq. (2), we get the following relation,

$$\langle \Psi | H | \Psi \rangle = \sum_i \int dr\, \psi_i^*(r)U(r)\psi_i(r) + \frac{1}{2}\sum_{i \neq j} \int dr \int d\acute{r}\, V(r,\acute{r})|\psi_i(r)|^2 |\psi_j(\acute{r})|^2$$
$$- \frac{1}{2}\sum_{i \neq j} \int dr \int d\acute{r}\, V(r,\acute{r})\delta_{s_i,s_j}\psi_i^*(r)\psi_i(\acute{r})\psi_j^*(\acute{r})\psi_j(r).$$ (5)

Considering the normalization constraint of the single-particle wave function (Eq. (4)), we minimize Eq. (5) with respect to the variation in the single-particle wave function. This leads to the following Hartree-Fock equation,

$$U(r)\psi_i(r) + \sum_j \int dr' V(r,r')\left|\psi_j(r')\right|^2 \psi_i(r)$$
$$- \sum_j \int dr' V(r,r')\psi_j^*(r')\psi_i(r')\psi_j(r)\delta_{s_i s_j} = \varepsilon_i \psi_i(r)$$ (6)

The third in the left side of the above equation is called exchange term.

CALCULATION OF A QUASI-ONE-DIMENSIONAL INTERACTING ELECTRON GAS IN THE PRESENCE OF MAGNETIC FIELD WITH THE HARTREE-FOCK METHOD

We consider a system including the interacting electrons confined in a cylindrical container with length L and R ($R \ll L$). For this system, we also consider the effect of ions as a uniform positive background. We compute some properties of this system by Hartree-Fock method as follows.

By applying the magnetic field, a spin-polarized system is given with $N^{(+)}$ spin-up and $N^{(-)}$ spin-down electrons. The

number density of spin-up and spin down electrons is characterized by $\rho^{(+)} = N^{(+)}/L$ and $\rho^{(-)} = N^{(-)}/L$, respectively. The spin-polarization parameter is defined as follows,

$$\xi = \frac{\rho^+ - \rho^-}{\rho} \tag{7}$$

where $-1 \le \xi \le 1$ and $\rho = N/L = \rho^{(+)} + \rho^{(-)}$ is the total number density of system.

In the presence of magnetic field, for our system, the single-particle Hamiltonian $U(r)$ includes the kinetic energy of each electron, the interaction energy between each electron and total positive background ($u^{ion}(r)$), and the interaction energy between each electron and magnetic field (B),

$$U(\boldsymbol{r}) = \frac{-\hbar^2}{2m}\nabla^2 + u^{ion}(r) - \boldsymbol{\mu}.\boldsymbol{B}, \tag{8}$$

where μ is the electron magnetic dipole moment and

$$u^{ion}(r) = \frac{-e^2}{4\pi\epsilon_0}\int\frac{\rho^{ion}(\acute{r})}{|r-\acute{r}|}\,d\acute{r}. \tag{9}$$

In above equation, ρ^{ion} is the density of positive background. The potential energy due to the interaction between electrons, $V(r,r')$, is as follows,

$$V(\boldsymbol{r},\acute{\boldsymbol{r}}) = \frac{1}{4\pi\epsilon_0}\frac{e^2}{|r-\acute{r}|} \tag{10}$$

Considering the charge neutrality condition ($\rho^{ion} = \rho^{el}$) and using Eqs. (8), (9) and (10), according to Eq. (6), we get the following Hartree-Fock equation for the system,

$$\frac{-\hbar^2}{2m}\nabla^2\psi_i(\boldsymbol{r}) - \boldsymbol{\mu}.\boldsymbol{B}\psi_i(\boldsymbol{r})$$
$$-\frac{e^2}{4\pi\epsilon_0}\sum_j\int d\acute{r}\,\frac{1}{|r-\acute{r}|}\psi_j^*(\acute{r})\psi_i(\acute{r})\psi_j(r)\delta_{s_is_j} = \varepsilon_i\psi_i(\boldsymbol{r}) \tag{11}$$

As also mentioned in the previous section, the third term in

the left side of Eq. (11) is called exchange term.

