Temperature driven metal-insulator transition in thin films

R.K. Brojen Singh
School of Computational and Integrative Sciences,
Jawaharlal Nehru University, New Delhi-110067, India.

We present the results of electron delocalization in thin films of finite thickness at finite temperature induced by thickness of the film and temperature. The two dimensional results show temperature induced metal-insulator transition (MIT) obtaining both insulating and metallic solutions. The localization length in insulating regime and zero frequency conductivity in metallic regime are found to be as a function of temperature and disorder parameter. Similarly, in thin films of finite thickness, delocalization of electronic states takes place induced by temperature as well as film thickness. Further, we could able to get critical temperature $T_c$ for fixed thickness and critical thickness, $b_c$ for fixed temperature. In metallic regime, conductivity is found to be as a function of film thickness, temperature and disorder.

I. INTRODUCTION

The scaling theory of localization proposed that all single particle quantum states of an electronic band in two dimensional noninteracting electrons solid are localized for any disorder however week but in three dimensional system there is a critical disorder above which all the states are localized, and below which some states are delocalized [1]. The temperature dependence of Drude conductivity in two dimensional system which comes from phase breaking time was studied in 2D-Anderson model of noninteracting electron gas [1, 2] and 2D metal-insulator transition scenario in the charged trap model [3]. Numerically at finite temperature it was found logarithmic dependence of temperature of 2D conductivity and $T^{p/2}$ dependence to the conductivity correction in 3D, where $p$ is phase breaking exponent [4]. Signature of weak localization correction to resistivity in thin metallic films at low temperatures was seen [5]. Experimentally conductance fluctuation in quasi-one-dimensional inversion layers in Si-MOSFETs was also observed at low temperatures [6].

However, the electron transport mechanism in thin films in the presence of temperature is still unclear specially in weak disorder regime. The quantum interference effects in these systems play an important role in the study of metal-insulator transition. But a systematic study showing clear understanding of electron localization in these systems are still remain unfinished. We address these questions and examine transport behavior of noninteracting electrons in weakly disordered quasi-two dimensional layers or thin films induced by temperature.

Our work is planned as in the following. In section 2 we briefly review self consistent theory of localization in disordered thin films. The systematic derivation of localization length as a function of various parameters, such as film thickness, disorder parameter and temperature is done in this section. Section 3 provides the two dimensional solutions both in insulating and metallic regimes induced by temperature are presented. The thin film solution both in insulating and metallic regime are discussed in section 4. In section 5 we draw some conclusion based on our results obtained in the respective sections.

II. SELF-CONSISTENT THEORY IN THIN FILMS

The scaling ideas at the microscopic level, have been supported by the self-consistent theory of localization due to Vollhardt and Wolfe [7, 8] (VW). This theory is very convenient technique to study metal-insulator transition specially to deal with weak disorders. In this theory one calculates the density response function, which is related to particle-hole pair propagator. The density fluctuations propagate diffusively due to particle number conservation, with a diffusion constant $D(q, \omega)$, which gets strong size and dimension dependent quantum corrections from the vertex in the particle-particle channel. These corrections are account for the enhanced interference between the time reversed paths and also have the same diffusive character when time-reversal invariance is present. VW theory was extended by Yoshioka, Ono and Fukuyama [9] to situations when the time reversal invariance is absent. It was argued that when the time-reversal invariance is not present the particle-hole and particle-particle channels are not related and one needs two diffusion constants. In this case self-consistent relation of VW gets replaced by a set of two relations between the diffusion constants of the two channels. Whereas in the absence of time-reversal invariance the two diffusion constants becomes equal and VW theory explains the situation. The theory was then extended to thin film of finite thickness in the absence of any field [10] and in the presence of perpendicular magnetic field [11].

The equation for the frequency dependent diffusion constant, $D(\omega)$ incorporating quantum diffusion due to backscattering, can be derived self consistently [7, 8] to
arrive at,
\[
\frac{D(\omega)}{D_0} = 1 - \lambda dk_F^{2-d} \int_0^{1/l} dq \frac{q^{d-1}}{\omega/\tilde{D}(\omega) + q^2}
\]  
(1)

where, \( \lambda = (2\pi E_F \tau)^{-1} \) is disorder strength in terms of Fermi energy \( E_F \) and the collision time \( \tau \) and \( k_F \) is Fermi wave number. \( D_0 \) is bare diffusion constant. The integration is restricted to momenta smaller than the inverse of the mean free path, 1/l. This equation for \( D(\omega) \) gives rise to metallic solution when \( D(\omega) \to D_0 \) as \( \omega \to 0 \), is a positive number, whereas insulating solution if \(-D(\omega)/i\omega = \xi^2(\omega) \to \xi^2(0)\), a real positive number.

