Indian J. Res. Found., (2015) 3, 11-14. ISSN 2454-6577

INDIAN JOURNAL OF RESEARCH FOUNDATION
www.indianjournal.net

RESEARCH ARTICLE

Metal – insulator transition and electron–electron interaction under intense magnetic fields in silicon

M. Muthukrishnaveni[1], N. Srinivasan[2,*]

[1]*Sri Ramakrishna Institute of Technology, Pachapalayam-641010, Coimbatore, Tamil Nadu, India*
[2]*Department of Physics, Thiagarajar College, Madurai-625015, Tamil Nadu, India*

Received 8 August 2015; Accepted 30 October 2015
Available online 30 October 2015

Abstract

Using a D^- ion model in an N-type semiconductor and a product Gaussian wave function with two variational parameters, closed analytical expressions are obtained for binding energy when the system is subjected to intense magnetic fields. The important results obtained are enhancement in ionization energy as the magnetic field (B) increased, reduction in (e - e) interaction energy as B increased, and enhancement in (e – e) – interaction energy with an increase in donor concentration. The quantitative estimates of the (e – e) – interaction in a magnetic field is a new result, which is discussed in the light of MIT and superconductivity.

Keywords
Semiconductor
Binding Energy
Magnetic Field
MIT
Superconductivity

Introduction

Magnetic field is an important probe in the investigations on properties of materials for a long time [1]. A renewed interest has recently been observed, especially in doped semiconductors, with a view to understand Metal – Insulator Transition (MIT) which is seen as a precursor to superconductivity [2, 3]. MIT occurs primarily due to two different mechanisms. One is the Mott transition driven by electron – electron (e – e) interactions and the other is the Anderson transition occurring due to randomness in impurity distribution [4, 5]. Another interest stems from the observation of MIT in low dimensional semiconductor systems such as quantum wells in hetero structures [6, 7], which contradicts the celebrated scaling theory [8, 9]. Recently a new Mott criterion for MIT in intense magnetic fields has been proposed [3]. Randomness and correlation effects were introduced as a consequence of the Hubbard model results [10, 11]. The theoretical field formulations with approximations in the evaluation or computer simulations [9, 12] were published earlier. In the present work, we considered a simple D^- ion model in doped semiconductors and include (e - e) – interaction in the Hamiltonian in a strong magnetic field.

Experimental

Model and calculations

The effective mass theory (EMT) of Kohn and Luttinger is fairly successful in providing the shallow donor

*Corresponding author
E-mail : mmkrishna.veni83@gmail.com

Published by GM SOFTWARE

spectra in semiconductors [13, 14]. Though several attempts have been made in the past to overcome certain short comings of the EMT, especially in many – valley semiconductors, no satisfactory theory free from criticism has emerged yet [14, 15]. Within the EMT, a D^- ion (ie., a donor with an additional electron presumably from a neighboring donor) as shown in **Fig 1** is described by the Hamiltonian

$$H_0 = -\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\hbar^2}{2m}\nabla_2^2 - \frac{e^2}{\varepsilon_0 r_1}e^{-\lambda r_1} - \frac{e^2}{\varepsilon_0 r_2}e^{-\lambda r_2} \quad (1)$$

where λ is the Thomas – Fermi screening parameter, ε_0 is the static dielectric constant of the semiconductor and m is the effective mass pertinent to the conduction band minimum. The (e - e) – interaction is described by

$$H_1 = \frac{e^2}{\varepsilon_0|\overline{r_1}-\overline{r_2}|} \quad (2)$$

omitting the spin – spin interaction. When the impurity concentration is high, the adjacent impurity orbits overlap forming an impurity band and the Hubbard model explains how correlation effects lead to MIT [16]. In a magnetic field, Eq (1) becomes

$$H_2 = \sum_{i=1}^{2}\left\{-\left(\frac{\partial^2}{\partial\rho_i^2}+\frac{1}{\rho_i}\frac{\partial}{\partial\rho_i}+\frac{1}{\rho_i^2}\frac{\partial^2}{\partial\rho_i^2}+\frac{\partial^2}{\partial z_i^2}\right)+\frac{L_{z_i}}{2}+\frac{\rho_i^2}{16}-\left(\frac{\gamma}{2}\right)^{\frac{-1}{2}}(\rho_i^2+z_i^2)^{\frac{-1}{2}}e^{-\lambda r_i}\right\} \quad (3)$$

In writing the above Hamiltonian we have used (i) cylindrical coordinates and (ii) a system of units in which $l = \left(\frac{\hbar}{2m\omega_c}\right)^{\frac{1}{2}}$ is the unit of length and $E = \hbar\omega_c$ is the unit of energy. The ω_c is the cyclotron frequency given by $\omega_c = \frac{eB}{mc}$ We have also defined a dimensionless parameter for magnetic field, $\gamma = \frac{\hbar\omega_c}{2R}$, where R is the effective Rydberg in a semiconductor, given by $R = \frac{me^4}{2\hbar^2\varepsilon_0^2}$.

