J. Sci. Soc. Thailand 13 (1987) 221-229

GROUND STATE ENERGY IN THE SCREENED POTENTIAL OF TWO-DIMENSIONAL ELECTRON GAS AT FINITE TEMPERATURES

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(Received 7 October 1987)

Abstract

The effect of screening on ground state energy of bound system of hydrogenic impurity and electron in a homogeneous two-dimensional electron gas (2-DEG) is studied within the linear response theory. The temperature and density dependent Lindhard function has been used. The long wavelength value of this function shows maximum in both high and low temperature limits. The ground state energy can be approximately calculated using the long wavelength limit in both low and high temperatures by the variational method. The result is in agreement with the work done by Stern and Howard[1], especially in the high temparature limit.

Introduction

The problem of screening of an impurity charge in an electron gas of density n, in thermal equilibrium at a temperature T, has attracted considerable attention in recent years. The effective potential due to the impurity charge as modified by the polarization of electron gas has to be solved. In the three-dimensional electron gas, the effective screened impurity potential goes over to the Debye-screened potential in the limit of high temperature and low density, and to the Thomas-Fermi potential in the opposite limit of low temperature and high density of the gas. In the intermediate degeneracy region where neither the Debye nor the Thomas-Fermi model is valid, Gupta and Rajagopal[2] calculated the potential within the framework of linear response theory via the temperature - and density-dependent Lindhard dielectric function. They compared their screened potential with the traditionally employed Debye potential and computed the ground-state energy of an electron trapped by this impurity potential. In the two dimensional system, Stern and Howard[1] have given a graph of binding energy versus the screening constant. They find a screening constant $\bar{s} = 4/a^*$ where $a^* = K \hbar^2/m^* e^2$ and K is the dielectric constant. The variation of $\bar{s}$ seen by them is due to K. Because of a peculiar nature of the function χ $(\bar{q}, n, T)$, the retarded part of the time-ordered density correlation function, appearing[3] in the dielectric function. The variation of $\bar{s}$ can also be viewed as being due to the temperature.

In this work, the screening effects of a static impurity charge on the ground state energy of two-dimensional electron system (2-DES) will be studied in analogy with three-dimensional case. The long wavelength value of the temperature-dependent response function

$\chi\,(\bar{q}. n, T)$ has been used to calculate the ground state energy at low and high temperatures. This approximation is reasonable because the response function is maximum in both low and high temperature limits.

The effective screened potential

Consider a static impurity charge $+Ze$ imbedded in a homogeneous 2-DEG of density $n(\bar{r})$ in thermal equilibrium at a temperature T. A uniform background of positive charges is assumed for charge neutrality. The external impurity charge polarises the medium and brings about a redistribution of the electronic charge density $n(\bar{r}, T)$ around it. The basic temperature dependent Kohn-Sham equations for the effective potential (neglecting the exchange-correlation effects and trying $Z = 1$) is,

$$V_{eff}\,[\bar{r}, n, T] = \frac{-e^2}{r} + e^2 \int \frac{n(\bar{r}', T)\, d\bar{r}'}{|\bar{r} - \bar{r}'|} \tag{1}$$

or in momentum space,

$$V_{eff}\,[\bar{q}, n, T] = \frac{-2\pi e^2}{q} + \frac{2\pi e^2}{q} \cdot n(\bar{q}, T) \tag{2}$$

In the linear response theory, the density deviation $n(\bar{q}, T)$ is approximated as responding linearly to the effective potential

$$n(\bar{q}, T) = \chi\,(\bar{q}, n, T)\, V_{eff}\,[\bar{q}, n, T] \tag{3}$$

where $\chi\,(\bar{q}, n, T)$ is the temperature-dependent response function. The screened potential is given by

$$V_{eff}\,[\bar{q}, n, T] = \frac{-2\pi e^2}{q}\, \frac{1}{1 - (2\pi e^2/q)\,\chi\,(\bar{q}, n, T)} \tag{4}$$

