MAGNETIC INTERACTIONS IN THE HUBBARD MODEL

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ABSTRACT

The Hubbard model is treated with the binary self consistent approximation. Within this approximation magnetic moments are introduced self consistently. The Ising type interactions were calculated explicitly in the limit of small temperature. Relaxing the static character of the approximation the interactions are transformed to Heisenberg type and are renormalized in their size. The renormalization is necessary in order to satisfy certain sum rules. The results are in good agreement with existing exact results 1-d.

By introducing a magnetic field the values of short range order and of the moments change. The self consistent bands are displaced and distorted.

For small magnetic field several approximations are applied. The change of the moments is found proportional to H^2 . The negative magnetoresistance of extrinsic semiconductors is explained as an elimination of moments. The persisting disagreements with certain experimental data are explained as effects of metastability.

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I. INTRODUCTION

Many body effects are important for the explanation of magnetism, metal insulator transitions and other phenomena.[1]

The field theoretical treatment of many particle systems is very difficult for practical purposes, and this leads us to seek a model that will be easy enough to understand and be amenable to approximations. First was tried the jellium model but it was found inadequate to explain insulating behavior for materials that we expect to have metallic behavior on the basis of Bloch-Wilson theory.[2] The ground state of many materials which are insulators is also antiferromagnetic. This was explained by Slater[3] by the fact that antiferromagnetism introduces cells of double size than before in the real space and this leads to gaps at the edges of the reduced first Brillouin zone.[2,3]

An objection to this explanation is the fact that many of these materials remain insulating for temperatures greater than the Neel temperature where according to this idea we should have metal.[2 3] Mott[1,2] noted that starting with Bloch states we should have conducting bands no matter how big the interatomic distance is. So for this case it is better to start with Wannier functions which are localized around sites.[1,2,3]

This idea was employed in treating semiconductors, impurities, etc. An electron may jump from one site to another and this depends on the effective Coulomb repulsion,U, that the electron feels on the next site. If the electron on the next site has the same spin as the electron which jumps to this site then by virtue of Pauli's principle it will stay away from it and the jumping electron will not feel the repulsion; otherwise it pays a lot of energy to move to the next site if the repulsion is big. So we see that the spin of the electron on the next site is very important. The correlations as we see are important in determining the nature of the material, i.e. if it is metal or insulator. Another important effect of the correlations between sites is the appearance of magnetic order.[1,3] The magnetic order is related to the appearance of localized moments[3]. Magnetic moments are formed when it is favorable energetically. This depends on the value of U and the transfer matri elements V_{ij} for jumps from site i to site j and the temperature. Cyrot[3] and more recently Economou and others [4,5] have studied extensively the case of $V_{ij} = V$ if ij nearest neighbors and zero otherwise. They found that for one dimensional lattices and for lattices which do not have closed loops moments appear for $U/V \rightarrow 0$. For 3-d there is a critical value of $U/V = u_3$ such that moments appear only for $U/V \geq u_3$. By studying the temperature behavior

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of such systems they found that there exist temperatures which depend on U/V at which the moments disappear.[5] The moments can be ordered or disordered so we can have ferromagnetism,[1] antiferromagnetism[3, 4, 5] and paramagnetism. They also scatter electrons and so contribute to the resistance. As was found experimentally the application of magnetic field on some extrinsic semiconductors produces negative magnetoresistance.[6,7] This is due to the fact that moments become ordered or tend to disappear with the application of a magnetic field. To describe the above effects we need a model which can give rise to correlations between sites, and includes parameters like coulomb repulsion U and transfer elements between sites $V_{i,j}$;thus depending on U/V we can have either metallic or insulating behavior. For U → 0 we should get back the free electron gas results. To include coulomb repulsion Hubbard[8] proposed a term $U\hat{n}_{i\uparrow}\hat{n}_{J\downarrow}$ where $\hat{n}_{i\uparrow},\hat{n}_{J\downarrow}$ are occupation operators for site i spin up (↑) or down (↓). This is a good approximation for many cases.

Hubbard formalized the above by writing the hamiltonian of the system:[8] 8

$$\hat{H} = \sum_{i\sigma} \epsilon_0\, \hat{n}_{i\sigma} + \sum_{ij\sigma} V_{ij\sigma}\, \alpha^{+}_{i\sigma} a_{j\sigma} + U \sum_{i} \hat{n}_{i\uparrow}\hat{n}_{J\downarrow} \qquad (1.1)$$

where the sites {i} form a lattice, σ = +1 for spin up and

-1 for spin clown; V_{ij} is the transfer matrix for hopping from i to j, and U is the Coulomb repulsion, $\alpha_{i\sigma}^{+}$ $\alpha_{j\sigma}$ are creation, annihilation operators of an electron at the Wannier state |i>, with spin σ; $\hat{n}_{i\sigma}$ is the corresponding number operator. We considered the case $V_{ij}= V$ for ij nearest neighbors and zero otherwise.

The Hubbard model is soluble only .in 1 dimension;[9] otherwise we need to find approximate solutions which behave reasonably. The first approximation we made was to restrict ourselves to the case where the sites {i} form a Bethe lattice (Cayley tree) i.e. a lattice containing no closed loops and completely characterized by the number of nearest neighbors Z or connectivity K = Z - 1. The second approximation we employed is the so called binary self consistent static approximation as developed by Economou and others in a series of papers.[4, 5]

In the binary, self-consistent, static approximation [3,4,5] one replaces the term $U\hat{n}_{i\uparrow}\hat{n}_{j\downarrow}$ by $\epsilon\hat{n}_{i\sigma}$, where the probability distribution of the random variables $\{\varepsilon_{i\varsigma}\}$ is given by

$$p(\in_{i\uparrow},\in_{i\downarrow}) = \frac{1}{2}\delta\left(\in_{i\uparrow}-\frac{1}{2}U(n-\mu)\right)\delta\left(\in_{i\downarrow}-\frac{1}{2}U(n+\mu)\right) + \tfrac{1}{2}\delta\left(\in_{i\uparrow}-\tfrac{1}{2}U(n+\mu)\right)\delta\left(\in_{i\downarrow}-\tfrac{1}{2}U(n-\mu)\right) \quad \mathbf{(1,2)}$$

n is the number of electrons per lattice site and y is a quantity to be determined self-consistently from the equation

$$\mu = \langle \bar{n}_{i\uparrow}\rangle_{\iota-\theta} - \langle \bar{n}_{i\downarrow}\rangle_{\iota-\theta} \qquad (1.3)$$

where the bar indicates quantum mechanical average and the brackets indicate average over the random variables $\{e_{j\sigma}\}$;the subscript i = u indicates a partial averagew here $\epsilon_{\iota\uparrow,}$ $\epsilon_{\iota\downarrow}$ are kept equal to U (n - μ) / 2 , U(n + μ)/2 respectively.

The quantity μ can be interpreted as the magnitude of a local moment.

In a series of recent papers [4,5] the binary, static Approximation was generalized as to incorporate the possi-Bility of magnetic ordering: A quantity P was introduced giving the probability of having $(\epsilon_{\iota\uparrow,}\epsilon_{\iota\downarrow}) = (U(n - \mu)j2,$ $U\{n + \mu)/2$ under the condition that $\epsilon_{j\uparrow,}\epsilon_{j\downarrow}) = (U(n + \mu)/2,$ $U(n - \mu)/2)$,where j is a nearest neighbor site of i. In other words, P gives the probability of the local moment at the site I being up under the condition that the moment at the site j is down. The quantity P was determined by minimizing the free energy of the system:

$$\frac{\partial F}{\partial P} = 0 \quad (1.4)$$

The free energy is found from the relation:

$$F = \ <\bar{H}> \ - \ \mathrm{TS}$$

<^H^>is thetotal energy, S the entropy. The entropy is composed From two parts:The electronic entropy S and the lattice enentropy S_1.The latter is equal to NK_BT In Ω where Ω is the number of arrangements of momentfor a given P and N is the number of sites.

The electronic part of the entropy per site

$$S_e' = -2\kappa_B \int dE\ [flnf + (1-f)\ln(1-f)]\rho + k_B \frac{U\mu}{4}\int \frac{dE}{E}(\rho_A - \rho_B)[flnf + (1-f)\ln(1-f)] \quad (1.6)$$

and the energy per site is

$$\mathbf{H'} = \mathbf{2}\int \mathrm{d}E\, E\, f(E)\rho(E) - \frac{1}{2}U(n^2 - \mu^2) \qquad (1.7)$$

In (1.6) and (1.7) ρ is he density of states per site, f is the fermi function, ρ_A, ρ_B are the partial DOS for spin up for the sites with potentials $\varepsilon\uparrow = \frac{U}{2}(n-\mu)$; $\varepsilon\downarrow = \frac{U}{2}(n+\mu)$ respectively.

From 1.4 we have:

$$\frac{\partial F'}{\partial P} = \frac{\partial}{\partial P}(\langle H'\rangle - TS_e') - T\frac{\partial S_l'}{\partial P} = 0$$

S_l' depends only on **P**: $S_l'(p)=f_1(P)$ **F**or 1 - d we have $S_l'(P) = k_B\{PlnP + (1-P)\ln(1-P)\}^5$. In ref. 5 it is argued that the determination of P is mathematically equivalent to solving the Ising model with nearest neishbor coupling only. P then is a function of BJ where J is the nearest neighbor coupling, β = 1/T:

$$P = \frac{1}{2} + f_2(\beta J) \qquad (1.8a)$$

For Izing systems $\frac{|\partial S_l}{\partial P} == ZJ/T$ (Z is the number of the nearest neighbors). So finally eq. (1.4) is rewritten

$$J = \frac{1}{Z}\frac{\partial F'_e}{\partial P} = \frac{1}{Z}\left(\frac{\partial\left(\langle H'\rangle - TS'_e\right)}{\partial P}\right) \qquad - \qquad (1.8b)$$

So instead of one equation(1.4) we have a system of equations: (1.8a, 1.8b).

In what follows we examine the special case n = 1 (one electron per site) for which the chemical potential is zero for all T.

For the n= 1 case examined here, it has been shown[5] that, at T = 0, P = 1, i.e. in the ground state the moments arrange themselves antiferromagnetically. Then Eq. (1.5) can be rewritten[5] as

$$J \to_{T\to 0} -\frac{\Delta\bar{H}_m}{2m} \qquad (1.9)$$

where $\Delta\bar{H}_m$ is the change in the total ground state energy when m of the NZ/2 antiparallel pairs of nearest neighbor moments change to a parallel configuration.

For the quantity J to be well defined the right hand side of Eq. (1.9) must be independent of m. We shall return to this point.

It was further demonstrated[4'5] that relaxing the static approximation results in changing the character of the magnetic interactions from Ising-like to Heisenberg-like. This change affects the various quantities of physical interest (such as the thermodynamic ones) both directly and indirectly through the modification (renormalization) of the self-consistently obtained u, J, $\rho(E)$. It was shown[4,5] that the renormalization of J is significant.

In the present work we calculate first in Section II the quantity J according to Eq. (1.9) for two values of m: (a) m = 1, corresponding to an improper joining of two perfectly antiferromagnetic semi-infinite segments (the corresponding J is denoted by J_b); (b) m = Z, corresponding to flipping one local moment (the corresponding J is denoted by J_F). We find that $J_F \neq J_B$ This discrepancy is attributed to additional interactions among non nearest neighbor moments. We generalized Eq. (1.9) to obtain an expression for the general coupling J_{nm}, where n, m are arbitrary sites. Explicit analytic results for all J_{nm} are obtained in the limit $T \rightarrow 0$. In this limit the quantities J_b, J_F can be easily expressed as a proper sum over all J_{nm}. It is shown that these sum rules are not satisfied in general. This discrepancy is attributed to the static approximation. In Section III we present an approximate scheme for renormalizing the various J's as a result of relaxing the static approximation. In some limiting cases where this renormalization is zero the sum rules are satisfied exactly. Furthermore, this renormalization greatly reduces the discrepancies in the sum rules over the whole range of U/B, where B is the half-width of the unperturbed (U = 0) band. We are thus led to propose that the various J's when properly renormalized are satisfying exactly the sum rules.

In Section IV we generalize our work to finite temperatures and we present explicit results for the temperature dependence of J_F. In Section V, using our results for the various J's, we calculate certain physical quantities for which exact results are available. Excellent quantitative agreement is obtained, which strongly indicates that the low lying excitations of the Hubbard model are identical with those of a system of local moments μ of spin 1/2 coupled through Heisenberg type interactions.

In Section VI we generalize our formulation to incorporate the presence of an extra magnetic field. We study in some detail the important case of small fields when several approximations can be employed. In Section VII we apply the formalism in an attempt to .explain the above mentioned negative magnetoresistance of some extrinsic semiconductors,

•II. CALCULATION OF J's AT T = 0

A. Basic Formulae

As was mentioned in the introduction in the ground state the moments arrange themselves antiferromagnetically, i.e. in an alternating up (u), down (d) configuration (see Figure la): The effective Hamiltonian H^, describing the motion of a spin cr electron in the static self-consistent approximation is

$$\hat{H} = \sum_{i\sigma} (\epsilon_0 + \epsilon_{I\sigma}) \hat{n}_{i\sigma} + \sum_{ij} V_{ij}\, \alpha_i^{+} a_j \qquad (2.1)$$

where the site energy $\varepsilon_0 + \varepsilon_{i\sigma}$ is

$$\varepsilon_0 + \varepsilon_{i\sigma} = \varepsilon_0 + \frac{U}{2} \pm \frac{U\mu}{2} \qquad (2.2)$$

For simplicity we choose $\varepsilon_0 + U/2 = 0$; then the site energies for a spin up electron ($\sigma = +1$) are as shown in Figure lb, where

$$x = U\mu/2 \quad ' \qquad (2.3)$$

The site energies for a spin down electron (a = -1) are shown in Figure 1C.

Because of the periodicity, there are only two different diagonal matrix elements of the Green function

$G_{i\sigma}(E) = <(ij(E-\overline{H}_{\sigma})^{-1}|\, iy$: one corresponding to site 0 of Figure lb and denoted by G_A and the other corresponding to site 1 of Figure lb and denoted by G_B. As shown in Appendix I G_A, G_B are given by

$G_AE) = 2K(E + x) [(K-1] (E^2 - X^2) + (K+1) (E^2 - x^2)^{1/2} (E^2 - x^2 - B^2/^2]^{-1}$ (2.4)

$G_R (E) = 2K(E - x) [(K-1) (E - x) + (K+1) (E - x) \quad (E - x - B) \quad]^{-1}$ (2.5)

where

$B = 2K^{1/2}V$ (2.6)

The corresponding site DOS ρ_A, ρ_g are given by

$$\rho_\alpha = - \frac{I}{p} \text{ Im } G_a(E^+), \quad a = A, B \qquad (2.7)$$

where E^+ denotes the limit of $G_a(E + is)$ as $s \to 0^+$. The self-consistency Eq. (1.3) for the size of the moment u becomes

$$\mu = \int_{-\infty}^{0} [\rho_B(E) - \rho_A(E)] \delta E \qquad (2.8)$$

For practical calculations we start with a chosen x; we evaluate then, G_A, $_{GB}$, ρ_A, ρ_B and mfrom Eq. (2.8). Having thus x and μ we obtain the corresponding U from Eq.. (2.3).

The ground state energy is given by

$$<\bar{H}'>_G = 2\int_{-\infty}^{0} \mathrm{d}E\, E\, f(E)\, p(E) - \frac{1}{2}U(n^2 - \mu^2) \qquad (2.8)$$

where

$$\rho(E) = \frac{1}{2}(\rho_A(E) + \rho_\beta(E)) \qquad (2.9)$$

B. Calculation of J_b

According to Eq. (1.9) the quantity ' can be written as $\frac{1}{2}(H_G - H_{\alpha'})$ where $\bar{H}_G$ is the total energy of the ground state configuration shown in Figure $\bar{H}_{\alpha'}$ la and is the energy of the configuration shown in Figure la^1. The difference $\bar{H}_G - \bar{H}_\alpha$, can be written as

$$\bar{H}_G - \bar{H}_{\alpha'} = \sum_{n\varsigma} \int_{-\infty}^{0} dE\, (\rho_{n\sigma}(E) - \rho_{n\sigma}{}^+(E))$$

$$= \sum_{n\varsigma} (-\frac{Im}{\pi}) \int_{-\infty}^{0} dE\, (G_{n\sigma}(E^+) - G_{n\sigma}{}^+(E^+)) \qquad (2.10)$$

where the unprimed quantities refer to the ground state configuration and the primed to the configuration shown in Figure la^1. Separating the contributions from the spin up ' (σ = 1) and the spin down (σ = -1) and the contributions from the left semi-infinite segments (I, III,I^1, III") from the right semi-infinite segncnts (II, IV, II', IV') (see Figure 1] we can write

$$\bar{H}_G - \bar{H}_{\alpha'} = (\bar{H}_I - \bar{H}_{I'}) + (\bar{H}_{II} - \bar{H}_{IV'}) + (\bar{H}_{III} - \bar{H}_{III'}) + (\bar{H}_{IV} - \bar{H}_{IIV'}) =$$

=

$$2(\bar{H}_I - \bar{H}_{I'}) + 2(\bar{H}_{II} - \bar{H}_{VI'}) \qquad (2.11)$$

where, e.g.

$$\bar{H}_I - \bar{H}_{I'} = \sum_{n\varsigma} (-\frac{Im}{\pi}) \int_{-\infty}^{0} dE\ (G_{n\uparrow}(E^+) - G_{n\uparrow}{}^{+}(E^+)) \qquad (2.12)$$

To evaluate the sum $\sum_i G'_{n\uparrow}(E^{=})\mathrm{E}^{+})$ we replace the configuration of Figure (lb') (reproduced in Figure 2a) by the configuration in Figure 2b, where the quantity e is determined in such a way that

$$G^{I}{}_{n\uparrow}(E^+) = G^{II}{}_{n\uparrow}(E^+) \qquad (2.13)$$

for all n belonging to I' or I". Equation (2.13) is written for site 0

$(E - e - (K + l)t_A)^{-1}$ « $(E - x - Kt_A - t_B)^{1}$

So

$$\tilde{\varepsilon} = x + t_A(E) - t_B(E) \qquad (2.14)$$

where the quantities $t_A(E)$, $t_B(E)$ are defined by

$$(K+1)t_B(E) = E - x - G_A^{-1} \qquad (2.15a)$$

$$(K+1)t_A(E) = E + x - G_B^{1} \qquad (2.15b)$$

(See Appendix I).

$G_{n\uparrow}$ and $G^{II}{}_{n\uparrow}$ correspond to Hamiltonians having only one site energy different, namely the one at site 0. Hence the difference $G_{n\uparrow} - G^{II}{}_{n\uparrow}$ can be expressed as:

$$G_{n\uparrow} - G^{II}{}_{n\uparrow} = G_{n0\uparrow}G_{0n\uparrow}\frac{x-\tilde{\varepsilon}}{1-(\tilde{\varepsilon}-\chi)G_A} \qquad (2.16)$$

where G_{nm+} is the n,m matrix element of G corresponding to the periodic configuration of Figure 1b. Taking into account Eqs. (2.12, 2.13, 2.14, 2.16) we obtain

$$\bar{H}_I - \bar{H}_{I'} = \bar{H}_I - \bar{H}_{I'} = \sum_{n\varsigma}\left(-\frac{Im}{\pi}\right)\int_{-\infty}^{0} dE\, \frac{t_B - t_A}{1-(t_A-t_B)}\sum_{n\varepsilon I} G_{n0\uparrow}\,G_{0n\uparrow} \qquad (2.17)$$

The sum

$$\sum_{n\varepsilon I} G_{n0\uparrow}\,G_{0n\uparrow}$$

can be evaluated explicitly (see Appendix II)

$$\sum_{n\varepsilon I} G_{n0\uparrow}\,G_{0n\uparrow} = (G_A^2 - k\dot{G}_A)/(\dot{K}+1) \qquad (2.18)$$

where $\dot{G}$ is the derivative with respect to energy of G_A.