The backscattering corrections in weak scattering regime for restricted geometries can be calculated systematically using path integral method [12]. This method assumes that the classical paths in the presence of randomly placed impurities can be taken as random walks [5, 13, 14]. Then the quantum corrections are related to the probability of return of the walk to its origin, which assumes that the classical paths in the presence of random disorder.

The boundary condition to be applied is that the current vanishes. The solution of this result is given by,
\[
P(\vec{r}, z, t) = \frac{2}{Ab} \sum_{n=0}^{\infty} \sum_q \cos^2 \left( \frac{n\pi z}{b} \right)
\times \exp \left[ -D_0 \left( q^2 + \frac{n^2 \pi^2}{b^2} \right) t \right]
\]  
(2)

where \( A \) and \( b \) are area and thickness of the film respectively. \( \vec{q} \) is two dimensional wave vector. For self-consistency, \( D_0 \) is replaced by \( D(\omega) \) and incorporating this result one obtains the following equation,
\[
\frac{D(\omega)}{D_0} = 1 - 2\lambda \int_0^{1/l} dq \sum_{n=0}^{\infty} q^2 + \frac{1}{\omega/\tilde{D}(\omega)}
\]  
(3)

For finite size of the system, the lower limit of the integration in equation (3) is replaced by 1/L. If we define, \(-D(\omega)/i\omega = \xi^2(\omega)\) and using the following summation formula,
\[
\sum_{n=0}^{\infty} \frac{1}{c^2 + n^2 \pi^2} = \frac{1}{2} \left( \coth(c) + \frac{1}{c^2} \right)
\]  
(4)

and by performing wave vector integration, one can easily able to get integral equation for \( \xi(\omega) \). The result is given by,
\[
\frac{1}{\lambda} = \log \left[ \sqrt{\frac{1 + \xi(\omega)^2 - L^{-2} + \xi(\omega)^2}{L^{-2} + \xi(\omega)^2} \times \frac{\sinh b\sqrt{1 + \xi(\omega)^2}}{\sinh b\sqrt{L^{-2} + \xi(\omega)^2}}} \right]
\]  
(5)

where, \( \tilde{\xi}(\omega) = \xi(\omega)/l \), \( b = b/l \) and \( L = L/l \) which are dimensionless parameters. Here \( l \) is the elastic mean free path. This situation is physically relevant at finite temperatures. Due to inelastic scattering, the electron looses its phase coherence over a distance \( L_\phi \), the inelastic phase coherence length. Quantum interference effects are believed to be observable only at low temperature [15].

The coherence regime can be defined by the condition \( L_\phi \geq L \). So we replace \( L \) in this equation by \( L_\phi \). This \( L_\phi \) depends upon temperature which can be taken as \( L_\phi \approx L_0(T/T_0)^{-p} \), where \( p \) is a parameter depending on scattering mechanism, dimensionality, etc. \( L_0 \) and \( T_0 \) are constants having the dimensions of length and temperature respectively. To study cross-over from two to three dimensions we need to scale the disorder parameter, \( \lambda \)

such that \( \lambda^{-1} = hN_F(2)D_0 \) and \( 4/(3\pi lL^2) = hN_F(3)D_0 \)

where, \( N_F(2) \) and \( N_F(3) \) are density of states at Fermi level at two and three dimensions respectively [10, 11, 16].

In this situation, we study Metal-Insulator transition induced by temperature in two-dimensional as well as in thin films respectively.

III. MIT IN 2D ELECTRON SYSTEM

We obtain two dimensional insulating solution as \( \omega \to 0 \) and by taking the limit \( b \to 0 \) in equation (5) and replacing \( L \) by \( L_\phi \). In this limit one can approximate sinh function as exponential and \( \lambda \to \lambda_2 \). Then solving for \( \xi(0) = \tilde{\xi} \), we get
\[
\tilde{\xi}(\lambda_2, \tilde{L}_\phi) = \tilde{L}_\phi \sqrt{e^{1/\lambda_2} - \frac{1}{L_\phi^2 - e^{1/\lambda_2}}} \]

(6)

