often triplet excitons. In that case the new phase i' will have a magnetic order, as will the subsequent phases. Similarly, starting from the metallic side, the first Overhauser instability may well be a spin-density instability,[7] so that the new phase m' will be magnetic, as will subsequent phases. Obviously all kinds of combinations of nonmagnetic and magnetic instabilities are possible.

We suggest that the above considerations provide a framework for the interpretation of distortive and/or magnetic phase transitions of small-gap solids. A fuller account is in preparation.

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[2]J. Zittartz, Phys. Rev. (to be published); also Office of Naval Research Technical Report No. 45, NONR-2216-(11), Project No. NR 017-630, 1967 (unpublished).

[3]For the moment we consider, for simplicity, only the lowest exciton band of each family. At the end we come back briefly to the excited bands.

[4]Of course a real solid will respond to this potential by a lattice distortion which the present model, with fixed nuclei, does not take into account.

[5]A. W. Overhauser, Phys. Rev. Letters 4, 415 (1960).

[6]It could happen that in passing from, say, m'' to m''', the density fluctuation w' disappears. This would lead to a somewhat different phase diagram than Fig. 3(b).

[7]A. W. Overhauser, Phys. Rev. Letters 4, 462 (1960).

FORMATION OF LOCAL MAGNETIC MOMENTS IN METALS*

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Current theories of local magnetic moment formation in metals are essentially Hartree-Fock theories[1,2] and certain improvements thereon.[3] These theories generally lead to implausibly sharp threshold conditions, and raise certain difficulties due to violation of rotational invariance.

In this note we suggest the possibility of calculating directly the quantities susceptible to measurement, in particular, spin susceptibility, using only standard many-body perturbation theory. The model is a degenerate electron gas described by a Hamiltonian consisting of the kinetic energy, Coulomb interaction, and a structureless impurity potential V.

The spin susceptibility at wave number $\vec{q}$ and frequency Ω, due to a periodic magnetic field of wave number q' and frequency Ω, is the analytic continuation to $\Omega + i\delta$ $(\delta > 0)$ of the function

$$\chi(q,q',\nu_n) = \frac{2(g\mu_B)^2}{\beta^2} \sum_{\omega_1\omega_2} \int \frac{d\vec{p}_1 d\vec{p}_2}{(2\pi)^6} \mathcal{G}^{II}(\vec{p}_1\omega_1, \vec{p}_2\omega_2; \vec{p}_1+\vec{q}, \omega_1+\nu_n; \vec{p}_2-\vec{q}', \omega_2-\nu_n) \qquad (1)$$

from the even points $i\nu_n = 2n\pi i/\beta$, where $\beta = 1/kT$, T is the temperature, and k Boltzmann's constant. $\mathcal{G}^{II}$ is the two-particle Green's function with a "triplet" assignment of spin subscripts (see below). The ω's are the "odd" points $(2n+1)\pi/\beta$. (The notation is that of Abrikosov, Gor'kov, and Dzyaloshinski.[4])

Wolff[2] has treated a "single-band" version of the present Hamiltonian in Hartree-Fock approximation, replacing the total potential $(V + \text{Hartree-Fock})$ by an average over one band. This results in an s-wave scattering problem with a zero-range force. He found a threshold condition on the parameters of the problem, beyond which "up"- and "down"-spin electrons see different Fock fields. We shall eventually perform a similar averaging, but begin with an exact formulation.

The analog of the Wolff condition in many-

body theory is that the Bethe-Salpeter equation for a certain reducible vertex $\Gamma(\vec{k}_1\omega_1, \vec{k}_2\omega_2, \vec{k}_1+\vec{q}, \omega_1+\nu, \vec{k}_2-\vec{q}', \omega_2-\nu)$ should have a divergent solution. (As the coupling strength is increased the divergence first occurs at $\nu=0$.) Our main point is that such an instability will occur only if uncorrected propagators are used in the Bethe-Salpeter equation: When Γ becomes large, so does the self-energy, so that the propagators diminish, inhibiting the instability.