In a similar way one can prove that $\bar{H}_{II} - \bar{H}_{II'}$ is given by an expression resulting from Eqs. (2.17, and 2.18) by replacing A -* B and B ->• A. Thus the final expression for $J_b = \frac{1}{2}(\overline{H}_G - \overline{H}'_G)$) is

$$J_b = -\frac{1}{2\pi} Im\left\{ \int_{-\infty}^{0} dE \cdot E \left[\frac{2(t_{B-}t_A)}{1-(t_{A-}t_B)G_A} \cdot \frac{G_A^2 - K\dot{G}_A}{K+1} + \frac{2(t_{A-}t_B)}{1-(t_{B-}t_A)G_A} \cdot \frac{G_B^2 - K\dot{G}_B}{K+1} \right] \right\} \tag{2.19}$$

he functions $t_A(z)$, $G_A(z)$, a = A, B are analytic for Im z ≠ 0 with

$$t_B^*(-E + iy) = -t_A(E+iy) \tag{2.20a}$$

$$G_B^* (-E+ iy) = -G_A(E+ iy) \tag{2.20b}$$

Moreover the sign of Im t^ and Im G^ is opposite to the sign of Imz. The integrand in Eq. (2.19) has two branch cuts, one from $\sqrt{s^2+B^2}$ to -x and the other from x to $\sqrt{s^2+B^2}$; it exhibits two isolated poles at ±E^, (0 £ E^ <_ x) given by

$$t_A(E_b) - t_B(E_b) = G_A^{-1}(E_b) \tag{2.21a}$$
$$t_B(-E_b) - t_B(-E_b) = G_B^{-1}(-E_b) \tag{2.21b}$$

Two more poles may appear at $\pm\overline{E_b}$ ($(x^2 + \mathbf{B^2})^{1/2} < \overline{E_b}$)) as a second root of Eqs. (2.21a, 2.21b). For the 1-D case (K=1) the poles at $\pm\overline{E_b}$ are always present.

$$J_b = \frac{1}{2}\lim_{s\to 0^+} -\frac{1}{\pi} Im\left(\int_{-(x^2+B^2)^{1/2}-s}^{-x+s} dE \cdot E\,\varphi_n\,(E^+) \right) + \frac{1}{2}\sum_i R_{bi}E_{bi} \quad (2.22)$$

Where $\varphi_b(E)$ is the quantity in parentheses in Eq (2.19),

And E_{bi}, R_{bi} are its poles and residues;the summation in

Eq(2.22)runs over the poles with $E_{bi} \leq 0$. The poles

Are the zeros of the expression $1-(t_A - t_B)G_A$. Using

The formulae AI.3a,3b (Appendix I) we get:

$$|E_g| = ((V^2(K + I)^2 + 4Vx(K-1) + x^2)^{1/2} - V(K+l))/2 \qquad (2.23)$$

The residues of φ_b are ½ because at E_b $t_A = E - x - Kt_b$ and

From AI.2a, 2b, $\frac{d}{dE}(E - x - kt_B) + t_A(1 - k\dot{t}_G) = 0$ so

$$\dot{t}_A(E - \dot{x} - kt_B) + t_A(1 - k) = 0$$

Or

$$\dot{t}_A + 1 - k\dot{t}_B = 0 \text{ -}$$

$$\frac{d}{dE}(G_A^{-1} - t_A + t_B) = \frac{d}{dE}(E - x - kt_B - t_A) = 2(1 - k\dot{t}_B) = 0$$

$$= \left(1 - \frac{K}{K+1}\frac{\dot{G}_A}{G_A^2} - \frac{K}{K+1}\right) = 2\frac{G_A^2 - K\dot{G}_A}{(K+1)G_A^2}$$

So the residue at the zero of $1-(t_A-t_B)G_A$ is

$$\frac{(t_A - t_B)G_A^{-1}}{\frac{d}{dE}(G_A^{-1}(t_A - t_B))}\frac{G_A^2 - K\dot{G}_A}{(K+1)} = \frac{1}{2} \qquad (2.24)$$

A simpler way to evaluate the integral in (2.19) is to consider a closed contour consisting of the negative real semiaxis, the positive imaginary semiaxis and the portion on a circle at infinity. The latter gives no contribution because $\phi_b(Z)\ \alpha\ z^{-3}$ as $z\to\infty$ • Hence

$$J_b = -\frac{1}{2\pi} Im\left(\int_{-\infty}^{0} dE\cdot E\,\varphi_b(E)\right) = \frac{1}{2\pi} Im\left(\int_{0}^{\infty} d(iy)\cdot iy\,\varphi_b(iy)\right)$$

$$= -\frac{1}{2\pi} Im\left(\int_{0}^{\infty} dy\cdot y\,\varphi_b(iy)\right) \qquad (2.25)$$

Since the function $\varphi_b(z)$ is analytic for Imz f 0 and has symmetric branch cuts and poles on the real axis it can be expressed as

$$\varphi_b(z) = \frac{2z}{\pi}\lim_{z\to 0^+}\int_{-s'-s}^{-x+s}\frac{Im\varphi_n(E^+)dE}{z^2-E^2} + \frac{1}{2}\sum_{E_{bi}<0}\frac{2zR_{bi}}{z^2-E^2} \qquad \mathbf{(2.26)}$$

Eq. (2.26) is useful for the discussion of the renormalization of j"k. in Section III. To obtain explicit results for we have used Eq. (2.25) with ^(iy) expressed in terms of G^ and as follows:

$$Im\varphi_b(iy) == Im\frac{2(G_B - G_A + 2G_BG_A)\left(G_A - \frac{K}{G_A}\frac{dG_A}{idy}\right)}{(KG_B + G_A - 2xG_BG_A)}\frac{1}{K+1} \qquad (2.27)$$

where

$$G_A(iy) = -2K(x+iy)/D \quad ; \quad G_B(iy) = 2K(x-iy)/D \quad ,(2.23)$$

$$D = (K-1)(x^2+y^2) + (K+1)*(x^2+y^2)^{1/2}(x^2+y^2+B^2)^{1/2}$$

(2.29)

The quantity x equals Uy/2.

J_b, is negative for all values of U/B and for all K; this verifies that the antiferromagnetic arrangement of the local moments is a local energy minimum. In the limit U/B → ∞ we obtain from Eqs, (2.23, 2.25 , 2. 26, 2.27 that

$$J_{b\ U/B\to\infty} \to -V^2/U \qquad (2.30)$$

which is independent of K. Eq. (2.30) is the standard result in this limit. 3 In the metallic limit, U/B -* 0, we have

$$J_{b\ U/B\to 0} \to -\frac{x}{K+1} \qquad (2.31)$$

Note that as U/B → 0, x approaches zero as exp(-cB/U), where c is a constant. In Fig. 3 we present our results for J_b vs U/B for various values of K. We observe that the quantity $(K+1)J_b/B$ is weakly dependent on K (except for. the K = 1 case) for not so large U/B. $|J_b|$ vs U/B exhibits a maximum for U/B ≈ 1.25.

C. Calculation of J_F

As was mentioned in the introduction the quantity Jp is defined by

$$J_F = -\frac{\Delta\hat{H}_F}{2(K+1)} \qquad (2.32)$$

where $\Delta\bar{H}_F = \bar{H}_F - \bar{H}_G$ with $\bar{H}_G$ the total energy of the ground state and Hp the total energy of a state resulting from the ground state by flipping one local moment. Thus

$$\Delta\breve{H}_F = -\sum_{n\sigma}\frac{1}{\pi}Im\left(\int_{-\infty}^{0} dE\cdot E\,[G^F_{nm_b}(E^+) - G_{nm}(E^+)\right)$$

Assuming (without loss of generality) that the site of the flipped moment is the 0 site (see Fig. la) we have

$$G^F_{n\sigma} = G_{n\sigma} + G_{n0\sigma}G_{0n\sigma}\frac{-2x\sigma}{1+2xG_A} \qquad (2.34)$$

Thus

$$\Delta\breve{H}_F = -\frac{1}{\pi}Im\left(\int_{-\infty}^{0} dE\cdot E\,\frac{-2x}{1+2xG_{0\uparrow}}\sum_n G_{0n\uparrow}G_{n0\uparrow} + \frac{2x}{1-2xG_{0\downarrow}}\sum_n G_{0n\downarrow}G_{n0\downarrow}\right) \qquad (235)$$

The summation $\sum_n G_{0n\sigma}G_{n0\sigma}$can be performed explicitly (see Appendix II) giving 1

$$\sum_n G_{0n\sigma}G_{n0\sigma} = -\frac{dG_{0\sigma}}{dE} \quad (2{,}36)$$

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hence

$$\Delta\widetilde{H_F} = \frac{1}{\pi} Im\left(\int_{-\infty}^{0} dE\cdot E\left[\frac{-2x(dG_A/dE)}{1+2xG_A}+\frac{2x(dG_B/dE)}{1-2xG_B}\right]\right) \tag{2.37}$$

Eq. (2.37) can be rewritten after integrating by parts as

$$J_F = \frac{1}{2\pi}\int_{-\infty}^{0} dE\cdot ln|[1+2xG_A][1-2xG_B| \tag{2.38}$$

One can change the integration path to the positive imaginary halfaxis as before; then Jp can be expressed as

$$J_F = \frac{1}{2\pi(K+1)}\int_{o}^{\infty} dy\cdot ln|[1+2xG_A(iy)][1-2xG_B(iy)]| \tag{2.39}$$

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If Eq. (2.37) is used for the calculation of Jp one should keep in mind that contributions are made by the poles of the quantity in parentheses. One such pole is at -Ep, where 0≤ Ep < x, with a residue equal to -1; this pole coincides with the zero of $1 - 2xGp$ when $x \leq x_C$, and with the zero of $1 + 2xG_A$ when x _≥ x_c; when $x \approx x_c \equiv (K+1)B/2\sqrt{K(2K+1)}$, $E_F = 0$. As can be seen from Eq. (2.39) J_F vs x is expected to develop a singularity when $E_F = 0$, i.e. when $x = 0, x_c$. Note that the quantity $\delta_c = 2x_c/B$ is weakly depending on K (for K = 1 $6_c = 2/\sqrt{3} \approx$ 1.154 and for K →∞ $\delta_C = 1//2 \approx .707$). Another pole at

$-\ddot{E}_F$ $(\ddot{E}_F > \sqrt{x^2 + B^2}\}$ ay appear for large enough x coming from the zero of $1 + 2xG_A$; in the 1 - D this pole is always present.

One can express J_F in a form analogous to Eq. (2.22), l-e.

$$J_F = \lim_{s\to 0} \frac{-Im}{2\pi(K+1)} \left(\int_{-(x^2+B^2)^{\frac{1}{2}}-s}^{-x+s} dE \cdot E\, \varphi_F(E^+) + \frac{1}{2(K+1)}(E_F + \breve{E}_F) \right) \qquad (2.40)$$

where the quantity φ_F (i.e. the quantity in parenthesis in Eq. (2.37)) can be written in a way similar to Eq. (2,24). In arriving at Eq. (2.40) we have taken into account that the residues of φ_F at the $-E_F$, $\overset{\approx}{-\dot{E}_F}$ poles are equal to -1, For K = 1 (1 - D case) Eq. (2.40) can be rewritten after one integration by part as

$$(2K+1)\,J_F = E_F - x + \tilde{E}_F - (x^2 + B^2)^{\frac{1}{2}} - \frac{1}{\pi}\left(\int_{-(x^2+B^2)^{\frac{1}{2}}}^{-x} dE\, Im\, ln[(1+2xG_A)(1-2xG_A)] \right) \qquad \mathbf{(2.41)}$$

Eq. (2.41) is valid for K > 1 and x large enough £so that the pole $-\overset{\cdot v}{\tilde{E}_F}$ is present); for small x the terms $\tilde{E}_F$ and $--(X^2 + B^2)^{1/2}$are absent.

For explicit calculations Eq. (2.39) is more convenient. One can easily show that ^

$$J_F \to_{U/B\to\infty} -\frac{V^2}{U} \qquad (2{\cdot}42)$$

for all K, which agrees with the same limit for J_b. The limit U/B → 0 (i.e. x → 0) requires some care, because the pole at -Ep approaches the integration range in Eq. (2.39). We found that the leading contribution to Jp as U/B -> 0 is

$$\mathrm{j_r} = -\frac{4\mathrm{k}}{\pi(\mathrm{K}+1)}\frac{\mathrm{x}^2}{\mathrm{B}}\ln\frac{\mathrm{B}}{2\mathrm{x}} + \mathrm{O}\left(\frac{\mathrm{x}^2}{\mathrm{B}}\right) \qquad (2.43)$$

Note that J_F approaches zero as U/B→0 much faster than J_b,| J_b| vs x exhibits a maximum at x = x_c where dJ_b/dx is discontinuous. Explicit results for J_F vs U/B are shown in Figure 4 for various values of K. We observe again that the quantity $(K+1)J_F/B$ is not so strongly depended on K.

Comparing Figures 3 and 4 one sees that $J_F \infty J_b$ (except in the limiting case U/B → ∞). Furthermore the difference is more pronounced in the 1 - D case (K = 1). One can attempt to attribute this difference to interactions among non-nearest neighbor pairs. In this case the equivalent Ising coupling will have the form

$$\mathrm{H}_I = -\frac{1}{2}\sum_{nm} J_{nm}\sigma_n\sigma_m \qquad (2.44)$$

where each σ_n can be +1 (local moment up) or -1 (local moment down). in a Bethe lattice $J^\wedge{}_m$ depends only on the distance p between sites n and m measured by the number of non retracting steps between n and m, i.e. J_{nm} = Jp (p = 1,2,3...). The quantity Jp can be expressed in terms of Jn_m as

$$J_F = \frac{1}{Z}\sum_{n} \pm J_{0n} \qquad (2.45)$$

where the +(-) sign is taken when n is the same (other) sublattice as (than) the 0 site. For a Bethe lattice Eq. (2.45) simplifies to

$$J_F = \sum_{p=1}^{\infty} (-1)^{P-1} K^{p-1} J_p \quad (2.46)$$

since there are $(K+1)K^{p-1}$ pth nearest neighbors. The quantity J_b can be written as

$$J_F = \sum_{p=1}^{\infty} (-1)^{P-1} pK^{p-1} J_p \quad (2.47)$$

Thus, if Jp = 0 for p ≥2, then $J_b = J_F = J_1$; on the other hand for $J_p \neq 0$ (p = 1,2,3,...) $J_F \neq J_b$
We will n/>w generalize Eqy (1.9) to obtain explicit formulae forin terms of thej quantities G_A, G_B. Let us

&

call $\overline{H}_{Io}$ the value of H_I in!Eq. (2.44) when all σ are antiferromagnetically arrariged (ground state); $\overline{H}_{In}$ when only σ_n is flipped; $\overline{H}_{Im}$ when only σ_m is flipped and when both σ_n and σ_m are flipped. Using Eq. (2.44) we can easily show that

$$-4J_{nm}\sigma_n^o\sigma_m^o = \overline{H}_{Io^t} + \overline{H}_{Inm} - \overline{H}_{In} - \overline{H}_{Im} \qquad (2.48)$$

where σ_n^o σ_m^o are the values' of σ_n σ_m in the ground state, The quantity $A = \overline{H}_{Io^t} + \overline{H}_{Inm} - \overline{H}_{In} - \overline{H}_{Im}$ can be expressed in terms of the G^ corresponding* to the Hamiltonian H . We have

$$A = \sum_{i\sigma} \int_{-\infty}^{0} dE\, E\, (\rho_{i\sigma}^{m} + \rho_{i\sigma}^{n} - \rho_{i\sigma}^{nm} - \rho_{i\sigma})$$

$$-\frac{Im}{\pi} \sum_{i\sigma} \int_{-\infty}^{0} dE\, E\, (G_{i\sigma}^{m} + G_{i\sigma}^{n} - G_{i\sigma}^{nm} - G_{i\sigma}) \qquad (2.40)$$

$G_{i\sigma}$ is the periodic Green function corresponding to the configuration shown in Figure (lb, lc); $G_{i\sigma}^{m}, G_{i\sigma}^{n}, G_{i\sigma}^{nm}$ result from $G_{i\sigma}$ when site m or site n or both are flipped. We have already used the relation

$$G_{i\sigma}^{\rho} = G_{i\sigma} + G_{ir\sigma} t_{r\sigma} G_{ri\sigma} \qquad (2.50)$$

connecting $G^{r}_{i\sigma}$ with $G_{iς}$ and the t-matrix $t_{r\sigma}$,

$$t_{r\sigma} = 2\mathrm{x}\sigma\sigma_r^{O}/(1 - 2\mathrm{x}\sigma\sigma_r^{O}\mathrm{G\,rr\sigma}) \qquad (2.51)$$

In the case of two defects at n and m repeated application of Eq. (2.51) yields

$$G_i^{nm} = G_i + \frac{1}{C_{nm}}[G_{in}t_nG_{ni} + G_{im}t_mG_{mi} + G_{in}t_nG_{nm}t_mG_{mi} + G_{im}\,t_m\,G_{mn}t_nG_{ni}] \qquad (2.52)$$

with

$$C_{nm} = 1 - t_nG_{nm}t_mG_{mn} \qquad (2.53)$$

We have temporarily dropped the subscript σ. The quantity $\sum_i(G_i^m + G_i^n - G_i^{nm} - G_i)$ can be expressed in a closed formula by employing Eqs. (2.50-2.53) and Eq. (2.36):

$$\sum_i(G_i^m + G_i^n - G_i^{nm} - G_i) = \frac{t_nt_m}{C_{nm}}[G_{nm}\dot{G}_{mn} + G_{mn}\dot{G}_{nm} + t_nG_{nm}G_{mn}\dot{G}_n + t_m\,G_{mn}\&G_{nm}\dot{G}_m] -$$

$$= \frac{d}{dE}\ln C_{nm} \qquad (2.54)$$

where the dot indicates differentiation with respect to E. Thus we obtain the desired expression for J_{nm} , i.e.

$$4J_{nm}\sigma_n^0\,\sigma_m^0 = \frac{1}{\pi}Im\left(\int_{-\infty}^{0} dE\;E\frac{d}{dE}\sum_{\sigma} lnC_{nm\sigma}(E)\right) \qquad (2.55)$$

integrating by parts we have

$$4J_{nm}\sigma_n^0\,\sigma_m^0 = \frac{1}{\pi}\int_{-\infty}^{0} dE \sum_{\sigma} ln(1 - t_n G_{nm} t_m G_{mn}) \qquad (2.56)$$

transforming to an integration along the imaginary axis as before we obtain

$$4J_{nm}\sigma_n^0\,\sigma_m^0 = \frac{1}{\pi}\int_{-\infty}^{0} dy \sum_{\sigma} ln|1 - t_n(iy)G_{nm}(iy)t_m(iy)G_{mn}(iy)| \quad (2.57)$$

In the metallic limit, x → 0, and $t_{m\sigma}$ → $2x\sigma\sigma_m^o$ thus Eq. (2.57) can be written approximately as

$$J_{nm} \approx -\frac{x^2}{\pi}\sum_{\sigma}\int_{0}^{\infty} dy\, Re(G_{nm\sigma}(iy)G_{mn\sigma}(iy) \qquad (2.58)$$

Note that Eq. (2.58) is a good approximation in the opposite (atomic) limit, U/B→∞, as well. The reason is that G_{nmo} → 0 as U/B → ∞ for n≠m and furthermore $t_{n\sigma} t_{m\sigma \to_{U/B\to\infty}} 4x^2\sigma_m^o\sigma_n^o$t

should be mentioned that Eq.~t2.58) was obtained before by Lacour-Gayel and Cyrot[10]; these authors have shown that Eq. (2.5S) leads to the well known RXKY formula for the interaction of local moments in a metal.

In the metallic limit, U/B. → 0, the leading term is proportional to x^2 with a proportionality constant given in Eq. (2.58) with $G_{nm\sigma}$ replaced by $G^0_{nm\sigma}$ where the superscript zero indicates that x = 0, i.e. y = 0. If μ = 0 we obtain a periodic system for all T and consequently the limiting Eq. (2.58) can be used for non-zero T as well (apart from a fermi factor whose inclusion will be discussed later).