The numerator inside the square root of this equation is always positive number for any values of \( \lambda_2 \). The solution of \( \xi \) as a function of \( L_\phi \) for various values of \( \lambda_2 \) is shown in Fig.1. The plots show that as \( L_\phi \) decreases i.e. temperature, \( T \) increases \( \xi \) remains almost stationary for some range of \( L_\phi \) and then \( \xi \) increases monotonically (showing divergence of \( \xi \) at different \( L_\phi \) values for different \( \lambda ) \) as \( T \) increases. This provides the signature of metal insulator transition in 2D system induced by \( T \) for different values of \( \lambda_2 \). The critical values \( L_\phi^2 \) and \( \lambda_2^2 \) can be calculated at \( \tilde{\xi} \to \infty \) from equation (6), and is given by, \( \frac{1}{\lambda_2^2} = 2\log(L_\phi^2) \). The dotted line is the approximate critical line which separate extended and localized regimes in 2D electron system. Then from equation 6 we get real positive solution of \( \xi \) only when the denominator is greater than one. So we get insulating phase as long as
\[
\frac{L_\phi^2}{L^2} > e^{1/\lambda_2}
\]  
(7)

With increasing temperature \( T \), \( L_\phi \) decreases and at a certain critical temperature \( T_c(\lambda_2) \), this inequality is not
In metallic phase we solve for real and positive value of words, metallic solution in two-dimensional case is obtained as well as disorder in two-dimensional system. Thus obviously we get a metal to insulator transition induced by temperature, one can also obtain these two insulating and metallic phases induced by $\lambda$ which can be seen from equation (6). In this situation taking $\xi \rightarrow \infty$ we obtain critical disorder, $\lambda_c$ from equation (6) as, $\lambda_c = 1/(2\log(L_\phi))$. Then we calculate two dimensional zero frequency conductivity, $\sigma_2$ using Einstein’s relation, $\sigma_2(\omega) = e^2N_F(2)D(\omega)$ as $\omega \rightarrow 0$ and substituting the value of $\lambda_c$. The result is $\sigma_2(\lambda_2, \tilde{L}_\phi) = \sigma_{02} \left[ 1 - 2\lambda_2 \log(\tilde{L}_\phi) \right] = \sigma_{02} \left[ 1 - \frac{\lambda_2}{\lambda_c^2} \right]$ (10)

where, $\sigma_{02} = e^2N_F(2)D_0$ is zero frequency Drude’s conductivity in two dimensional system. Thus obviously we get a metal to insulator transition induced by temperature as well as disorder in two-dimensional system.

IV. MIT IN THIN FILM

The insulating solution of thin film can be obtained by scaling $\lambda$ given by, $4/(3\pi t \lambda_3^2) = hN_F(3)D_0$ and using the relation (5) as $\omega \rightarrow 0$ by

$$\frac{1}{\lambda_3} = \frac{3\pi}{4b} \log \left( \frac{1 + \xi^2}{\tilde{L}_\phi^{-2} + \xi^2} \times \frac{\sinh \left( \tilde{b} \sqrt{1 + \xi^2} \right)}{\sinh \left( \tilde{b} \sqrt{\tilde{L}_\phi^{-2} + \xi^2} \right)} \right)$$

$$= \frac{3\pi}{4b} \log \left( \frac{1 + \xi^2}{\tilde{L}_\phi^{-2} + \xi^2} \right), \quad \tilde{b}(1) \quad (11)$$

The behaviour of $\xi$ with respect to $\tilde{b}$ is shown in the Fig.(2). In this figure we found that, for a fixed value of $\lambda_3$, $\xi$ diverges at different values of $\tilde{b}$ for various values of $\tilde{L}_\phi$ ((10) as shown in Fig. 2. Whereas for large values of $\tilde{L}_\phi$ ((10), $\xi$ saturates with $\tilde{b}$ showing the signature of existence of insulating phase driven by $T$. Further, the equation (11) indicates that $\xi$ always does not have solution for any values of $\tilde{b}$, $\lambda_3$ and $\tilde{L}_\phi$. This shows the possibility of metal insulator transition in thin films induced by $T$.

The critical disorder, which can be defined as the disorder at which phase transition takes place, can be obtained from equation (11) by taking $\xi \rightarrow \infty$ and the critical disorder $\lambda_c$ is given by,

$$\frac{1}{\lambda_c^2(b, L_\phi)} = \frac{3\pi}{4b} \log \left( L_\phi \times \frac{\sinh(\tilde{b})}{\sinh(b/L_\phi)} \right)$$

$$= \frac{3\pi}{2b} \log \left( \tilde{L}_\phi \right), \quad \tilde{b}(1) \quad (12)$$

