

SESSION V—THE HUBBARD HAMILTONIAN

Self-Consistent Pair Correlations in Narrow Energy Bands

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The Mott-insulator and paramagnetic metal ranges of the half-filled energy band, governed by the Hubbard Hamiltonian, are discussed in terms of an electron-hole picture.

About 20 years ago a simple model was introduced by Mott for the insulator-metal transition. He considered a lattice of hydrogen atoms arranged in a regular lattice. With only one electron per atom, but two 1s states available for them, such a system constitutes a half-filled band, according to band theory. Thus it should be a metal. It is physically clear, however, that for large values of the lattice constant we have a system of independent hydrogen atoms and this should be an insulator. Band theory alone cannot describe the insulating state. Some generalization is necessary.

We may imagine this system as a lattice of electrons and holes. The holes are all the atomic states not occupied by electrons. If an electron wants to leave its atom, or rather its hole, it feels an attractive potential. For a large lattice constant this is a Coulomb attraction which can keep the electron and the hole bound. Also the overlap of wavefunctions from one atom to the next is small, so the electron and the hole are not much inclined to move. As the lattice constant diminishes, the Coulomb attraction becomes screened and also the atomic wavefunctions overlap more. So the electron-hole attraction is diminished while their motion is enhanced. Eventually a bound state cannot be maintained and the material becomes a metal. By considering bound states we go beyond band theory.

This conceptually simple model is mathematically very complicated. Its investigation with the complete Coulomb interaction is hopelessly difficult. Therefore it is preferable to investigate it with the simplest Hamiltonian that exhibits the most important features of the model. This Hamiltonian was introduced by Hubbard for hydrogenlike atoms.¹ Hubbard himself and also many other people have investigated the consequences of this Hamiltonian. Some approaches are given later in the conference. We discuss here only one particular

approach to this problem. The Hamiltonian is given by

$$H = \sum_{ij\sigma} T_{ij} c_{i\sigma}^+ c_{j\sigma} + J \sum_i n_{i+} n_{i-}. \quad (1)$$

The subscripts indicate lattice sites and spins. Electrons can hop between nearest neighbors. This is described by the first term. The interaction term shows that two electrons repel each other on the same atom. If we describe the negative spin states by holes, but continue to describe the positive spin states by electrons, the Hamiltonian appears in the form

$$H = \sum_{ij} (h_{ij+} \psi_{i+}^+ \psi_{j+} + h_{ij-} \psi_{i-}^+ \psi_{j-}) - J \sum_i n_{i+} h_{i+}, \quad (2)$$

where

$$h_{ij-} = -h_{ij+}. \quad (3)$$

The hopping energy of the holes is negative and the interaction between electron and hole is attractive.

The physical content of this transformation can be seen on Figs. 1 and 2. In Fig. 1 each atom has one electron and one hole. This we use as a reference state. Figure 2 shows that an electron moved from its own atom to another atom. It experiences a repulsion there. In fact it would experience a repulsion on any atom but on its own. This is equivalent to saying that it would be attracted to its own atom. If this attraction is strong enough, a bound state forms. Mathematically speaking, we are looking for an isolated pole of the t matrix or of the two-particle Green's function or, in more conventional terms, for a bound-state solution of the two-particle Schrödinger equation.

The bound state can be considered an exciton. It can be described in terms of the difference coordinate and the center-of-mass momentum. The energy and the binding energy of the exciton depend on the choice of this center-of-mass momentum. This is very important. We choose it such that the energy should be minimum. Then we find, for a simple cubic lattice in the tight-binding approximation, that the binding energy vanishes when the bandwidth/potential-energy

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¹ References to the literature can be found in G. Kemeny and L. G. Caron, *Phys. Rev.* **159**, 687 (1967).

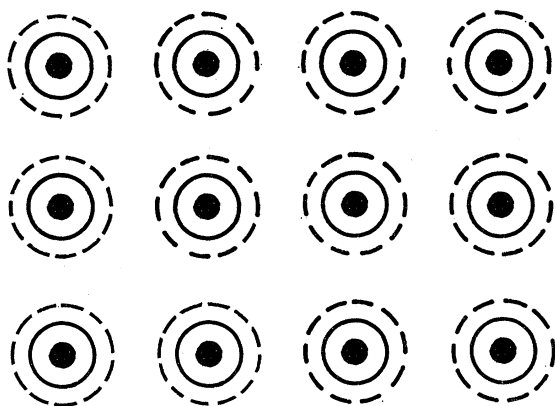


FIG. 1. The reference state with one electron and one hole on each atom.

ratio reaches the value 1.5. The wave function of the bound state decays essentially exponentially as a function of the difference coordinate. The electron and the hole can be very far from each other and still be bound, because the exponential decay can be very slow if the binding energy is small.

