G. Gladstone, Phys. Rev. 172, 302 (1968).
[7]D. Golibersuch and A. J. Heeger, Phys. Rev. 182, 584 (1969).
[8]B. Dreyfus, J. Souletie, J. L. Tholence, and R. Tournier, J. Appl. Phys. 39, 846 (1968).
[9]P. Monod, Phys. Rev. Lett. 19, 1113 (1967).
[10]W. M. Star and G. J. Nieuwenhuys, Phys. Lett. 29A, 26 (1969).
[11]J. C. F. Brock, J. C. Ho, C. P. Schwartz, and N. E. Phillips, in *Proceedings of the Eleventh International Conference on Low Temperature Physics, St. Andrews, Scotland, 1968,* edited by J. F. Allen, D. M. Finlayson, and D. M. McCall (St. Andrews University, St. Andrews, Scotland, 1969), p. 1229.
[12]C. M. Hurd, J. Phys. Chem. Solids 28, 1427 (1967).
[13]G. Chouteau, B. Manhes, and R. Tournier, in *Proceedings of the Eleventh International Conference on Low Temperature Physics, St. Andrews, Scotland, 1968,* edited by J. F. Allen, D. M. Finlayson, and D. M. McCall (St. Andrews University, St. Andrews, Scotland, 1969), p. 1316.
[14]B. Caroli, J. Phys. Chem. Solids 28, 1427 (1967).
[15]R. Tournier and A. Blandin, Phys. Lett. 24, 397 (1970).
[16]Antiferromagnetic interactions at a distance $<r_c$ are not destroyed even by a field of 60 kOe, so that the saturation value measured is only due to ferromagnetic pairs. The Curie constant is nearly the same for $4N$ impurities with spin S or N superparamagnetic pairs with spin $2S$ plus N pairs with spin 0.

PHASE TRANSITION IN HUBBARD MODEL

M. Cyrot
Laboratoire de Physique des Solides, Faculté des Sciences de l'Université de Paris, 91 Orsay, France*
(Received 16 March 1970; revised manuscript received 4 August 1970)

We investigate the appearance of magnetism in the Hubbard model. In the limit of large value of the interaction U, we show that localized moments appear below a critical temperature T_L. We find a Ruderman-Kittel interaction between these moments, which gives an ordered magnetic phase at a critical temperature T_c smaller than T_L.

For many years, there has been important activity in the fields of itinerant ferromagnetism, metals which exhibit localized-moment behavior above the transition temperature and the Mott transition. A particularly important start for this problem is the Hubbard Hamiltonian,[1] where one assumes a nondegenerate band of width Δ studied in tight binding and where electrons interact only when they are on the same atom, i.e., on the same Wannier state, the interaction being U, in that case.

In this Letter, we want to show that for this model magnetism can occur in two stages. For large values of the ratio U/Δ, there exists a first critical temperature T_L below which localized moments appear on each site. These localized moments interact and one can take into account only a two-body interaction which is a Ruderman-Kittel type. As a result of this interaction one can have a transition to a ferromagnetic or antiferromagnetic state at a second critical temperature T_c smaller than T_L. For small values of U/Δ, $T_L = T_c$ and the appearance of localized moments is connected with the appearance of magnetism if any. These results are in qualitative agreement with a model for magnetism in transition metals suggested by Friedel, Leman, and Obsewski.[2] The differences in approach and in choice of model have made if difficult to compare the present results in detail with previous works. However our results are different from the Hartree-Fock calculation of Blandin and Lederer,[3] although we agree with the qualitative features.

We support these conclusions with the calculation of the free energy using a functional integral representation.[4] This replaces the interaction U by an arbitrary magnetic field varying from site to site and having a Gaussian probability. We show that the free energy can be written as a series $F_1 + F_2 + \cdots$ of functions of the local field on one, two, $\cdots$ sites. For large U/Δ, the main term is the first one and F_1 is strongly peaked over two symmetrical values of the local field for temperature smaller than T_L. This shows the existence of local moments. This magnitude is a function of temperature and gives a susceptibility which deviates from a Pauli law. The second term of the series gives the interaction between moments. So one obtains an ordering temperature of these local moments of the order of $T_c \cong F_2$. For small U/Δ, F_1 and F_2 are comparable and greater than the remaining terms. We obtain $T_L = T_c$ when magnetism can occur.

