

LOCAL MOMENTS NEAR THE METAL-INSULATOR TRANSITION

Subir Sachdev

Center for Theoretical Physics, P.O. Box 6666
Yale University, New Haven, CT 06511

This paper reviews recent progress in understanding the metal-insulator transition in a system of spin-1/2 interacting electrons in the presence of a non-magnetic random potential. Using results of recent experiments in doped semiconductors, it is argued that the metallic state near the transition can be described by a phenomenological two-fluid model of local moments and itinerant quasiparticles. A mean-field calculation on a disordered Hubbard model which justifies this two fluid model is described. Recent advances in the non-linear sigma model description of the transition are also discussed.

The subject matter of the lecture presented by the author overlapped considerably with previous talks by the author [1] and R.N. Bhatt [2]. We will not repeat here the material covered in these talks which has been published elsewhere [1, 2]; we will concentrate, instead on reviewing some recent theoretical work. Upon combining the present paper with these previous reviews [1, 2], the reader will have a fairly complete record of the talk presented by the author.

The experimental motivation for this investigation comes from experiments in doped semiconductors like $Si : P$ and $Si : B$. The dopant electrons (or holes) in these materials can be described quite accurately by the following Hamiltonian

$$H = - \sum_{i,j} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_i (\epsilon_i - \mu) c_{i\sigma}^\dagger c_{i\sigma} \quad (1)$$

Here the sites i, j represent the donor orbitals and are placed at positions $\mathbf{R}_i, \mathbf{R}_j$ distributed randomly in a system of volume V . The hopping matrix elements t_{ij} are exponentially decaying functions of $|\mathbf{R}_i - \mathbf{R}_j|$

$$t_{ij} = t_0 \exp(-|\mathbf{R}_i - \mathbf{R}_j|/a_B) \quad (2)$$

where the Bohr-radius a_B is approximately 20 \AA . The Hubbard repulsion U acts between two electrons on the same site. The on-site energy ϵ_i is also a random variable. The chemical potential μ is adjusted to control the filling factor of the system. Uncompensated doped semiconductors are at or very close to half-filling. The quantity which is varied experimentally is the concentration n of the electrons. At a critical concentration $n = n_c$ the system is observed to undergo a transition from an insulator ($n < n_c$) to a metal ($n > n_c$).

REVIEW OF EXPERIMENTS

The experimentally observed properties of this transition have been reviewed elsewhere ([1, 2] and references therein). For completeness, we recall here a few important features. The most striking feature of the experimental data [3] is the difference in the properties of the conductivity and spin-susceptibility in the metallic system. The conductivity, which vanishes at $T = 0$ and $n = n_c$ is only weakly temperature dependent, changing by about 15% between $10K$ and $0.1K$. In contrast the spin-susceptibility increases by a factor of 10 between

$T = 10K$ and $T = 0.1K$ for $n = 1.09n_c$. The temperature dependence of the susceptibility is in fact rather similar to that of the insulator, which has an even greater enhancement. This difference leads one to suspect rather different physical effects are responsible for the apparent continuous vanishing of the conductivity at $n = n_c$, and for the enhancement of the spin-susceptibility. In fact, it was found that all of the thermodynamic data on the metal near $n = n_c$ could be described by a phenomenological two-fluid model. The two fluids are (i) an itinerant fermi liquid of quasiparticles and (ii) localized electrons spins interacting with each other via an antiferromagnetic exchange. The spin-susceptibility χ and specific heat C are predicted to have the following temperature dependences

$$\begin{aligned}\frac{C}{T} &= N(E_F) + \left(\frac{T}{T_0}\right)^{-\alpha} \\ \chi &= N(E_F) + \beta(\alpha) \left(\frac{T}{T_0}\right)^{-\alpha}\end{aligned}\quad (3)$$

The two terms represent the contributions of the itinerant fluid and the local moments respectively. The temperature dependence of the local moment susceptibility and specific heat are deduced from the Bhatt-Lee model [4] of the insulating state. The density of states $N(E_F)$ and β are known constants and the only unknown is T_0 , which is a measure of the fraction of electrons in localized moments. With this one adjustable parameter, the equations above provide a surprisingly good fit to the experiments [3]. An important *prediction* of these phenomenological equations is that the Wilson ratio $T\chi/C$ remains *finite* at $T = 0$: the experimental data agree well with this prediction. Nuclear magnetic resonance experiments of Alloul and Dellouve [5] have also provided direct experimental evidence for the presence of localized moments at densities $n < 2n_c$.

