Int. J. Chem. Sci.: 10(1), 2012, 331-341
ISSN 0972-768X
www.sadgurupublications.com

AN EVALUATION OF EFFECTIVE MASS (m^*/m_O) OF ELECTRON AS A FUNCTION OF CONCENTRATION OF ELECTRONS IN n-CHANNEL INVERSION LAYER

A. KUMAR[a], M. K. SINGH and L. K. MISHRA[*]

Department of Physics, Magadh University, BODH GAYA – 8247234 (Bihar) INDIA
[a]C/o Dr. Paras Nath Singh, Vill. & P.O.- Kakhanpar, PUNPUN (Patna) – 804453 (Bihar) INDIA

ABSTRACT

Using two theoretical models (Ando formalism and Vinter formalism) an evaluation of effective mass (m^*/m_o) of electron as a function of N_s (concentration of electrons) in n-channel inversion layer has been performed. Our theoretical result of (m^*/m_o) decreases with Ns as per experimental observation. However, the theoretical values evaluated from Ando formalism are in better agreement with the experimental data

Key words: Effective mass, n-Channel inversion layer, Quasi-particle, Electron Concentration.

INTRODUCTION

In this paper, we have presented the method of evaluation of effective mass (m^*/m_o) as a function of concentration of electron in n-channel inversion layer Ns. Inversion layer is a two-dimensional system. As we know that in two dimensional system, electrons are confined to move within a plane placed in vacuum, the Fourier transform V (q) of electron-electron interaction is given by $2\pi e^2/q$ in contrast to $4\pi e^2/q^2$ in three dimension.

The electron-electron interaction affects various properties of the two-dimensional electron gas. Among them are the quasi-particle properties such as effective mass and the g factor. These quantities have attracted much attention because these are directly observable experimentally. The g-factor was first obtained by Fang and Stiles[1] in n-channel inversion layer on Si (100) and was found to be enhanced from the bulk value close to 2. Smith and Stiles[2] determined the effective mass in the same system and showed that effective mass first enhanced then decreased with the electron concentration.

[*]Author for correspondence; E-mail: muphysicslkm@gmail.com

The theoretical studies of effective mass of electron in 2D electron gas starts with Landau Fermi liquid theory[3] in which the so-called *f* function plays a central role. Random phase approximation[4] has been used to calculated *f*-function as a function of electron concentration. In this approximation the quasi particle energy of an electron with a spin (±1) and valley index *v* is obtained from the total energy by taking the functional derivative with respect to the Fermi function. The quasi particle energy is related with the Green's function and the dielectric function is obtained by further taking propagator π (q, ω). The *f* function is obtained by further taking the functional derivative of quasi particles energy with respect to Femi derivation function. One obtains m/m^* and g/g^* with respect to f function. Such scheme for two dimensional system was given by Suzuki and Kawamoto[5] and Ting, Lee and Quninn[6].

m^* and g^* were also calculated from different approximation schemes[7-14]. In these approximation schemes, one treats the self-energy shift to the lower order by screened Coloumb interaction, taking the image effect in the electron-electron interaction by neglecting the dynamical screening and replacing ε (q, ω) by ε (q, o). One also determines the difference of exchange interactions of up and down spin electron in the vicinity of the Fermi surface where the effective mass is determined by virtual excitation of electron-hole pairs and plasmons with wide range of energy. The effective mass were also calculated with the renormalization constant Z which is defined as –

$$Z = \left[1 - \frac{\partial \Sigma(H,\omega)}{\partial E}\right]^{-1} \qquad \ldots(1)$$

Where Σ (H, ω) is the self-energy evaluated to the lower order in the dynamically screened interaction.

$$1 - \frac{m}{m_D^*} = Z\left|1 - \frac{m}{m_R}\right| \qquad \ldots(2)$$

The subscripts D and R refer to the results obtained by the Dyson equation[8] and Rice's approximation[9] written in the following equation, respectively.

$$E(k) = \varepsilon(k) + \Sigma(k, \varepsilon(k)) \qquad \ldots(3a)$$

and

$$E(k) = \varepsilon(k) + \Sigma(k, E(k)) \qquad \ldots(3b)$$

with

$$\varepsilon(k) = \frac{\hbar_2 k_2}{2m} \qquad \ldots(3c)$$

Since Z varies from 0.3 to 0.8 in the density range 10^{11}-10^{13} cm^{-2} in the n-channel inversion layer on the Si (100) surface therefore the different between m_D^* and m_R^* are important. A density functional formulation[15,16] has also been used to calculate the effective mass and the g-factor.