The function χ is the retarded polarization and at zero temperature it is a wellknown Lindhard function. The Lindhard function generalized to non-zero temperature is

$$\chi\,(\bar{q}, n, T) = -2 \int \frac{d^2p}{(2\pi)^2}\, \frac{f(\bar{p} + \bar{q}) - f(\bar{p})}{\varepsilon_{\bar{p}} - \varepsilon_{\bar{p}+\bar{q}}} \tag{5}$$

with $\varepsilon_{\bar{p}} = \hbar^2 p^2/2m$ and $f(\bar{p})$ is the Fermi function for the electrons :

$$f(\bar{p}) = \frac{1}{\exp\,[\beta\,(\varepsilon_{\bar{p}} - \mu)] + 1} \tag{6}$$

The chemical potential μ appropriate to the temperature T and electron density $n(\bar{r})$ must be determined from the condition

$$n = 2 \int \frac{d^2k}{(2\pi)^2} \frac{1}{\exp\left[\beta\left(\frac{\hbar^2 k^2}{2m} - \mu\right)\right] + 1} \tag{7}$$

Thus μ / E_F is a function of T only, and does not depend separately on n and T. Our task in this section is to calculate $\chi(\bar{q}, n, T)$ analytically. Making transformations, $\bar{p} + \bar{q} \rightarrow \bar{k}$ for $f(\bar{p} + \bar{q})$ and $\varepsilon_{\bar{p}+\bar{q}}$, and $\bar{p} \rightarrow -\bar{p}$ for $f(\bar{p})$ and $\varepsilon_{\bar{p}}$, using the fact that $\varepsilon_{-\bar{p}} = \varepsilon_{\bar{p}}$ and $f(-\bar{p}) = f(\bar{p})$, we get

$$\chi(\bar{q}, n, T) = \frac{4}{(2\pi)^2} \int d^2p \frac{f(\bar{p})}{\varepsilon_{\bar{p}} - \varepsilon_{\bar{p}-\bar{q}}}$$

$$= \frac{2m}{\pi^2 \hbar^2 q} \int_0^\infty p\, f(\bar{p}) dp \int_0^{2\pi} \frac{d\theta}{2p\cos\theta - q} \tag{8}$$

Consider the angular integral, $I(\theta)$;

$$I(\theta) = \int_0^{2\pi} \frac{d\theta}{2p\cos\theta - q} = \frac{1}{q} \int_0^{2\pi} \frac{d\theta}{a\cos\theta - 1}$$

where $a = 2p/q$. Let $z = e^{i\theta}$, $\cos\theta = \frac{1}{2}(z + \frac{1}{z})$, it follows that

$$I(\theta) = \frac{-2i}{aq} \oint_{/z/=1} \frac{dz}{(z - \frac{1}{a})^2 + (1 - \frac{1}{a^2})}$$

with the poles at $\frac{1}{a} \pm i(1 - \frac{1}{a^2})^{1/2}$ for $a^2 > 1$ and $\frac{1}{a} \pm (\frac{1}{a^2} - 1)^{1/2}$ for $a^2 < 1$. Since the sum of residues in case of $a^2 > 1$ is zero, there is no contribution to the integration from $a^2 > 1$. For $a^2 < 1$, only the pole at $\frac{1}{a} - (\frac{1}{a^2} - 1)^{1/2}$ lies inside the unitcircle $| z | = 1$ and the maximum value of a is unity. It follows that the upper limit of the p-integration in eq. (8) is q/2. Since the residue of the pole is $-\frac{1}{2}(\frac{1}{a^2} - 1)^{1/2}$, the value of $I(\theta)$ is, then, $I(\theta) = -2\pi/(q^2 - 4p^2)^{1/2}$ and eq.(8) becomes

$$\chi(\bar{q}, n, T) = \frac{-4m}{\pi \hbar^2 q} \int_0^{q/2} \frac{p f(\bar{p}) dp}{\sqrt{q^2 - 4p^2}} = \frac{-4m}{\pi \hbar^2 q} h(\bar{q}, n, T) \tag{9}$$

with $$h(\bar{q}, n, T) = \int_{0}^{q/2} \frac{pf(\bar{p})dp}{\sqrt{q^2 - 4p^2}} \qquad (10)$$