Using our explicit results for J_{nm}, J_F, J_b s we can show that that the sum rules (2.46), (2.47) are not satisfied in general. This proves that the interaction of the local moments cannot be described self-consistently through an Ising type coupling. We shall return to this matter in the next section.

One can express the quantities G_{NM} in terms of G_A, G_B (t_A, t_B) as shown in Appendix III. Then the expresion for Jp (P = n - m) becomes

$$J_{2l+1} = -\frac{1}{2\pi}\int_0^\infty dy\ ln\left|1+\frac{4G_AG_B\theta^{2l+1}x^2}{(1+2xG_A)(1-2xG_B)}\right| \qquad l=0,1,2,\ldots \tag{2.59}$$

where

$$\theta(iy) = t_A(iy)t_B(iy)/V\^{} \tag{2.60}$$

and

$$J_{2l} = \frac{1}{4\pi}\int_0^\infty dy\ ln\left|\left(1-\frac{4x^2{G_B}^2\theta^{2l}}{(1-2xG_B)^2}\right)\left(1-\frac{4x^2{G_A}^2\theta^{2l}}{(1+2xG_A)^2}\right)\right| \qquad l=0,1,2,\ldots \tag{2.61}$$

As we have shown before, in both the atomic (U/B→∞) and metallic (U/B→ 0) limits the logarithms in Eqs. (2.60, 2.61) can be expanded up to the first non vanishing term, in which case we obtain

$$J_{2l+1} \approx -\frac{2x^2}{\pi}\int_0^\infty dy\, G_A(iy)G_B(iy)\theta^{2l+1} \qquad (2.62)$$

$$J_{2l} \approx -\frac{x^2}{\pi}\int_0^\infty dy\left[{G_A}^2(iy) + {G_A}^2(iy)\right]\theta^{2l} \qquad (2.63)$$

Eqs. (2.62, 2.63) in the atomic limit, U/B→∞ yield the following explicit results for J_P

$$J_{2l+1} \approx -\frac{1\cdot 3\cdots(4l+1)V^{4l+2}}{2\cdot 4\cdots(4l+2)x^{4l-1}} + O\left(\frac{V^{4l+2}}{x^{4l+3}}\right) \qquad (2.64)$$

$$J_{2l} = -\frac{1\cdot 3\cdots(4l-1)4lV^{4l}}{2\cdot 4\cdots 4l(4l+2)x^{4l-1}} + O\left(\frac{V^{4l+4}}{x^{4l+1}}\right) \qquad (2.65)$$

where, in the same limit,

$$x \approx \frac{U}{2} - \frac{K+1}{4K}\frac{B^2}{U} + O\left(\frac{B^4}{U^3}\right) \qquad (2.66)$$

In particular

$$J_1 \approx \frac{V^2}{U} + O\left(\frac{V^4}{U^3}\right) \qquad (2.67)$$

$$J_2 \approx -2V^4/U^3 \quad ; J_3 \approx -`10V^6/U5 \qquad (2.68)$$

Note that the sum rules (2.46, 2.47) are valid to order V^2/U but they are violated to the next order V^4/U^3 ,

In the metallic limit the lowest order in x^2 can be found by putting x = 0 in the integrand of Eqs. (2.62, 2.63); then $G_A(iy) = G_B(iy) = G_0(iy) = 2Ki/[(K-1)y + (K+1)(y^2+B^2)^{1/2}]$ and J_p becomes

$$J_{p_{x\to 0}} \approx -\frac{2x^2}{\pi}\int_0^{\infty} dy\, G_0^2(iy)\theta^p \quad p = 1,2,3,\ldots \qquad (2.69)$$

The quantity J_p multiplied by the number of pth nearest neighbors, $(K+1)K^{P-1}$, and expressed in units of B is weakly dependent on K (for not so large U/B). We obtain explicitly

$$\frac{(K+1)K^{p-1}J_p}{B} \approx \left(\frac{2x}{B}\right)^2 (-1)^p C_{p,K} \ as \quad x \to 0 \quad (2.70)$$

where

$$C_{p,K} = \frac{2K}{\pi(K+1)}\int_0^{\infty\infty} dt \left[\frac{K-1}{K+1}t + (1+t^2)^{\frac{1}{2}}\right]^{-2}\left[t + (1+t^2)^{\frac{1}{2}}\right]^{-2p} \qquad (2.71)$$

From Eqs. (2.7) and (2.71) we see that as x → 0, J_p for odd p is negative while for even p is positive. Remember that Jp is negative for all p as x →≈.Actually each

J_{2p+1} is negative over the whole range $0 < U/B < \infty$, while the J_{2P} are negative for large values of U/B, change sign at U/B ~ 1, and remain positive below this value.

For K =∞ the quantity $C_{p,K}$ can be obtained as

$$C_{p,\infty} = \frac{1}{\pi}\frac{4(p+1)}{(2p+1)(2p+3)} \approx \frac{1}{\pi}\frac{1}{p+1} \qquad (2.72)$$

For K = 1 one can easily show that

$$\frac{1}{2p+1}\frac{1}{\pi} < C_{p,1} < \frac{1}{2p}\frac{1}{\pi} \qquad (2.73)$$

in particular

$$C_{1,1} = \frac{2}{\pi} - \frac{1}{2}, \quad C_{2,1} = \frac{1}{2} - \frac{4}{3\pi} \qquad (2.74)$$

If we have kept the x dependence of θ(iy) in Eq. (2.69) we would have obtained

$$\frac{(K+1)K^{p-1}J_p}{B} \approx \left(\frac{2x}{B}\right)^2 (-1)^p C_{p,K} \; as \quad x \to 0 \qquad (2.75)$$

with $\alpha_{x\to 0} \to Cx/B$; this shows that the interaction range $1/\alpha$ approaches infinity as x → 0; note that $C_{p,K}$ ~ 1/p as p→∞ Next we check whether or not the sum rules (2.46), (2.47) are satisfied in the limit x→ 0. For this purpose we substitute Eq. (2.69) in ihe fight hand side of Eqs.

(2.46) and (2.47) (keeping the x-dependcnce in0(iy)); the summation can easily be performed under the integral and we finally obtain

$$\sum_{p=1}^{\infty}(-1)^{p-1}K^{p-1}J_{p_{\overrightarrow{x\to 0}}}-\frac{4K}{\pi(K+1)^2}\frac{x^2}{B}ln\frac{B}{2x}+O(x^2/B)$$

(2.76)

$$\sum_{p=1}^{\infty}(-1)^{p-1}pK^{p-1}J_{p_{\overrightarrow{x\to 0}}}-x\frac{K}{\pi(K+1)^2}\frac{x^2}{B}ln\frac{B}{2x}+O(x^2/B)$$

(2.77)

Equations (2.76) and (2,77) can be obtained also from Eq. (2.75) allowing thus an explicit determination of the value of the constant C, as being equal to $4\gamma_K(K+1)/K$, where $\gamma_K = \lim_{p\to\infty} pC_{K,p}$ (for K = ∞, C = 4/π). Comparing Eqs. (2.43) and (2.76) we see that the sum rule (2.46) is obeyed in the limit $x \to 0$. On the other hand, comparison of Eqs. (2.31) and (2.77) shows that, although the functional dependence is the same, J_b is larger than the sum by a factor (K+1)/K; this factor/has the maximum value for the 1 - D case and is equal to one for the K = ∞ case. We will discuss in the next paragraph the physical significance of these results.

In Figure 5 we plot $(K+1)K^{p-1}J_p/B$ vs U/B for p = 1,2, 3; these results were obtained from Eqs. (2.59 - 2.61) by performing the integrals numerically. Note that an anomalous behavior is exhibited for U/B ~ 1; this anomaly is associated with the" poles of γ_K $\varphi_{nm}(E)\equiv(-1)^{n-m+1}\frac{d}{dE}\sum_n lnC_{nm\sigma}(E)$

approaching the origin, E = 0. This last statement can be justified by noticing that Eq. (2,55) can be written as

$$J_{nm} = -\frac{1}{4\pi}\int_{0}^{\infty} dy\ y\ Im\,\varphi_{nm}(iy)$$

The factor $\varphi_{nm}(iy)$ integrand tends to become very large for small y as the poles of $\varphi_{nm}(E)$ approach the origin. We mention also that around U/B~0 the sum rules are strongly violated as a result of the anomalous behavior of J_{nm} .

III THE ROLE OF DYNAMICAL PROCESSES

Up to now we have presented results within the framework of the static binary alloy approximation. As was pointed out by Economou and White[4] in the static approximation the configuration of the local moments is frozen, while in reality there exists the possibility of dynamical processes (DP) where an up moment turns down while at another site a down moment turns up. Such DP can be incorporated a posteriori by adding to our static Hamiltonian a term $\Delta\hat{H}$, where

$$\Delta\hat{H} = \sum_{ij} t_{ij}\sigma_{\iota}{}^{+}{}_{*}\sigma_{j}$$

(3.1)

If $\Delta\hat{H}$ is added to the Ising part $\hat{H}_{\mathrm{I}}$ of the static Hamiltonian , which taking into account the isotropy of our model, can be written as:

$$\Delta\hat{H} = -\frac{1}{2}\sum_{nm} J_{nm}^{H}\,\vec{\sigma}_{n}\vec{\sigma}_{m}$$

(3.2)

As a result $\hat{H}_{\mathrm{I}}\rightarrow\hat{H}_{\mathrm{H}}$ the effective one-particle potential $\hat{H}_{\sigma}$ will be modified, and consequently the density of states $-\frac{Im}{\pi}G_{i\sigma}(E)$ will change. As a result the self-consistnently determined values of μ J_b J_F and J_p (p= 1, 2 , …) will be renormalized; we denote the new values by a superscript H. In general, it is quite difficult to find $G_{i\sigma}^{H}$, however, it is possible to make reasonable estimates of $G_{i\sigma}^{H}(z)$ for z around the poles of $G_{i\sigma}^{H}(z)$.

The poles of the Green function give the eigenenergies corresponding to localized eigenstates. Thus the poles $\pm E_F$ are the levels associated with an electron trapped around the reversed local moment, i.e. around the magnetic excitation; similarly the poles $\pm E_b$ correspond to sates localized around the "wrong" joining of the two semi-infinite segments, and so on for the poles associated with J_p. In the presence of the Hamiltonian (3.1) such magnetic excitations (which trap electrons around them) can propagate through the crystal dragging the trapped electron with them. This propagation will broaden the "defect" level to a subband of width Z^*t where Z^* is an effective number of nearest neighbors and t is a typical value for the matrix element t_{ij}. The complex entity of an electron trapped around a propagating magnetic excitation (i.e. propagating electron bound to magnetic excitations) can be called magnetic polaron because of the obvious analogy with ordinary polarons.

Thus DP causes magnetic polaron to propagate; such propagation broadens the sharp structure (such as δ-functions) of the quantities $\mathrm{Im}\varphi_\alpha(E)$ (α=b, F, nm,); this broadening in turn modifies the values of $\varphi_\alpha(iy)$ (see e.g. Eq (2.24),

Which determines the magnetic coupling J_α (α=b, F, nm; se the e.g. Eq. (2.23)). As Can be seen from Eq. (2.24) the most serious modification of $\varphi_\alpha(iy)$ will take place when the poles of $\varphi_\alpha(E)$ are very close to the orgin, E = 0 .
On the other hand if the poles and the branch cuts of $\varphi_\alpha(E)$ are far away from the origin, the changes in Im $\varphi_\alpha(E)$ will hardly affect $\varphi_\alpha(iy)$, which implies that $J_a^H \approx J_\alpha$ when U/B is very large.

Here we have attempted an approximate calculation of the broadening of those pairs of $\varphi_\alpha(E)$ which are in the range [-x , x] and are expected to have a more pronounced effect on J_α. The poles appear in pairs symmetrically located around the origin, E = 0. In calculating the broadening of each pair of poles, $\pm|E_{\alpha i}|$, we have omitted the broadening of each pair of poles and of the branch cuts. This approximation is reasonable when the pair $\pm| E_{\alpha i} |$ in not locate very close to other states. Then the question of broadening becomes equivalent to finding the tight binding bands of two levels $\pm| E_{\alpha i}|$ in the presence of a transfer matrix element $t_{\underline{ij}} = 2J_{ij}^H$. We have assumed further that the two levels are arranged in an alternating configuration and that $t_{ij} = 0$ for i, j non nearest neighbors. Under these approximations the quantity $\varphi_\alpha(z)$ for z around the poles $\pm|E_{\alpha i}|$ will become $\tilde{\varphi}_{\alpha i}(z)$ where

$$\tilde{\varphi}_{\alpha i}(z) = R_{\alpha i} * K_\alpha z \left[(K_\alpha - 1)(z^2 - E_{\alpha i}^2) - (K_\alpha + 1)(z^2 - E_{\alpha i}^2)^{\frac{1}{2}}(z^2 - E_{\alpha i}^2 - B_\alpha^2)^{\frac{1}{2}}\right]^{-1} \tag{3.3}$$

Eq. (3.3) is derived by adding the expressions for G_A and G_B with K+1 replaced by the coordination number K_α+1 corresponding to th4e propagation of the magnetic polaron and B replaced by $B_{\alpha}\nexists\approx 4\sqrt{K_{\alpha}}|J_b^H|$ and multiplying by the residue Rαi at the poles ±$|E_{\alpha i}|$. The modification of the quantities J_α due to the broadening of the poles at in the range [-x , x] is then

$$\Delta \mathrm{J}_{\alpha} = A_{\alpha}\frac{-Im}{\pi}\int_{-\infty}^{0} dE\ E\left[\sum_{i}\tilde{\varphi}_{\alpha i}(E) - \varphi_{\alpha}(E)\right] =$$

$$A_{\alpha}\sum_{\iota} R_{\alpha i}\frac{-Im}{\pi}\int_{-\infty}^{0} dE\ E\left[\frac{\tilde{\varphi}_{\alpha i}(E)}{R_{\alpha i}} - E_{\alpha i}\right] \qquad (3.4)$$

where the summation extends over the poles in the range [-x , 0] and A_a= 1/2, 1/2{K+1) 1/4 for α = F. b. p respectively (see Eq. (2.18k 2.30, 2.55) Equation (3.6) can be written as

$$\frac{\Delta \mathrm{J}_{\alpha}}{B_{\alpha}} = -A_{\alpha}\sum_{i} R_{\alpha i}\, g(x_{\alpha i}; K_{\alpha})\ ; \alpha = b, F, p \qquad (3.5)$$

where

$$x_{\alpha i} = |R_{\alpha i}|/B_{\alpha} \qquad (3.6)$$

$$g(x; K)\ = \int_{x}^{x'} y\ \sigma(y; x, K)\, dy\ - c\ \ x, \qquad (3.7)$$

$$\sigma(\mathrm{y};\mathrm{x},\mathrm{K}) = \frac{K}{(K+1)\pi}\frac{y(1+x^2-y^2)^{1/2}}{(y^2-x^2)^{1/2}[1+4K\,(x^2-y^2)/(K+1)^2]} \tag{3.8}$$

$$x' = (1 + x^2)^{1/2} \tag{3.9}$$

g can be expressed in terms of elliptic functions; g(x; K) is a decreasing function of x which approaches zero as x^{-1} as $x \to \infty$ and goes to constant C_K for $x \approx 0$ (e.g. $C_1 = 2/\pi \approx .6366$, $C_\infty = 4/3\pi \approx .4244$). Given the various approximations utilized in obtaining Equation (3.5) it is not unreasonable to write

$$g(x;\ K) \approx \frac{1}{2}(x^2+1)^{1/2} - x/2 \tag{3.10}$$

Our explicit results reported below were obtained by using Eq. (3.7) for g(; K); we found that the approximation (3.10) leaves our results essentially unaffected (except when $x_{\alpha i} \to 0$).

The desired quantity J_α^H can be obtained from Eq. (3.5) by taking into account that $\Delta J_\alpha = J_\alpha^H - J_\alpha$ and that $B_\alpha \approx 4\sqrt{K_\alpha}|J_b^H| \approx \sqrt{K_\alpha}|J_F^H|$.

For α= b, F there is only one pole in the range [-x,0] which has a residue -1; then Eq. (3.5) simplifies to:

$$\Delta J_\alpha/B_\alpha = A_\alpha\ g(x_\alpha;\ K_\alpha)\ ;\quad \alpha = b,\ F \tag{3.11}$$

For α= b and K = 1 (1-D case) the magnetic excitation propagates to the next nearest neighbor so that $K_b = 1$ and $B_b=4\ |J_b^H|$ then for K =1

$$\Delta J_b^H/4|J_b^H| = \frac{1}{2}\ g\left(\frac{|E_b|}{4|J_b^H|}, 1\right) \qquad (3.12)$$

Where $|E_b|=(V^2+x^2\}^{1/2}= V$. because g(x, K) is a decreasing function of x, and $|E_b|/4|J_b^H|$ increases with U/B. it follows that the relative correction $\Delta J_b/|J_b^H|$ is largest when U/B → 0 (then $\Delta J_b^H/|J_b^H| \approx 1.27$) and decreases monotonically with increasing U/B.

For α= b and K ≠ 1 the magnetic excitation associated with E_b does not propagate under the influence of $\Delta\hat{H}$; it is transformed to more complicated excitations. Thus the general formula (3.5) is not applicable. We propose later an empirical way to obtain ΔJ_b in this case. We expect however, that $\Delta J_b/J_b$ is considerably smaller for K ≠ 1.

For α = F, K_F can be taken as K and $B_F = \sqrt{K}|J_F^H|$
Then Eq. (3.11) becomes

$$\Delta J_F^H/|J_F^H| = \frac{4\sqrt{K}}{2(K+1)}g(x_F; K) \qquad (3.13)$$

Where $x_F = |E_F|/4\sqrt{K}|J_F^H|$. Note that $\Delta J_F^H|J_F^H|$ becomes maximum for Y/B such that $E_F = 0$ and tends to zero as U/B → ∞ or as U/B → 0. As we see below, $\Delta J_p/|J_p|$ also approahes zero

As U/B approaches zero or infinity. It is worthwhile to note that in the limit U/B → 0 where neither J_F nor any J_p are modified by DP the sum rule (2.46) is satisfied. On the other hand the sum rule (2.47) is not satisfied in this limit for arbitrary K. In particular for K = 1 $|J_b|$ is by a factor of two larger than the sum. In this case DP will reduce $|J_b^H|$ by a factor of 2.27 and the sum rule will not be violated by only 13.5%. (If approximation (3.10) was used the sum rule for $|J_b^H|$, K =1 will be satisfied exactly as U/B → 0. Thus DP tend to eliminate the anomalies in J's and tend to make the sum rules (2.46, 2.47) sati= sfied. We conjecture that the DP, if correctly incorporated, will make the sum rules satisfied eatly and that when the sum rules are satisfied exactly the dynamicl corrections are zero. On this basis we expect that J_b^H should be equal to $KJ_b/(K+1)$ as U/B → 0. This indicates that $J_b \approx J_b^H$ for large K, since the largest discrepancy is expected for U/B = 0 and is only (K+1)/K. For large K, $J_F \approx J_F^H$, as can be seen from Eq. (3.13). Of course this is an expected feauture, since for large K the role of dynamical fluctuation should diminish and should disappear as K → ∞.