A recent calculation of renormalization factor (constant) Z and effective mass of the two-dimensional electron gas was performed by Holdzman *et al.*[17] They calculated the momentum distribution of the Fermi liquid phase of the homogeneous two-dimensional electron gas. They showed that close to the Fermi surface, the momentum distribution of a finite system with N electron approaches its thermodynamic limit slowly, with leading order correction scaling as $N^{-1/4}$. These corrections dominate the extrapolation of the renormalization factor Z and the single particle effective mass m^* to the infinite system size. They showed that in the range $1 \leq r_s \leq 10$, one gets a lower renormalization factor Z and the higher effective mass $m^* > m$ compared to the perturbative random phase approximation value[18,19]. Here $r_s = \left(\pi n a_B^2\right)^{-\frac{1}{2}}$ is the Wigner-Seitz density parameter, n is the density and $a_B = \hbar^2/me^2$ is the Bohr radius. Similar type of calculation was also performed by Asgari and Tanatar.[20] They calculated many body effective mass as a function of r_s for $0(r_s \leq 8)$ for quasi two dimensional electron as (Q_{2D}) confined in a GaAs/A1GaAs triangular quantum well. Their results show that effective mass enhancement is smaller in the Dyson equation calculation than in the OSA (On Shell Approximation). When results, were compared with the experimental data of Tan *et al.*[21,22], the following conclusions were drawn.

(a) RPA and the local field factors beyond the RPA are similar in the weak coupling ($r_s \leq 1$).

(b) Theoretical calculations in the strong coupling region are not so close to experimental data.

De Palo *et al.*[23] have a similar calculations in the same range of coupling strengths.

In this paper, we have evaluated (m^*/m_0) of electrons as a function of N_s (concentration of electrons in n-channel inversion layer). We have used two theoretical formalism (Ando formalism) and (Vinter formalism). Experimental results show that (m^*/m_0) of electron decrease with N_s. The evaluated results in both formalism indicate that (m^*/m_0)

decrease with N_s. However, the value calculated under Ando formalism are in better agreement with the experimental data.

Mathematical formula used in the evaluation

One starts with the quasi particle enerty[24,25] $E_{\sigma v}$ (k) of an electron with a spin σ (±1) and valley index *v*

$$E_{\sigma v}(k) = \varepsilon(k) - \int \frac{d\omega}{2\pi i} \sum_q \frac{V(q)}{\varepsilon(q,\omega)} G^0_{\sigma v}(k-q, \varepsilon(k)-\omega) \quad \ldots(4)$$

with $\varepsilon(k) = \hbar^2k^2/2m$. Green function is given by –

$$G^0_{\sigma v}(k,E) = \frac{n_{\sigma v}(k)}{E-\varepsilon(k)-i0} + \frac{1-n_{\sigma v}(k)}{E-\varepsilon(k)+i0} \quad \ldots(5)$$

$n_{\sigma v}$ (k) is the Fermi distribution function. ε (q, ω) is the dielectric function, given by-

$$\varepsilon(q,\omega) = 1 + V(q)\,\Pi\,(q,\omega) \quad \ldots(6)$$

with

$$\Pi\,(q,\omega) = -\sum_{\sigma v} \int \frac{dE}{2\pi i} \sum_k G^{(0)}_{\sigma v}(k,E)\, G^{(0)}_{\sigma v}(k+q, E+\omega) \quad \ldots(7)$$

$$V(q) = \left(2\pi e^2 \Big/ \tilde{k}_{ins}\right) F(q) \quad \ldots(8)$$

Where

$$\left(2\pi e^2 \Big/ \tilde{k}_{ins}\right) F(q)$$

$$\tilde{k} = \tilde{k}_{sc} + \tilde{k}_{sc}/2 \quad \ldots(9)$$

Here $\tilde{k}_{ins}$ is the dielectric constant of semiconductor and $\tilde{k}_{ins}$ is that of insulator. One consider a 2 D model in which half z > 0 space is filled with semiconducting medium and other half z < 0 is filled with insulating medium.