For calculating the energy of system, we must compute the single particle energy ε_i by solving the Hartree-Fock equation (Eq. (11)). For this purpose, we take the single-particle wave function $\psi_i(r_i)$ in the cylindrical coordinates [21].

$$\psi_{mnk}(\rho,\varphi,z) = \frac{1}{\sqrt{\pi R^2 L}J_{m+1}(\gamma_{mn}R)}J_m(\gamma_{mn}\rho)e^{im\varphi}e^{ikz}$$
$$\tag{12}$$

where $J_m(\gamma_{mn}\rho)$ is the Bessel function of order m. The single-particle states are described by the quantum numbers m, n and k is the wave number of electrons along the axis of cylinder. Using the above single particle wave function (Eq. (12)), we get the following expression for the exchange term,

$$Exchang\ Term = -\frac{e^2}{4\pi\epsilon_0}\sum_j\int d\acute{r}\,\frac{1}{|r-\acute{r}|}\psi_j^*(\acute{r})\psi_i(\acute{r})\psi_j(r)\delta_{s_is_j}$$
$$= -\frac{e^2}{4\pi\epsilon_0}\left(\frac{2}{\pi R^2}\right)\frac{1}{(\pi R^2 L)^{\frac{3}{2}}}\sum_j\sum_m\sum_n\int_{-\infty}^{+\infty}dk$$
$$\times\frac{e^{im\varphi}e^{ikz}J_m(\gamma_{mn}\rho)e^{im_j\varphi}e^{ik_jz}J_{m_j}\left(\gamma_{m_jn_j}\rho\right)}{J_{m+1}^2(\gamma_{mn}R)(k^2+(\gamma_{mn})^2)J_{m_j+1}^2(\gamma_{mn}R)J_{m_i+1}\left(\gamma_{m_in_i}R\right)}$$
$$\times\int_0^R\acute{\rho}J_m(\gamma_{mn}\acute{\rho})J_{m_i}(\gamma_{m_in_i}\acute{\rho})J_{m_j}\left(\gamma_{m_jn_j}\acute{\rho}\right)d\acute{\rho}$$
$$\times\int_0^{2\pi}e^{i(m_i-m_j-m)\acute{\phi}}\,d\acute{\phi}\int_{-\infty}^{+\infty}e^{i(k_i-k_j-k)\acute{z}}d\acute{z}\,,$$
$$\tag{13}$$

where we have inserted the following Fourier transformation for expression $\frac{1}{|r-r'|}$,

$$\frac{1}{|r-\acute{r}|} = \frac{2}{\pi R^2}\sum_m\sum_n\int_{-\infty}^{+\infty}dk\,\frac{e^{im(\varphi-\acute{\varphi})}e^{ik(z-\acute{z})}J_m(\gamma_{mn}\acute{\rho})J_m(\gamma_{mn}\rho)}{J_{m+1}^2(\gamma_{mn}R)(k^2+(\gamma_{mn})^2)}$$
$$\tag{14}$$

The aim of this paper is to obtain the ground state energy of this system, therefore we assign $n = n_i = n_j = 1$ have $m = m_i = m_j = 0$. Now, we solve the above integrals numerically using the MAPLE software, and finally the following relation is obtained for the exchange term,

$$Exchange\ Term = \frac{-e^2}{4\pi\varepsilon_0}\frac{0.021}{LR^2(0.078)}\sum_j\frac{1}{(k_i-k_j)^2+(\gamma_{01})^2}\psi_i(r)$$

$$(15)$$

By inserting Eqs. (12) and (15) in Eq. (11), we get the following relation for single particle-energy ε_i,

$$\varepsilon_i = \frac{\hbar^2}{2m}((\gamma_{01})^2+k_i{}^2)-\mu B-\frac{0.021\,e^2}{4\pi\epsilon_0 LR^2(0.078)}\sum_j\frac{1}{(k_i-k_j)^2+(\gamma_{01})^2}$$