A major question has been left unresolved in the phenomenological discussion of the experimental results: how can a metallic system in which all states near the Fermi-level are extended, support the existence of localized moments? Density fluctuations leading to islands of insulating sites cannot be the answer; simulations show that at densities near $n = n_c$, the fluctuations strong enough to create localized states do not occur often enough to account for the experimental results. It is this question which the bulk of the rest of the paper will attempt to address. The discussion is a review of results contained in Ref [6]

SINGLE-IMPURITY

To set the stage let us consider a simplified version of the Hamiltonian $H = H_i$ with a *single* impurity at a site \mathbf{R}_0 . All the sites are placed on a regular lattice and the hopping matrix elements are given by

$$t_{ij} = \begin{cases} t & i, j \text{ nearest neighbors, } \mathbf{R}_i \neq \mathbf{R}_j \neq \mathbf{R}_0 \\ w & \mathbf{R}_i \neq \mathbf{R}_j \text{ and } \mathbf{R}_i = \mathbf{R}_0 \text{ or } \mathbf{R}_j = \mathbf{R}_0 \\ 0 & \text{otherwise} \end{cases} \quad (4)$$

The on-site energies ϵ_i are all chosen equal and the chemical potential is chosen so that the system is close to half-filling. We assume that U is always small enough, or the temperature T large enough so that the system is in a metallic state and all spin-density wave instabilities can be safely ignored. The model under consideration is closely related to the Anderson-Wolff [7] models of local moment formation in transition metals. By analogy with these models and subsequent work [8] we can understand the properties of H_i .

A mean-field diagonalization of H gives rise to a *resonance* near the Fermi-level. The width, Γ , of this resonance is of order

$$\Gamma \sim \frac{w^2}{t} \quad (5)$$

for small w . The consequences of the existence of this resonance can be elucidated by considering the temperature dependence of χ_0 , the local spin susceptibility of the impurity site. At very high temperatures $T \gg U$ we have

$$\frac{\chi_0}{(g\mu_B)^2} = \frac{1}{8kT} \quad (6)$$

where g is gyromagnetic ratio, μ_B is the Bohr magneton. At lower temperatures, two different types of behavior can occur depending upon the value of U/Γ :

(a) *Local moment regime* For $U/\Gamma > \alpha$ (where α is a numerical constant of order unity) we find

$$\frac{\chi_0}{(g\mu_B)^2} = \frac{1}{4kT} \quad (7)$$

This susceptibility is a factor of 2 larger than the high-temperature result and is simply the Curie susceptibility of a single free spin. At very low temperature $T \sim T_K$, the Kondo effect takes over and the susceptibility is quenched.

(b) *Fermi liquid regime* For $U/\Gamma < \alpha$ the local moment does not form and the susceptibility becomes temperature independent

$$\frac{\chi_0}{(g\mu_B)^2} \sim \frac{1}{\Gamma} \quad (8)$$

The crucial point for our purposes is that measurements on all of the doped semiconductors are performed at temperatures well above T_K . Thus the enhancement of the susceptibility in the local moment regime is very relevant. We emphasize that no localized state was necessary for the development of the local moment. Instead all that was required was a sufficiently narrow resonance at the Fermi level. Moreover the Anderson-Clogston compensation theorem [7] implies that the *spin density* associated with the local moment is strongly localized at the impurity site.

FULLY DISORDERED SYSTEM

We will now use the insight gained from the single-impurity system to investigate the properties of the fully random H . A suitable mean-field formalism is provided by the effective field method of Feynman and de Gennes [9]. This involves finding the best single-particle effective Hamiltonian

$$H_{eff} = - \sum_{ij} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i\sigma} (\tilde{\epsilon}_i - \mu) c_{i\sigma}^\dagger c_{i\sigma} + \sum_i \mathbf{h}_i \cdot \mathbf{S}_i \quad (9)$$

where \mathbf{S}_i is the spin of the electron at site i . The on-site energy $\tilde{\epsilon}_i$ and magnetic field \mathbf{h}_i are variational parameters. A non-zero value of \mathbf{h}_i implies the formation of a local moment at the site i . We shall be particularly interested in the spatial distribution of \mathbf{h}_i . The variational parameters must be determined by minimizing the following quantity

$$-kT \ln \text{Tr} \exp \left(- \frac{H_{eff}}{kT} \right) + \langle H - H_{eff} \rangle_{eff} \quad (10)$$

where the second expectation value is taken in the canonical ensemble defined by H_{eff} . This problem is too complicated to be solved numerically in the present form. As we are interested in the initial instability to local moment formation, we expand the effective free energy in powers of \mathbf{h}_i . For U small enough, \mathbf{h}_i is zero, and the saddle point condition reduces to

$$\tilde{\epsilon}_i = \epsilon_i + U \sum_{\alpha} |\Psi_{\alpha}(i)|^2 f(\lambda_{\alpha}) \quad (11)$$

which is simply the familiar Hartree-Fock equation for the Hubbard model. Here $\Psi_\alpha(i)$ is the exact eigenstate of H_{eff} with $\mathbf{h}_i = 0$, and λ_α is the eigenvalue.