This can hardly be an adequate approximation. There are many pairs between an electron and a hole if they are widely separated. The motion of these inbetween pairs would disrupt a bound state.

In order to find a better approximation let us examine Fig. 3. Each atom, except the two at the center, has one electron and one hole. At the center one atom has two electrons, the other has two holes. Let us concentrate on these two atoms. If we consider one of the electrons and one of the holes to form an exciton, then we should consider the other electron and other hole also to form an exciton. The spatial wave function of these two excitons should be the same and their spins should be opposite. We have here a requirement of self-consistency. Each exciton is described by a pair wave function, or pair correlation and two such pair correlations must be determined self-consistently.

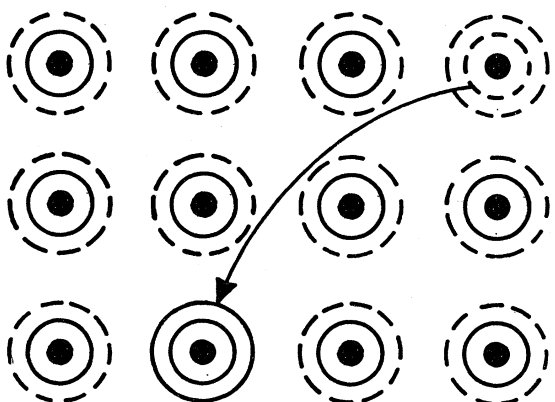


FIG. 2. One electron transferred to another atom.

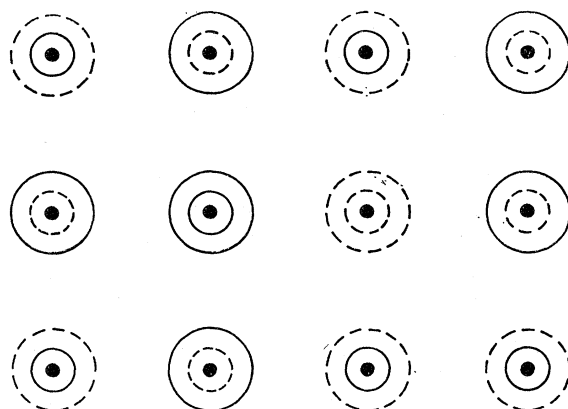


FIG. 3. The two atoms at the center have two electrons and two holes, respectively. The other atoms have one of each.

Figure 3 shows a configuration in which the selected electron-hole pair feels the entire attractive potential. This is due to the fact that the other electron-hole pair occupies exactly the same two atoms. But there are other configurations possible. On Fig. 4 we show such configurations. In configuration 1 the selected electron and hole are on the same atom and the other atom has two holes. In configuration 2 the electron and the hole are on different atoms. We see that the electron gains no potential energy by returning to the left atom. These two configurations would not occur if the medium did not move. The medium consists of excitons similar to the selected one. Thus the total potential energy of a pair should contain a term which reflects the fact that the motion of the medium reduces the attractive potential. The medium has to be represented by a wave function similar to the wave function of the selected pair, since the medium also consists of excitons.

Let us now see what mathematical tools are required to handle this problem. We require an equation of motion for an electron and a hole interacting with each other and the medium. The two-particle Green's function equation is

$$\begin{aligned}
 & [i(\partial/\partial t_1) - h_{1+}] [i(\partial/\partial t_2) - h_{2-}] L_2(1_+ 2_-; 1_+' 2_-') \\
 & \quad + iJ\delta(1-2) G_2(1_+ 2_-; 1_+' 2_-') \\
 & = -J^2 \{ G_4(1_+ 2_- 1_- 2_+; 1_+' 2_-' 1_- + 2_+ +) \\
 & \quad - G_2(1_+ 1_-; 1_+' 1_- +) G_2(2_- 2_+; 2_-' 2_+ +) \}, \quad (4)
 \end{aligned}$$