As a start we have a Hubbard Hamiltonian:

$$H = \sum_{ij\sigma} T_{ij\sigma} C_{i\sigma}^{\dagger} C_{j\sigma} + \tfrac{1}{2} U n_{i\sigma} n_{i-\sigma}. \tag{1}$$

We will calculate the partition function using a functional integral formalism. Z can be written[3]

$$Z=\int(\Pi d\xi_{is})\exp(-\sum_{is}\xi^2\,\mathrm{Tr}\,T_s e^{-\beta H_s}), \tag{2}$$

$$H_s=\sum_{ij\sigma s}T_{ij}C_{i\sigma s}^{\dagger}C_{j\sigma s}+\left[\tfrac{1}{2}U-\mu-\left(\frac{2U}{\beta}\right)^{1/2}\sigma\xi_{is}\right]n_{i\sigma s}. \tag{3}$$

The main interest of this formulation is to eliminate the two-body potential. We have to calculate a partition function of noninteracting particles moving in an arbitrary scattering potential $Z(\{\xi_i\})$.

In this paper we will only deal with the static approximation which is exact for $T_{ij}=0$ and for $U=0$ and gives a smooth interpolation through the region $U/\Delta\sim 1$. That is, we neglect the s dependence of our scalar field ξ_i. As usual we introduce a coupling constant λ_i for the potential ξ_i. Taking the logarithmic derivative of the partition function, we have

$$\frac{1}{Z\{\xi\}}\frac{\partial Z}{\partial\lambda_i}=\sum_{\sigma}(2\beta U)^{1/2}\sigma\xi_i\langle n_{i\sigma}\rangle.$$

$\langle n_{i\sigma}\rangle$ is given by the one-electron Green's function in the field ξ_i:

$$n_{i\sigma}=G_{ii}(\tau=0^-).$$

In the absence of the random field ξ_i we have

$$G_{ij}^{0}(\omega_\nu)=\frac{1}{N}\sum_k\frac{\exp[ik(R_i-R_j)]}{i\omega_\nu-\epsilon_k+\mu-\frac{1}{2}U}. \tag{4}$$

To calculate G_{ii} we have to solve an alloy problem. Introducing the notation $G_{ij}(\omega_\nu,\xi_1,\xi_2,\cdots,\xi_n)$, it is straightforward to show that

$$G_{ij}(\omega_\nu,\xi_1,\cdots,\xi_l,\cdots,\xi_n)=G_{ij}(\omega_\nu,\xi_1,\cdots,\xi_l=0,\cdots,\xi_n)+G_{il}(\omega_\nu,\xi_1,\cdots,\xi_l=0,\cdots,\xi_n)\times\frac{\xi_l}{1-\xi_l G_{ll}(\omega_\nu,\xi_1,\cdots,\xi_l=0,\xi_n)}G_{lj}(\omega_\nu,\xi_1,\xi_l=0,\cdots,\xi_n). \tag{5}$$

Then we obtain for the partition function

$$\ln\frac{Z(\xi_1,\cdots,\xi_i,\cdots,\xi_n)}{Z(\xi_1,\cdots,\xi_i=0,\cdots,\xi_n)}=\sum_\sigma\sum_{\omega_\nu}e^{-i\omega_\nu 0^-}\ln[1+(2U/\beta)^{1/2}\sigma\xi_i G_{ii}^{\sigma}(\omega_\nu,\xi_1,\cdots,\xi_i=0,\xi_n)]. \tag{6}$$

Let us assume for the moment that we can neglect all terms which connect the local field on different sites, that is,

$$Z(\xi_1,\cdots,\xi_n)=\Pi_i Z_i,$$

$$Z_i=\exp\{\textstyle\sum_\sigma\sum_{\omega_\nu}e^{-i\omega_\nu 0^-}\ln[1+(2U/\beta)^{1/2}\sigma\xi_i G_{ii}^{\sigma 0}]\}.$$

The partition function can be written

$$Z=\int(\Pi_1 d\xi_i)\exp\{\textstyle\sum_i F_1(\xi_i)\}, \tag{7}$$

$$F_1(\xi_i)=\xi_i^2-\sum_\sigma\beta\int\frac{d\omega}{\pi}\frac{1}{1+e^{\beta\omega}}\arctan\frac{(2U/\beta)^{1/2}\sigma\xi_i\pi n(\omega)}{1+(2U/\beta)^{1/2}\sigma\xi_i\mathrm{P}\int[n(\omega')/\omega'-\omega]d\omega'}; \tag{8}$$

$n(\omega)$ is the density of states. If we want to evaluate this integral by means of the saddle-point method we have to look at the minimum of F_1. This is an even function. For large values of T, $F(\xi)$ has a single minimum at the origin so that states near $\xi=0$ are most heavily weighted. For T smaller than T_L there arise two symmetric minima $\pm\xi_0$. This is a localized-moment regime with $\pm\xi_0$ corresponding to spins up and spins down.[5] As one can see, the susceptibility corresponding to these two regimes changes with temperature from a Pauli law to a Curie law with a varying moment. The critical temperature is given by

$$1+2U\int d\omega\int d\omega'\frac{f(\omega)-f(\omega')}{\omega-\omega'}n(\omega)n(\omega')=0. \tag{9}$$

Assuming a constant density of states of width Δ, one obtains localized moments only if

$$U/\Delta > 1/4 \ln 2.$$

At large values of U, T_L is proportional to U: $T_L \sim \frac{1}{2}U$.