The critical disorder is found to be as a function of $\tilde{b}$ and $L_\phi$. So for a finite temperature, one can obtain thickness induced delocalization of states in thin films. The behaviour of $\lambda_c^2$ as a function of $\tilde{b}$ for different values of $L_\phi(T)$ is shown in Fig. 2 (lower left panel) separating localized and extended states in the phase diagram. From this figure one can able to see that as temperature increases, the critical disorder increases and saturates. Since we have a phase transition in this case, it is possible to obtain zero frequency diffusion constant in extended regime. We can calculate it from equation (3) first by taking the limit $\omega \rightarrow 0$ and then doing the summation and integration respectively. Then using equation (12) we get the following result,

$$D_3(\lambda_3, \tilde{b}, \tilde{L}_\phi) = D_0 \left[ 1 - \frac{3\pi}{4b} \lambda_3^2 \log \left( \tilde{L}_\phi \times \frac{\sinh(\tilde{b})}{\sinh(b/L_\phi)} \right) \right]$$

$$= D_0 \left[ 1 - \left( \frac{\lambda_3}{\lambda_c(b, \tilde{L}_\phi)} \right)^2 \right] \quad (13)$$

where, the finite thickness zero frequency diffusion constant, $D_3$ is found to be as a function of $\tilde{b}$, $\lambda_3$ and $\tilde{L}_\phi$. We can also get metallic solution only when $\lambda_3 < \lambda_c$. Fig. 2 (lower right panel) shows the solution of $D_3$ with respect to $\tilde{b}$ for different values of $\tilde{L}_\phi$ and fixed $\lambda_3$. The curves monotonically increases as $\tilde{b}$ increases and then starts.
where, $\sigma_{03} = e^2N_F(3)D_0$ is zero frequency Drude’s conductivity in three dimensional system. So clearly in the finite system size, there is a Metal-Insulator transition driven by temperature, thickness of the film and disorder.

V. CONCLUSION

We have extended self-consistent theory of localization due to Vollhardt and Wölfle to thin films incorporating temperature $T$ and studied the role of temperature in metal-insulator transition in 2D and thin layered films. We analyzed the phase transition when phase relaxation length $\tilde{L}_\phi$ is finite.

In two dimensions, we found localization length as a function of disorder as well as temperature. We obtain metal-insulator transition in 2D induced by disorder as well as temperature. Further, we could able to get critical disorder as a function of temperature in 2D system. We also calculated zero frequency diffusion constant and conductivity in metallic regime. In the case of thin films, we found a critical disorder which depends on thickness of the film and temperature. In this case we obtained a transition from insulator to metal driven by thickness and temperature. In insulating regime, the localization length increases rapidly as a function of thickness as temperature $T$ increases for a fixed value of disorder. But for small $T$, the localization length saturates to some value as we increase thickness. We calculated the zero frequency conductivity for the disorder smaller than the critical value (metallic regime). We claim that for non-zero temperature, there is possibility of insulator to metal transition induced by thickness of the film as well as temperature.

[1] E. Abrahams, P.W. Anderson, D.C. Licciardello and T.V. Ramakrishnan, Phys. Rev. Lett. 42, 673 (1979). D.J. Thouless, Phys. Rep. 13C, 93 (1974); F. J. Wegner, Z. Phys. B25, 327 (1976).
[2] A. Gold and V.T. Dolgopolov, Phys. Rev. B 33, 1076 (1986); S. Das Sarma, Phys. Rev. B 33, 5401 (1986).
[3] B.L. Altshuler and D.L. Maslov, Phys. Rev. Lett. 82, 145 (1999);
[4] A. MacKinnon and B. Kramer, Z. Phys. B-Cond. Matt. 53, 1 (1983).
[5] G. bergmann, Phys. Rep. 107, 1 (1984).
[6] A.B. Fowler, A. Hartstein and R.A. Webb, Phys. Rev. Lett. 48, 196 (1982).
[7] D. Vollhardt and P. Wölfle, Phys. Rev. Lett. 46, 842 (1980); Phys.Rev. B 22, 4666 (1980).
[8] D. Vollhardt and Wölfle, in Electronic Phase Transitions, edited by W. Hanke and Yu.V. Kopaev (Elsevier Science, Amsterdam, (1992)p. 1.
[9] D. Yoshioka, Y. Ono and H. Fukuyama, J. Phys. Soc. Japan, 50, 3419 (1981). Y. Ono, D. Yoshioka and H. Fukuyama, J. Phys. Soc. Japan, 50, 2143 (1981).
[10] R.K. Brojen Singh and D. Kumar, Phys. Rev. B66, 75123 (2002).
[11] R.K. Brojen Singh and D. Kumar, Phys. Rev. B69, 115420 (2004).
[12] S. Chakravarty and A. Schmid, Phys. Rep. 140, 193 (1986).
[13] D.E. Khmelnitskii and A.I. Larkin, Sov. Phys. Usp. 25, 185 (1982).
[14] D.E. Khmelnitskii Physica B and C 126, 235 (1984).
[15] R.K. Brojen Singh, Ph.D. Thesis, ‘Localization in thin films’ (2004).