F (q) is the form factor given by[26] –

$$F(q) = \frac{1}{2}\int_0^\infty dz' g(z)g(z')\left\{\left[1+\frac{\tilde{k}_{ins}}{\tilde{k}_{sc}}\right]e^{-q|z-z|}+\left[1-\frac{\tilde{k}_{ins}}{\tilde{k}_{sc}}\right]e^{-q|z-z|}\right\} \quad \ldots(10)$$

g (z) is the charge distribution for inversion[27].

$$g(z) = \frac{b^3}{2}z^2e^{-bz} \quad \ldots(11)$$

Where b is the adjustable parameter. The Landau *f*-function is obtained by taking the functional derivative of equation (4) with respect to nσ'v' ($\bar{k}'$)

$$f_{\sigma v;\,\sigma' v'}(\bar{k},\bar{k}') \; f_0(\bar{k},\bar{k}') + \delta_{\sigma\sigma'}\delta_{vv'} f_e\,(\bar{k},\bar{k}') \quad \ldots(12)$$

Then one gets

$$m/m^* = 1 - \frac{m}{2\pi\hbar)^2}\sum_{\sigma\sigma'}\sum_{vv'}\int d\theta\; f_{\sigma v;\sigma' v'}(\theta)\cos\theta \quad \ldots(13)$$

and

$$g/g^* = 1 + \frac{m^*}{2\pi\hbar)^2}\int d\theta\; f(\theta) \quad \ldots(14)$$

Where $f(\theta) = f(\bar{k},\bar{k}')$ with $k = k' = k_F$ and $k.k' = k_F^2\cos\theta$. The effective mass m* and effective g factor g* are defined as usual by -

$$\frac{1}{m^*} = \frac{1}{\hbar^2 k_F}\frac{\partial}{\partial k}E_{\sigma v}(k)\big|k = k_F \quad \ldots(15)$$

With

$$E_{\sigma v}(k_F) = E(k_F) - \frac{1}{2} * \sigma\mu_B H \quad \ldots(16)$$

H is a weak magnetic field and μ_B is the Bohr magneton.

In the density function formalism[15,16], the quasi particle effective mass is given by -

$$m^*/m_l = \int_0^\infty dz \frac{m^*(n(z);z)}{m_{op}} n(z) [\int_0^\infty dz n(z)]^{-1} \quad \ldots(17)$$

Where m*(z (z); z) is the effective mass of the homogeneous three dimensional electron gas m_{op} is an isotropic mass defined by -

$$m_{op}^{-1} = (2m_\tau^{-1} + m_l^{-1})/3 \quad \ldots(18)$$

m_t and m_l are transverse and longitudinal mass, respectively.

One also calculates effective mass of 2D electron gas by calculating quasi particle excitation energy $\delta\varepsilon_{QP}$ (k), which is the quasi particle energy measured from the chemical potential μ of the interacting system by solving self-consistency the Dyson equation[28,29].

$$\delta\varepsilon_{QP}(K) = \varepsilon_K + R\sum_{rel}{}^R(k,\omega)/\omega = \delta\varepsilon_{QP}(K)/\hbar \quad \ldots(19)$$

Where

$$R\sum_{rel}{}^R(k,\omega) = R\sum_{rel}{}^R(k,\omega) - \sum_{rel}(k_F,0) \quad \ldots(20)$$

This is called on shell approximation (OSA). Once the QP (quasi particle) excitation energy is known, the effective mass m*(k) can be calculated by means of the relationship

$$\frac{1}{m^*(k)} = \frac{1}{\hbar^2 k}\frac{dz_{Qp}(k)}{dk} \quad \ldots(21)$$

Evaluating m*(k) at $k = k_F$, one gets the QP effective mass at the Fermi surface.

RESULTS AND DISCUSSION

In this paper, we have presented a method of evaluation of effective mass (m^*/m_o) of electron in n-channel inversion layer on Si (100) surface as a function of concentration of electrons in the inversion layer N_S. The calculation has been performed with the help of two theoretical models theo^I (Vinter Formalism)[8,9] and theo^{II} (Ando formalism)[15,16] and the results are compared with the experimental results of Smith and Stiles[2]. These results have been given in Table 1. In the first theoretical model, (m^*/m_o) is rather low as compared to the experimental data for each value of N_S. The theoretical results evaluated from Ando Formalism[15,16] is rather in better agreement with the experimental data. However, the