$$(16)$$

Since the system is spin-polarized, the total energy of system is

$$E = \sum_i \varepsilon_i^{(+)} + \sum_i \varepsilon_i^{(-)} \tag{17}$$

where $\varepsilon_i^{(+)}\left(\varepsilon_i^{(-)}\right)$ is the single particle energy of spin-up (spin-down) electrons. After some algebra, we obtain the total energy per particle as the following relation,

$$\frac{E}{N} = \frac{L}{2\pi}\{\frac{\hbar^2}{2m}\left(\gamma_{01}{}^2 k_F^{(+)}+\frac{k_F^{3(+)}}{3}+\gamma_{01}{}^2 k_F^{(-)}+\frac{k_F^{3(-)}}{3}\right)-\mu B(k_F^{(+)}-k_F^{(-)})$$

$$-\frac{e^2}{4\pi\epsilon_0}\frac{8\times0.021}{3\pi^2 R(0.078)}[k_F^{(+)}\arctan\left(\frac{k_F^{(+)}}{\gamma_{01}}\right)-\frac{1}{2}\gamma_{01}\ln\left(1+\frac{k_F^{2(+)}}{\gamma_{01}^2}\right)$$

$$+k_F^{(-)}\arctan\left(\frac{k_F^{(-)}}{\gamma_{01}}\right)-\frac{1}{2}\gamma_{01}\ln(1+\frac{k_F^{2(-)}}{\gamma_{01}^2})]\}.$$

$$(18)$$

For this system, $k_F^{(+)}$ and $k_F^{(-)}$, the Fermi momenta of spin-up and spin-down electrons, are obtained as follows [7],

$$N^{(+)} = \sum_{mnk} = \frac{L}{2\pi}\int_0^{k_F^{(+)}}dk = \frac{Lk_F^{(+)}}{2\pi}$$

$$\Rightarrow k_F^{(+)} = \frac{2\pi}{L}N^{(+)} = \frac{\pi}{L}N(1+\xi) = \pi\rho(1+\xi)$$

$$(19)$$

$$N^{(-)} = \sum_{mnk} = \frac{L}{2\pi}\int_0^{k_F^{(-)}}dk = \frac{Lk_F^{(-)}}{2\pi}$$

$$\Rightarrow k_F^{(-)} = \frac{2\pi}{L}N^{(-)} = \frac{\pi}{L}N(1-\xi) = \pi\rho(1-\xi)$$

$$(20)$$

According to Eqs. (7), (19) and (20), we can rewrite the total energy per particle as follows,

$$\frac{E(\rho,B)}{N} = \frac{\hbar^2}{2m}\left(\left(\frac{3\pi}{4R}\right)^2+\frac{(\pi\rho)^2(1+\xi)^3}{6}+\frac{(\pi\rho)^2(1-\xi)^3}{6}\right)-\mu\xi B$$

$$+E_{exch},$$

$$(21)$$

where E_{exch} is the contribution of energy related to the exchange term (exchange term),

$$E_{exch} = -\frac{e^2}{4\pi\epsilon_0}\frac{8(0.021)}{6\pi^2 R(0.078)}\left[(1+\xi)arctan\left(\frac{4R\rho}{3}(1+\xi)\right)\right.$$

$$+(1-\xi)arctan\left(\frac{4R\rho}{3}(1-\xi)\right)$$

$$-\frac{3}{16R\rho}\left(ln\left(1+\frac{16R^2\rho^2(1+\xi)^2}{9}\right)\right.$$

$$\left.\left.+ln\left(1+\frac{16R^2\rho^2(1-\xi)^2}{9}\right)\right)\right]$$

$$(22)$$

Using the above relation, we can compute the total energy per particle for the system at various densities and magnetic fields.

RESULTS AND DISCUSSION

In this section, we present our results for some properties of a quasi-one-dimensional interacting electron gas in the presence of magnetic field for $R = 10$ nm.