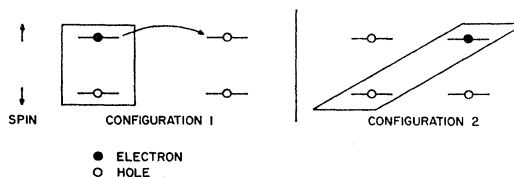


FIG. 4. Electron-hole configurations illustrating the effect of the medium.

where

$$L_2(1_+2_-; 1_+'2_-') = G_2(1_+2_-; 1_+'2_-') \\ - G_1(1_+; 1_+')G_1(2_-'2_-'). \quad (5)$$

Here 1_+ and 2_- are the space, time, and spin coordinates of the electron and hole, respectively. Equation (4) contains the possibility of free-electron and hole motion due to the presence of the so-called inhomogeneous terms. We do not need these in discussing the range of bound pairs. So the G_1G_1 product can be omitted and so can the G_2G_2 product. The terms left over have the following meaning: $\partial/\partial t_1$ and $\partial/\partial t_2$ are the time derivatives; h_1 and h_2 are the hopping energies; $J\delta$ is the direct interaction of the electron and the hole forming the pair, if they are on the same atom; the right hand side differs from zero only if 1 and 2 are not the same atom. In that case we must consider four states, hence the four-particle Green's function.

If we utilize the requirement of self-consistency, the four-particle Green's function can be expressed in terms of two-particle Green's functions. After some manipulations we arrive at the self-consistent equation for the pair wave function:

$$[\omega - h_1 - h_2 - J\delta_{\mathbf{R}_1\mathbf{R}_2}]\psi(\mathbf{R}_1\mathbf{R}_2) \\ = \frac{1}{4}J^2[|\psi(\mathbf{R}_1\mathbf{R}_1) |^2 - |\psi(\mathbf{R}_1\mathbf{R}_2) |^2] \\ \times [(\frac{1}{2}\omega - h_1)^{-1} + (\frac{1}{2}\omega - h_2)^{-1}]\psi(\mathbf{R}_1\mathbf{R}_2). \quad (6)$$

Here we substituted the eigenvalue in place of the time derivative. If we omit the right-hand side, we get back the approximation we discussed at the beginning. The influence of the medium is ignored. This is the nonself-consistent approximation. Only the direct electron-hole interaction is considered. The right-hand side vanishes, as required, if the electron and the hole are on the same atom because then neither is in contact with the medium. If they are not on the same atom, it represents the influence of the medium by the self-consistent potential and the motion of the medium.

The solution of Eq. (6) shows two features. First that the transition from insulator to metal occurs at a smaller value of the bandwidth/potential-energy ratio, namely at 1.26 rather than at 1.5. We anticipated this when we said that the motion of the medium reduces the attractive potential.

The second feature is that even at the weakest binding, more than 94% of the pair-wave-function amplitude corresponds to the electron and the hole being on the same atom, and the amplitude for being on different atoms is less than 6%. This result is much more satisfactory than what we obtained before, where the amplitude could decrease very slowly for weak binding. Thus the excitons, if they can exist at all, are very compact. This calculation then shows that the binding energy goes to zero continuously, as Professor Mott has stated, but the wave function changes discontinuously at the transition.

We have shown how the self-consistent pair-correlation approach can be applied in the Mott-insulator range. Let us discuss now the application of this method in the metallic range. Our problem can be usefully compared with the Brueckner theory of nuclear matter.²

In nuclear matter, as in a narrow energy band, fermions interact with strong short-range repulsive forces. This excludes the application of the Born series. In the nucleus the noninteracting Fermi sea is always used as the reference state. This involves the assumption that there is no clustering in the nucleus. We just saw that clustering does occur in the narrow energy band in the form of excitons. But the metallic range is presumably characterized by the absence of clustering and the noninteracting Fermi sea can be used at the reference state.

Nuclear matter has a low density. Therefore two nucleons separating after a collision will probably not collide again before their relative wave function can resume its precollision asymptotic form. The pre- and post-collision asymptotic forms are identical, because collision with phase shift is impossible for particles in a Fermi sea. This means that the particles must end up in the same state they started from, since all other states with the same energy are occupied. At small distances the relative wave function has a decreased amplitude because of the repulsive interaction. The distance at which the relative wave function first resumes the value it would have in the absence of repulsion is called the healing distance.³ The healing distance is somewhat smaller than the average distance between nucleons and thus subsequent collisions are independent of each other in a good approximation. This is made possible by the small radius of the repulsive potential, which in the nucleus is taken to be a hard core. The ratio of the average interparticle distance to the radius of the potential is almost 4. In a half-filled narrow band the same ratio is 1, since there are enough particles present to cause interaction virtually everywhere. There is no "free flight." Thus the half-filled narrow band is a high-density system compared to a nucleus. (Not in the sense of the electron gas.)