evaluated results decrease with N_S as per experimental observations. Vinter for formalism (theo^I)[8,9] is based on a model in which a semiconductor, with a dielectric constant K_{SC} fills the half space $z > 0$ and other half space $z < 0$ is filled with an insulating medium of dielectric constant K_{ins}. Using the dielectric function $\varepsilon(q,\omega)$ given by equation (6) one obtains the effective mass equation (13). By computing Eq. (13) as a function of N_S, one obtains the values of (m^*/m_o) as a function of N_S shown in Table 1. On the other hand, the Ando formalism is a density functional formalism. In the density functional formalism, the density distribution of an interacting electron gas under an external field can be obtained by a one body Schrödinger type equation containing an exchange correlation potential in addition to the usual Hartree potential and external potential. One can take the exchange correlation potential U_{xc}. The exchange correlation potential is obtained by a functional derivative of the exchange correlation part of the ground state energy $E_{xc}[n(\overline{R})]$ is not known and is replaced by a product $n(\overline{R})\,E_{xc}[n(\overline{R})]$ in the usual local approximation where $E_{xc}(\overline{R})$ is the exchange-correlation energy per electron of a uniform electron gas with the density n. In this approximation, $U_{xc}(\overline{R})$ becomes the exchange-correlation part of the chemical potential μ_{xc} of the uniform electron gas. In the density function formalism, the quasi-particle effective mass is given by equation (17) and (18).

Table 1: An evaluated results of effective mass (m^*/m_o) of electron in n-channel inversion layer on Si (100) surface as a function of concentration of electron in the inversion layer N_S. The calculation has been performed with the help of two theoretical models theor^I and theor^{II} and are compared with experimental results

N_s (10^{12} cm^{-2})	(m^*/m_o)		
	Theo^I	**Theo^{II}**	**Expt.**
0.5	0.226	0.246	0.268
1.0	0.220	0.232	0.259
1.2	0.206	0.228	0.255
1.4	0.200	0.217	0.248
1.6	0.187	0.212	0.244
1.8	0.172	0.208	0.240
2.0	0.160	0.205	0.238

Cont…

N_s (10^{12} cm^{-2})	(m^*/m_o)		
	Theo^{I}	**Theo^{II}**	**Expt.**
2.1	0.155	0.202	0.232
2.6	0.152	0.200	0.230
2.8	0.147	0.197	0.227
3.0	0.142	0.195	0.227
3.2	0.140	0.192	0.222
3.5	0.132	0.187	0.220

In Table 2, we have shown the theoretical results of the renormalization factor z and effective mass (m^*/m_o) calculated from VMC (Variational quantum Monte Carlo)[30] and perturbative RPA[31] calculations as a function of r_s (Winger-Seitz density parameter) in the calculation, it appears that in the range $1 \leq r_s \leq 10$, one gets a lower renormalization factor Z and a higher effective mass (m^*/m_o) compared to the perturbative random phase approximation value. In Table 3, we have reported the many-body effective mass (m^*/m_o) as a function of r_s for a Q_{2D} electron gas confined in a GaAs/AlGaAs triangular quantum well with four theoretical formalism I (OSA), II (Dyson), III (OSA-RPA) and IV (Dyson-RPA)[32]. Theoretical results[20] were compared with the recent experimental data[21,22]. After comparison it appears that III (OSA-RPA) and IV (Dyson-RPA) are in right trend with experimental data although the values are quite less. In Table 4, we have given experimental results of effective mass or band mass of electrons of some two dimensional systems[33-35]. These results show band mass of electron m^*/m_o (bare mass) in hetro -structures and quantum well systems. These results are very similar to QMC results[36] of 2D electron gas for $r_s = 1$.

Table 2: Theoretical results of renormalization function Z and effective mass (m^*/m_o) calculated from VMC (Variational quantum Monte Carlo)[31] and pertubative RPA calculation[32] as a function of r_s

r_s	Z_{VMC}	Z_{RPA}	$(m^*/m_o)_{VMC}$	$(m^*/m_o)_{RPA}$
1	0.627	0.663	1.267	1.025
3	0.348	0.442	1.398	1.116
5	0.225	0.348	1.547	1.168
8	0.165	0.272	1.686	1.195
10	0.090	0.247	1.729	1.219

Table 3: Many-body effective mass (m^*/m_o) as a function of r_s for a Q_{2D} electron gas confined in a GaAs/AlGaAs triangular quantum well with four theoretical I (OSA), II (Dyson), III (OSA-RPA) and IV (Dyson-RPA). Theoretical results[20] were compared with experimental data[21,22]

r_s	(m^*/m_o)				
	I (OSA)	**II (Dyson)**	**III (OSA-RPA)**	**IV (Dyson-RPA)**	**Expt.**
0.5	0.987	0.962	0.992	0.976	0.852
1	0.923	0.978	1.023	0.985	0.985
3	0.974	1.038	1.086	1.049	1.125
4	1.085	1.052	1.102	1.054	1.224
5	1.110	1.063	1.184	1.067	1.358
6	1.168	1.077	1.238	1.078	-
7	1.248	1.084	1.339	1.087	-
8	1.369	1.092	1.386	1.096	-