In Fig. 1, we have plotted the ground state energy per particle E/N *vs.* density for different magnetic fields. The results show that the ground state energy increases by increasing the density. There is no minimum point in the energy curve, therefore we can conclude that the system does not have any bond state. Our results also indicate that for each density, the energy reduces by increasing the magnetic field leading to a more stable system. This results is in agreement with that of Olszewski calculation [23]. We have also found that the magnitude of exchange energy (Eq. (22)) decreases by increasing the radius. For example at
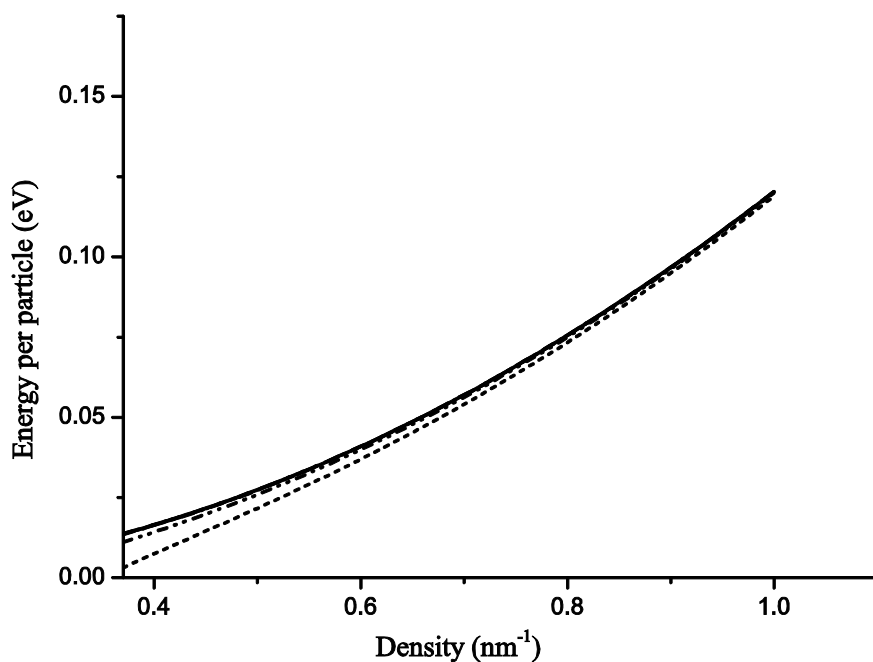
Fig. 1. The ground state energy per particle as a function of density at $B = 0.5$ (solid curve), 400 (dashed-dotted-dotted curve) and 800 T (short-dashed curve) for $R = 10$ nm.
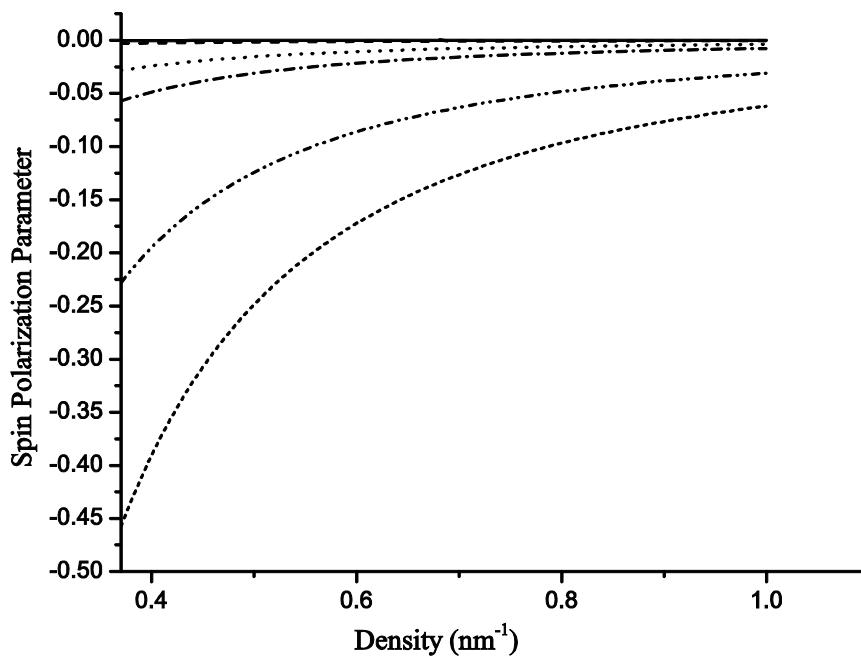

Fig. 2. The spin-polarization parameter at the equilibrium state of system as a function of the density at $B = 0.5$ (solid curve), 50 (dashed curve), 100 (dotted curve), 400 (dashed-dotted curve) and 800 T (dashed-dotted-dotted curve) for $R = 10$ nm.