The validity of this approximation will be discussed in considering the coupling between localized moments. The next approximation in Eq. (6) is to take into account site j in the Green function G_{ii}. The logarithmic term becomes[6]

$$\ln\left[1+\left(\frac{2U}{\beta}\right)^{1/2}\sigma\xi_i G_{ii}^{0\sigma}-\frac{2U}{\beta}\xi_i\xi_j\frac{G_{ij}^{0\sigma}G_{ji}^{0\sigma}}{1+(2U/\beta)^{1/2}\sigma\xi_j G_{jj}^{0\sigma}}\right]. \tag{10}$$

This approximation will be valid in the limit of either U/Δ or Δ/U small. It is easy to see that one can write

$$Z=\int(\Pi_i d\xi_i)\exp[-\textstyle\sum_i F_1(\xi_i)-\sum_{ij}F_2(\xi_2,\xi_i,\xi_j)-\sum_{ijk}F_3(\xi_i,\xi_j,\xi_k)+\cdots]. \tag{11}$$

The ratio of two successive terms is the small parameter U/Δ or Δ/U.

For large values of U/Δ we have shown that $F_1(\xi_i)$ has two symmetric minima $\pm\xi_0$ for $T \ll T_L$. F_2 is much smaller than F_1 and F_3 is smaller than F_2 so one can neglect all interactions of order greater than two. In F_2, we approximate ξ_i and ξ_j by $\xi_0\sigma_i$ and $\xi_0\sigma_j$ with $\sigma_i=\pm1$, $\sigma_j=\pm1$ so we can write F_2 as

$$F_2=-(1/T)J_{ij}\sigma_i\sigma_j \tag{12}$$

with

$$J_{ij}=-2\xi_0^2 U\sum_i\sum_{\omega_\nu}e^{-i\omega_\nu 0^-}\frac{1}{N^2}\sum_{kk'}\frac{\exp i(k-k')(R_i-R_j)}{(i\omega_\nu-\epsilon_k)(i\omega_\nu-\epsilon_{k'})}\frac{1}{(1-A^2\xi_0^2)} \tag{13}$$

and

$$A^2=\frac{2U}{\beta}\int d\omega\int d\omega'\frac{n(\omega)n(\omega')}{(i\omega_\nu-\omega)(i\omega_\nu-\omega')}.$$

For large values of U and for $A^2\xi_0^2 \ll 1$, one obtains a Ruderman-Kittel interaction between localized moments. This yields a transition temperature T_c given by the equation

$$1=U_{\text{eff}}\frac{1}{N}\sum_k\frac{\partial f}{\partial\epsilon_k}(T). \tag{14}$$

U_{eff} is an effective interaction which depends on temperature and is given by

$$U_{\text{eff}}=2\xi_0^2 U.$$

For small values of U/Δ there is no localized-moment regime with magnetic disorder. We will show that one can have a transition to a magnetic state with the appearance of localized moments on each site, i.e., $T_L=T_c$. One can neglect terms F_3 and following. We restrict ourselves to the value of $\xi_k=\sigma_k\xi$, $\sigma_k=\pm1$, and look at the minimum of F_1+F_2 as a function of ξ. We have first to sum on values of σ_k. This sum is the free energy of an Ising model $\mathcal{F}(\xi)$ with an interaction given by[13]

$$Z=\int d\xi\exp[-NF_1(\xi)-N\mathcal{F}(\xi)].$$

This integral can be done by the saddle-point method and one obtains a nonzero value of ξ for the minimum if the energy gained by magnetic ordering is larger than the energy needed to create a localized moment.

In both cases we have reduced the calculation of the partition function to the partition function of an Ising model. It is obvious that it would have been better to linearize the interaction with a vectorial field so we would not have broken the symmetry.[4] It is likely that one would have obtained a Heisenberg model instead of an Ising one. Details about this calculation and applications will be published soon.

We wish to thank Professor J. Friedel for helpful discussions and Professor J. R. Schrieffer for comments and for sending his preprint on the two-center problems.