Using δ-function normalization of the plane-wave eigenfunctions, it is possible to write the thermodynamic Green's functions, self-energies, and vertex functions as sums of two parts: one with a diagonal singularity (a momentum-conserving δ function), and another without such singularity but with off-diagonal elements in momentum space. An important simplification occurs in the limit of zero impurity concentration: The diagonally nonsingular part does not enter the equations for the diagonally singular parts (for finite concentrations this is no longer true). A formal process for solving the zero-concentration problem is given in the following definitions (D) and derived equations (E): Total Green's function (E) (Dyson's equation),

$$\mathcal{G}(\vec{k}\vec{k}', \omega_n) = (2\pi)^3\delta(\vec{k}-\vec{k}')g_0(\vec{k}, \omega_n) + g_0(\vec{k}\omega_n)\int \frac{d\vec{k}''}{(2\pi)^3}\Sigma_t(\vec{k}\vec{k}'', \omega_n)\mathcal{G}(\vec{k}'', \vec{k}', \omega_n), g_0(\vec{k}, \omega_n) = 1/(i\omega_n - \epsilon_k + \epsilon_F). \quad (2)$$

Total self-energy (D),

$$\Sigma_t(\vec{k}\vec{k}', \omega_n) = (2\pi)^3\delta(\vec{k}-\vec{k}')\Sigma(\vec{k}\omega_n) + \Sigma(\vec{k}\vec{k}', \omega_n). \quad (3)$$

Dyson equation for pure medium propagator (E),

$$g(\vec{k}, \omega_n) = g_0(\vec{k}\omega_n) + g_0(\vec{k}\omega_n)\Sigma(\vec{k}\omega_n). \quad (4)$$

T matrix (D),

$$T(\vec{k}, \vec{k}', i\omega_n)g(\vec{k}'\omega_n) = \int \frac{d\vec{k}''}{(2\pi)^3}\Sigma(\vec{k}\vec{k}'', \omega_n)\mathcal{G}(\vec{k}''\vec{k}'\omega_n). \quad (5)$$

Nonsingular part $g(\vec{k}\vec{k}'\omega_n)$ (D),

$$\mathcal{G}(\vec{k}\vec{k}'\omega_n) = (2\pi)^3 g(\vec{k}\omega_n)\delta(\vec{k}-\vec{k}') + g(\vec{k}\vec{k}', \omega_n). \quad (6)$$

Then (E)

$$g(\vec{k}\vec{k}'\omega_n) = g(\vec{k}\omega_n)\Sigma(\vec{k}\vec{k}'\omega_n)g(\vec{k}'\omega_n) + \int \frac{dk''}{(2\pi)^3}g(\vec{k}\omega_n)\Sigma(\vec{k}\vec{k}''\omega_n)g(\vec{k}''\vec{k}'\omega_n). \quad (7)$$

From Eqs. (5)-(7) we get (E)

$$T(\vec{k}\vec{k}'i\omega_n) = \Sigma(\vec{k}\vec{k}'\omega_n) + \int \frac{d\vec{k}''}{(2\pi)^3}\Sigma(\vec{k}\vec{k}''\omega_n)g(\vec{k}''\omega_n)T(\vec{k}''\vec{k}'i\omega_n). \quad (8)$$

Finally, from perturbation series it is seen that

$$\Sigma(\vec{k}\vec{k}'\omega_n) + V(\vec{k}\vec{k}') + \Sigma^m(\vec{k}\vec{k}'\omega_n),$$

where $V(\vec{k}\vec{k}')$ is the bare-impurity potential, and Σ^m is constructed exactly as for the uniform gas out of vertex functions and propagators [with $\mathcal{G}(\vec{k}\vec{k}'\omega_n)$ replacing $g(\vec{k}\omega_n)$, etc.], and with the (one and only) diagonally singular term subtracted off.

We assume the uniform gas to be nonmagnetic. Then the BS equation for the diagonally singular part Γ_D of Γ has a finite solution for v, zero included. The local moment singularity, if any, must show up in the nondiagonal part Γ_{ND}. The detailed structure of the BS equation will be discussed in a forthcoming paper; here we state it only schematically with primed indices summed over, and a given index denoting energy, momentum, and spin orientation. The BS equation for the Γ reducible in the

channel relevant for the calculation of $\mathcal{G}^{II}$ reads [1 and 2 ingoing particles, 3 and 4 outgoing, see Fig. 1(a)]

$$\Gamma(12;34)=\Gamma^{(i)}(12;34)+\Gamma^{(i)}(13';31')\mathcal{G}(1'4')\mathcal{G}(2'3')\Gamma(4'2;2'4) \tag{9}$$

where $\Gamma^{(i)}$ is the sum of all vertices irreducible in the channel presently under consideration. $\mathcal{G}$ is the exact one-particle Green's function. It is advantageous to effect a separation with respect to spin subscripts[5]:

$$\Gamma_{\sigma_1\sigma_2\sigma_3\sigma_4}(12;34)=\tfrac{1}{2}\Gamma_a\delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4}+\Gamma_b(\delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_3}-\tfrac{1}{2}\delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4})$$