In the above system of units H_1 becomes

$$H_{e-e} = \left(\frac{\gamma}{2}\right)^{\frac{-1}{2}}\frac{\varepsilon_0}{r_{12}} \quad (4)$$

Hence the total Hamiltonian for the D^- ion is

$$H_{new} = H_2 + H_{e-e} \quad (5)$$

The Thomas – Fermi screening parameter λ contains the donor concentration , $\lambda = \left(\frac{4\pi e^2\eta}{\varepsilon_0}\right)^{\frac{1}{2}}$, where $\eta = \frac{3}{2}\left(\frac{N}{E_F}\right)$ is the density of electron states at the Fermi energy E_F. In our system of units, $\lambda = \left(\frac{12\pi^2e^2N^{\frac{1}{3}}}{\hbar\varepsilon_0\omega_c}\right)^{\frac{1}{2}}(3\pi^2)^{\frac{-1}{3}}$. We solve the Schrödinger equation with Eqo(5) as the Hamiltonian, choosing the variational method. The variational ansatz is chosen as

$$\psi = N\prod_{i=1,2}e^{\frac{-\rho_i^2}{8a^2}}e^{\frac{-z_i^2}{8b^2}} \quad (6)$$

extending the calculations [2, 3]. Here a and b are the variational parameters which extremalise the ground state energy. The normalization constant N and the ionization energy are given by $N = \left(8\pi^{\frac{3}{2}}a^2b\right)^{-1}$ and

$$E(\gamma) = \gamma - 2\gamma\langle H_{new}\rangle_{min} \quad (7)$$

Note that the energy is now in units of effective Rydberg. The ionization energy is the energy required to push the electron from the lowest binding energy level into the lowest Landau level. The effect of the electron spin is to shift the lowest Landau level, $\frac{1}{2}\hbar\omega_c$, by $-\mu B$, where μ is a Bohr magneton. Hence Eqo (7) is modified to

$$E_{ion}(\gamma,\lambda) = \left(1-\frac{2\mu m}{e\hbar}\right)\gamma - 2\gamma\langle H_{new}\rangle_{min} \quad (8)$$

After a lengthy calculation, we obtain

$$\langle H_{new}\rangle = \left(\frac{1}{2a^2}+\frac{1}{4b^2}+\frac{a^2}{2}\right)-\frac{1}{2a^2b}\frac{e^{\frac{\lambda^2R_0^2}{8}}}{(\pi\gamma)^{\frac{1}{2}}}\left(\frac{R_0^2}{2\sqrt{2}}-\frac{\pi^{\frac{1}{2}}\lambda R_0^3}{8}\right)+\frac{2.235\times10^{-3}}{(a^2b)^{\frac{1}{3}}}\gamma^{\frac{-1}{2}} \quad (9)$$

where $R_0 = \left(\frac{3}{4}a^2b\right)^{\frac{1}{3}}$. In evaluating certain integrals we have used the mean value theorem of calculus [17, 18].

Results and discussion

For every donor concentration and for different magnetic fields, $E_{ion}(\gamma,\lambda)$ has been computed and the results are presented in **Fig 1.** We notice that the 'ionization energy' increases in a magnetic field. As the donor concentration increases this energy decreases. These results are similar to those obtained earlier [2, 3], except for the contribution from electron spin. The spin contribution itself is small, 0.316R,