Table 4: Experimental results of effective mass of electrons or band mass of electron (m^*) of two dimensional system[32-34]

Systems	**Effective mass or band mass of electron (m^*)**
H_xGa_{1-x}/GaN $x = 0.13$	$0.215 \pm 0.006\ m_0$
Undoped AlGaN/GaN heterostructures	$0.2 \pm 0.01\ m_0$
Modulation doped $In_{0.65}\ Ga_{0.35}\ As/\ n_{0.52}Al_{0.48}As$ single quantum well	$0.05869\ m_0$

REFERENCES

1. F. F. Fang and P. J. Stiles, JETP Lett., **31**, 208 (1980).

2. J. L. Smith and P. J. Stiles, Sov. Phys. JETP, **5**, 361 (1982).

3. L. D. Landau, Sov. Phys. JETP, **3**, 920 (1957).

4. P. Nozieres and D. Pines, Phys. Rev. IIL, 442 (1958).
5. M. Suzuki and S. Kawamoto, J. Phys. Soc. Japan, **30**, 325 (1975).
6. N. Ting, D. M. Lee and J. J. Quinn, Surf. Sci., **73**, 40 (1978).
7. J. F. Janak, Phys. Rev., **178**, 1416 (1970).
8. F. J. Olkawa, Surf. Sci., **98**, 350 (1980).
9. T. M. Rice, Ann. Phys. (N.Y.), **31**, 100 (1961).
10. J. Hubbard, Proc. R. Soc. London Ser A, **240**, 539 (1957).
11. J. Hubbard, Proc. R. Soc. London Ser A, **243**, 336 (1958).
12. B. K. Lundqvist, Phys. Londons, Mater, **6**, 196 (1967).
13. A.W. Overhauser, Phys, Rev. B, **18**, 2884 (1978).
14. M. B. Pogrebinski, Sov. Phys. Semicond., **31**, 372 (1987).
15. B. Vinter, Surf. Sci., **110**, 947 (1988).
16. B. Vinter, Surf. Sci., **118**, 248 (1990).
17. M. Holtzmann, T. Alm, P. Schuck and R. Cote, Phys. Rev. B, **79**, 041308 (R) (2009).
18. H. J. Schulze, P. Schnck and N. Van Giai, Phys. Rev. B, **61**, 8026 (2000)
19. R. Asgari, B. Davondi, M. Polini, G. F Giulani M. P. Tosi, and G. Vignale, Phys. Rev. B, **71**, 045323 (2005).
20. R. Asgari and B. Tanatar, Pramana J. Phys., **70**, 285 (2008).
21. Y. W. Tan, D. H. Kobe, D. M. Lee, J. O. Sofo and M. Randeria, Phys. Rev. Lett. (PRL), **94**, 016405 (2005).
22. Y. W. Tan, D. H. Kobe, D. M. Lee, J. O. Sofo and M. Randeria, Phys. Rev. B, **73**, 045334 (2006).
23. S. De. Palo, A. Griffin, A. N. Bloch, R. Minas and R. M. Quick., Phys. Rev. Lett. (PRL), **94**, 226405 (2005).
24. T. Ando, A. B. Fowler and F. Stern., Rev. Mod. Phys., **54**, 437 (1984).
25. T. Ando, J. Phys. Soc. Japan, **5**, 2978 (1981).
26. F. F. Fang and W. E. Howard, Phys. Rev., **174**, 823 (1966).
27. F. F. Fang, A. B. Fowler and A. Hartstein, Surf. Sci., **73**, 269 (1978).

28. S. Yarlagadda and G. F. Gialiani, Phys. Rev. B, **61**, 12556 (2000).

29. H. M. Bohm and K. Schorkhuser, J. Phys. Condens, Matter, **12**, 2007 (2000).

30. M. Holtzmann, Phys. Rev. B, **68**, 046707 (2003).

31. G. F. Giuliani and G. Vignali, Quantum Theory of the Electron Liquid, Cambridge University Press, Cambridge (2005).

32. R. Asgari, Phys. Rev. B, **74**, 155319 (2006).

33. C. R. Elsass, Appl. Phys. Lett., **74**, 3528 (1999).

34. A. M. Kurakin, J. Appl. Phys., **105**, 073703 (2009).

35. P. N. Hai, Mater. Sci. Engg., **43**, 82, 218 (2001).

36. R. Asgari, B. Davondi and B. Tanakar, Solid State Commun., **130**, 13 (2004).

Accepted : 27.09.2011