We have used the same approach to renormalize J_1 and J_2. We obtain

$$\frac{\Delta J_1}{|J_1^H|} \approx 2\sqrt{2K-1}\left[g\left(x_{F1};\sqrt{2K-1}\right) - g\left(x_1;\sqrt{2K-1}\right)\right] \qquad (3.14)$$

where

$$x_{F1} = \frac{|E_F|}{4\sqrt{2K-1}|J_1|}\ x_1 = \frac{|E_1|}{4\sqrt{2K-1}|J_1|} \qquad (3.15)$$

and |E_1| is the zero of C_{01}(E) in the range [0,x]/ Similarly .

$$\frac{\Delta J_2}{|J_2^H|} \approx \sqrt{K}\left[g(x_2;K) + g\left(x_{\frac{1}{2}};K\right) - 2g\,(x_{F1};K)\right] \qquad (3.16)$$

where

$$x_2 = \frac{|E_2|}{4\sqrt{K}|J_1^H|} \qquad x'_2 = \frac{|E'_2|}{4\sqrt{K}|J_1^H|} \qquad (3.17)$$

|E_2|, |E'_2| are the two zeros of C_{02}(E) in the range [0,x]/

In Figure 6 we plot some of our results for J_α^H We see that (a) DP tend to elminate the anomalous behavior of the static approximation (expecially around U/B ~ 1 for J_1, J_2, etc; compare with Figure (5)). (b) For U/B $\gtrsim$ 3, $J_1^H \approx J_F^H \approx J_b^H$, thus the magnetic propery cn be descrobed by a signle nearest neighbor J; probably the most reliable J to use in this range is J_α^H because its value is affected less by errors in the way we introduced the dynamical corrections. (c) For $1 \lesssim$ U/B $\lesssim 3$ the presence of J_2^H is felt to some extent and as U/B becomes smaller more and more of the longer range couplings become significant. For small values of U/B (U/B ≈ .5), the quantities J_p are give by Eq (2.75) with $\alpha = 4\gamma_K(K+1)\, x/KB$, and $C_{p,K} = \gamma_K/p$ for large p.

It should be pointed out that the present way of calculating the effects of DP on the various J's is not rigorous; nevertheless, it contains the basic physical ingredients and produces results which are in good agreement with exact calculations, as we shall show in a later section.

IV EXTENSION TO FINITE TEPERATURES

As the temperature is raised from zero the various J’s may change because (a) the parameters $x \equiv U\mu/2$ amd p, which characterize the effective random medium, are temperature dependent; (b) one should defferentiate the “electronic” free energy (see Eq. (1.5)) and not the energy with respect to P. In this section we calculate the various J’s in terms of x, P and T, i.e.e $J_\alpha = f_\alpha(x,P,T)$. To obtain J_α as a function of T for a constant U/B one should obtain x, P from the equations

$$J_F = fF(x,P;T) \qquad (4.1)$$

$$P = \varphi(J_F/RBT) \qquad (4.2)$$

$$x \equiv U\mu/2 = UR(x, P) \qquad (4.3)$$

In describin the system by a single P the following assumptions were made: (a) $J_b \approx J_F \approx J_1$ (i.e. $J_p \approx 0$, $p = 2, 3\dots$). (b) The static approximation is adequate. We have seen already in the T=0 that these assumptions are not valid everywhere. With increasing temperature (b) above is reasonable because the thermal fluctuations tend to mask the dynamical fluctuations. Assumption (a) is reasonable except around the temperature $T_\mu(U/B)$ where the local moments μ disappear. [4,5]

Eq. (4.2) can be obtained from the solution of the Ising model; e.g. in the 1-D case, $P = \varphi(J_F/k_BT) \equiv \exp(-J_F/k_BT)/[\exp(-J_F/k_BT) + \exp(J_F/k_BT)]$; in 2-D case Onsager's solution can be used [4,5] while in 3-D one can employ the Bethe Peierls approximation which is exact in a Bethe lattice. Eq. (4.3) is obtained from the self-consistency equation (1.3). Finally the function $J_F = f_\alpha(x, P, T)$ can be obtained from Eq. (1.5) (or its generalizations) as will be shown below.

To simplify the algebra we will omit the second term in the right hand of Eq. (1.8). This term is small for not so high T. One can show then[5] that

$$F'_e = \frac{U}{4}(\mu^2 - 1) - \frac{1}{N}\sum_{n\sigma} \int dE\ f(E)\langle D_{n\sigma}(E)\rangle \qquad (4.4)$$

where

$$D_{n\sigma}(E) = \frac{-Im}{\pi}\int_{-\infty}^{E} G_{n\sigma}(E^{+'})dE' \qquad (4.5)$$

If one reverses one local moment of the site 0 the change in the quantity $\sum_{n\sigma} G_{n\sigma}(E)$ will be equal to

$$\sum_{n\sigma} \delta G_{n\sigma}(E) = \frac{d}{dE} ln[(1 - 2x\sigma_0 G_{0\uparrow})1 + 2x\sigma_0 G_{0\downarrow})] \qquad (4.6)$$

where $\sigma_0 = 1$ (-1) if the local moment at the site 0 is up (down). Eq. (4.6) is proved as in Section II From Eq. (4.6) one can obtain immediately that $\sum_{n\sigma} \delta D_{n\sigma} = -\frac{Im}{\pi} \ln Q_F$ where Q_F is the quantity in parentheses in Eq. (4.6). Thus

$$\delta F'_e = -\frac{Im}{N\pi} \int_{-\infty}^{\infty} dE\, f(E) \langle ln\ Q_F(E^+) \rangle \qquad (4.7)$$

By reversing a local moment, P changes by $\delta P = -Z(2P-1)/(NZ/2)$, since Z(2P-1) antiferromagnetic bonds are destroyed on the average out of a total NZ/2. Thus

$$J_F = \frac{1}{Z}\frac{\partial F'_e}{\partial P} = \frac{1}{Z}\frac{\delta F'_e}{\delta P} = -\frac{1}{2(K+1)(2P-1)}\frac{Im}{\pi} \int_{-\infty}^{\infty} dE\, f(E) \langle ln\ Q_F(E^+) \rangle \quad (4.8)$$

The integration path can be transformed to one starting from infinity towards 0 just to the left of the imaginary semiaxis and returning to infinity form the right side; one picks up this way the contribution from the poles of f€ and Eq. (4.8) can be rewtitten as

$$J_F = \frac{k_B T}{(K+1)(2P-1)} \sum_{l=0}^{\infty} \langle ln\ |Q_F(iy)|_l \rangle \qquad (4.9)$$

where

$$y_l = (2l+1)\pi k_B T \qquad l = 0, 1, 2, \ldots \qquad (4.10)$$

Thus the expression for J_F at $T \neq 0$ can be obtained from that at $T = 0$, Eq. (2.39), by replacing the integral by a sum, by taking the average of the integrand and by dividing by (2P-1) (See Appendix IV for calculational details).

Similarly J_{nm} for $T \neq 0$ can be obtained from Eq. (2.57) by replacing the integral by a sum at the points y_l, given by Eq. (4.10) and, by averaging with sides of Eq. (2.57). Finally the quantity J_b for $T \neq 0$ can be expressed as follows

$$J_b = \frac{k_B T}{(2P-1)} \sum_{l=0}^{\infty} \langle ln\ |Q_b(iy)|_l \rangle \qquad (4.11)$$

where $Q_b(z)$ is defined from the relation

$$-\frac{d \ln Q_b(z)}{dz} = \varphi_b(z)\ ; \qquad (4.12)$$

$\varphi_b(z)$ has been defined in Section II. Note tht the sum rules are now modified

$$J_F = \sum_{p=1}^{\infty} (1-2p)^{p-1} K^{p-1} J_p \qquad (4.13)$$

$$J_b = \sum_{p=1}^{\infty} (1-2p)^{p-1} p K^{p-1} J_p \qquad (4.14)$$

For large x/B the easiest quantities to calculate are the various Jmn which can be obtained from the approximate equations (2.58) (by averaging and replacing the integral by a sum). These operations affect the value of J_{mn} very little when x/B is high. Thus in the regime x/B>>1, $J_b(T) \approx J_F(T) \approx J_1(T) \approx J_b(0) \approx J_F(0) \approx J_1(0)$. Correction to J_F and J_b can be found from the sum rules (4.13), (4.14). We have verified that J_F, J_1 are essentially temperature independent by calculating them directly from Eq. (1.5) or (4.9).

When x/B << 1 one can use Eq. (2.69) (with the integral replaced by the sum; there is no reason to average the integrand since for x = 0 the effective potential is periodic). Furthermore for $k_BT << B$ the effects of replacing the integral by a sum are very small Thus for x/B << 1 and $k_BT << B$, J_p are given by Eq. (2.75). In this regime one can obtain Jb and J_F from the sum rules (4.13, 4.14) . Note though that, for x/B << 1, J_b and J_F have no physical significance and one should use the complete set of { J_p } to obtain quantities of physical interest.

We have obtained also the temperature dependence of various J_α for intermediate values of x/B. In figure 7 we present results for J_F vs T for K = 5 and U/B ≈ 1.38. These results were obtained by solving Eqs. (4.1 - 4.3) self - consistently with $f_F(x, P, T)$ determined from Eq. (4.9(and (J_F/k_BT) obtained by using the Bethe - Peierls approximation.[11] We should mention that the actual temperature dependence of J_F is considerably less that the one shown in Figure 7. At very low temperatures the rise in $-J_F$ results from the static approximation and is spurious. We have indicated by dot the corrected values of J_F at T = 0 as a result of DP. Furthermore the higher tempera= tures, where DP have a negligible effect on J_F, Eq. (4.9) is not accurate any more because the omitted second term in the LHS of Eq. (1.8) becomes appreciable; inclusion of this term will add to $-J_F$ given by (4.9) a positive term which increases with increasing T. On the basis of these arguments we have estimated that J_F vs T behaves like the dotted line in Figure 7.

To summarize our findings we can state that (a) Over the U-T plane area, where the thermodynamic properties are determined by th magnetic excitations, the latter are described by a Heisenberg Hamiltonian $\widehat{H}_H = -\frac{1}{2}\sum_{nm} J_{nm}^H \vec{\boldsymbol{\sigma}}_{\boldsymbol{n}} \vec{\boldsymbol{\sigma}}_{\boldsymbol{m}}$ J_{nm}^H can be considered to be good approximation as temperature independent and hence can be replaced by their values at T = 0 as determined in the present work. (b) For values of U/B and T such that μ is larger than about .7, one can take $J_b \approx Jf \approx J1$ and omit Jnm for $|n-m| \geq 2$ i.e. one can describe the magnetic excitations by a single J; the most appropriate is J_b because it is more reliably determined

(c) For values of U/B and T corresponding to very small μ the couplings J_{nm} become of long range and as $\mu \to 0$ $K^{|m-n-1|}$ $|J_{nm}|/|J_1| \sim |n-m|^{-1}$ for large $|n = m|$

V. COMPARISON WITH EXACT RESULTS IN THE 1-D (K=1) CASE

In 1-D there exist results for the ground state energy,[9] the zero temperature susceptibility [12] and some properties of the excitation spectrum [12,13,14] of the 1 – D half – filled Hubbard model. These results can serve as a check for the present approximation. To achieve this comparison we need the corresponding quantities for the Heisenberg model (Eq. (3.2)). The particular case, $J_{nm} = 0$ for $|n-m| \geq 2$, has been studied extensively[15]; the general case has been examined by Ziman[16] in the framework of the spin wave approximation. The latter is not quantitatively reliable for the 1 – D case and in the case of long range J_{nm} it fails even qualitatively, the reason being that the excitations tend to become Ising-like rather than spin wave for long range coupling.[17] In the regime of long range coupling one can use the following qualitative analysis. Separate the chain of local moments into adjacent lusters each of length l_c equal to the range of the coupling, $l_c = a/\alpha$, where a is the lattice spacing and α is defined by Eq. (2.48). Within each cluster there are no spin waves since the coupling is long range. The interaction among clusters is short range and consequently can be represented to a good approximation by the nearest neighbor cluster coupling only, which is of the order of

J_b. As a result of these considerations we obtain the following picture. The intracluster excitations are Ising like and make a negligible contribution to the thermodynamic quantities as $T \rightarrow 0$; the intercluster excitations are those of a Heisenberg Hamiltonian with nearest neighbor coupling, J_b, and an effective lattice spacing equal to l_c; these excitations dominate the thermodynamic quantities as $T \rightarrow 0$.

For $U/B \gtrsim 3$ our results (see e.g. Figure 4) show that the couplings beyond the nearest neighbors are small; hence the results by Bonner and Fisher[15] can be used with the nearest neighbor coupling taken as J_b. We have chosen J_b and not J_F or J_1 because (i) J_b is more reliably determined and (ii) spin wave theory shows that the effect of a small next nearest coupling, J_2 can be incorporated by replacing J_1 by $J_1-2J_2 \approx J_b$. At very low U/b we have used the cluster argument presented above to obtain a rough order of magnitude estimate of the quantities of interest.

Below we discuss separately the various quantities for which comparison of our results with exact results is made.

(i) *E_g energy gap at $T = 0$* Our result for E_g within the static approximation is $E_{gs} = U\mu$. Dynamical processes by changing the coupling to Heisenberg type introduce zero point spin waves at $T = 0$, i.e. an effective disorder, which broadens the static sub - bands and reduces the gap. Thus we expect that $E_g = U\mu$. Furthermore because the number of spin waves is suppressed at low U/B we expect that the reduction of the static gap should be smaller at low U/B. Comparing with the exact results of Musurkin and Ovchinnikov[14] we find that the inequality $E_g < U\mu$ is satisfied everywhere. As $U/B \to \infty$, $E_{gs} \equiv U\mu \to U + O(V^2/U)$ while the exact result is $E_g \to U - 4V + O(V^2/U)$ Note that for any $P \neq 1$ E_{gs} would become $U - 3V + O(V^2/U)$ in the $U/V \to \infty$ limit. In the opposite limit $U/V \to 0$, $E_{gs} \to 16V\exp(-2\pi V/U)$ vs $[8(UV)^{1/2}/\pi]\exp(-2\pi V/U)$ for the exact result. Note that the exponential dependence is predicted correctly although the prefactor is different.

(ii) EG ground state energy. Economou and White [4,5] compared the ground state energy with the result of Lieb and Wu. [9] They found excellent agreement for all values of U/B, with a minor discrepancy for U/B around 1 / 2. Probably this discrepancy cannot be attributed to the approximations involved in using the single J expression for Heisenberg ground energy. Our expression for the ground state energy $|E_G| = \bar{H}_G^i + (4\ln 2 - 2)\,|J_b^H|$ tends to $(4 - \ln 2)V^2/U$ in the limit, which agrees exactly with the corresponding limit of the exact formula. The same exact agreement is obtained in the opposite metallic limit, where $|E_G| \to 4v/\pi - U/2v$, as $U/B \to 0$.

(iii) Vg, zero energy ground velocity. For large U/B ($U/B \gtrsim 3$) where the single J approximation is reasonable we can use Cloizeaux and Pearson [18] result, $v_g = 2\pi a|J_b|$, to express v_g in terms of our J_b. Our results are displayed in Figure 8c (for U/B >2) together with the exact results. In the atomic limit our asymptotic expression v_g/a, $V_g/a \rightarrow 2\pi V^2/U$, coincides with the exact result. For $U/B \lesssim 3$ we cannot obtain U_g reliably because no accurate formula expressing v_g in terms of J_{nm} is available. In the small U/B limit one can check our results qualitatively by employing the cluster argument, which yields $v_g \approx 2\pi l_c|J_b^H| = 2\pi a|J_b^H|/\alpha$. Using our previous results for $|J_b^H|$ and α we obtain $V_g \sim \pi^2 V/4$. This rough estimate is denoted by a dot in Figure 8c; it is surprisingly close to the exact result, $v_g \rightarrow 2V$ as $U \rightarrow 0$.

(iv) $\chi(0)$, zero temperature susceptibility. For large U/B, where the single J approximation is reasonable, $\chi(0)/\mu_B^2 N$ can be expressed in terms of our $|J_b^H|$ as $1/\pi^2|J_b^H|$.[19] In the atomic limit, $\chi(0)/\mu_B^2 N \sim \alpha/\pi^2|J_b^H| \rightarrow 1/\pi V$. Explicit results are shown in Figure 8b.

(v) C_1 linear coefficient of the speific heat. As $T \rightarrow 0$, the specific heat $C \rightarrow C_1 T$. In the region where a single J is a good approximation $C_1 = .175\ N\ K_B^2/|J_b^H|$.[15] This formula combined with our results for $|J_b^H|$ yields the dashed line shown in Figure 8a. Again for $U/B \lesssim 3$ we cannot obtain reliable results because of the lack of an accurate formula expressing C_1 in terms of J_{mn}. In the metallic limit our cluster argument yields $C_1 \sim .175N\ K_B^2/|J_b^H| \rightarrow .446\ K_B^2/V$ against $\pi N K_B^2\ /V = 1.047\ NK_B^2/V$ for the exact result. In figure 61 we display also the numerical per turbative results of Seitz and Klein[20] and our estimates based upon the numerical work of Shiba[21] on fineit Hubbard rings.

On the basis of the above results it is reasonable to state that the low lying excitations of a half - fille Hubbard model can be successfully approximated for all U/B by the spin waves of a Heisenberg model, $H_H = -\frac{1}{2}\sum_{nm} J_{nm}^H\, \vec{\boldsymbol{\sigma}}_{\boldsymbol{n}}\vec{\boldsymbol{\sigma}}_{\boldsymbol{m}}$ with the coupling J_{2m}^H determined as in the present work.

VI. MAGNETIC FIELD

A. Self Consistence Relations

In the presence of a Magnetic Field the Hubbard Hamiltonian (1.1) will be written

$$\hat{H} = \sum_{i\sigma}(\epsilon_0 - \sigma\mu_0 H)\,\hat{n}_{i\sigma} + V\sum_{<ij>\sigma}\alpha^{+}_{i\sigma}a_{j\sigma} + U\sum_{i}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \qquad (6.1)$$

where i denotes sites, <ij> denotes that the summation is restricted over nearest neighbors only, μ_0 is the Bohr magneton. As in the case of H = 0 we make a static self consistent binary approximation, i.e. the term $U\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$ is replaced by $\varepsilon_{i\sigma}\hat{n}_{i\sigma}$[5] where $\{\varepsilon_{i\sigma}\}$ have a binary distribution[5]

$$(\epsilon_{i\uparrow}, \epsilon_{i\downarrow}) = x(\epsilon_{i\uparrow} - \epsilon_{A\uparrow})\delta(\epsilon_{i\downarrow} - \epsilon_{A\downarrow})$$

$$+(1-x)\delta(\epsilon_{i\uparrow} - \epsilon_{B\uparrow})\delta(\epsilon_{i\downarrow} - \epsilon_{B\downarrow}) \qquad (6.2)$$

x is the concentration of sites of type A, $\varepsilon_{\alpha\sigma}$, α = A or B, will be calculated self consistently. We have to addition the conditional probability P = $P_{A/B}$; probability of a site being of type A given that a nearest neighbor site is B. In the binary self consistent approximation the electron with spin σ is described by a hamiltonian:

$$\hat{H}_\sigma = \sum_{i\sigma}(\epsilon_0 - \sigma\mu_0 H + \varepsilon_{i\sigma})\,\hat{n}_{i\sigma} + V\sum_{<ij>}\alpha^{+}_{i\sigma}a_{i\sigma} \qquad (6.3)$$

Eq. 6.3 represents a random alloy with its energies:

$$E_{i\sigma} = \varepsilon_0 = \sigma\mu_0 H + \varepsilon_{i\sigma} \quad (i = \text{A or B}) \qquad (6.4)$$

We first find the partial density of states[5] for the hamlltonian 6.3 and we demand for self consistency:

$$\varepsilon_{\alpha\sigma} = U\langle n_{\alpha-\sigma}\rangle \qquad (6.5)$$

where α = A or B. So we have to solve two hamiltonians.

The up: With scaterring $\delta_\uparrow = E_{B\uparrow} - E_{A\uparrow}$, concentration of A:x; correlation coefficient P, and center of band $E_{B\uparrow}$, and the down hamiltonian with scattering $\delta_\downarrow = E_{A\downarrow} - E_{B\downarrow}$, concentration of A:x, correlation coefficient P and center of band $E_\downarrow$. By redefining the zero of energy we can change the values of $E_\uparrow$ and $E\downarrow$ by a constant; we can put them symmetrically around the origin. Their difference is $\Delta = E_\uparrow - E\downarrow$. Since $U > 0$ it is unlikely that charge will accumulate in certain sites so $n_{\alpha\uparrow} + n_{\alpha\downarrow} = 1$ for α = A or B. This leads to $\delta_\uparrow = \delta\downarrow$ and Fermi level at $E_f = 0$.