The hard-core repulsion does not allow nucleons to approach within the radius of this potential. Thus if the amplitude of the noninteracting wave function is unity, then the change introduced by the hard core is also unity. It has been shown in the theory of nuclear matter that this precludes an expansion in terms of the t matrix. By inserting one more t matrix into any diagram between two nucleon lines one finds that the ratio of the new and the old diagrams is unity and thus there is no convergence. This is the consequence of the complete expulsion of the wave function from the hard core. Expansion in terms of the density,

² A very good review of this subject was given by B. D. Day, *Rev. Mod. Phys.* **39**, 719 (1967).

³ The figures in L. C. Gomez, J. D. Walecka, and V. F. Weisskopf [*Ann. Phys. (N.Y.)* **3**, 241 (1958)] are very instructive.

however, proves to be possible because the density is low.

We wish to argue that in the metallic range of the half-filled narrow band the situation is just the reverse. Expansion in terms of the density is obviously not possible, but expansion in terms of the t matrix could be convergent. In the electron-hole representation the interaction term becomes attractive. A hard-core repulsion would transform into an infinite attractive potential. Even if the attractive potential is not infinitely strong, but only strong enough for electron-hole pairs to form, the system is an insulator by the formation of excitons. In this range the Fermi sea is unstable and cannot be used as a reference state. So the analogy to nuclear matter breaks down. But this is not the range we are talking about, anyway. The potential has to be sufficiently weak not to cause instability and allow the Fermi sea to be used as a reference state. Still it may be strong enough not to allow the application of the Born series. In this range, expansion in powers of the t matrix seems to be the only possible course of action.

It seems likely that not too many terms in such an expansion need be taken into account and that the treatment can be based on Eqs. (4) and (5). This time we need the inhomogeneous terms, i.e., the entire equation, because we are dealing with free particles. The self-consistent pair-correlation approach to this problem appears to be useful again. Because of the attraction between electrons and holes the configuration on Fig. 5(a) has more than average amplitude. Now as the electron and the hole on, let us say, the left atom separate after collision, configurations like the one in Fig. 5(b) occur, which have lesser amplitudes because the potential energy is unfavorable. If we compare the wave functions in the absence and in the presence of interaction, we expect the wave-function amplitude to increase for small separations due to electron-hole attraction. This increase, however, is

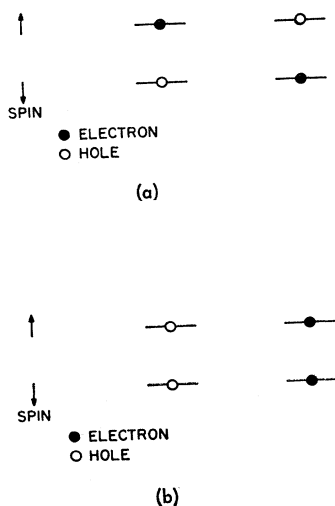


FIG. 5. (a) A configuration of more than average amplitude in the metal. (b) A configuration of less than average amplitude.

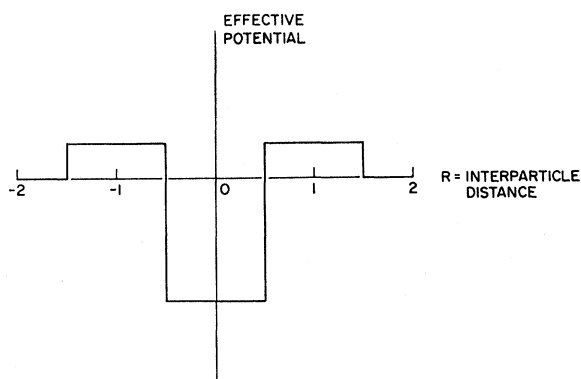


FIG. 6. The effective potential for an electron-hole pair in the metal.

going to be diminished by the unfavorable effective potential energy at separations by one lattice site, which comes about by the correlations in the medium. So the effective potential energy for a pair ought to have the form of Fig. 6. It seems likely that the healing distance, which must exist in view of the Fermi sea, should not be more than two lattice constants. The equation describing this situation is the inhomogeneous version of that exhibited for the Mott insulator in Eq. (6) and we do not dwell on it.