$$H_{eff}(\mathbf{h}_i = 0)\Psi_\alpha = \lambda_\alpha\Psi_\alpha \quad (12)$$

The same set of exact eigenstates were introduced by Abrahams *et. al.* [10] in their analysis of interaction effects in disordered systems. Expanding the effective free energy in powers of \mathbf{h}_i , we obtain

$$F_{eff}(\mathbf{h}_i) = F_{eff}(\mathbf{h}_i = 0) + \sum_{ijk} \chi_{ij}(\delta_{jk} - U\chi_{jk})(\mathbf{h}_i \cdot \mathbf{h}_k) + \dots \quad (13)$$

where

$$\chi_{ij} = - \sum_{\alpha,\beta} \Psi_\alpha(i)\Psi_\beta^*(i)\Psi_\beta(j)\Psi_\alpha^*(j) \frac{f(\lambda_\alpha) - f(\lambda_\beta)}{\lambda_\alpha - \lambda_\beta} \quad (14)$$

where χ_{ij} is the susceptibility matrix of free electrons described by $H_{eff}(\mathbf{h}_i = 0)$. The local magnetic field \mathbf{h}_i will acquire a non-zero expectation value when the quadratic form in Eqn (13) first has a negative eigenvalue. It is clear from the expression for F_{eff} that the eigenvectors of the quadratic form are the eigenvectors of the spatial matrix χ_{ij} :

$$\sum_j \chi_{ij}m_a(j) = \kappa_a m_a(i) \quad (15)$$

Expanding the \mathbf{h}_i in term of the complete set $m_a(i)$ we see from Eqn (13) that the system first becomes unstable to local moment formation when the largest susceptibility eigenvalue κ_a exceeds $1/U$. Moreover the spatial distribution of the magnetization will be proportional to the corresponding eigenvalue $m_a(i)$.

This is as far as general considerations can carry us. We now have to use numerical simulations to study the behavior of the system. The results of such a numerical study are presented in Ref. [6] and the reader is referred to that paper for greater details. The mean field equation (11) for a random Hamiltonian H was solved by iteration. The corresponding susceptibility matrix χ_{ij} was diagonalized exactly and the structure of its eigenvectors studied. The eigenvectors of χ_{ij} and $H_{eff}(\mathbf{h}_i = 0)$ were characterized by the inverse participation ratio

$$\begin{aligned} P_H &= \langle |\Psi_\alpha(i)|^4 \rangle \\ P_\chi &= \langle |m_a(i)|^4 \rangle \end{aligned} \quad (16)$$

Here the average is taken over several samples over states near the Fermi level for P_H and over the largest 5 eigenvalues of χ for P_χ . System sizes as large as 400 sites were studied. The results unambiguously showed that the eigenvalues of $\chi_{ij} - m_a(i)$ were much more strongly localized than the one-electron eigenstates $\Psi_\alpha(i)$. In particular the $m_a(i)$ were essentially localized on a few sites, while the extent of the $\Psi_\alpha(i)$ was limited by the system size. This localization of the $m_a(i)$ may be viewed as a generalization of the Anderson-Clogston compensation theorem [7].

The physical implication of the results above is clear. Weakly disordered systems contain very local instabilities towards the formation of local moments. These instabilities are associated with the eigenvalues of χ_{ij} and do not require a localized Hartree-Fock eigenstate. The local moments, once formed will lead to a dramatic enhancement of the spin-susceptibility and specific heat of the disordered metal. Moreover since the same spins are responsible for both enhancements, the Wilson ratio $T\chi/C$ is expected to be finite at $T = 0$.

FIELD THEORETIC RESULTS

While the results discussed above do clarify the physical picture they do not make any specific predictions on the critical properties of the metal-insulator transition. The only available method is the field-theoretic non-linear sigma model of interacting electrons in weak disorder [11]. As the method is intrinsically a weak disorder expansion in $d = 2 + \epsilon$ dimensions it will be difficult for it to properly capture the local moment instabilities discussed above: these instabilities can occur at weak disorder and require the use of exact eigenstates.