This is prove as follows: The total density of states is

$$\rho(E) = \rho_\uparrow(E) + \rho_\downarrow(E) \qquad (6.6)$$

with

$$\rho_\sigma(E) = x\rho_{A\sigma}(E) + (1-x)\rho_{B\sigma}(E) \qquad (6.7)$$

with $\rho_{\alpha s}(E) = -\frac{1}{\pi} Im \ll i\sigma|(E + is - H_\sigma)^{-1}|i\sigma \gg_{i=\alpha}$ with $s \to 0^+$,

To find the fermi level we observe that we have the following symmetry between σ and - σ: [5]

$$\rho_{\alpha\sigma}(E) = \rho_{\alpha-\sigma}(E) \qquad (6.8)$$

$$\int_{-\infty}^{+\infty} \rho\, dE = 2 = 2 \int_{-\infty}^{0} \rho\, dE$$

so $E_F = 0$. Then

$$E_{A\downarrow} - E_{B\downarrow} = U(n_{A\uparrow} - n_{B\uparrow}) = \delta_\downarrow$$

and

$$E_{B\uparrow} - E_{A\uparrow} = U(n_{B\downarrow} - n_{A\downarrow}) = \delta_\uparrow \qquad (6.9)$$

and equal. The difference of the centers of the bands Δ is equal to:

$$\Delta = E_\uparrow - E_\downarrow = (E_{A\uparrow} + E_{B\uparrow})/2 - (E_{A\downarrow} + E_{B\downarrow})/2 =$$

$$\mu_0 H + \frac{U}{2}(n_{A\uparrow} + n_{B\uparrow} - 1) \qquad (6.10)$$

So we need to determine for a given H and U the self consistent values of δ and Δ from Eqs (6.9) and (6.10).

As we saw earlier the minimization of the free energy of the system with respect to P leads to $J=\frac{1}{Z}\left(\frac{\partial F_c'}{\partial P}\right)$ where J is the interaction of moments in the equivalent Ising system[5]. In the presence of H the concentration of the sites will change from ½ tp x such that

$$\left(\frac{\partial F}{\partial x}\right)_{P,H}=0;\ \left(\frac{\partial F}{\partial P}\right)_{x,H}=0;(P=\ P_{A/B})$$

Now as Ising system the energy per site is:

$$H_I'=-2J\left(\frac{1}{2}-2*(1-x)\cdot P\right)-\mu H(2x-1)$$

So in the presence of magnetic field we have with a method similar to ref. 5

$$J=\frac{1}{2(1-x)Z}\left(\frac{\partial F_e'}{\partial P}\right)_{x,H};\mu H=\ -ZJP-\frac{1}{2}\left(\frac{\partial F_e'}{\partial x}\right)_{P,H}$$

As mentioned in ref. 5 the lattice determines the details of the relation between P, x and μH, βJ. This relation is derived as in ref. 5 by observing that the relation between J and P is the same as given by an Ising system of interacting moments. The Ising model in 3 dimentions is not solvable and we employ an approximation which is a Bethe Peierls approximation. Details of this method (specific heat and susceptibility) are given in the following section and in Appendix V. In the next subsection we will find the relations $P = f_1(\beta J, \beta\mu H)$ and $x= f_2(\beta J, \beta\mu H)$ employing this modified Bethe – Peierls approximation.

B. Ising Model

In the following paragraphs the relations between P and x and βJ and βμH will be found with the aid of Bethe Peierls approximation using a method proposed by T. Eggarter[11] for the ferromagnetic case. The antiferromagnetic case is more complicated since all sites are not equivalent but are divided into two sublattices. At $T = 0$ a moment either belongs in the "up" sublattice or in the "down" sublattice. For $T \neq 0$ we have reversals of some moments and as T increases it reaches a critical value T_c at which the long range order (LRO) disappears but short range order (SRO) is maintained. (LRO is destroyed when $P(\alpha_0|\alpha_n) \rightarrow x$ as $n \rightarrow \infty$. $P(\alpha_0|\alpha_n)$is conditional probability of having moment of type A at site n given moment α_0 at 0).

Let us call the up sublattice by plus, + and the "down" sublattice by minus, - . The we use $P_s(\alpha)$ to mean probbility of finding moment of type α at a given site in sublattice s where $\alpha = A$ or B and $s = \pm$. For $T = 0$ $P_+(A) = 1$, $P_+(B) = 0$. The probability of having α without knowledge of sublattice is

$$P(\alpha) = \frac{1}{2}(P_+(\alpha) + P_-(\alpha)) \tag{6.11}$$

The probability $P_s(\alpha,\alpha')$ is the joint probability of having α on the s sublattice and α' on the –s. So the probability of having α, α' moments without knowledge in which sub-lattice moment α probability for nearest neighbors.)

$$P(\alpha,\alpha') = \frac{1}{2}(P_+(\alpha,\alpha') + P_-(\alpha,\alpha')) \tag{6.12}$$

From 6.11 and 6.12 we find the conditional probability of having α given that a nearest neighbor is α':

$$P(\alpha/\alpha') = P(\alpha,\alpha')/P(\alpha') \tag{6.13}$$

It is also possible to define conditional probabilites pertaining to a particular subblattice (α on s)

$$P_s^C(\alpha/\alpha') = \frac{P_s(\alpha,\alpha')}{P_{-s}(\alpha')} \tag{6.14}$$

The probability of having α on a particular sublattice can be thought of as a sum over pair probabilites:

$$\mathrm{P_s}(\alpha) = \sum_{a'} \mathrm{P_s}(\alpha,\alpha') = \sum_{a'} \mathrm{P_{-s}}(\alpha,\alpha') \tag{6.14}$$

For a lattice with γ nearest neighbors we can define conditional probability of having α_1, α_2,… α_γ in the neighbors and α in the central site: $P_s^C(\alpha/\alpha_1, \alpha_2, \cdots \alpha_\gamma)$.

At this point the central approximation of the present approach is introduced.

$$P_s^C(\alpha/\alpha_1, \alpha_2, \cdots \alpha_\gamma) = P_s^C(\alpha/\alpha_1) \qquad (6.16)$$

A consequence of this approximation is that one an easily determine the probability of having α, in the central atom and α_1, α_2,… α_γ on its γ nearest neighbors.

$P_s(\alpha, \alpha_1, \alpha_2, \ldots \alpha_\gamma) = P_s(\alpha) P_{-s}(\alpha_1|\alpha) P_{-s}(\alpha_2|\alpha\alpha_1) . . . P_{-s}(\alpha_\gamma|\alpha\ldots\alpha_{\gamma-1})$

Assuming there are n_A nearest neighbors A and m_B B we can write the right hand of the above equations as

$$\frac{\gamma!}{n!\,m!} P_s(\alpha)(P_{-S}^c(A|\alpha))^{n_A}(P_{-S}^c(B|\alpha))^{m_B}$$

The expression of $P_s(\alpha, \alpha_1, \alpha_2, \ldots \alpha_\gamma)$ in terms of conditional probabilites together with basic statistical physics results allows us to determine all probabilities. Thus by flipping the central moment which is surrounded by n_A A moments and m_B B moments we obtain

$$\frac{P_+(A, n_A, m_B)}{P_-(B\ n_A, m_B)} = \exp\big(-\beta(2J(n_A - m_B) + 2\mu H)\big) \qquad (6.17)$$

where J is the coupling constant, H the magnetic field and µ is the magnetic moment in the Ising hamiltonian

$$H_1 = J \sum_{<ij>} \mu_i \mu_j + H \sum_i \mu_i \qquad (6.18)$$

The symbol <ij>restricts the sum over nearest neighbors only. Eq. (6.17) is valid by changing s to -s and thus we have from 6.17 two equations. In the present work we have expressed everything in terms of $P_+(\alpha,\alpha')$

The following symmetry helps us express 6.17 with the aid of $P_+(\alpha,\alpha')$

$$P_+(\alpha,\alpha') = P_-(\alpha,\alpha') \qquad (6.19)$$

So equations 6.17 can be written with the aid of (6.19, 6.14, 6.15, 6.11) as

$$\left[\frac{P_+(B,B) + P_+(B,A)}{P_+(A,A) + P_+(A,B)}\right]^{\gamma-1} \cdot \left[\frac{P_+(A,A)}{P_+(B,A)}\right]^{\gamma} = \exp\left(2\beta(\mu B + \gamma J)\right) \qquad (6.20)$$

From the equality

$$\frac{P_+(A,n_A,m_B)}{P_+(B,n_A,m_B)} = \frac{P_-(A,n_A,m_B)}{P_-(B,n_A,m_B)}$$

we get

$$\left[\frac{P_+(A,A)}{P_+(B,A)}\right]^{\gamma} = \left[\frac{P_+(A,B) + P_+(A,A)}{P_+(B,B) + P_+(B,A)} \cdot \frac{P_+(B,B) + P_+(A,B)}{P_+(A,A) + P_+(B,A)}\right]^{\gamma-1} \qquad (6.21)$$

Now instead of flipping the central moment we flip a neighbor so that $n_A \rightarrow n_A + 1$ and $m_B \rightarrow m_B - 1$. By demanding that (6.17) is valid for every n_A. we have

$$\frac{P_+(A,n_A+1,m_{B-1})P_-(B,n_A,m_B)}{P_+(B,n_A,m_B)P_-(B,n_A+1,m_{B-1})} = \exp(4J\beta) \qquad (6.22)$$

This can be expressed as:

$$\frac{P_+(A,A)P_+(B,B)}{P_+(B,A)P_+(A,B)} = \exp(4JB) \qquad (6.23)$$

and so (6.20, 6.21, 6.23) with

$P_+(A,A) + P_+(A,B) + P_+(B,A) + P_+(B,B) = 1$ (6.24)

form a complete set of equations which an be solved numerically in the general case. For $H = 0$ and $T \geq T_c$ we can solve the set analytically since then $P_+(A,A) = P_+(B,B)$ and $P_+(B,A) = P_+(A,B)$. So (6.21) and (6.22) are identities and we have

$P = P_{A/B} = (\exp(2J\beta)+1)^{-1}$ for $H = 0$, $T>T_c$ (6.25)

For the general case the results are given in Figures 9,10. As we see the curves x vs H/kT and P vs H/kT have a discontinuity in the slope at the critical temperatures for the phase transition from antiferromagnett to ferromagnet. For $T \to 0$ the transition is sharper. At $T \to 0$ the critical value of μH is γJ but it is reduced as the temperature increases to become zero at $T = 2|J|/\ln(\gamma/(\gamma-2)) = 4.93$ in our case where $\gamma = 6$. The curves P vs $\mu H/kT$ reflect the fact that $\frac{dP}{dH}(A,B) = 0$ for $H \to 0$. For larger values of H, $P(A,B) \to 0$ but $P(B) \to 0$ also and so $P = P(A,B)/P(B)$ approaches 1 asymptotically.

C. Equations and Approximations

Taking into account the results of subsections A and B we can conclude that the binary self consistent approximation consists of the following equations

$$U = 2\delta/(\langle n_{A\uparrow}\rangle - \langle n_{B\uparrow}\rangle) \qquad (6.26a)$$

$$\Delta = \mu_0 H + \frac{U}{2}(\langle n_{A\uparrow}\rangle + \langle n_{B\uparrow}\rangle - 1) \qquad (6.26b)$$

$$x = f_1(\beta J,\ \beta\mu H) \quad \text{(B.P.A.)} \qquad (6.26c)$$

$$P = f_2(\beta J,\ \beta\mu H) \quad \text{(B.P.A.)} \qquad (6.26d)$$

$$J = \frac{1}{2(1-x)}\left(\frac{\partial F'_e}{\partial P}\right)_{\mu,x} \quad (P = P_{A/B} = P(A|B) \qquad (6.26c)$$

$$\mu H = -\,ZJP - \frac{1}{2}\left(\frac{\partial F'_e}{\partial x}\right)_{PH} \qquad (6.26f)$$

so we have a system of six equations 6.26 that should be solved to get self consistent values of δ, Δ, μ, J, x, P.

Equation (6.26f) gives the correct behavior for T = 0 as H → 0, i.e. $\left(\frac{\partial \overline{H'}}{\partial x}\right) = -2ZJP$) $(H'$ = average energy per site).
This can be proved using the relation

$$\rho_{A\uparrow}(E,\ x,\ P) = \rho_{B\downarrow}(E,\ 1-\chi,\ \frac{1-x}{x}P)$$

This relation is derived by demanding that the physics should not change if we interchange the roles of A and B.
Then

$$\frac{1}{Z}\frac{\partial \overline{H}}{\partial x} + ZJP = \frac{1}{Z}\frac{\partial \overline{H}}{\partial x} + \frac{P}{(1-x)^2}\frac{\partial \overline{H}}{\partial P}$$

$$= \Big(\lim x$$

$$= \frac{1}{2}\Big) \left\{ \int_{-\infty}^{0} EdE (P \frac{\partial}{\partial P}(\rho_A + \rho_B) + \frac{1}{2}\frac{\partial}{\partial x}(\rho_A + \rho_B)) \right.$$

$$\left. + x \int_{-\infty}^{0} dE (P \frac{\partial}{\partial P}\big(\rho_{A\uparrow}(E) - \rho_{B\uparrow}(E)\big) + \frac{1}{2}\frac{\partial}{\partial x}\big(\rho_{A\uparrow}(E) - \rho_{B\uparrow}(E)\big) \right\} = 0$$

($\varepsilon = \frac{U\hat{\mu}}{2}$). The last statement is true because:

$$\frac{\partial \rho_A}{\partial P} = \frac{\partial}{\partial P}(\rho_{A\uparrow} + \rho_{A\downarrow}) = \frac{\partial \rho_B}{\partial P};\ \frac{\partial \rho_{A\sigma}}{\partial P} = -\ \frac{\partial \rho_{B-\sigma}}{\partial x} - 4P\frac{\partial \rho_{B-\sigma}}{\partial P}$$

Where σ = ↑ or ↓ We see that (6.26e, 6.26f) give us values of μH, J for various values of x, P, similarly equations c, d give values of μH, and J for various values of x, P. These give us self consistent values of μH, J from the intersetion of the appropriate curves. To simplify we can take for J the same value as for H = 0. Then we have to find only the value of μH self consistently. For very small fields we used more approximations. By studying the results of (6.26c, 6.26d) we see that the lines x vs μH and P vs μH are always following the rule ΔP=2PΔx,

So for very small fields the probability of pairs remains the same: dP(A,B) = 0 as H varies and only the probability P(B) (P(A)) changes appreciably. Then

$$dP_{A/B} = d(P(A,B)/P(B)) = +\frac{P(A,B)dx}{(1-\frac{1}{Z})^2}$$

So $dP_{A/B}=\frac{P_{A/B}}{1/z}dx$ (or since we use the notation $P_{A/B}=P$)

$$\Delta P = 2P\,\Delta x \qquad (6.28)$$

(dP(A,B) = 0 as H varies because ofr the symmetry P(A,B) = P(B, A)).

If we have a small H we expect that $n_{A\uparrow}+n_{B\downarrow}$ will differ a little from unity. Then (6.26c) can be expanded around values of H = 0. To make this expansion we need an expansion of the density of states. Let u call ρ^H the density of states with a magnetic field. Then $\rho_\sigma^H(E) = \rho_\sigma^H(E+\sigma\Delta)$ where $\rho_\sigma^\delta(E)$ is the density of states with the same σ, δ, x as $\rho_\sigma^H(E)$ bu withour displacement Δ so

$$\rho_\sigma^\delta(E+\sigma\mathit{\Delta}) = \rho_\sigma^\delta\left(E+\sigma\mathit{\Delta}, P_0+dP, \frac{1}{2}+dx, \delta^0+d\delta\right) \qquad (6.29)$$

where P_0, δ^0 are values of P, δ for H = 0. The differences inside the parentheses in (6.29) are small so we can expand in a Taylor series:

$$\rho_\sigma^H = \rho_\sigma^\delta(E+\sigma\mathit{\Delta}) + \frac{\partial\rho_\sigma^\delta}{\partial P}\left(P_0+\frac{1}{2}, \delta^0\right)dx + \frac{\partial\rho_\sigma^\delta}{\partial\delta}\left(P_0, \frac{1}{2}, \delta^0, d\delta\right)$$

By expanding also in terms of E + σΔ we get (keeping in mind that $\rho_A(0) = \rho_B(0)$ for x = $\frac{1}{2}$)

$$n_{A\uparrow} + n_{B\uparrow} = n_{A\uparrow}^0 + n_{AB\uparrow}^0 + 2\Delta(\rho_A + D\rho_A) +$$
$$\left(d\delta\frac{\partial}{\partial\delta} + dx\frac{\partial}{\partial x} + dP\frac{\partial}{\partial P}\right)(n_A' + n_B') \qquad \left(at\ x = \frac{1}{2}\right)$$

For x=.5 always $n_{A\uparrow} + n_{B\uparrow} = 1$ so

$\frac{\partial}{\partial x}(n_{A\uparrow} + n_{B\uparrow}) = 0$ *and* $\frac{\partial}{\partial P}(n_{A\uparrow} + n_{B\uparrow}) = 0$

For $\frac{\partial}{\partial x}(n_{A\uparrow} + n_{B\uparrow})$ we observe that the quantity f(x) = $n_{A\uparrow} + n_{B\uparrow}$ as a function of x has the following symmetry (by interchanging the roles of A and B)

$$f(x) = f(1-x)$$

So $\frac{\partial}{\partial x}(n_{A\uparrow}+n_{B\uparrow})=0$ at x~1/2. In first order then

$n_{A\uparrow}+n_{B\uparrow}=1+\Delta\cdot\rho(E_F)$; $E_F=0$ (6.30)

$$\rho(0)=\rho(E_F)=x\rho_A(0)+(1-x)\rho_B(0)=\rho_A(0)$$

at x = .5. So substituting in (6.10) we obtain

$$\Delta=\frac{\mu_0 H}{1-U\rho(E_F)} \qquad (6.31)$$

Eq. (6.31) is similar to the relation for the susceptibility derived in many body theories. Here we do not have the case of

$$1-U\rho(E_F)=0$$

because the phase transitions have already taken plae in our formalistm. So Eq. (6.31) is always true. For small magneti fields we can prove that the self consistent value of μ does not change in first order in the magnetic field but only on second order: Dμ $=H^2$.