and similarly for $\Gamma^{(i)}$. Equation (9) is then seen to hold separately for Γ's with subscripts a and b. Only Γ_b is needed in Eq. (1) and only Γ_b shows a tendency to instability. We now extract the nonsingular part (9ND) from Eq. (9) assuming weak, zero-range, electron-electron coupling v. The bare vertex is diagonally singular, and has spin components a,b proportional to $\frac{1}{2}v$ and $-v$, respectively. The lowest order contribution to the kernel $\Gamma_b{}^i\mathcal{G}\mathcal{G}$ of (9ND) comes from this bare vertex. The lowest order nonsingular contribution to the driving term of (9ND) is $O(v^2)$ and comes from two sources: (1) the integral term of 9 with $\Gamma_b{}^{(i)}$, $\Gamma_b\sim v$, and the singular part removed, giving $v(\mathcal{G}\mathcal{G}-\mathcal{G}_D\mathcal{G}_D)v$, and (2) second-order contributions to $\Gamma_b{}^{(i)}$. The "other" particle-hole channel [Fig. 1(b)] contributes nothing to $\Gamma_b{}^{(i)}$. Particle-particle channels do contribute but their temperature dependence raises special problems outside the scope of this Letter. $\mathcal{G}$ must now be made consistent with Γ. The dominant contribution Σ^m is shown in Fig. 2(a).

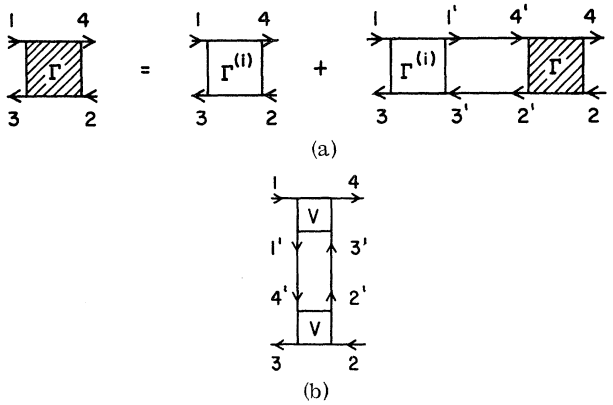

FIG. 1. (a) The Bethe-Salpeter equation in the relevant particle-hole channel. (b) The "other" particle-hole channel does not contribute to Γ_b.

Evidently, in lowest approximation to the kernel of (9ND) this diagram may be obtained by closing the 3 tail of the integral term in (9ND) onto the 2 tail, with acquisition of a minus sign and some numerical factors. Hence, neglecting some small terms $O(v^2)$, Σ^m is also given by the diagram in Fig. 2(b). Finally, in the present approximation Γ depends on the four-momentum transfers 1-3, 2-4 only. In particular, Γ_b depends on ν only, and not on ω_1,ω_2.

Going over to the one-band, zero-range model of Wolff[4] we make the replacement

$$\frac{1}{V_p}\int g(\vec{k}\omega)\frac{d\vec{k}}{(2\pi)^3}=\mathcal{F}(i\omega),$$

where V_p is the volume occupied in k space by one band. ($V_p{}^{-1}=V_a$ the volume of one atomic cell.) Retaining only s-wave amplitudes and assuming a zero-range bare potential $V(\vec{k}\vec{k}')$ $=V$(independent of k), it is seen that Σ^m loses its k dependence, provided T does. But that is indeed consistent with (8). Henceforth, we write $V_a\Sigma(i\omega)$ for $\Sigma(kk'\omega)$, $V_aT(i\omega)$ for $T(kk'i\omega)$, etc., because in the present normalization they are proportional to the atomic volume. Thus (8) becomes

$$T(i\omega)=\Sigma(i\omega)+\Sigma(i\omega)\mathcal{F}(i\omega)T(i\omega).$$

Also, introducing

$$V_a h(i\omega)=\frac{1}{V_p{}^2}\int \mathcal{G}(\vec{k}\vec{k}',\omega)\frac{d\vec{k}\,d\vec{k}'}{(2\pi)^6},$$

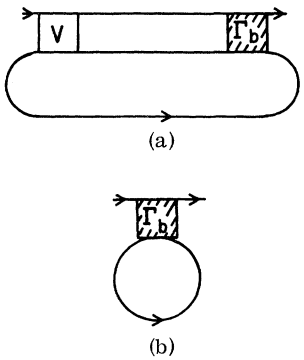

FIG. 2. (a) The dominant contribution to Σ^m when Γ_b becomes large. (b) Aside from terms $O(v^2)$, Σ^m is also given by this diagram.