The one-loop renormalization group results of Finkelstein and the physical arguments of Castellani *et. al.* can be encapsulated in the following scaling form for the conductivity σ

$$\sigma(\omega, \xi) = \frac{1}{\xi^{d-2-\theta}} F(\omega \xi^{d+x}) \quad (17)$$

where $\xi \sim (n - n_c)^{-\nu}$ is the correlation length and F is a universal function. At finite temperature we expect that ω can be replaced by T . An attempt to fit the temperature dependent conductivity in $Si : P$ with this scaling form was unsuccessful [12]. The spin diffusivity D_s , χ and C/T have the leading divergences

$$\chi \sim \xi^{\theta+x} \quad D_s \sim \xi^{-\theta-x} \quad \frac{C}{T} \sim \xi^x \quad (18)$$

Note that the Wilson ratio is predicted to diverge as ξ^θ , which is also not in accord with experiments. The one-loop values of the exponents are $\nu = 1/\epsilon$, $\theta = \epsilon$ and $x = 3\epsilon$.

Recently Belitz and Kirkpatrick [13] have analyzed the higher order corrections to the Finkelstein field theory. They found two important results

(i) the metal-insulator fixed point of Finkelstein and Castellani *et. al.* is in fact *suppressed* and does not describe the ultimate critical behavior. The system however does not notice the suppression until it is exponentially close (for small ϵ) to the ‘fixed’ point. Thus *e.g.* the temperature would have to be of order

$$T \sim \exp\left(-\frac{c}{\epsilon^{3/2}}\right) \quad (19)$$

The ultimate fixed point theory remains inaccessible in the ϵ expansion.

(ii) Because the suppression is exponentially small, the scaling equations (17) and (18) can meaningfully define *effective* exponents. Belitz and Kirkpatrick [13] found that

$$\theta = d - 2 \quad (20)$$

to all orders in ϵ . Comparing with Eqn (17) this indicates that the conductivity σ is *not* driven towards zero. Thus in the scaling region, the spin diffusivity is suppressed, the spin susceptibility enhanced, but the conductivity remains finite. This picture is remarkably similar to that developed in the mean-field calculations discussed above. However it is not clear that the critical region will be large when $\epsilon = 1$, which is necessary for the exponents to have any meaning.

CONCLUSIONS

It is heartening that the two rather different approaches discussed in this review appear to obtain similar results. Neither of the approaches has however so far come up with a theory of the metal insulator transition. It is clear, however, that an important part of the physics of the dirty metallic state is the formation of localized magnetic moments. The length scale associated with the formation of these moments is much smaller than the correlation length ξ . It is clear that the ultimate theory of the transition will have to incorporate this length scale at an initial stage.

I would like to acknowledge contributions of my collaborators M. Milovanovic and R.N. Bhatt.

References

- [1] S. Sachdev, R.N. Bhatt, and M.A. Paalanen, J. Appl. Phys. **63**, 4285 (1988)
- [2] R.N. Bhatt, M.A. Paalanen, and S. Sachdev, Journal de Physique, Colloque C8, 1179 (1988).
- [3] M.A. Paalanen, J. Graebner, R.N. Bhatt and S. Sachdev, Phys. Rev. Lett. **61**, 597 (1988).
- [4] R.N. Bhatt and P.A. Lee, Phys. Rev. Lett. **48**, 344 (1988).
- [5] H. Alloul and P. Dellouve, Phys. Rev. Lett. **59**, 578 (1987).
- [6] M. Milovanovic, S. Sachdev and R.N. Bhatt, Phys. Rev. Lett. **63**, 82 (1989).
- [7] P.W. Anderson, Phys. Rev. **124**, 41 (1961); P.A. Wolff, Phys. Rev. **124**, 1030 (1961).
- [8] F.D.M. Haldane Phys. Rev. Lett. **40**, 489 (1978); H.R. Krishnamurthy, J.W. Wilkins and K.G. Wilson, Phys. Rev. **B 21**, 1003 (1980); **B 21**, 1044 (1980).
- [9] R.P. Feynman, *Statistical Physics*, (Benjamin, New York, 1972); P. G. de Gennes, *Superconductivity of Metals and Alloys*, (Benjamin, New York, 1972).
- [10] E. Abrahams, P.W. Anderson, P.A. Lee, and T.V. Ramakrishnan, Phys. Rev. **B 24**, 6783 (1981).
- [11] A.M. Finkelstein Zh. Eksp. Teor. Fiz. **84**, 166 (1983) [Sov. Phys. JETP **57**, 97 (1983)]; Z. Phys. B **56**, 189 (1984); C. Castellani, B.G. Kotliar, P.A. Lee, Phys. Rev. Lett. **56**, 1179 (1986).
- [12] S. Sachdev, unpublished.
- [13] D. Belitz and T.R. Kirkpatrick, Nucl. Phys. **B 316**, 509 (1989); T.R. Kirkpatrick and D. Belitz, Phys. Rev. **B 40**, 5227 (1989); D. Belitz and T.R. Kirkpatrick, Phys. Rev. Lett. **63**, 1296 (1989); T.R. Kirkpatrick and D. Belitz, U. of Maryland preprint.