$B = 0$, the exchange energy of system for $R = 10$ nm is $E_{exch} = $ -0.00592 eV and for $R = 5$ nm is $E_{exch} = $ -0.0065 eV. This behavior has been also concluded by Olszewski [23].

The spin-polarization parameter as a function of density for various magnetic fields has been drawn in Fig. 2. This figure shows that the magnitude of spin-polarization parameter decreases by increasing the density, while it increases by increasing the magnetic field, especially at low densities. From Fig. 2, we also see that at high magnetic fields, the decreasing rate of magnitude of spin-polarization parameter becomes very large. In Fig. 3, the spin-polarization parameter of a quasi-one-dimensional interacting electron gas has been plotted versus the magnetic field for different values of density. This figure shows that the spin-polarization parameter is almost zero for the magnetic fields less than $B \sim 30$ T. It is seen that for the magnetic fields greater than about 100 T, the magnitude of spin-polarization parameter rapidly increases by increasing the magnetic field, and finally at high magnetic fields it becomes unity. Figure 3 shows that the value of magnetic field in which the spin-polarization becomes unity increases by increasing the density.

Magnetic susceptibility is calculated by the following relation,

$$\chi(\rho,B) = \left(\frac{\partial M_2(\rho,B)}{\partial B} \right)_\rho \tag{23}$$

In Fig. 4, the magnetic susceptibility of a quasi-one-dimensional interacting electron gas $\chi/N/\mu|$ has been plotted versus the magnetic field for three different values of density. It is seen that for each density, the ratio $\chi/N/\mu|$ has a maximum showing a ferromagnetic phase transition induced by the magnetic field at high fields. The magnitude of magnetic field in transition point depends on the density.

We can calculate the pressure of system from the total energy per particle,

$$P(\rho,B) = \frac{\rho^2}{\pi R^2} \left(\frac{\partial (E(\rho,B)/N)}{\partial \rho} \right)_B \tag{24}$$

The pressure of a quasi-one-dimensional interacting

electron gas *vs.* density for different values of magnetic field is presented in Fig. 4. It shows that as the density increases, the pressure of system increases. However, the pressures at small magnetic fields are nearly identical.

Incompressibility κ of the system is calculated using the following formula,

$$\kappa(\rho,B) = \rho \frac{\partial p(\rho,B)}{\partial p} \tag{25}$$

In Fig. 5, the incompressibility *vs.* density has been given for several magnetic fields. We see that the incompressibility increases as the density increases. By increasing the magnetic field, the difference between the incompressibility of different magnetic fields increases.