Finally we wish to add that after completing the work on the metallic range, which is paramagnetic, we intend to generalize the method to antiferromagnetism. This will probably require only slight generalization. The amplitude of incoming waves with either spin will have to take on different values on the two different sublattices. Such distinction is unnecessary for the paramagnetic solution.

Discussion of Kemeny and Caron's Paper

J. B. GOODENOUGH (M.I.T.): As one who has been concerned from the experimental side to see what we can learn about this transition, I find it useful to construct an electronic phase diagram. We consider only that cut in the phase diagram corresponding to a single electron in interacting orbitals. We plot temperature T versus the transfer integral b_{ij} , which you had written as T_{ij} . I would like to distinguish two critical regions, not just one. In one limit ($b_{ij} < b_c$) we talk about a "localized-electron regime" in which we use crystal-field theory to describe electrons localized at specific atoms. In this limit we use superexchange theory to describe the interactions between the atoms. According to superexchange theory, we expect an increase in the Néel temperature with increasing b_{ij} . At the opposite limit ($b_{ij} > b_m$) we are in the broad-band region, and in this collective-electron region we have Pauli paramagnetism with, at lowest temperatures, a possible transition to the superconducting state. As b_{ij} decreases in this limit, there should be a band criterion for a transition from a nonmagnetic to a spontaneously magnetic state, a band criterion of the Stoner type for ferromagnetism or, for the case of a half-filled band under consideration here, the point $b_{ij} = b_m$ where the band becomes split into two discrete bands, one filled and one empty, as has been derived from the Hubbard Hamiltonian. In the intermediate interval $b_c < b_{ij} < b_m$, we expect the Néel temperature to decrease with increasing b_{ij} or decreasing band gap, since thermal excitation across the gap

destroys increased stabilization due to antiferromagnetic ordering. Now I mention this because it seems that $b_o < b_{ij} < b_m$ represents a transition region. If the electrons go from a semiconducting state (a nonconducting state) having localized electrons directly to a metallic state, they must pass directly through this intermediate region. The transitional region $b_o < b_{ij} < b_m$, on the other hand, represents a region of spontaneous band antiferromagnetism. If this is included, the electrons pass, with increasing b_{ij} , from a semiconducting state with localized electrons, where we can use crystal-field theory, to a semiconducting state with collective electrons and spontaneous magnetism, where we should use a band theory that includes electron correlations, to a metallic state with collective electrons and no spontaneous magnetism, where Hartree-Fock theory may be sufficient above T_c .

G. KEMENY: Well, what I would like to say about this intermediate range is that the question of antiferromagnetism in a narrow band has been handled before several times, and there is one conclusion which comes out of those calculations which is the following: If the temperature is at absolute zero, then no matter how weak this interaction may be, you always get antiferromagnetic order. Maybe a very weak antiferromagnetism, but some. We were trying with Laurent Caron to make an improvement on this calculation and we wanted to simplify things and after a lot of work we came out with the same result that people came out with before. Then we realized that we were such eager beavers that we made the same approximation in the end that other people made before. What happens is very much like the case of superconductivity. You put your electrons into certain k states and just each electron into one k state without any spread. Then you come up with the superconductive type of solution which is that at absolute-zero temperature you get these superconductive pairs no matter how small the interaction may be. Now the trouble is that one does not take scattering into account correctly and what I mentioned at the end of my talk about antiferromagnetism is, that next time we want to do better, but we first have to have the metallic solution. The trouble with the prediction of these previous theories is that the result would be that you would always have antiferromagnetism at absolute-zero temperature. I don't think that is correct. I mean, there should be a certain minimum interaction required to get antiferromagnetism and, as I say, all of these previous theories because of approximations do not give rise to such a minimum. I hope that when we will be able to do this better, we will come up with a minimum.