For small fields we can expand $\tilde{\mu}=\frac{\delta}{U}$ (6.7) around the value at H = 0. With the applications of H we have μ(H) = $\mu(P^0+\Delta P,\frac{1}{2}+\Delta x,\Delta)$ where ΔP, Δx are the corresponding changes in P and x from the value at H = 0, Δ is the displacement of the bands (given by (6.3100. Expanding we have

$$\mu(P,x,\Delta) - \mu\left(P^0,\tfrac{1}{2},0\right) = \mu(P,x,0) - \mu\left(P^0,\tfrac{1}{2},0\right)$$

$$+\left.\frac{\partial\mu}{\partial\Delta}\right|_{P,x}\cdot\Delta + \frac{1}{2}\left.\frac{\partial^2\mu}{\partial\Delta^2}\right|_{P^0,\frac{1}{2}}\cdot\Delta^2 \quad (6.32)$$

The last terms is calculated at zero filed since we are interested only to order H^2

$$\left.\frac{\partial\mu}{\partial\Delta}\right|_{P,x} = \frac{\partial}{\partial\Delta}\left[\int\left(\rho_{A\uparrow}(E,x,P) - \rho_{B\uparrow}(E,x,P)\right)dE\right]$$

$$-\int_{-\infty}^{E_F}\left(\frac{d\rho_{A\uparrow}}{dE} - \frac{d\rho_{B\uparrow}}{dE}\right)dE = \rho_{A\uparrow}(E_F) - \rho_{B\uparrow}(E_F)|_{x,P}$$

similarly

$$\frac{\partial^2\mu}{\partial\Delta^2} = \frac{\partial}{\partial E}\rho_{A\uparrow}\left(P^0,\frac{1}{2}\right) - \frac{\partial}{\partial E}\rho_{B\uparrow}\left(P^0,\frac{1}{2}\right)$$

Thus

$$\mu(P,x,\Delta) - \mu\left(P^0,\frac{1}{2}\right) = \mu(P,x,0) - \mu\left(P^0,\frac{1}{2},0\right)$$

$$+(\rho_A^+(x,P) - \rho_B^+(x,P))\Delta + \frac{\partial\rho_A(E_F)}{\partial E}\cdot\Delta^2 \qquad (6.33)$$

(The last line is true because $\frac{\partial\rho_A^+(E_F)}{\partial E} = -\frac{\partial\rho_B^+(E_F)}{\partial E}$)

The difference $\rho_{A\uparrow}(x,P) - \rho_{B\uparrow}(x,P)$ can be expanded:

$$\mathrm{\rho_{A\uparrow}(x,P) - \rho_{B\uparrow}(x,P) = \rho_{A\uparrow}\left(\tfrac{1}{2}, P^0\right) - \rho_{B\uparrow}\left(\tfrac{1}{2}, P^0\right)}$$

$$+\frac{\partial \rho^+_{A\uparrow}}{\partial x} - \frac{\partial \rho^+_{B\uparrow}}{\partial x}\bigg|_{x=\frac{1}{2},\boldsymbol{P^0}} \Delta x + \frac{\partial \rho^+_{A\uparrow}}{\partial P} - \frac{\partial \rho^+_{B\uparrow}}{\partial P}\bigg|_{x=\frac{1}{2},\boldsymbol{P^0}} \Delta P$$

or since $\rho_A(E_F) = \rho_B(E_F)$ and this holds true for every P at $x = \frac{1}{2}$, then

$$\mathrm{\rho_{A\uparrow}(x,P) - \rho_{B\uparrow}(x,P)} = \left(\frac{\partial \rho^+_{A\uparrow}\left(\frac{1}{2}, \mathrm{P^0}\right)}{\partial x} - \frac{\partial \rho^+_{B\uparrow}\left(\frac{1}{2}, \mathrm{P^0}\right)}{\partial x}\right) \cdot \Delta x$$

We expand

$$\mu(P,x,0) - \mu\left(P^0, \frac{1}{2}, 0\right)$$

$$= \frac{\partial \mu}{\partial P}\Delta P + \frac{\partial \mu}{\partial \mathrm{x}}\Delta x + \frac{1}{2}\frac{\partial^2 \mu}{\partial x^2}\Delta x^2 + \frac{1}{2}\frac{\partial^2 \mu}{\partial P^2}\Delta P^2 + \frac{\partial^2 \mu}{\partial x \partial P}\Delta x \Delta P$$

$$= \frac{\partial \mu}{\partial P}\Delta P - 2P\frac{\partial \mu}{\partial \mathrm{P}}\Delta x + \frac{1}{2}\frac{\partial^2 \mu}{\partial x^2}\Delta x^2 + \frac{1}{2}\frac{\partial^2 \mu}{\partial P^2}\Delta P^2 + \frac{\partial^2 \mu}{\partial x \partial P}\Delta x \Delta P$$

$$= \frac{1}{2}\frac{\partial^2 \mu}{\partial x^2}\Delta x^2 + \frac{1}{2}\frac{\partial^2 \mu}{\partial P^2}\Delta P^2 + \frac{\partial^2 \mu}{\partial x \partial P}\Delta x \Delta P \qquad (6.34)$$

So Dμ changes only as $(\Delta x)^2$. First orders Dμ is zero because $\frac{\partial \mu}{\partial P}\Delta P + \frac{\partial \mu}{\partial \mathrm{x}}\Delta x = \frac{\partial \mu}{\partial P}(\Delta P - 2P\Delta x) = 0$

From $\mathrm{\rho_{A\downarrow}(E, x, P_{\mathit{A,B}}) = \rho_{B\uparrow}(E, 1-x, P_{\mathit{B/A}})}$, we get

$$\frac{\partial^2 \rho_{A\downarrow}}{\partial x^2} = \frac{\partial^2 \rho_{B\uparrow}}{\partial x^2} + \frac{2P}{x^2}\frac{\partial^2 \rho_{B\uparrow}}{\partial x \partial P} + \frac{2P}{x^3}\frac{\partial \rho_{B\uparrow}}{\partial P} + \frac{P^2}{x^4}\frac{\partial^2 \rho_{B\uparrow}}{\partial P^2}$$

$$\frac{\partial^2 \rho_{B\downarrow}}{\partial x^2} = \frac{\partial^2 \rho_{A\uparrow}}{\partial x^2} + \frac{2P}{x^2}\frac{\partial^2 \rho_{A\uparrow}}{\partial x \partial P} + \frac{2P}{x^3}\frac{\partial \rho_{A\uparrow}}{\partial P} + \frac{P^2}{x^4}\frac{\partial^2 \rho_{A\uparrow}}{\partial P^2}$$

By integration from $-\infty$ to E_F and subtraction we get

$$\frac{P}{x^2}\frac{\partial^2\mu}{\partial x\partial P}+\frac{P}{x^3}\frac{\partial\mu}{\partial P}+\frac{P^2}{2x^4}\frac{\partial^2\mu}{\partial P^2}=0$$

Substituting this in (6.34) we get

$$\mu(P,x,0)-\mu\left(P^0,\frac{1}{2},0\right)=\frac{\partial\rho_{A\uparrow}(E_F)}{\partial E}\Delta^2+\left(\frac{\partial\rho_{A\uparrow}}{\partial x}-\frac{\partial\rho_{B\uparrow}}{\partial x}\right)_{E_F}\Delta\cdot\Delta x$$
$$-\left(4P\frac{\partial\mu}{\partial P}+2P^2\frac{\partial^2\mu}{\partial P^2}-\frac{1}{2}\frac{\partial^2\mu}{\partial x^2}\right)(\Delta x)^2 \qquad (6.35)$$

So for small fields (up to 20 KG) the correction to the self consistent value of μ is proportional to H^2. This changes in μ , P, with the magnetic field allowing us to calculate the changes in the density of states and in transport properties. In other words we have developed here a formalism which can be used for calculating magnetoresistance. In the next section we will apply this formalism to the question of negative magnetoresistance observed in impurity bands in crystalline semiconductors.

VII. APPLICATIONS – NEGATIVE MAGNETORESISTANCE

Negative magnetoresistance is observed in extrinsic semiconductors.[6,22,23] These are formed by doping semiconductors with n or p type impurities. If the density of the impurities is high enough an impurity band is formed whiich is located near the conduction band for n-type semiconductors or near to the valene band for p-type. The fermi level lies on the middle of the impurity band.[6] The impurities occupy random positions on the lattice. The on site potential U can be calculated as the energy pf a pair of electroms on the same center.[6] The hopping matrix element V is calculated from an overlap integral <i|H|j> where i, j are nearest neighbor sites and |i> is a Wannier state. Since the position of the impurities is random, the ratio $u = U/V$ will be random. We may subdivide the semiconductor into grains over which U/V is constnt. For each grain we may apply Economou's[5] self consistent binary approximation and find the self consistent values of μ and P. As was found by Cyrot[3] and Economou[5] μ is zero for a given T if $u<u_T$ where u_T is found in the binary self consistent approximation of the Hubbard model. Thus the grains with $u < u_T$ do not contribute to the scatering of electrons. This scattering of electrons from moments was first proposed by Toyozawa[24] to explain negative magnetoresistance. With the application of a magneti field u_T becomes $u_T(II)$

And we will sow $u_T(H) > u_T$. Thus the region of u where $\mu = 0$, is increased by an interval $\Omega = u_T(H) - u_T(0)$. If the probability distribution of u is $\wp(u)$ and this will give us a measure of how much the magnetoresistance dropped. If we assume $\wp(u)$ broaad enough then the negative magnetoresistance is proportional to $\Omega = u_T(H) - u_T(0)$. In Toyozava's theory the moments are formed from localized eletrons only, and the he considers the scattering of Bloch electrons. Economou's theory [4,5] builds the moments self consistently.

The scattering of the electrons in Economou's theory[5] is due to the difference in the self consistent site levels δ. The quantity δ is related to μ by the self consistency relation

$$\mu = \delta/u \qquad (7.1)$$

For each δ and P the quantity μ was calculated.[5] So we have a relation

$$\mu = f_1(\delta, P) \qquad (7.2)$$

(see ref. 5). The short range order parameter p is a function of βJ

$$P = f_2(\beta J) \qquad (7.3)$$

On the other had J can be expressed as a function of δ, p

(see earlier results)

$$J=f_3(\delta,\ J) \qquad (7.4)$$

The above function can be approximated by

$$f_1(\delta,P) = (1-\exp(-\delta^2/u_P^2))^{1/2} \qquad (7.5)$$

where

$$u_p = u_1 + 2(1-P)(u_{.5} - u_1) \qquad (7.6)$$

is the value of $u = U/V$ at which $\delta = 0$ if $u < u_p$ for a given P. u_1, u_5 are the respective values of u_P for P = 1, .5 respectively. Relation (7.3) was calculated in a Bethe Peierls approximation. A good fit is

$$P = 1 - \frac{1}{2}\exp(-z^* J/kT) \qquad (7.7)$$

where $Z^* \cong 10$. Relation (7.3) was calculated for P =1 before. A fit is

$$J \cong 16\delta^2 \qquad (7.8)$$

With the above approximations we can find the value of u_T Eq. (7.1) is written

$$\mu = \frac{\delta}{u} = \frac{\delta}{u_P} - \frac{\delta^3}{{u_P}^3} \qquad (7.9)$$

$$\frac{u - u_P}{u u_P} = \frac{\delta^2}{4u_P^3}$$

If we put $\frac{1}{u u_P}$ and $\frac{1}{u_P^3} = 1$ we have

$$u - u_1 = \frac{\delta^2}{4} + \Delta u \exp(-Z^* \delta^2/kT\ ) \qquad (7.10)$$

$(\Delta u = u_{.5} - u_1)$. For δ = 0, u= $u_{.5}$. For δ increasing from 0, u passses from a minimum u_T and then increases again (See figure 11). The lower values of δ are discarded as giving a greater free energy.[5] Thus δ drops abruptly at u_T from a finite value

$$\Delta - (T/(10Z)*\ln(4Z'\ \Delta u/T))^{1/2} \qquad (7.11$$

to zero. So for every T we find the appropriate u_T such that $\frac{du_T}{d\delta} = 0$.

The corresponding equation to (7.10) for the case of a magnetic field is found by observing that for H small the self consistently found μ will change to μ(H = 0)+Dμ where Dμ is calculated as in (6.35). Then we have a new reltion between u and δ. This gives a $u_T(H)$. From (6.35) we have

$$D\mu = -(\Delta x)^2 4P \frac{\partial \mu}{\partial P} \qquad (7.12)$$

where

$$\frac{\partial \mu}{\partial P} = \frac{\partial}{\partial P}\left(\frac{\delta}{u}\right) \cong \frac{\partial}{\partial P}\left(\frac{\delta}{u_P}\right) = \delta^2 \frac{\Delta u}{{u_P}^2}$$

and

$$\Delta x \cong \frac{\mu H}{2kT} \exp(-Z^* J/2kT) \qquad (7.13)$$

With these approximations we have

$$u - u_1 = \frac{\delta^2}{4{u_P}^3} + \left(C\,(\frac{H}{T})^2 \delta^2 + \Delta u\right) \exp(-Z^* \delta^2/kT\ ) \qquad (7.14)$$

From this equation we can find the value of $u_T(H)$ from $\frac{\partial u}{\partial \delta} = 0$. The results of this procedure are depicted in Figure 11 where we give the difference $\Delta m = u_T(H) - u_T$. We see that for $H \rightarrow 0$ $\Delta m = u_T(H) - u_T \propto H^2$. This is a characteristic that exists also in Toyozawa's theory.[23,24]

Many experimental results show that the behavior of Δm is $\propto H^c$ where $c \simeq 1$. This cannot be explained by introducing dynamical effects. Existing theories with dynamical effects give $\Delta m \propto H^3$.[23] This anomalous behavior can be explained with the following considerations: As we saw earlier $D\mu \propto (\Delta x)^2$. This change of μ is the sum of $D\mu_\uparrow \propto D(n_{A\uparrow} - n_{B\uparrow})$ and $D\mu_\downarrow \propto D(n_{B\downarrow} - n_{A\downarrow})$. These partial $D\mu_\sigma$ are also zero in first order of Δx. This is due to the symmetry of the bands around the fermi level. Actually the bands are asymmetric around Fermi level.[6] This is due to the nearness of the conduction band. Then $D\mu_\uparrow \propto (\Delta x) > 0$;

$D\mu_{\downarrow} \propto (\Delta x) < 0$;but $D\mu = 0$ so again $D\mu \propto (\Delta x)^2$. The linearity is explained then as an effect of metastability. The grain where $\Delta\mu_{\uparrow} \propto (\Delta x) > 0$ may be remote so it will be difficult to build up moments where they were absent. This will give a total $D\mu \propto (\Delta x)$.

VIII CONCLUSIONS

A) The low lying excittions of a half - filled 1-D Hubbard model are spin waves which can be described by a Heisenberg Hamiltonian, $H_H = -\frac{1}{2}\sum_{nm} J_{nm} \vec{\boldsymbol{\sigma}}_{\boldsymbol{n}} \cdot \vec{\boldsymbol{\sigma}}_{\boldsymbol{m}}$ for all U/B. For large U/B ($\geq$ 3) J_{nm} ($|n-m| \geq 2$) can be omitted in front of $J_1 = J_{n,n+1}$, For small U/B (<<1), $J_{nm}/B \sim \alpha^2 |n - m|^{-1} \exp(-\alpha|n - m|)$, where α^{-1}, the range of the interaction (in units of lattice spacing), approaches infinity as U → 0.

Higher in energy lies the quasiparticle - quasihole spectrum, which exhibits a gap at T = 0 and is renormalized with increasing T. The quasiparticles (quasiholes) are composite entities (which can be appropriately termed spin polarons) consisting of an electron (hole) bound to a cloud of spin waves.

At high U/B the spin wave and the quasihole-quasiparticle bands are well separated in energy and they equally share the degrees of freedom of the system. For low U/B ($\lesssim 1$) the two bands merge together to form a composite band. The character of the excitation within the composite band changes continously with increasing energy from spin wave to almost free electron passing through the mixed character spin polaron. As U → 0, only intercluster spin waves exist and as a result of the increasing size of the clus Sters, the number of degrees of freedom vested in spin waves approaches zero.

B) The application of a magnetic field displaces the bnds by $\Delta = \mu_0 H/(1 - U\rho(E_F))$. This result shows the effect of correlations between sites. The displacement is bigger than what we expect from a free electron gas. Our treatment gives E_F always at zero with the application of magnetic fields. As for the negative magnetoresistance it is explained as a result of elimination of magnetic moments. To explain further the low field behavior we observe that the combination of asymmetrical bands with metastability can explain the observed behavior of H^c where $c \sim 1$.

APPENDIX I

Let the configuration for P=1 be as in Figure 1a. As we see in this figure we have two kinds of sites characterized by the letters u and d. The site potentials have the values x at the sites d, and −x at the sites u. The diagonal matrix elements can be expressed through the Renormalized Perturbation Expansion (RPE).[25] This gives us explicit results because of the periodicity, as will be seen below. In RPE the diagonal matrix elements are:

$$\langle \mathrm{i}|\mathrm{G}|\mathrm{i}\rangle = {}^{1}\!/\!(E-\varepsilon_i-\Delta_i) \qquad \text{(AI . 1)}$$

where ε_i is the site potential at site I and Δ_i is the self energy at site i.

Economou and Cohen[26] expressed Δ_i in terms of continuous fraction in the case of 1 dimensional lattices. In the case of 1 dimensional lattices. In the case of 1 - d Δ_i is the sum of two continued fractions: $\Delta_i = t_i^+ + t_i^-$.

$$t_i^+ = \frac{V^2}{(E-\varepsilon_{i+1}-V^2/(E-\varepsilon_{i+2}-V^2/(E-\varepsilon_{i+3}-\ldots)))}$$

$$t_i^- = \frac{V^2}{(E-\varepsilon_{i-1}-V^2/(E-\varepsilon_{i-2}-V^2/(E-\varepsilon_{i-3}-\ldots)))}$$

If the lattice is periodical $\varepsilon_{i+1}=\varepsilon_{i-1}=\varepsilon_{i+3}=\varepsilon_{i-3}=\ldots=\varepsilon_1$, $\varepsilon_{i+2}=\varepsilon_{i-2}=\varepsilon_{i+1}=\varepsilon_{i-1}=\varepsilon_2$. Then $t_i^+ = t_i^-$

and Δ_i can be written as

$$\varDelta_i = 2t_i = \frac{2V^2}{(E - \varepsilon_1 - V^2/(E - \varepsilon_2 - V^2/(E - \varepsilon_1 - \dots)))}$$

So

$$t_i = \frac{V^2}{(E - \varepsilon_1 - V^2/(E - \varepsilon_2 - \dots)))}$$
$$= \frac{V^2}{(E - \varepsilon_1 - t_{i+1})} \quad \text{(A1,2a)}$$

where

$$t_{i+1} = \frac{V^2}{(E - \varepsilon_2 - V^2/(E - \varepsilon_1 - \dots)))}$$
$$= \frac{V^2}{(E - \varepsilon_2 - t_i)}$$

(AI.f2b)

So for 1-d t_i t_{i+1} can be found explicitly.

For Bethe lattices we can generalize the above procedure: A Bethe lattice is defined as a lattice with no closed loops and each atom is connected with Z neighbors. We may consider the 1-d as a special case of a Bethe lattice that corresponds to Z =2. For a general Z the site self energy is:

$$\Delta_i = Z\ t_i$$

where

$$zt_i = \frac{V^2}{(E - \varepsilon_{i+1} - (Z-1)V^2/(E - \varepsilon_{i+2} - (Z-1)\,V^2/(E - \varepsilon_{i+3} - \dots)))}$$

For periodic case

$$\varepsilon_{i+1}=\varepsilon_1,\ \ \varepsilon_{i+2}=\varepsilon_2$$

and

$$t_i = \frac{V^2}{(E-\varepsilon_1-(z-1)t_{i+1})} \qquad \text{(A1.2a)}$$

$$t_{i+1} = \frac{V^2}{(E-\varepsilon_2-(z-1)t_i)} \qquad \text{(A1.2b)}$$

Thus we have explicit formulas for general Z. In our case we have:

$t_0=t_B=V^2/(E+x-(Z-1)t_1)= V^2/(E+x-Kt_A)$

where

$K = Z-1$

$t_A= V^2/(E-x-Kt_B)$

So

$$t_B = V^2/(E+x-KV^2/(E-x-Kt_B)$$

$$t_B=V^2(E-x-Kt_B)/(E^2-x^2-Kt_B(E + x) - K V^2)$$

$$t_B^2(E+x)*K - t_B(E^2-x^2)+V^2 (E-x)=0$$

So

$$t_B =(E^2-x^2-(E^2-x^2)^{1/2}(E^2-x^2-B^2)^{1/2}/(2K(E+x))$$

(AI.3a)

$t_A = (E^2-x^2-(E^2-x^2)d^{1/2}(E^2-x^2-B^2)^{1/2}/(2K(E-x))$ (AI.3b)

where

$$B^2 = 4KV^2$$

So

$$\langle 1|\mathrm{G}|1\rangle = G_A(E)$$

$$= 2K(E+x)((K-1)(E^2-x^2)+(K+1)(E^2-x^2)^{1/2}(E^2-x^2-B^2)^{1/2})^{-1}$$

$$\langle 0|\mathrm{G}|0\rangle = G_B(E)$$

$$= 2K(E-x)((K-1)(E^2-x^2)+(K+1)(E^2-x^2)^{1/2}(E^2-x^2-B^2)^{1/2})^{-1}$$

APPENDIX II

We need to calculate sums of the form:

$$\sum \langle 0|G_\sigma|n\rangle\langle n|G_\sigma|0\rangle$$

We observe that:

$$\sum_{all\,n} \langle 0|G_\sigma|n\rangle\langle n|G_\sigma|0\rangle$$
$$= \langle 0|G_\sigma^2|0\rangle = \langle 0|(E-H_\sigma)^{-2}|0\rangle$$
$$= -\frac{d}{dE}\langle 0|(E-H_\sigma)^{-1}|0\rangle = -\frac{d}{dE}G_\sigma(E)$$

The sum over n lying on a part of a Cayley tree (as for example part I in Figure 1b) can be found by using the fact that

$$\sum_{overall\,n} \langle 0|G_\sigma|n\rangle\langle n|G_\sigma|0\rangle$$
$$= \langle 0|G_\sigma|0\rangle^2 + (K+1)\psi$$

where ψ is the sum over n lying entirely on one branch of Cayley tree. For example in Figure Ib ψ is the sum of <0|G|n><n|G|0> for n lying on the branch 01 or 02 or 03. Then a sum over n lying on all the branches except one is K*ψ.