we see that

$$h(i\omega)=\mathfrak{F}(i\omega)+\mathfrak{F}(i\omega)T(i\omega)\mathfrak{F}(i\omega).$$

Setting the momentum average of Γ_B equal to $\gamma(i\nu)$, we can solve the BS equation, obtaining

$$\gamma(i\nu)=\frac{v^2(1/\beta)\sum_\omega[h(i\omega)h(i\omega-i\nu)-\mathfrak{F}(i\omega)\mathfrak{F}(i\omega-i\nu)]}{1+(v/\beta)\sum_\omega h(i\omega)h(i\omega-i\nu)}. \quad (10)$$

$\Sigma^m(i\omega)$ is now given by the Dyson equation $\Sigma^m(i\omega)=V-\mathfrak{F}^{-1}(i\omega)-h^{-1}(i\omega)$, but, as briefly discussed above, it also equals $-\frac{3}{4}\sum_\nu\gamma(i\nu)h(i\nu+i\omega)$. Hence, if we define $h_0(i\omega)$ as the s-wave zero-range projection of the Green's function of an electron gas with impurity potential V, and with self-energy corrections (but not vertex corrections) included [i.e., if $h_0^{-1}(i\omega)=\mathfrak{F}^{-1}(i\omega)-V$], we finally get

$$\frac{1}{h_0(i\omega)}-\frac{1}{h(i\omega)}=-\frac{3}{4\beta}\sum_\nu\gamma(i\nu)h(i\nu+i\omega). \quad (11)$$

The two simultaneous nonlinear equations (10) and (11) for h and γ should not exhibit instability. From their solution one can find a susceptibility at zero frequency, averaged over all wave numbers of the applied field: From (1), and the relation between g^{II} and Γ,

$$\frac{\text{Average total moment on site}}{\text{Magnetic field}}=(g\mu_B)^2\gamma(0)\left\{\frac{1}{\beta}\sum_\omega[h(i\omega)]^2\right\}^2. \quad (12)$$

As a crude method of solving (10) and (11), which should be correct at moderately high temperatures, we note that if we were well below threshold, we would simply iterate (11), writing $h=h_0$ in the right-hand side. It is easy to show that each term of the sum is of order vkT/V. Suppose, however, we are near threshold so that $\gamma(0)$ is very large. Then we rewrite (11) as

$$\frac{1}{h_0(i\omega)}-\frac{1}{h(i\omega)}+\frac{3}{4\beta}\gamma(0)h(i\omega)=-\frac{3}{4\beta}\sum_{\nu\neq 0}\gamma(i\nu)h(i\omega+i\nu)$$

and begin by solving this equation with the right-hand side equated to zero.[6]

The h so obtained can then be used for beginning the iteration. Near threshold, γ can be simplified [assuming that the uniform medium is so nonmagnetic that $(v/\beta)\sum\mathfrak{F}(i\omega)\mathfrak{F}(i\omega)\ll 1$]. The initial h is then found from the quadratic equation

$$1/h_0-1/h=Qh,$$

whose solution is

$$h=(1/2Q)[h_0^{-1}-(h_0^{-2}-4Q)^{1/2}], \quad (13)$$

where

$$Q=\frac{3v}{4\beta}\left\{1+\frac{v}{\beta}\sum_\omega[h(i\omega)]^2\right\}. \quad (14)$$

The square root in (13) is defined as having a branch cut from $h_0=-(2Q)^{-1/2}$ to $+(2Q)^{-1/2}$; this ensures that h goes to h_0 as $\omega\to\pm\infty$. As an example consider the case of a V giving a resonance of width Δ at energy x_0. In the vicinity of x_0, we may write

$$h_0(x+i\delta)=\frac{\mathfrak{F}}{1-V\mathfrak{F}}\cong-\frac{1}{V}\frac{1}{1-V\mathfrak{F}},$$
$$=A/[(x-x_0)+i\Delta\,\mathrm{sgn}\delta],$$

where $A=-1/V^2F_{\gamma'}(x_0)$, $\Delta=F_i(x_0)/F_{\gamma'}(x_0)$, $\mathfrak{F}(x+i\delta)=F_\gamma+iF_i$, and x_0 is that root of $VF_\gamma=1$ at which $F_{\gamma'}$ is negative (neglecting self-energy effects of the uniform gas,

$$\mathfrak{F}(z)=\frac{1}{V_p}\int\frac{1}{z-\epsilon_k+\epsilon_F}\frac{d^3\vec{k}}{(2\pi)^3}$$

and so F_i is negative so that Δ is positive). Then from (14)

$$h(x+i\delta)=\frac{1}{2QA}\{(x-x_0+i\Delta\,\mathrm{sgn}\delta)-[(x-x_0+i\Delta\,\mathrm{sgn}\delta)^2-4QA^2]^{1/2}\}. \quad (15)$$