when $\gamma = 1$. The parameters chosen are $m = 0.3m_0$ and $\varepsilon_0 = 11.7$, where m_0 is the free electron mass. Two points that emerge from **Fig 1** are, (i) as the donor concentration increases the 'ionization energy' decreases leading to MIT at a critical concentration. Experimentally, for P donor in Si, the critical donor concentration (N_c) is 3.74 X 10^{18} cm^{-3} [19] , when $\gamma = 0$), and (ii) for any donor concentration, as the magnetic field increases the critical concentration also increases, showing that one requires a higher magnetic field to bring out MIT. The (e – e) interaction which is the third term in Eq (9) is plotted for different magnetic fields and donor concentrations in **Fig 2**. The interaction energy decreases as the magnetic field increases. This energy is of the order of 1 to 2% of E_{ion} , for donor concentrations less than 10^{16} cm^{-3}. Only for $N \geq N_c$ it is about 16%. Hence in intense magnetic fields, in the semiconductor region, the (e – e) – interaction may be dropped. The reason for this small value may be seen in the following way. The value of $\gamma = 1$ corresponds to a magnetic field of 154 T is Si, which is very high. The cyclotron radius for this magnetic field turns out to be 14 Å, approximately. However, for $N = 10^{15}$ cm^{-3}, the average separation between electrons, r_{12}, becomes $\sim$ 6000Å , if one equates $\frac{e^2}{\varepsilon_0 r_{12}}$ to 0.0062 R . −0.762

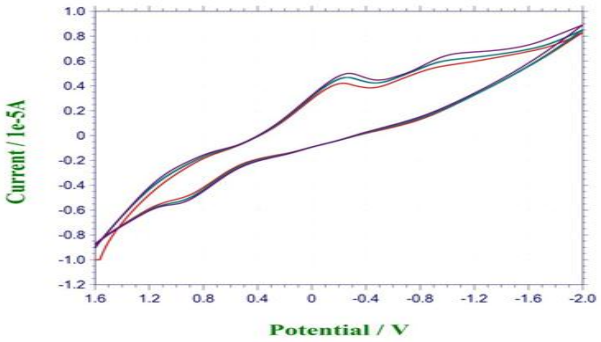

Fig 1 Ionization energy in effective Rydberg defined as the energy required to remove an electron from D^- ion in Si.

For a given magnetic field, as the donor concentration increases, the interaction energy also increases. From the above we observe that only for $N \geq N_c$, the interaction energy is appreciable, $\sim$ 10% or more. This shows that the effect of high donor concentration and the effect due to magnetic field are competing factors. While the former brings electrons closer due to overlap of orbits of neighbouring donor sites, the latter appears to keep them apart since all coulomb interactions (both repulsive and attractive) are small perturbations under intense magnetic fields. Ultimately, the effect due to concentration wins and MIT occurs.

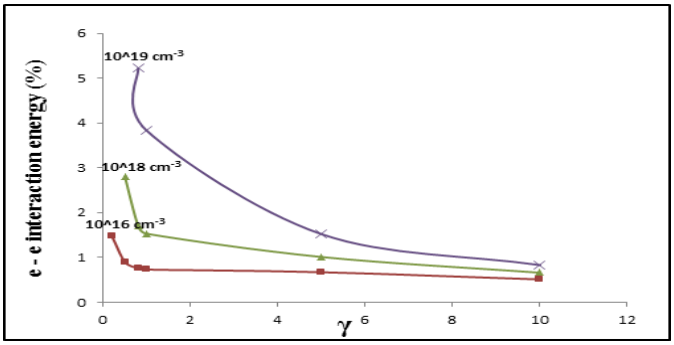

Fig 2 Electron – electron interaction energy as % of E_{ion}

The above results have a bearing on superconductivity [20, 21]. While the destruction of superconductivity in a strong magnetic field is known, several recent experiments have shown the occurrence of superconductivity in ferromagnetic materials [22, 23]. Interestingly, superconductivity in strong magnetic fields in heavily doped semiconductors has been predicted [24]. A typical value obtained by Rasolt [24] is Tc $\sim$ 0.5 K for N $\sim$ 10^{18} cm^{-3} in a magnetic field of 1 MG. which corresponds to $\gamma = 1$, approximately. Superconductivity in heavily doped semiconductors, both in bulk and in quantum well systems has been clearly established [25, 26]. However, it is the conjecture of Rasolt which is the motivation for the present work. It is the phonon assisted (e – e) interaction which is at the root of BCS theory for superconductivity. But we notice that in a strong magnetic field the electron – lattice interaction becomes weaker [27] and as the present work indicates the (e – e) interaction also becomes weak. This softening of the electron-lattice coupling has not been considered by Rasolt. Hence the phonon assisted BCS mechanism, and consequently the low value obtained for T_c is questionable. The triplet pairing (in a strong magnetic field) of electrons leading to superconductivity should occur by invoking other mechanisms.

The scenario that emerges from the present work is that we have a collection of nearly spin polarized free electrons influenced by a strong magnetic field, separated from each other by a large distance of about 6000 Å for $\gamma = 1$ when $N = 10^{15}$ cm^{-3}. After metallization occurs, superconductivity may

arise due to any non–phonon mechanism with a triplet paring of electrons.