G. J. HYLAND (University of Liverpool): Dr. Goodenough's suggestion of an intermediate (transition region) state between the localized and collective electron limits reminds me of an idea recently put forward by Fröhlich [in *Ferroelectricity*, E. F. Weller, Ed. (Elsevier Publ. Co., Amsterdam, 1967), pp. 9-15] that the onset of the metallic phase might be preceded by a ferroelectric or antiferroelectric phase. The electrons which, for large inter-center spacing a , are localized can carry out collective longitudinal and transverse vibrations with frequencies W_L and W_T , respectively; with decreasing a , however, overlap increases, the Coulomb attraction of the localized electrons to their centers becomes screened, and eventually the localization can no longer be maintained, i.e., $W_T \rightarrow 0$ as $a \rightarrow a_0$, say. This does not necessarily mean, however, that for $a \leq a_0$ the system is metallic, i.e., that the band model is now valid; such validity requires that the short-range interaction between electrons (left over after the long-range part has been treated in terms of a plasma—as can always be done) be negligible in comparison with the bandwidth; it might well be that this requires a much higher density a_1 , where $a_1 < a_0$. Now the vanishing of W_T (as $a \rightarrow a_0$ from above) implies a large increase in the static dielectric constant, such as is typical of the onset of the ferro/antiferro/electric state; there would then be three phases: the insulating phase ($a > a_0$), the ferroelectric phase ($a_1 < a < a_0$), and the metallic phase ($a < a_1$). It is of interest in this connection to point out that Umeda *et al.* [J. Phys. Soc. Japan **21**, 1461 (1966)] have observed a new phase (the T phase) in VO_2 in a narrow temperature range between the usual semiconductive and metallic phases, which as far as I know has not yet been investigated for ferroelectricity.

J. B. GOODENOUGH: If I may continue, I would like to mention some experiments. However, first I would like to distinguish the type of lattice instability that occurs in a collective-electron region ($b_{ij} > b_c$), the type of instability that Dr. Adler talked about yesterday where changes in the lattice periodicity stabilize the electrons, from the type of instability that occurs with localized electrons. This latter type of instability is illustrated by Jahn-Teller distortions or by spin-orbit coupling distortions below a magnetic-ordering temperature where the orbits are aligned by a collinear alignment of the spins. J. M. Longo, J. A. Kafalas, and myself have examined several oxides with the Perovskite structure. Briefly, let me mention a single series. In each ABO_3 compound of this series, the transition-metal B atom has two outer d electrons, so we are dealing with the same d -like band in all cases. These compounds, together with some physical properties, are listed in the table in the order of decreasing b_{ij} :

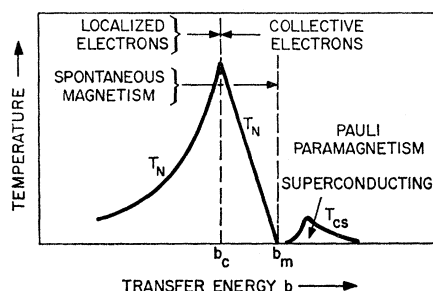
Physical properties of Perovskites with d^2 configuration at the B cations.

Compound	T_N (°K)	$d\rho/dT^b$	Symmetry 300°K	Remarks
BaMoO ₃	Pauli ^a	>0	Cubic	
SrMoO ₃	Pauli ^a	>0	Cubic	
CaMoO ₃	Pauli ^a	>0	Ortho.	
SrCrO ₃	Pauli ^a	>0	Cubic	
CaCrO ₃	90	<0	Ortho.	$dT_N/dP = -0.23^\circ\text{K/kbar}$
PbCrO ₃	240	<0	Cubic	Collinear-type-G order $T < T_N$
LaVO ₃	137	<0	(Cubic)	Tet. ($c/a < 1$) \rightleftharpoons Cubic at T_N
YVO ₃	110	<0	Ortho.	DTA anomaly at $T_i = 73^\circ\text{K}$

^a Pauli = temperature-independent χ_m and no spontaneous magnetic order.

^b ρ = electrical resistivity: Metallic ($d\rho/dT > 0$) vs semiconducting ($d\rho/dT < 0$).

In the Perovskite only 180° cation-anion-cation interactions are important, and $b_{ij} \sim \lambda_r^2$, where λ_r is the covalent mixing parameter. Clearly λ_r is larger for $4+$ than for $3+$ ions, for $4d$ orbitals than for $3d$ orbitals. In addition, λ_r is reduced by covalent A-O bonding, which increases in the order Ba, Sr, Ca, Pb. All the molybdates (BaMoO_3 and SrMoO_3 first examined by Brixner) are metallic and Pauli paramagnetic. So also is SrCrO_3 , which was first investigated by Chamberlain of Du Pont. This indicates that these materials all correspond to $b_{ij} > b_m$. All the rest are antiferromagnetic semiconductors corresponding to $b_{ij} < b_m$. In LaVO_3 we find that below the Néel temperature there is a spontaneous distortion of the crystal from cubic to tetragonal symmetry, characteristic of a spin-orbit coupling distortion where the electrons are localized ($b_{ij} < b_d$). PbCrO_3 , on the other hand, remains cubic below T_N . This has been investigated by Roth of G.E. with neutron-diffraction data, he found collinear spins, but no distortion of the crystal from cubic symmetry down to the lowest temperatures. Therefore with spontaneous distortion as a criterion for a localized electron regime versus a collective-electron regime, we place the critical transfer integral b_c between LaVO_3 and PbCrO_3 . Now, if we look at the Néel temperatures, we find a maximum in T_N about where we have placed the critical distance b_c , which corresponds to the general prediction of the figure:



Because the Perovskite structure is not indicative to cation-cluster formation, we are not plagued with narrow-band instability of the type found in VO_2 . As a result it is possible to obtain this good indication of a transition region $b_c < b_{ij} < b_m$. Certainly the d -like wave functions in PbCrO_3 are quite different from those in LaVO_3 insofar as the structural-instability criterion is concerned. However, these data also indicate that the transitional region is narrow, so that we should not be surprised to find spontaneous band magnetism a relatively rare phenomenon in the periodic table.

G. HORWITZ (Yeshiva University): I think it is rather important to clarify the relations within the model. I think that one has to realize the following: There is a possibility of metal-insulator transitions being associated with a magnetic state as well as nonmagnetic and these would, of course, imply different conditions. There might be a range of values in which this state would be antiferromagnetic and another range where not. Similarly, there is a possibility of the band-type antiferromagnet as an alternative to this localized kind of antiferromagnet and here again the question as to which states dominate or to whether there is some kind of intermediate region is another kind of problem which hasn't been explored. We'll have to look at these

alternative kinds of solutions as a function of the ratio of the parameters and then determine which is the most stable state. And then one could get a real phase diagram of the various regions in a meaningful way in terms of the model.

G. KEMENY: Well, I agree with this, except for possibly one point, which is this: I don't know whether in this model we could get something like band-type antiferromagnetism and localized-type antiferromagnetism. I don't see that one could reasonably make such a distinction because a solution of the problem would simply have to be that there is some up-spin sublattice and down-spin sublattice. I mean sublattices for just some preferential occupations. This has to build up somehow in terms of Bloch waves and I don't think that such a distinction can be made.

H. BROOKS (Harvard University): Can I comment on that? I think what you said is exactly right. As a matter of fact, if the antiferromagnetic state in the band approximation is described as a full band, as it will be, the localized model by the usual Wannier transformation is entirely equivalent to a band model, so I think the distinction is not a meaningful one.

G. HORWITZ: I do feel there is a distinction. Although in the one-electron description of the ordered state a full antiferromagnetic band is equivalent to the usual Wannier states, the correlations bring about a distinction. As first suggested by Mott, a criterion would be whether or not the Néel temperature is associated with the metal-insulator transition. If there is an antiferromagnetic transition when you go from insulator to metal, then either description will do, but if the Néel temperature is lower than the metal-insulator transition temperature, then there is, effectively, a distinction.

G. KEMENY: I think the point is that if we look at this as a function of temperature, we may come to the following conclusions, although you cannot demonstrate this mathematically: We start out with a system in which there is long-range order and therefore there is antiferromagnetism, but if we look at the short-range order, then we find that an electron and a hole, which are on the same atom, cannot separate from each other too far. So the long-range order is the magnetic order, the short-range order is, if you wish, a Mott-type order. But if you raise the temperature, it is possible that the long-range order, the antiferromagnetic order, cannot be maintained and you get a magnetically disordered system but you still have the bound pairs left. So in nickel oxide it is quite possible that this is the mechanism. The problem here is that one has to consider both the long- and the short-range order. What I was concerned with in my talk was only the short-range order and we assumed that there was no long-range order at all. Now on the other hand, when I said at the end of the talk, that after we get a solution for the metallic range we may look at the antiferromagnetic solution, what I implied there was that you start out assuming that you have a long-range antiferromagnetic order and then you put in the short-range correlations and then you would have both aspects of it. But that's not very easy.

T. ARAI (Argonne National Lab.): After the intermission, I will try to explain how I can get a metallic antiferromagnet from an insulating antiferromagnetic state by compressing the lattice, in other words, by decreasing the lattice constant.