*Laboratoire associé au Centre National de la Recherche Scientifique.
[1]J. Hubbard, Proc. Roy. Soc., Ser. A 276, 238 (1963), and 277, 237 (1963), and 281, 401 (1963).
[2]J. Friedel, G. Leman, and S. Obsewski, J. Appl. Phys. 32, 325S (1961).
[3]A. Blandin and P. Lederer, Phil. Mag. 14, 363 (1966).
[4]See, for instance, J. R. Schrieffer, presented at Canadian Association of Physists Summer School, Banff, Canada, 1969 (to be published).
[5]S. Q. Wang, W. E. Evenson, and J. R. Schrieffer, Phys. Rev. Lett. 23, 92 (1969).
[6]This is exactly the results obtained in the two-center problem by W. E. Evenson, S. Q. Wang, and J. R. Schrieffer, to be published.

EXCITATION OF THE GIANT RESONANCE IN ^{12}C BY INELASTIC ELECTRON SCATTERING

Y. Torizuka, A. Yamaguchi, T. Terasawa, Y. Kojima, K. Nakahara, M. Oyamada, K. Itoh, A. Nakada, S. Mitunobu, and M. Kimura
Laboratory of Nuclear Science, Tohoku University, Sendai, Japan
(Received 20 July 1970)

The longitudinal and transverse form-factor spectra for electroexcitation of the ^{12}C giant resonance were determined separately. Results are presented for an excitation energy range of from 15 to 30 MeV and for a momentum-transfer range of 0.84-1.56 F^{-1}. We have found levels with the following excitation energies (MeV), spins, and parities: 18.6 (3^-), 19.6 (4^-), 20.0 (2^+), 20.6 (3^+), 21.6 (3^-), 22.0 (1^-), 22.7 (1^-), and 23.8 (1^-). We have also found new evidence of the spin-isospin mode for the 22.7-MeV (1^-) excitation.

We have employed a new method of displaying the longitudinal and transverse form factors for electroexcitations [$|W_L(q,\omega)|^2$ and $|W_T(q,\omega)|^2$] as form-factor spectra. Such a procedure is useful particularly in the giant-resonance region as a means of isolating a complicated structure, since the form factors for some levels are almost completely either longitudinal or transverse. Results for ^{12}C are presented for the excitation energy range of from 15 to 30 MeV and for momentum transfers of 0.84, 1.04, 1.22, and 1.56 F^{-1} which are favorable for the excitations of $J=1$, 2, 3, and 4 states, respectively. We could find many peaks which were marginally apparent from previous studies. Such examples will be seen for the 18.6- (3^-), 20.0- (2^+), 20.6- (3^+), and 22.7-MeV (1^-) states.

In the Born approximation for the interaction of the electron with the nucleus, the cross section for electron scattering is given by [1,2]

$$\frac{d^2\sigma}{d\Omega d\epsilon_2}\frac{Z^2e^4\cos^2\frac{1}{2}\theta}{4\epsilon_1^2\sin^4\frac{1}{2}\theta}\frac{1}{1+2\epsilon_1\sin^2\frac{1}{2}\theta/M_T}|W(q,\omega)|^2, \tag{1}$$

$$|W(q,\omega)|^2=\frac{q_\mu^4}{q^4}|W_L(q,\omega)|^2+\left(\frac{q_\mu^2}{2q^2}+\tan^2\tfrac{1}{2}\theta\right)|W_T(q,\omega)|^2, \tag{2}$$

where $W_L(q,\omega)$ is the part of the total form factor $W(q,\omega)$ due to the Coulomb or the longitudinal interaction, and $W_T(q,\omega)$ is the part due to the transverse interaction. The four-momentum of the electron is $k_\mu=(\vec{k},i\epsilon)$; the subscripts 1 and 2 refer to the initial and final states, respectively. The momentum transfer is $q_\mu=(\vec{q},i\omega)=k_{1\mu}-k_{2\mu}$ and θ is the scattering angle of the electron. M_T is the mass of the target nucleus. The generalized form factor is related to the usual one by

$$|F(q)|^2=\int_\omega|W(q,\omega)|^2d\omega. \tag{3}$$

In order to separate the longitudinal and transverse parts from the total form factor, the spectra were taken at relatively forward and backward angles, keeping q constant.

Our measurements were carried out using the beams of the Tohoku 300-MeV electron linear accelerator. The forward-angle spectra corresponding to the q values of 0.84, 1.04, 1.22, and 1.56 F^{-1} were taken in the range 40°-80° at the incident energy of 250 MeV and the backward-angle spectra were taken at 135° by adjusting incident energies to give the same momentum transfers. In the present kinematical calculation, q is calculated by assuming an excitation energy of 25 MeV. The thickness of the graphite target was 104 mg/cm^2. In our electron spectrometer, the scattered electrons were