Using these equations, the effective potential in eq.(4) becomes

$$V_{eff}(\bar{q}, n, T) = \frac{-4\pi}{q + 8h(\bar{q}, n, T)/q} \qquad (11)$$

where the unit of $e^2 = 2$, $\hbar^2 = 2m = 1$ have been used. The Fourier transform of eq.(11) is

$$V_{eff}(\bar{r}, n, T) = \frac{-1}{(2\pi)^2} \int d^2q\, V_{eff}(\bar{q}, n, T)\, e^{i\bar{q}\cdot\bar{r}}$$

$$= -2 \int_{0}^{\infty} \frac{q^2\, Jo\,(qr)\, dq}{q^2 + 8h(\bar{q}, n, T)} \qquad (12)$$

where $J_0(x)$ is the Bessel function of order zero. The effective potential will be used to calculate the ground state energy of an electron trapped by the impurity potential in the next section. Variation of χ $(\bar{q}, n, T)$ with q at various values of T is shown in Fig. 1[3], where we use the unit that $\hbar^2 = 2m = 1$ and $e^2 = 2$. For low temperature limit, χ is approximately constant with the value of 0.159. This constant agrees quite well with that calculated by Maldague[4]. The curves are drastically change for $q \geqslant 2k_F$ and go to zero as $q \rightarrow \infty$. χ is exactly constant at $T = 0$ upto $q = 2k_F$, whereas it has a logarithmic slope at $q = k_F$ in 3-D case (see, for example, Ziman[5]). For $q > 2k_F$, it decreases as $1/q^2$ for the low temperature limit. At higher temperature the curves converge slowly and the sharpness near $q = 2k_F$ is disappears.

Ground state energy of bound system

The ground state energy of an electron trapped by the impurity potential can be evaluated by the variational method. The trial wavefunction is $\psi(\bar{r}) = Ae^{-\gamma r}$, where γ is a real positive parameter to be determined by minimising the energy. The normalization condition of ψ $(\bar{r})$ gives $A^2 = \frac{2\gamma^2}{\pi}$. The ground state energy, $E_0(\gamma)$, is

$$E_0(\gamma) = \langle \psi\ (\bar{r}) \,|\, -\nabla^2 + V_{eff}(\bar{r}, n, T) \,|\, \psi\ (\bar{r}) \rangle \qquad (13)$$

where $\nabla^2 = \frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr}$ is the kinetic energy operator. The expectation value of the kinetic energy is

$$< \psi(\bar{r}) | -\nabla^2 | \psi(\bar{r}) > = -\int d^2r\, \psi^*(\bar{r}) \left(\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} \right) \psi(\bar{r}) \tag{14}$$

$$= \gamma^2$$

and the expectation value of the effective potential is

$$< \psi(\bar{r}) | V_{eff}(\bar{r}, n, T) | \psi(\bar{r}) > = -16\gamma^3 \int_0^\infty \frac{q^2 dq}{[q^2 + 8h(\bar{q},n,T)]\,[4\gamma^2 + q^2]^{3/2}} \tag{15}$$

Since the long wavelengthvalue of $h(\bar{q}, n, T)$ is the maximum value of $\chi(\bar{q}, n, T)$ in both high and low temperature limits, we have

$$h(\bar{q}, n, T) \sim q/4 \qquad \text{for } q \to 0,\ T \text{—} 0$$
$$\sim q/4t \qquad \text{for } q \to 0,\ T \to \infty$$

where $t = T/T_F$. This is equivalent to taking Yukawa type potential. This approximation is not bad because $\chi(\bar{q}, n, T)$ remains constant in both the limits over a substantial range of q, as can be seen from Fig. 1. We, therefore, can calculate the ground state energy at low and high temperature with screening effect.

Low temperature limit

In this limit, eq. (15) becomes

$$< \psi(\bar{r}) | V_{eff}(\bar{r}, n, T) | \psi(\bar{r}) > = -16\gamma^3 I$$

where $$I = \int_0^\infty \frac{q\, dq}{(q + 2)(4\gamma^2 + q^2)^{3/2}}$$

Letting $q + 2 = z$ and $a = 4\gamma^2 + 4$, then

$$I = \frac{1}{a-4} - \frac{1}{a\gamma^2} + \frac{1}{a\gamma} + \frac{2}{a^{3/2}} \ln\left(\frac{\sqrt{\gamma^2 + 1} - 1}{\gamma^2 + \gamma\sqrt{\gamma^2 + 1}} \right)$$

$$= \frac{1}{4\gamma^2} - \frac{1}{4\gamma^2(\gamma^2 + 1)} + \frac{1}{4\gamma(\gamma^2+1)} + \frac{1}{4(\gamma^2+1)^{3/2}} \ln\left(\frac{\sqrt{\gamma^2 + 1} - 1}{\gamma^2 + \gamma\sqrt{\gamma^2+1}} \right)$$

