

On Metal–Insulator Transitions

NEVILL MOTT

Cavendish Laboratory, Cambridge CB3 0HE, United Kingdom

Received April 2, 1990

DEDICATED TO J. M. HONIG ON THE OCCASION OF HIS 65TH BIRTHDAY

It is a pleasure to make a small contribution to a *Festschrift* for Professor J. M. Honig. I am grateful for a substantial article which he wrote for one of mine¹; in fact, his article and others in this volume were a great help to me in preparing a second edition of my book (1), *Metal-Insulator Transitions*, which will appear in the summer of this year (1990).

I take this opportunity to comment on the nature of the so-called “Mott transition” and contrast it with the “Anderson transition.” In 1947, I published a paper (2) suggesting that, if the number of electrons per unit volume in a solid could be varied by volume change or by alloying, a *discontinuous* transition from nonmetallic to metallic behavior would occur; as applied to doped semiconductors it should be observed when for a concentration of electrons n given by $n^{1/3}a_H = 0.25$, where a_H is the Bohr radius for the donor. Both conclusions were correct, but the argument used in obtaining them was wrong. We now use a description due to Brinkman and Rice (3) in which the transition results from the overlap of the two

Hubbard bands. Moreover, the transition in doped semiconductors now seems to be of Anderson type, resulting from disorder, that is from the random positions of the donors (see Mott (4)). The Mott transition, as I see it, is a transition from an antiferromagnetic insulator to a metal, which *may* be antiferromagnetic. It occurs, as a result of intraatomic interaction, when

$$\frac{1}{2}(B_1 + B_2) \approx U,$$

where B_1, B_2 are the widths of the two Hubbard bands and

$$U = \langle e^2/\kappa r_{12} \rangle,$$

called the Hubbard U . The averaging is intraatomic, or within a donor, and κ a background dielectric constant. It is thus similar to a normal band-crossing transition, and in all cases such transitions are first order.

Professor Honig (footnote 1, p. 265) remarks that Mott transitions depend only on electron density effects, and so that the large hysteresis effects observed in vanadium oxides rule out these as transitions of this kind. I do not entirely agree, if I define the transition as I have here. Any first-order transition, in which the number of free electrons changes from zero to a finite number, is almost certain to change the volume and in

¹ Transitions in selected transition metal oxides, in *The Metallic and Non-metallic States of Matter*, (P. P. Edwards and C. R. N. Rao, Eds.), Taylor & Francis, London (1985).

noncubic structures also the ratio of the lattice parameters, or even the structure. So I would call a Mott transition any transition from an antiferromagnetic insulator to a metal, as one essentially involving the Hubbard U and of the same general type.

Now, since this kind of transition is essentially of first order, the actual value of the lattice parameter at which it occurs under pressure cannot be observed; there is a discontinuous change in volume. To observe the transition itself, quenched alloys must be used. In principle, the transition must occur in a solubility gap for the annealed alloy. I am therefore very interested in Fig. 2 of Professor Honig's article quoted (taken from Shrivashankar and Honig (5)). In this figure the logarithm of the resistivity of $(V_{1-x}Ti_x)_2O_3$ is plotted against $1/T$ for values of x between 0 and 0.05. From these curves it is clear that a first-order transition occurs from the semiconducting to the metallic state.

The metallic alloys of V_2O_3 with Ti_2O_3 have a resistivity of about $10^{-4} \Omega \text{ cm}$, little dependent on temperature. This implies that each titanium atom has an apparent scattering cross section of about seven times its cross-sectional area. This large value is, I believe, caused by the properties of the highly correlated gas, predicted for a metal near the transition by Brinkman and Rice (3). In this model most sites remain singly occupied, with the moment resonating between its several orientations; current is caused by a few doubly occupied or unoccupied sites, so the resistivity for a given number of scatterers is enhanced.

We turn now to the Anderson transition. This occurs only in the presence of some kind of disorder; the activation energy for conduction goes continuously to zero as the transition is approached from the insulating side, and the zero temperature conductivity goes continuously to zero as it is approached from the metallic side. Typical behavior is shown by the oxide $La_{1-x}Sr_x$

VO_3 , where with increasing x the activation energy for conduction decreases continuously to zero.

The present author (6) in 1972 put forward the concept of a minimum metallic conductivity $\sigma_{\min} = 0.03 e^2/\hbar a$, where a is the mean distance between electrons. This is now known to be false; both the scaling theory of Abrahams *et al.* (7) and the concept of quantum interference (Bergman (8)) show that the conductivity σ should, at a low temperature, tend to zero, normally linearly with changing composition. The present author (4) and Mott and Kaveh (9) have investigated the problem of why, as in $La_{1-x}Sr_xVO_3$ and in liquid systems, a minimum metallic conductivity is so often observed.

Metal-insulator transitions in oxides have recently become very fashionable as a subject of research, on account of the discovery of the high T_c superconductors. The first of these $La_{2+x}Sr_xCuO_4$, is, like $La_{1-x}Sr_xVO_3$, an antiferromagnetic insulator when $x = 0$. Both are doped, the Sr producing holes in the oxygen $2p$ band or among the magnetic ionized atoms (e.g., Cu^{2+}). Both materials, with increasing x , undergo a transition to the metallic state together with a disappearance of the magnetic order. In the case of the superconductor, as soon as the metallic state appears, so does superconductivity, T_c , increasing with x and then decreasing.

For the phenomenon, there are still as many theories as there are theorists. The present author believes that the carriers (oxygen $2p$ holes) move in an impurity band, forming spin polarons with the $Cu(3d)^9$ spins, and that these combine to form pairs (bosons). A degenerate gas of bosons is a superconductor. The quasi-two-dimensional structure of these oxides facilitates pair formation. The model suggests that current above T_c is carried by a nondegenerate gas of these bosons (spin bipolarons). Above T_c the resistivity-temperature curve differs strongly from that in the vanadate; in the latter the resistivity hardly depends on

temperature T up to 300 K while in the former it is usually proportional to T . The author has attempted to explain this in terms of the properties of spin polarons, arguing that the diffusion coefficient D of a spin polaron depends little on temperature and the conductivity σ is given by Einstein's relation as

$$\sigma = n e^2 D / k_B T,$$

where n is the constant number of carriers (see Mott (10), Micnas *et al.* (11), and de Jongh (12)).

I believe that the same kind of chemical insight that Professor Honig has contributed to metal-insulator transitions will be needed to unravel the problem of these oxide superconductors.

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