Conclusions

MIT in doped semiconductors in intense magnetic fields has been investigated within the simple EMT, considering a D^- ion model. The electron – electron interaction has been calculated variationally. Closed analytical expressions are obtained for the case of Thomas – Fermi potential and (e - e) - interaction. The interaction energy is usually less than 1.5% of the 'ionization energy' for all magnetic fields investigated when the donor concentration is less than about 10^{16} cm^{-3}. For higher concentrations the interaction energy becomes large, as much as 16.5% for < 1 . Even in this case, when $\gamma > 1$, the interaction energy is approximately 1%. Hence we conclude that the (e – e) – interaction may be dropped in the evaluation of the ground state energies of donors under intense magnetic fields. However, in the metallic region $(N \geq N_c)$, this becomes appreciable.

Acknowledgments

We thank Dr. K. Navaneethakrishnan and Dr. R. Joseph Xavier for their help and constant, encouragement.

References

[1] G. Landwwehr, *Applications of High magnetic fields in Semiconductor Physics, Springer, Berlin*, (1983).

[2] R. Suganya, K. Navaneethakrishnan, *Solid State Commun.*, 138, (2006), 99.

[3] M. Muthukrishnaveni, N. Srinivasan, *Phase Transition*, 85, (2012), 391.

[4] N. F. Mott, *Metal – Insulator Transition*, Taylor Francis, Philadelphia, 5, (1974), 5.

[5] P. W. Anderson, *Phys. Rev.*, 109, (1958), 1492.

[6] S. V. Kravchenko, W. Mason, J. E. Furneaux, V. M. Pudalov, *Phys. Rev. Lett*., 75, (1995), 910.

[7] E. Abrahams, S. V. Kravchenko, M. P. *Rev. Mod. Phys.*, 73, (2001), 251..

[8] E. Abrahams, P. W. Anderson, D. C. Licciardello, T. V. Ramakrishnan, *Phys. Rev. Lett.*, 42, (1979), 673

[9] P. A. Lee, T. V. Ramakrishnan, *Rev. Mod. Phys*., 57, (1985), 287.

[10] A. John Peter, K. *Phys. Stat. Solid* B, 220, (2000), 897.

[11] A. John Peter, K. Navaneethakrishnan, *Physica E*, 16, (2003), 223.

[12] M. Imada, A. Fujimori, Y. Tokura, *Rev. Mod. Phys*., 70, (1998), 1039.

[13] W. Kohn, *Solid State Phys*., 5, (1957), 257.

[14] R. Resta, *Crystalline Semiconducting materials and Devices, Eds*., Plenum Press, 217, (1986).

[15] M. Altarelli, W. K. Hsu, *Phys. Rev. Lett*., 43, (1979), 1346.

[16] B. K. Ridley, *Quantum Process in semiconductors*, Clarendon press, oxford, 78, (1982).

[17] A. Sivakami, K. Navaneethakrishnan, *Physica E*, 40, (2008), 649.

[18] R. Jeice, K. Navaneethakrishnan, *Braz. J. Phys,*. 39, (2009), 526

[19] M. A. Paalanen, T. F. Rosenbaum, G. A. Thomas, R. N. Bhatt, *Phys. Rev. Lett.*, 48, (1982), 1284.

[20] C. Nirmala Louis, K. Iyakutti, P. Malarvizhi, *J. Phys. Cond. Matt.*, 16, (2004), 1577.

[21] M. A. Kastner, R. J. Birgeneau, G. Shirane, Y.Endoh, *Rev. Mod. Phys*. 70, (1998), 897

[22] D. Aoki, et.al., *Nature*, 413, (2001), 613.

[23] F. Levy, I. Sheikin, B. Grenier, A. D. Huxley, *Science*, 309, (2005), 1343.

[24] M. Rasolt, *Phys. Rev. Lett*., 58, (1987), 1482.

[25] E. Bustarret, C. Marcent, P. Achatz, J. Kacmarcik, F. Levy, A. Huxley, L. Ortega, E. Bourgeos, X. Blase, D. Debarre, J. Boulmer, *Nature*, 444, (2006), 465.

[26] S. Adachi, *GaAs and Related materials: Bulk semiconducting and super lattice properties, World Scientific*, Singapore, (1994).

[27] G. Balasubramanian, K. Navaneethakrishnan, *Solid State Commun*., 49, (1984), 855.