Converting the sum in (14) to a contour integral around the real axis and neglecting its very weak temperature dependence we find

$$\frac{4\beta Q^2A^2}{3v}-A^2Q=\frac{\beta}{3\pi}\mathrm{Im}[\tfrac{2}{3}(-x_0+i\Delta)^3-4A^2Q(-x_0+i\Delta)-\tfrac{2}{3}\{(-x_0+i\Delta)^2-4A^2Q\}^{3/2}]. \quad (16)$$

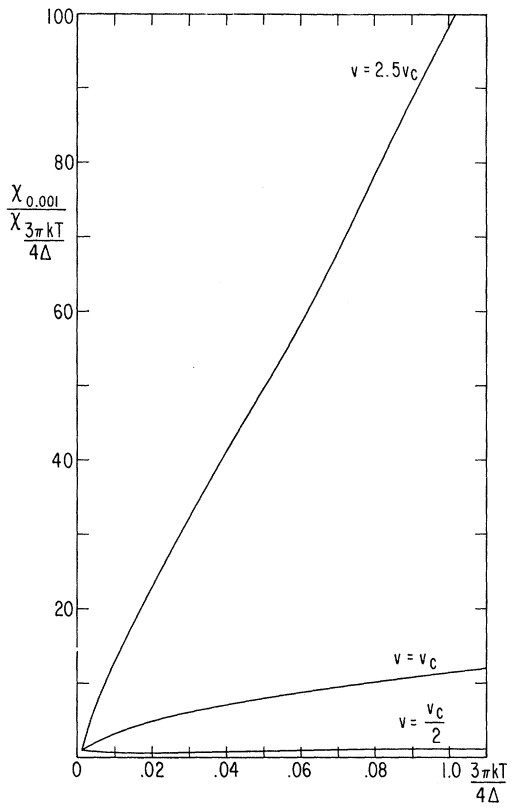

FIG. 3. Reciprocal susceptibility arbitrarily normalized to the susceptibility at $3\pi kT/4\Delta = 0.001$. For $v/v_c \ll 1$, the whole series in Eq. (12) should be taken into account.

Equations (15) and (16) are especially conveniently analyzed if the resonance is at the Fermi level, $x_0 = 0$. The following behavior is then found: Disregarding the term A^2Q, on the left-hand side, Eq. (16) has a root only if the initial curvature of the right-hand side near $Q = 0$ exceeds that of the left-hand side. This happens if $v > v_c = \pi\Delta/A^2$ holds (Wolff's condition). If $v \gg v_c$ the term A^2Q can be totally disregarded, Q becomes independent of β, $\gamma(0)$ which is $-\frac{4}{3}\beta Q$ goes like $1/kT$, and the susceptibility, which can be written $\simeq(g\mu_B)^2\frac{4}{3}Q\beta(3/4\beta Q - 1/v)^2$, will have a leading $1/T$ term. On the other hand, if $v \ll v_c$, (16) has a root only by dint of the $-A^2Q$ term on the left-hand side of (16). This root is of order $Q = v/\beta$. γ is then temperature independent, and so is M/H. The transition between the two regimes is, of course, smooth. Some computed results are shown in Fig. 3.

We note that there is no trace of the Kondo effect.[7] This may be due to one of several shortcomings. For example, the emphasis on the $\gamma(0)$ term in Eq. (11) obviously becomes unjustifiable at very low temperatures. Also, all particle-particle correlation effects, which frequently lead to logarithmic temperature dependence, have been neglected. Studies of these questions are still in progress.

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[5]The calculation was first done using the more familiar decomposition $\frac{1}{2}(\delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4} \pm \delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_3})$. The present more convenient form was suggested by D. R. Fredkin.

[6]A more accurate initial $h(i\omega)$ could be obtained by solving $h_0^{-1} - h^{-1} + (3/4\beta)h\sum_\nu\gamma(i\nu) = 0$, and substituting this h into $-(3/4\beta)\sum\gamma(i\nu)\,[h(i\omega + i\nu) - h(i\omega)]$ to obtain the correction. However, because of the presumably rapid convergence of $\sum\gamma(i\nu)$, this should not cause a serious quantitative change at high T.

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