Thus

$$< \psi(\bar{r}) \,|\, V_{eff}(\bar{r}, n, T) \,|\, \psi(\bar{r}) > = -4\gamma + \frac{(4\gamma - 4\gamma^2)}{\gamma^2 + 1} - \frac{4\gamma^3}{(\gamma^2 + 1)^{3/2}} \ln\left(\frac{\sqrt{\gamma^2 + 1} - 1}{\gamma^2 + \gamma\sqrt{\gamma^2 + 1}}\right)$$

The ground state energy in the low temperature limit is,

$$\underset{\substack{T \to 0 \\ q \to 0}}{E_0(\gamma)} \simeq \gamma^2 - 4\gamma + \frac{4\gamma - 4\gamma^2}{\gamma^2 + 1} - \frac{4\gamma^3}{(\gamma^2 + 1)^{3/2}} \ln\left(\frac{\sqrt{\gamma^2 + 1} - 1}{\gamma^2 + \gamma\sqrt{\gamma^2 + 1}}\right) \qquad (16)$$

The condition $\frac{\partial E_0}{\partial \gamma} = 0$ is a condition of minimum energy and it leads to the cubic equation which can be solved numerically to give $\gamma_0 \sim 1.2134$. The corresponding ground state energy is

$$E_0 \simeq -0.535568 \text{ Ryd.}$$

The condition $\left.\frac{\partial^2 E}{\partial \gamma^2}\right|_{\gamma_0} > 0$ has been checked to ensure minimum. This value should be compared with $E_0 = -4.0$ rydberg when there is no screening.

High temperature limit

A similar procedure of calculation in this limit leads to the expectation value of $V_{eff}(\bar{r}, n, T)$ being

$$< \psi(\bar{r}) \,|\, V_{eff}(\bar{r}, n, T) \,|\, \psi(\bar{r}) > = -4\gamma + \frac{4\gamma(1 - \gamma t)}{(\gamma^2 t^2 + 1)} - \frac{4\gamma^3 t^2}{(\gamma^2 t^2 + 1)^{3/2}} \ln\left(\frac{\sqrt{\gamma^2 t^2 + 1} - 1}{\gamma^2 t^2 + \gamma t\sqrt{\gamma^2 t^2 + 1}}\right)$$

Leading to the ground state energy

$$E_0(\gamma) = \gamma^2 - 4\gamma + \frac{4\gamma(1 - \gamma t)}{(\gamma^2 t^2 + 1)} - \frac{4\gamma^3 t^2}{(\gamma^2 t^2 + 1)^{3/2}} \ln\left(\frac{\sqrt{\gamma^2 t^2 + 1} - 1}{\gamma^2 t^2 + \gamma t\sqrt{\gamma^2 t^2 + 1}}\right) \qquad (17)$$

which is also a function of temperature. The condition $\partial E_0(\gamma)/\partial\gamma = 0$ leads to the equation

$$\frac{\gamma^3 t^3}{(\gamma^2t^2+1)^2}\left[\frac{\gamma t}{\sqrt{\gamma^2t^2+1}-1} - \frac{1}{\gamma^2t^2+\gamma t\sqrt{\gamma^2t^2+1}} - 2\right]$$

$$+ \frac{3\gamma^2 t^2}{(\gamma^2t^2+1)^{5/2}}\ln\left(\frac{\sqrt{\gamma^2t^2+1}-1}{\gamma^2t^2+\gamma t\sqrt{\gamma^2t^2+1}}\right) + \frac{\gamma^2t^2+2\gamma t-1}{(\gamma^2t^2+1)^2} + \left(1-\frac{\gamma}{2}\right) = 0$$

Numerical values of γ and the corresponding values of ground state energy at various high temperatures are listed in Table 1, and shown in Fig. 2. For $t > 4$, the approximation is reasonably treated quite well when compared with the result by Stern and Howard[1].