SUMMARY AND CONCLUSIONS

In this model, we have considered an interacting system of electrons in a uniform positive background, confined in a long cylindrical container with radius $R = 10$ nm. For this system, some properties are investigated in the presence of a uniform magnetic field using the Hartree-Fock formalism. Our calculations show that the energy of this system increases by increasing the density. With increasing the magnetic field, the system becomes more stable. Based on the results, the spin-polarization parameter is almost zero for magnetic fields less than about 30 T, while for the magnetic fields greater than about 100 T, its magnitude grows rapidly. Our results also indicate a ferromagnetic phase transition at high magnetic fields. Our calculation shows that the pressure of system increases by increasing both density and magnetic field. This behavior is also observed for the incompressibility of the system. One can use these results to study nanowires [7-9].
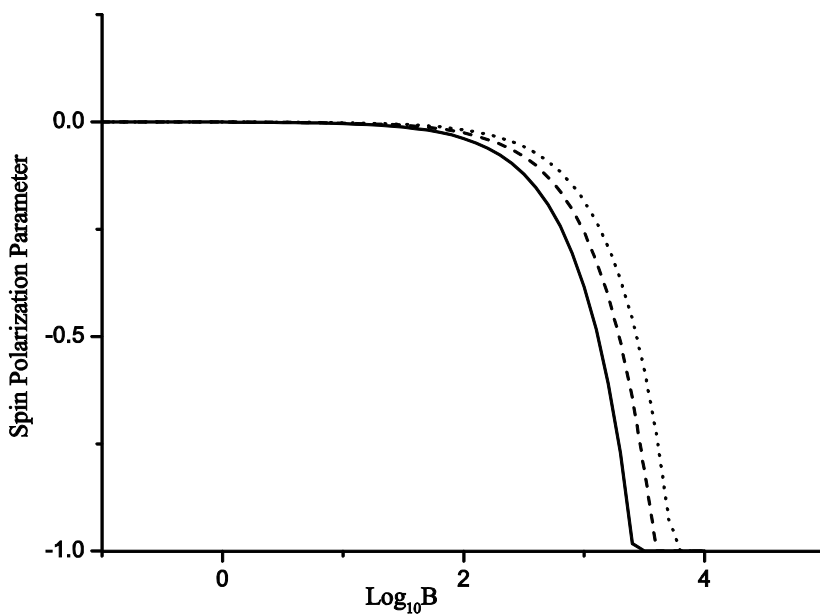
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Fig. 3. The spin-polarization parameter at the equilibrium state of system as a function of the magnetic field at $\rho = 0.45$ (solid curve), 0.55 (dashed curve) and 0.65 nm^{-1} (dotted curve) for $R = 10$ nm.
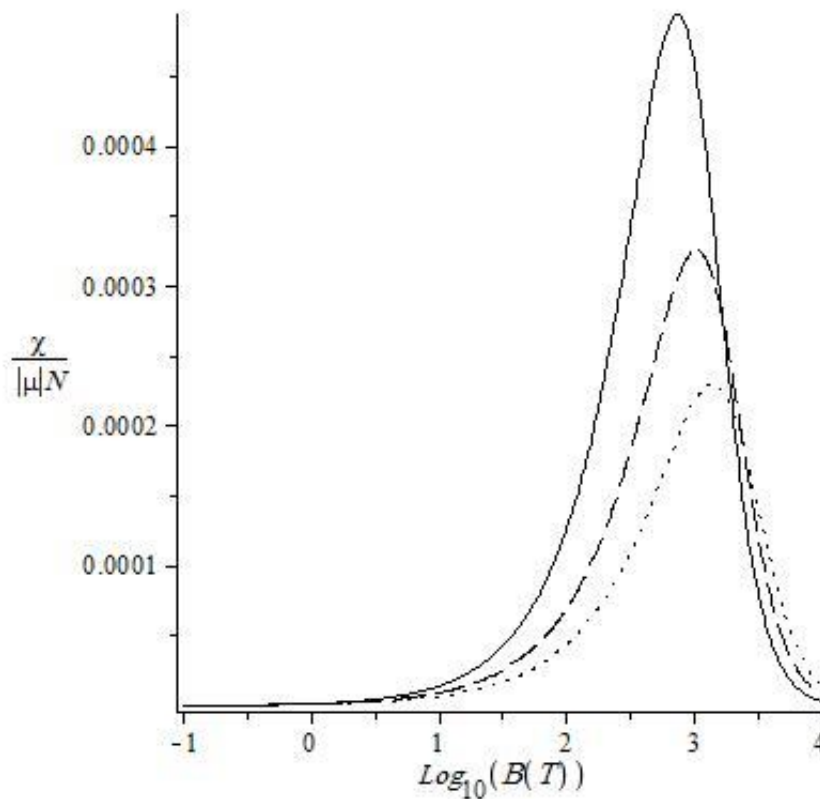