So

$$\sum_{n\in\mathrm{I}} \langle 0|G_\sigma|n\rangle\langle n|G_\sigma|0\rangle$$

$$= \ \langle 0|G|0\rangle^2 + K\psi$$

$$= \langle 0|G_\sigma|0\rangle^2 - \frac{K}{K+1}\left(\frac{dG_\sigma}{dE} + \langle 0|G_\sigma|0\rangle^2\right)$$

$$= \frac{\left(\langle 0|G_\sigma|0\rangle^2 - K\,\frac{dG_\sigma}{dE}\right)}{(K+1)}$$

APPENDIX III

We need to express G_{nm} in terms of G_A. G_B This can be done with the aid of Renormalization Perturbation Expansion.[25. 27]

$$<n|G|m> = <n|G|n>V<n+1|G^{\{n\}}|n+1>V... <n|G^{\{m=1\}}|m> \quad (AIII.1)$$

where the supersript (i) dentotes that the site (i) has infinite site potential: $\varepsilon_i = \infty$. The above RPE expression is true only for Bethe lattices.[26]

We call $\tilde{G}_A$ the Green's function corresponding to site G_A with one nearest neighbor having $\varepsilon_i = \infty$. Then

$$\tilde{G}_A = (E - \epsilon_A - K t_B)^{-1}$$

Similarly

$$\tilde{G}_B = (E - \epsilon_B - K t_A)^{-1}$$

If we want to calculate J_{nm} we need

$$G_{nm\sigma} G_{mn\sigma}$$

Let us take the n site with site energy t_A

$$G_{nn\sigma} = G_A = 1/(E - t_A - (K+1)t_B)$$

(see AI.1) then G_{nm} according to AIII.1 is

$$G_{nm} = G_A V \tilde{G}_B V \tilde{G}_A \cdots V \tilde{G}_m \qquad \text{(AIII. 2)}$$

$\tilde{G}_m = \tilde{G}_B$ if |n - m| odd

and

$\tilde{G}_m = \tilde{G}_A$ if |n - m| even

So from AIII.2 we have

a) | n - m | even

$$G_{nm} G_{mn} = {G_A}^2 (V^2 \tilde{G}_A \tilde{G}_B)^{|n-m|}$$

b) | n - m | odd

$$G_{nm} G_{mn} = G_A G_B (V^2 \tilde{G}_A \tilde{G}_B)^{|n-m|}$$

APPENDIX IV

The calculation of (4.9) involves an average over all possible configurations of the random variables $\{\varepsilon_{i\sigma}\}$ which were introduced in (1.1). This average is calculated with the aid of an extension of C.P.A.[28] as developed by E.N. Economou and C.T. White.[5] In this method they introduced an effective medium which is characterised by 2 site potentials placed periodically. These site potentials are determined self consistently (as in the case of C.P.A.). This method has the good feature that reproduces exactly the periodic limit which is expressed by $P_{A/B}$ (= conditional probability of a site being up given that next site is down) = 1.

To introduce currectly the effects of P = 1 the efffective medium is characterized now by 2 site potentials Σ_0, Σ_1. These have the property that for P = 1 reduce to $\varepsilon_A, \varepsilon_B$ respectively They are calculated self consistntly by demanding that average scatterin be zero at nearest and next nearest neighbors of site 0, The average scattering is calculated asusual from the T matrix:

$\langle T \rangle = 0$

In site 1 (nearest neighbor)

$$\langle T \rangle = \frac{\epsilon_A - \Sigma_1}{1 - (\epsilon_A - \Sigma_1)\langle 1|G|1\rangle} P^1_{A/\alpha} + \frac{\epsilon_B - \Sigma_1}{1 - (\epsilon_B - \Sigma_1)\langle 2|G|2\rangle} P^1_{B/\alpha} = 0 \quad \text{(AIV. 1)}$$

For site 2:

$$\langle T\rangle = \frac{\epsilon_A - \Sigma_0}{1-(\epsilon_A-\Sigma_0)\langle 2|G|2\rangle}P_{A/\alpha}^2 + \frac{\epsilon_B - \Sigma_0}{1-(\epsilon_B-\Sigma_0)\langle 2|G|2\rangle}P_{B/\alpha}^2 = 0 \qquad (AIV.2)$$

G is an effective hamiltonian whih depends on Σ_0, Σ_1. So the above equations are trancedental and they are solved numerically.

The solutions of (AIV.1, AIV.2) are behaving badly as E real inside the band. This is due to the sharp peaks of ImG, ReG. So we need to know the asymptotic solutions far away from the bands and proceed with caution if we are to solve (AIV.1, AIV.2) to get density of states. But for the purpose of (4.9) the method is very fast since then we can staart the calculation from a very far point and approach zero without any risk of divergence. This makes (4.9) very economical, so instead of first calculating density of states of their energies and then differences along the real axis we get J_F through (4.9) with one calculation.

APPENDIX V

The four equations (6.20, 6.21, 6.23, 6.24) can be reduced to one using:

$$\lambda = P_{+}(A,A)/P_{+}(A,B)$$

$$\omega = P_{+}(B,B)/P_{+}(B,A)$$

$$\eta = P_{+}(A,B)/P_{+}(B,A)$$

By using $\Omega = \exp(-2\beta(\mu H + \gamma J))$ the final equations is written as:

$$F(\lambda) = 1 - \Omega\lambda((1 + \Omega D f(\lambda)/(1+\Omega f))^{\gamma-1} = 0 \qquad (AV.1)$$

Where

$$D = \exp(4J\beta)$$

$$f(\lambda) = ((D+\lambda)/(1 + \lambda))^{(\gamma-1)}$$

γ = number of nearest neighbors. For $H = 0$ we use a simpler equation than (AV.1) because $P_{+}(B,B) = P_{+}(A,A)$, This leas to

$$\varphi(\lambda) = D\Omega\, f(\lambda) - \lambda = 0 \qquad (AV.2)$$

for $H = 0$.

From (AV.1) we find $\frac{\partial\lambda}{\partial H} = -\frac{\partial F/\partial H}{\partial F/\partial\lambda}$ and this gives by use of (AV.2)

$$\frac{d\lambda}{dH} = 2\beta\lambda/(1 + \Omega\mathrm{D} \cdot \frac{\partial f}{\partial \lambda})$$

And

$$\frac{dP(A)}{dH} = \frac{2P_+(A,A)}{1 + \Omega\mathrm{D} \cdot \frac{\partial f}{\partial \lambda}} \qquad (AV.3)$$

For T > T_i (AV.3) can be resritten

$$\chi = \frac{dP(A)}{dH} = \frac{\beta \exp(2\beta J)}{\gamma - (\gamma - 2)\exp(2\beta J))}$$

The susceptibility of T = T_C can be written

$$\chi(T_c) = \frac{dP(A)}{dH} = \frac{(\gamma - 2)\log\left(\frac{\gamma}{(\gamma - 2)}\right)}{8(\gamma - 1)}$$

To find the specific heat we use (AV.2). We have

$$\frac{d\lambda}{dT} = -\frac{J^2}{T^2}\frac{\lambda(\gamma - 4) - 3\gamma D}{\frac{(\gamma - 1)\lambda(1 - D)}{1 + \lambda} - (\lambda + D)} \qquad (AV.4)$$

At T_C $\frac{d\lambda}{dT} = \infty$

The spicifi heat is

$$C = \frac{dE}{dT} = -\gamma J \frac{\partial P}{\partial T}$$

$P = (D+\lambda^2)/(D+2\lambda D+\lambda^2)$

The specific heat in the Bethe Peierls approximation has a finite value at T_C[30] For T > T_C and J<0 we have

$$C = \left(\frac{J}{T}\right)^2 2\gamma \, \exp(2\beta J) \, /(1 + \exp(2\beta J))^2$$

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FIGURE CAPTIONS

Figure 1	Configurations of the moments described in the text for the calculation of the magnetic interaction J_B.(a), (b) , (c) correspond to perfect periodicity. (a'), (b'), (c') correspond to improper joining of two otherwise perfectly periodic Bethe lattices.
Figure 2	(a) Improper joining of 2 otherwise perfectly periodic Bethe lattices;(b) The configuration in I' has all $G''_{n\uparrow}$ (E) = $G'_{n\uparrow}$ (E) (see text).
Figure 3	Magnetic coupling J_b vs U/B for various Bethe lattices(B is half the U = 0 bandwidth) in thestatic approximation. The dots are the corresponding values according to the asymptotic expression (see text).
Figure 4	Magnetic coupling J_F vs U/B for various Bethe lattices in the static approximation. The dots are the corresponding values according to the asymptotic expression (see text).
Figure 5	Magnetic couplings J_1 ,J_2 ,J_3 vs U/B for two Bethe lattices in the static approximation. Bethe lattices in the static approximation. Dots represent values according to asymptotic expression
Figure 6	Renormalized magnetic couplings J_b^H, J_F^H, J_1^H U/B for two Bethe lattices.Dots represent the

corresponding values according to the asymptotic expression.

Figure 7 Magnetic interaction J_F vs K_BT/B for $K = 5$. Dot represents the renormalization due to dynamical processes magnetic interaction J_F^H. Dashed curve represents the estimated temperature dependence of J_F^H.

Figure 8 Linear coefficient of the specific heat, C_1; (a), zero temperature susceptibility $X(0)$; (b) and zero energy group velocity, $v_g(C)$ vs U/B. The dots at the $U/B = 0$ axis are rough order of magnitude estimates according to the cluster approach (see text). SK are the results of Seitz and Klein (see ref. 20) and S are estimates based upon Shiba's work (see ref. **21)** .

Figure 9 From top to bottom: Temperature dependence of short order parameter P, magnetic susceptibility X, and specific heat C. The dashed line on the plot of C does not mean that $C \to \infty$ at $KT_C/1J|$ (see ref. 30).

Figure 10. From top to bottom: Dependence of the short order parameter P and concentration of up x on the magnetic field for various values of temperature :

(a) |J}/KT = .2

(b) |J}/KT = .25

(c) |J}/KT = .3

(d) |J}/KT = .4

Figure 11. Schematic representation at a given T of δ vs. U. The upper curve corresponds to H = 0 the lower curve corresponds to H finite. The dashed lines give <5 which does not minimize the free energy (see ref. 5). $u_T(0)$, $u_T(H)$ are the values of u such that for $u < u_T$ $\delta = 0$

Figure 12. Negative magnetoresistance vs H (in K Gauss) for various temperatures.

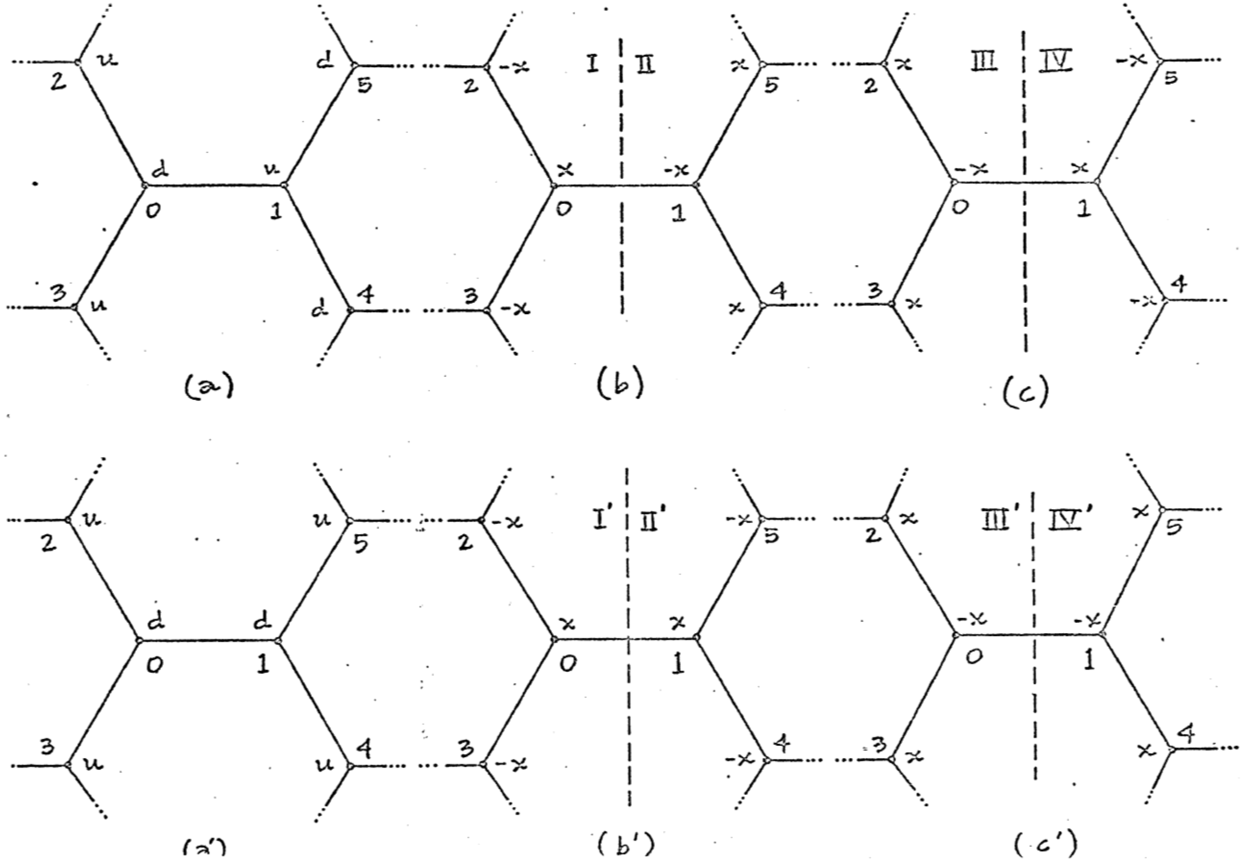

u
d
u
d
-x
I
II
x
x
III
IV
-x
2
5
2
5
2
5
d
u
x
-x
-x
x
0
1
0
1
0
1
3
u
d
4
3
-x
x
4
3
x
-x
4
(a)
(b)
(c)
v
u
-x
I'
II'
-x
x
III'
IV'
x
2
5
2
5
2
5
d
d
x
x
-x
-x
0
1
0
1
0
1
3
u
u
4
3
-x
-x
4
3
x
x
4
(a')
(b')
(c')