TABLE 1. VALUES OF γ AND THE CORRESPONDING VALUES OF E_0 AT VARIOUS HIGH TEMPERATURES

t	γ	E_0 (Rydbergs)
5	1.814	-2.311758
6	1.842	-2.600770
7	1.864	-2.806932
8	1.881	-2.960399
9	1.893	-3.079130
10	1.904	-3.173657

Discussion

My analysis is based on the linear response theory which would be valid for small Z impurities (in this case, Z = 1). For large Z impurities, a non-linear theory is needed. In 3-D case and at T = 0, such a non-linear screening theory was investigated by Almbladh *et al.*[6], which showed significant differences from the results of the linear theory. The density functional theory of Hohenberg-Kohn-Sham at finite temperatures can be applied for obtaining the energy spectrum of high Z ions. However, we must include the term $V_{xc}[n,T] = \delta\Omega_{xc}[n,T]/\delta n(\bar{r})$ in the effective potential given by eq.(1). Ω_{xc} is the thermodynamic potential due to exchange and correlation effects and V_{xc} is the corresponding exchange and correlation potential. In 3-D case, Gupta and Rajagopal[7] showed the effect of including V_{xc} on the bound state spectrum of neon nucleus (Z = 10) embedded in a plasma of electron density $n = 10^{24}$ electrons/cm^3 at a temperature T = 100 eV = 1.2×10^6 K. The effect was found to be very substantial. ε_{1s} is lowered by aboute 6 %, ε_{2S} by 20 % and ε_{2p} by as much as 30% compared to the self-consistent Hartree result. In 2-D case. Phatisena *et al.*[3] calculated the value of V_{xc} at various densities and temperatures. The finite temperature non-linear theory for two-dimensional system will be reported latter.