Fig. 4. $\chi/N/\mu_e|$ as function of the magnetic field at $\rho = 0.45$ (solid curve), 0.55 (dashed curve) and 0.65 nm^{-1} (dotted curve) for $R = 10$ nm.
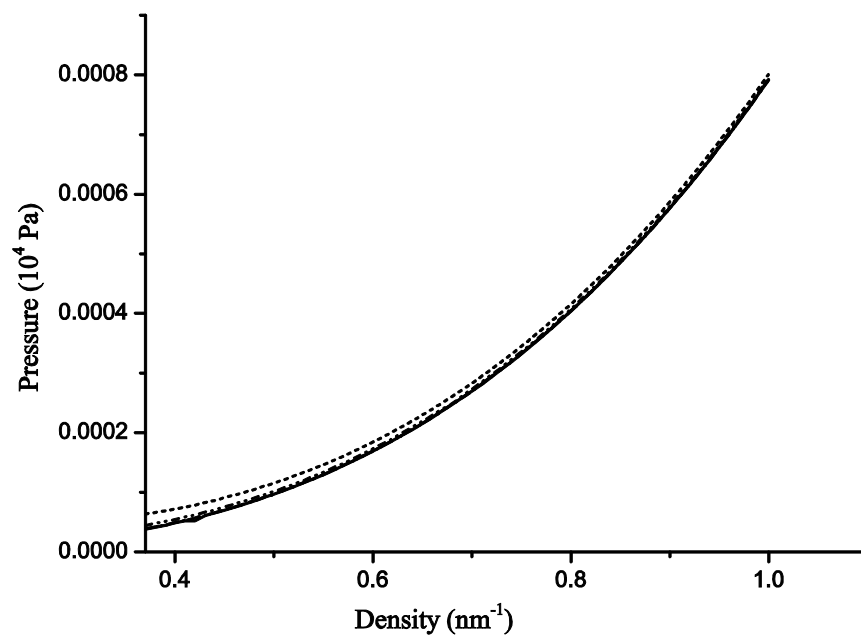
Fig. 5. The pressure of system as a function of density at $B = 100$ (solid curve), 400 (dashed-dotted-dotted curve) and 800 T (short dashed curve) for $R = 10$ nm.
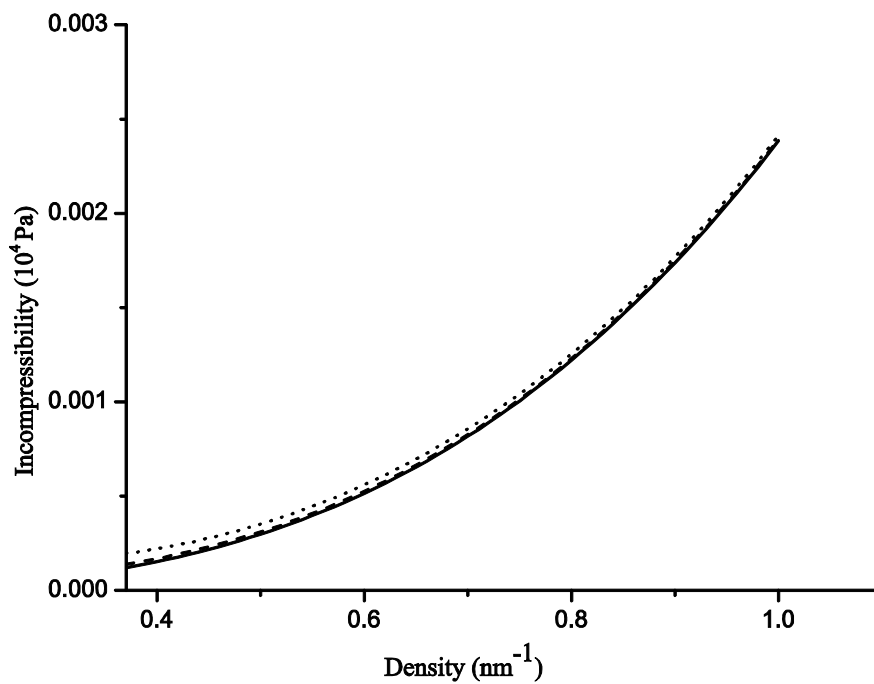

Fig. 6. The incompressibility of system *vs*. density at $B = 100$ (solid curve), 400 (dashed curve) and 800 T (dotted curve) for $R = 10$ nm.

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