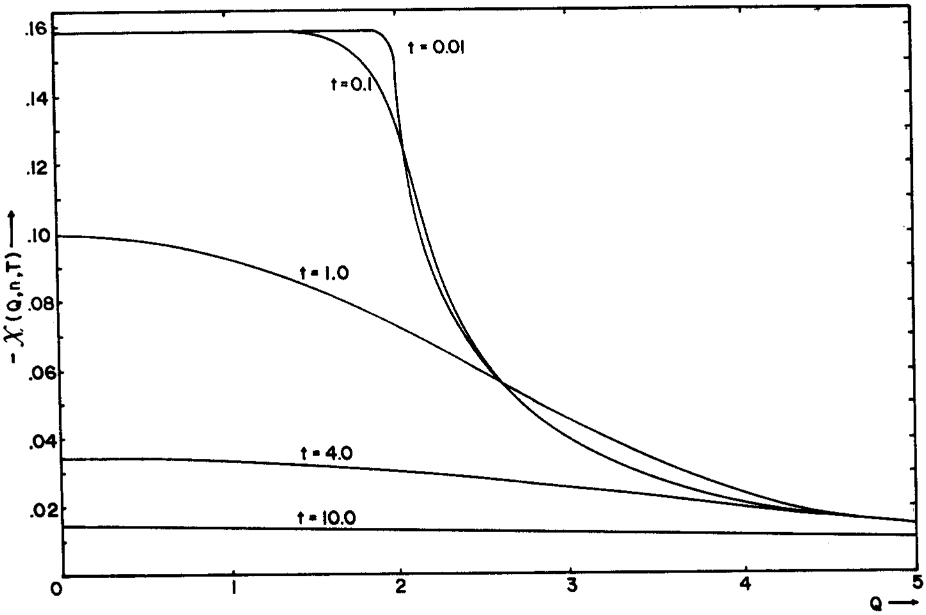

Figure 1. Variation of X (Q, n, t) with $Q = q/k_{FV}$ at various $t = T/T_F$

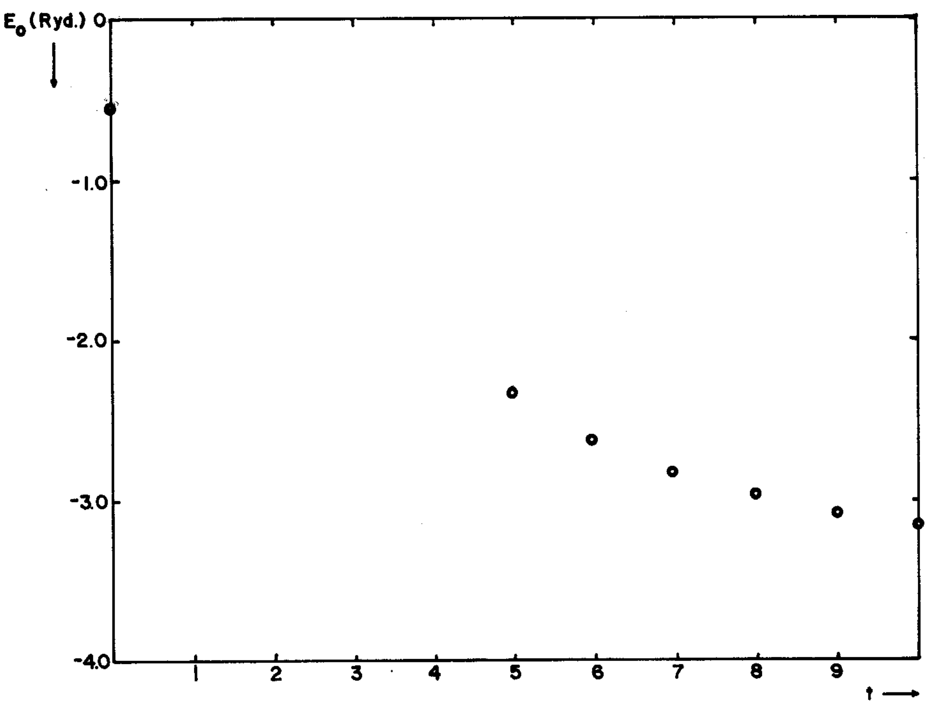

Figure 2. Ground state energy E_0 as a function of $t = T/T_F$ at high temperatu

Acknowledgment

The author would like to thank Dr. Panat and Dr. Amritkar of University of Poona, India, for numerous valuable discussions as well as for detailed comments on the manuscript.

References

1. Stern, F. and Howard, W.E. (1967). Properties of semiconductor surface inversion layers in the electric quantum limit. *Phys. Rev.* **163**, 816-835.
2. Gupta, U. and Rajagopal, A.K. (1979). Plasma screening effects in the intermediate degeneracy region. *J. Phys.* **B12**, L703-L709.
3. Phatisena, S., Amritkar, R.E., and Panat, P.V. (1986). Exchange and correlation potential for a two-dimensional electron gas at finite temperatures. *Phys. Rev.* **A34**, 5070-5079.
4. Maldague, P.F. (1978). Many-body corrections to the polarizability of the two-dimensional electron gas. *Surf. Sci.* **73**, 296-302.
5. Ziman, J.M. (1964). *Principles of the Theory of Solids,* Cambridge University Press, Cambridge, P. 155.
6. Almbladh, C.O., von Barth, U., Popovic, Z.D., and Stott, M.J. (1976). Screening of a proton in an electron gas. *Phys. Rev.* **B14**, 2250-2254.
7. Gupta, U. and Rajagopal, A.K. (1982). Density functional formalism at finite temperatures with some applications. *Physics Reports* **87**, 259-311.

บทคัดย่อ

ศึกษาผลของการกั้นที่มีต่อพลังงานที่สถานะพื้นของระบบแก๊สอิเล็กตรอนสองมิติที่มีสารเจือปน โดยใช้ทฤษฎีการสนองตอบเชิงเส้น เนื่องจากฟังชัน Lindhard ซึ่งขึ้นอยู่กับอุณหภูมิและความหนาแน่นของระบบ มีค่าสูงสุดที่ความยาวคลื่นมาก ๆ ทั้งอุณหภูมิสูงและอุณหภูมิต่ำ ดังนั้นจึงใช้ฟังชันนี้ที่ลิมิตดังกล่าวหาพลังงานที่สถานะพื้นของระบบโดยใช้วิธีการแปรผัน ผลที่ได้สอดคล้องกับผลงานของ Stern และ Howard โดยเฉพาะอย่างยิ่งที่อุณหภูมิสูง ๆ