Figure 1

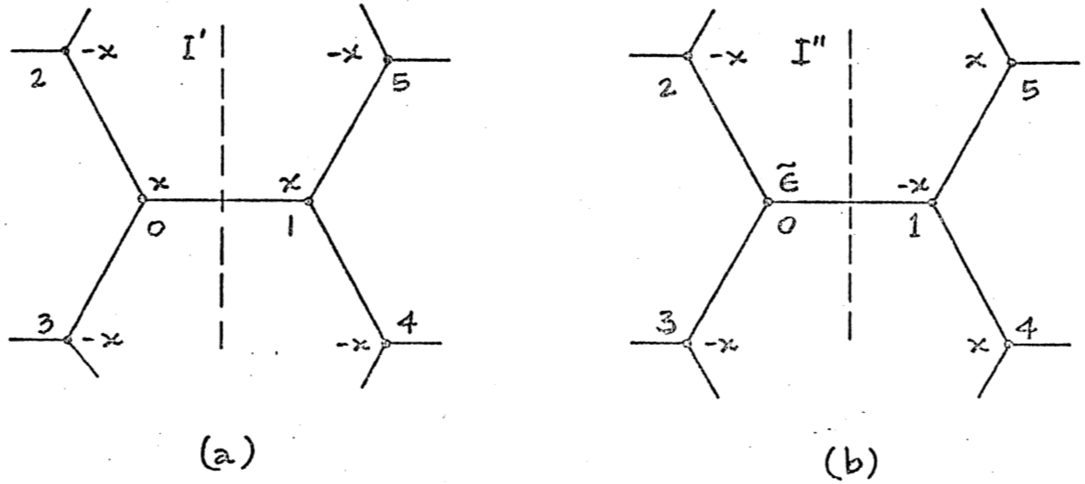


Figure 2

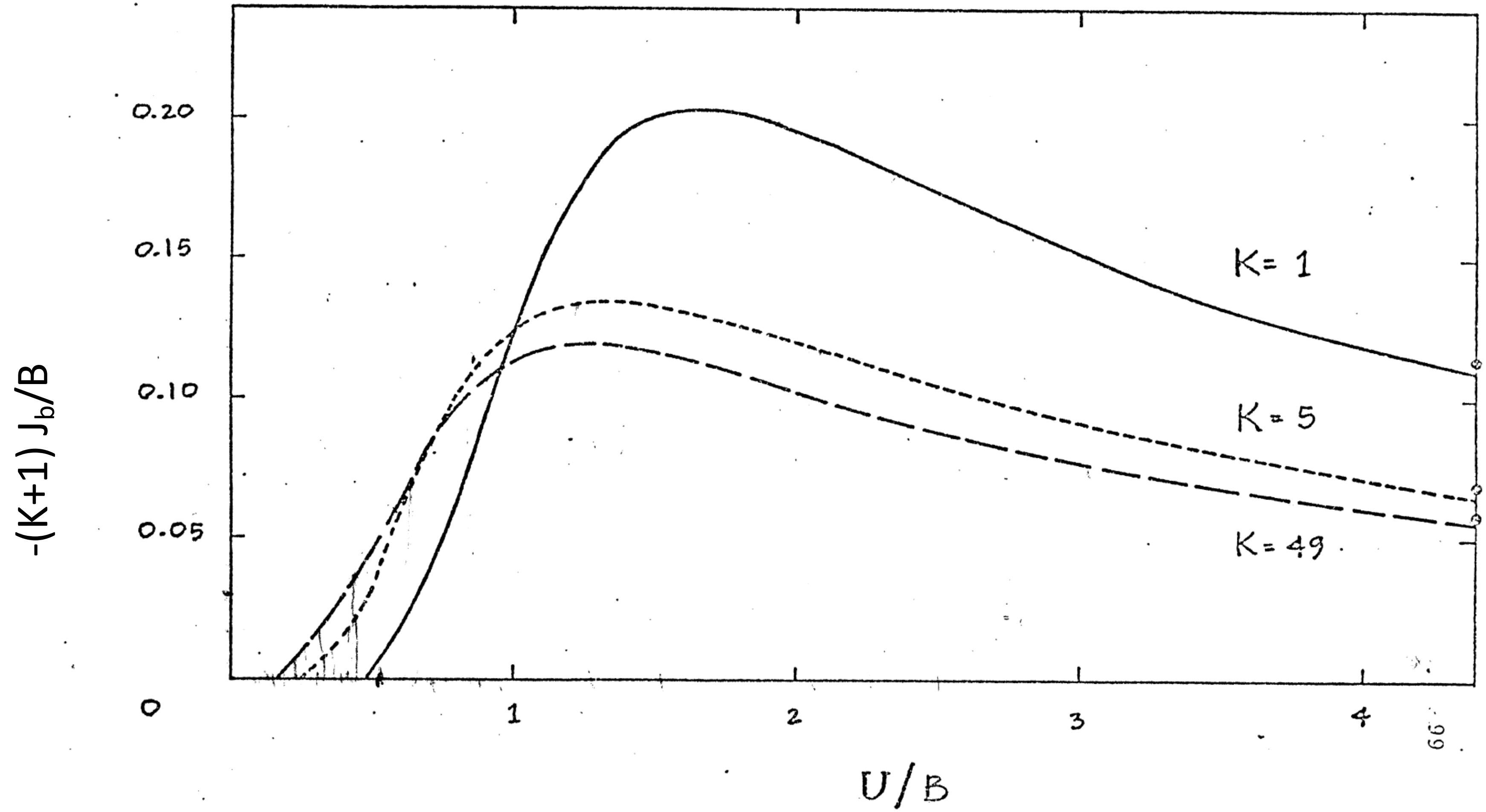


Figure 3

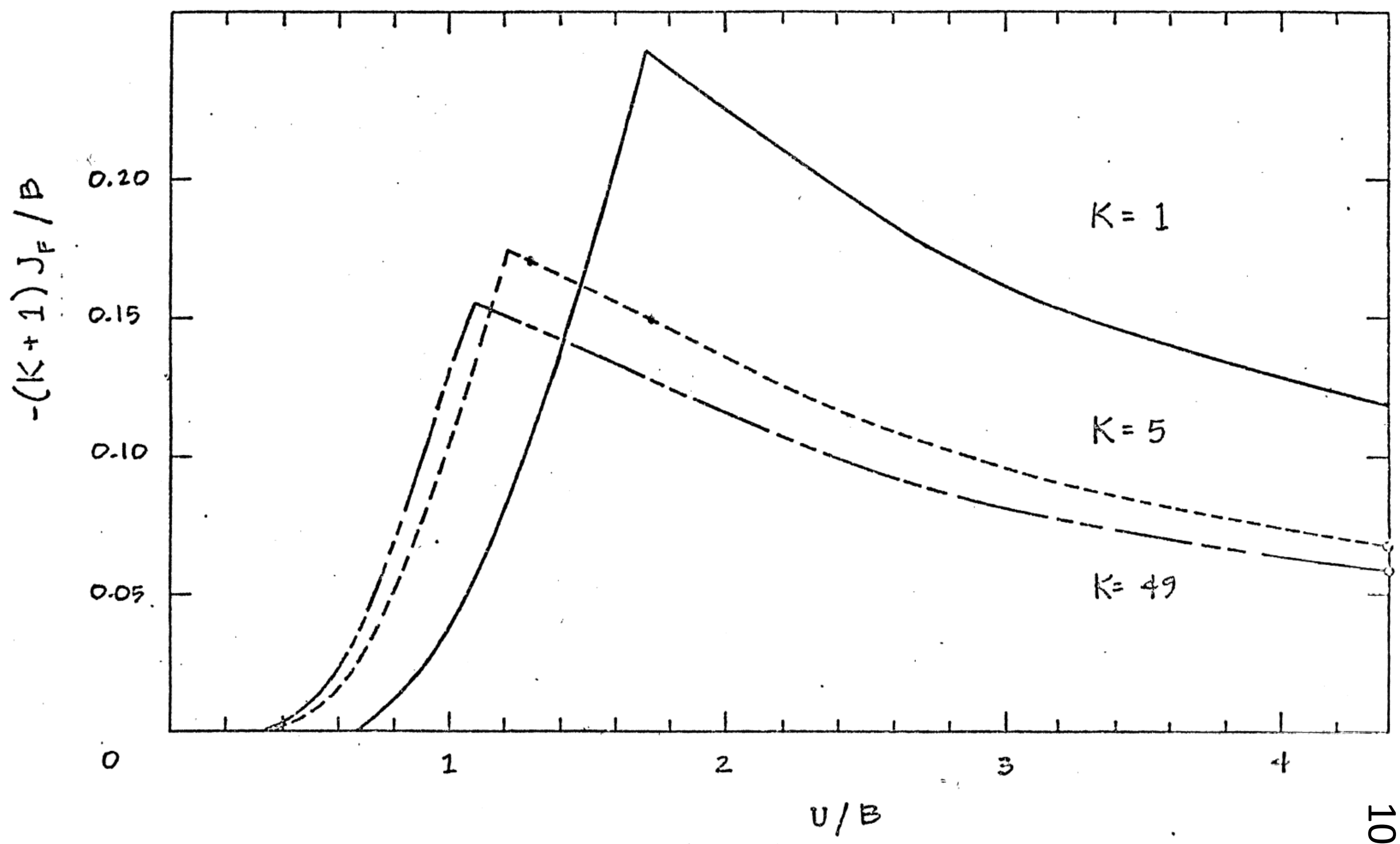


Figure 4

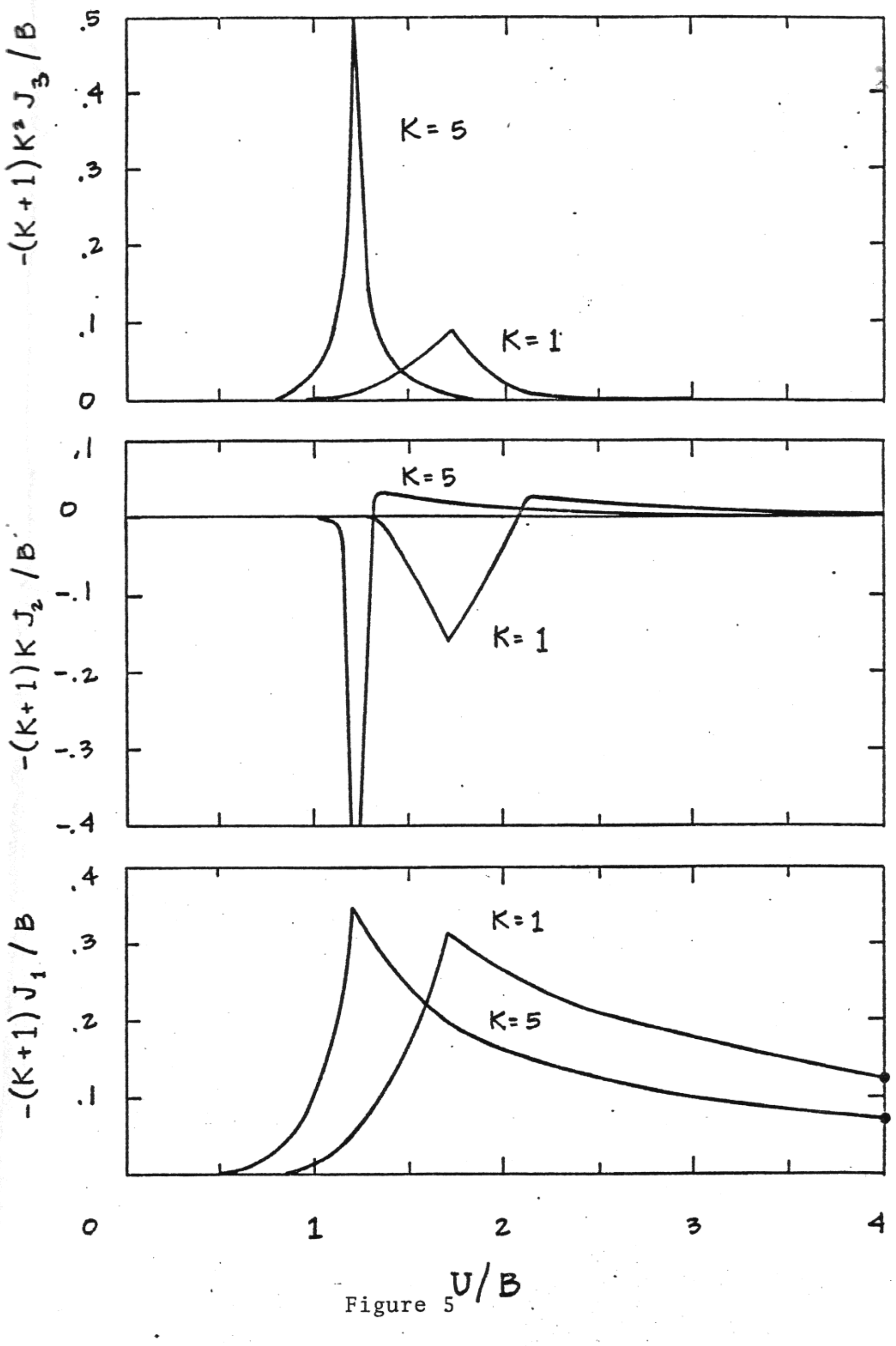

$-(K+1)K^2J_3/B$
.5
.4
.3
.2
.1
0
K= 5
K= 1
$-(K+1)KJ_2/B$
.1
0
-.1
-.2
-.3
-.4
K= 5
K= 1
$-(K+1)J_1/B$
.4
.3
.2
.1
K= 1
K= 5
0
1
2
3
4
U/B

Figure 5

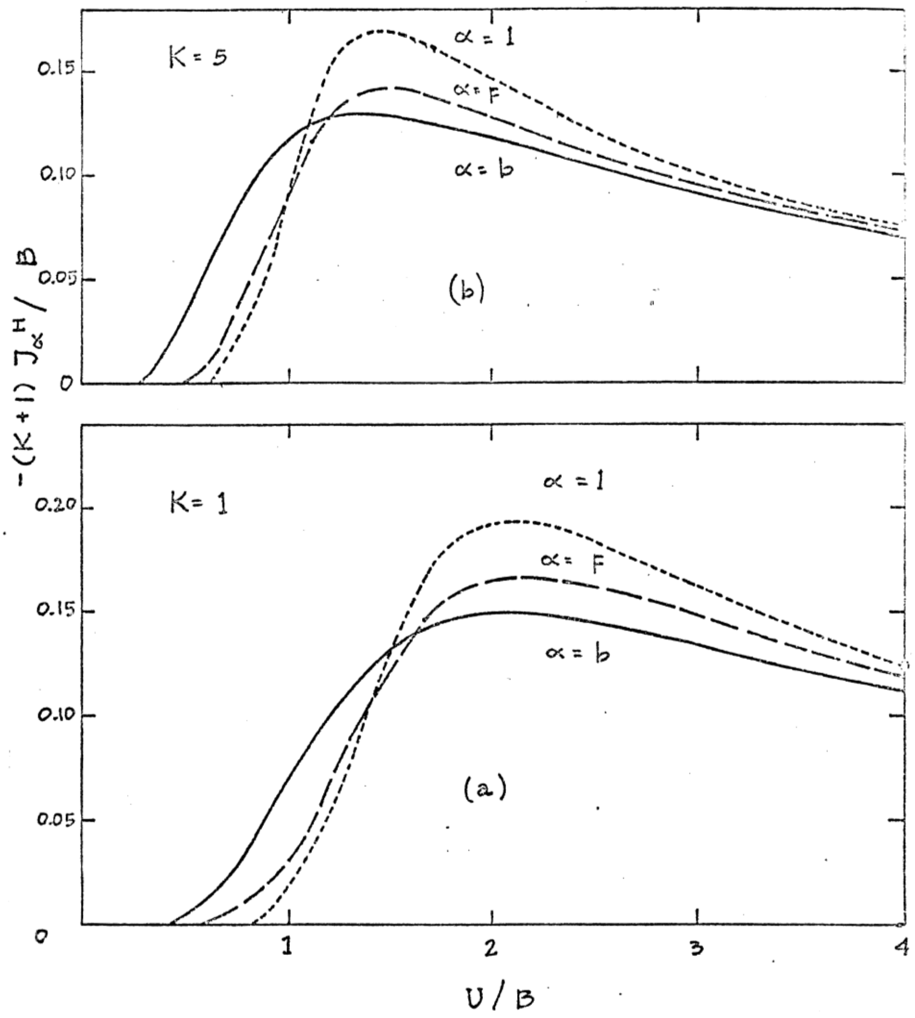

K= 5
α = 1
α = F
α = b
(b)
0.15
0.10
0.05
0
$-(K+1)\, J_\alpha^H / B$
K= 1
α = 1
α = F
α = b
(a)
0.20
0.15
0.10
0.05
0
1
2
3
4
U / B

Figure 6

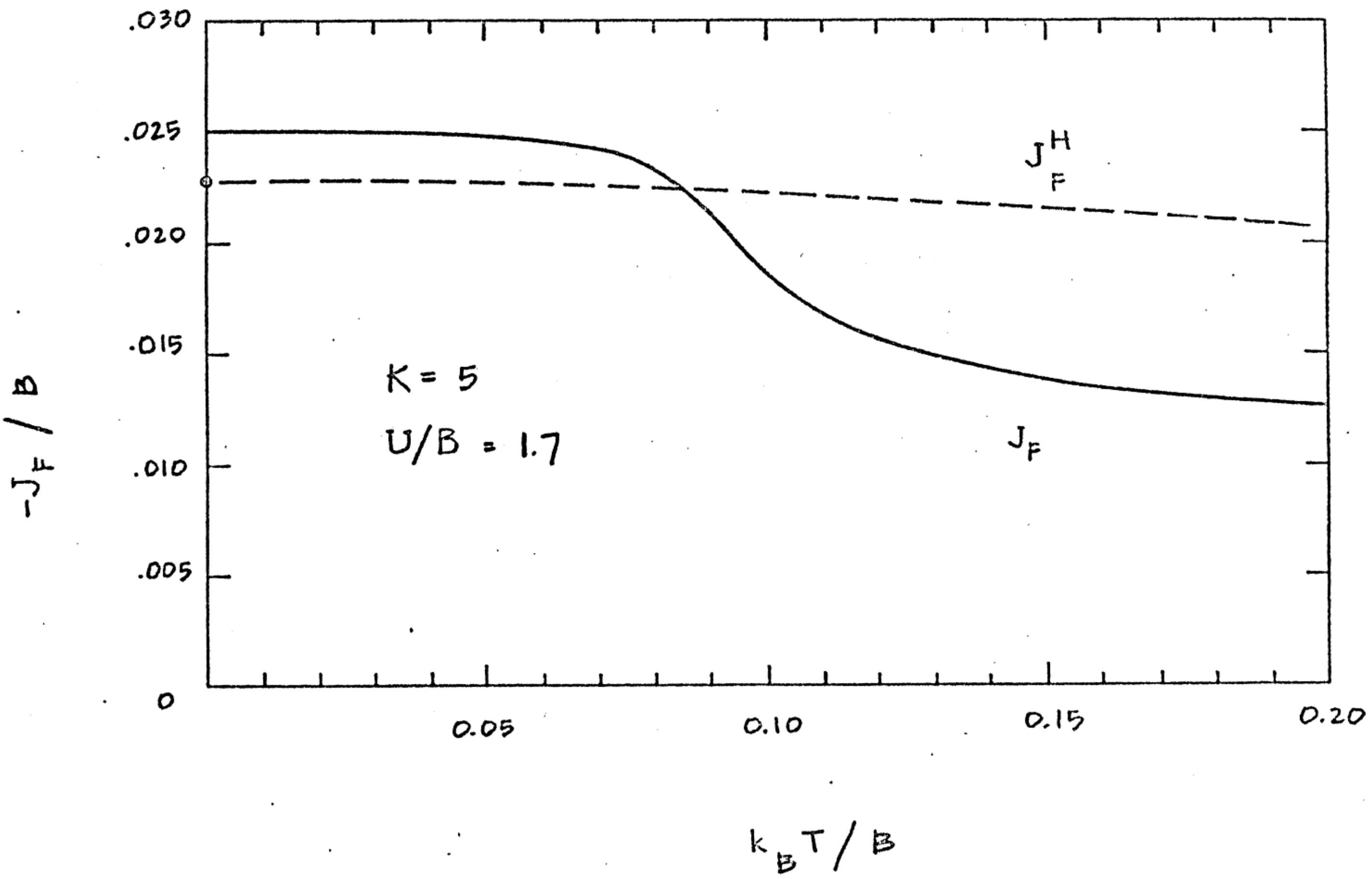
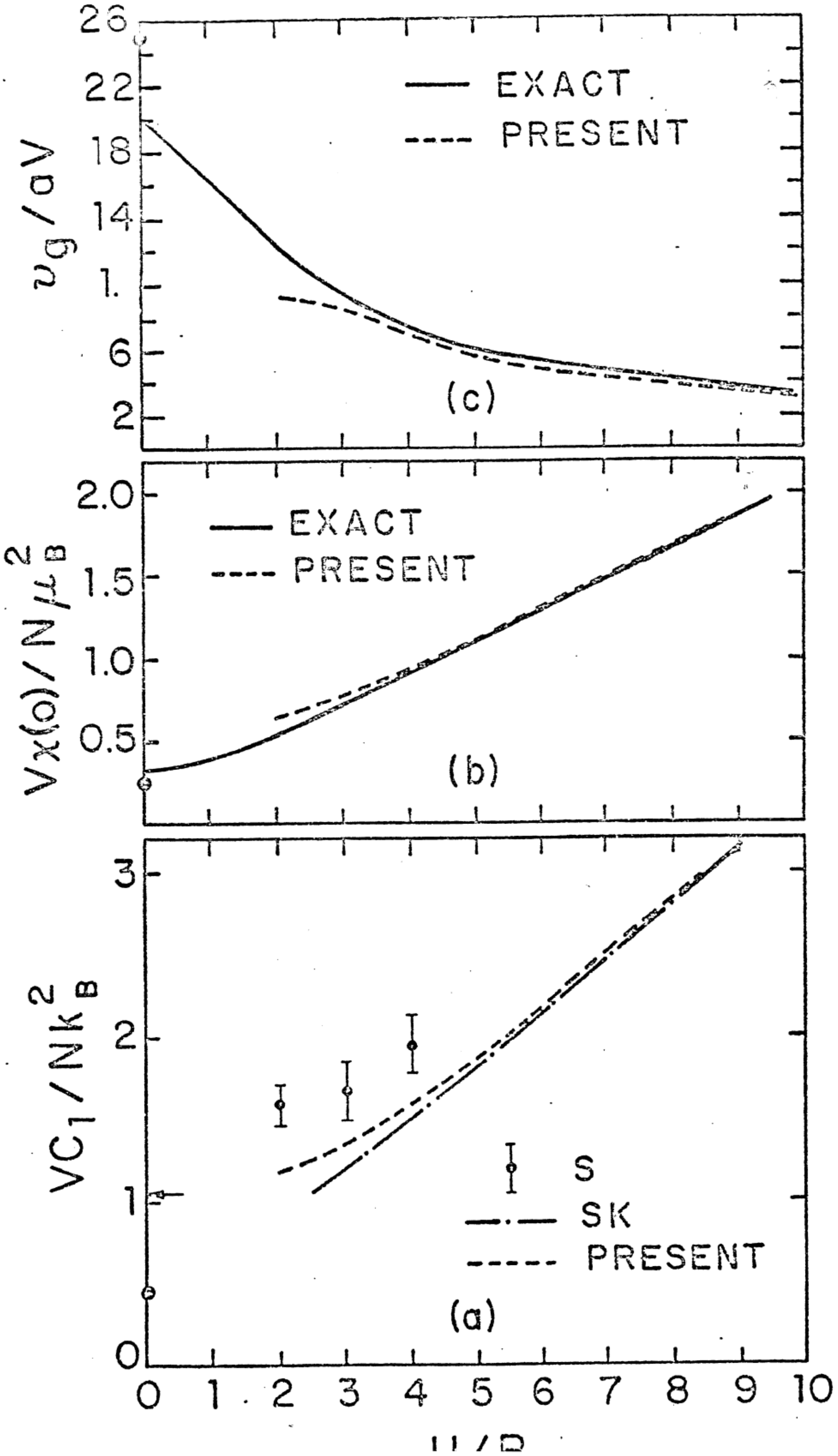


Figure 7


v_g/aV
26
22
18
14
1.
6
2
EXACT
PRESENT
(c)
$V\chi(0)/N\mu_B^2$
2.0
1.5
1.0
0.5
EXACT
PRESENT
(b)
VC_1/Nk_B^2
3
2
1
0
S
SK
PRESENT
(a)
0
1
2
3
4
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7
8
9
10
U/B

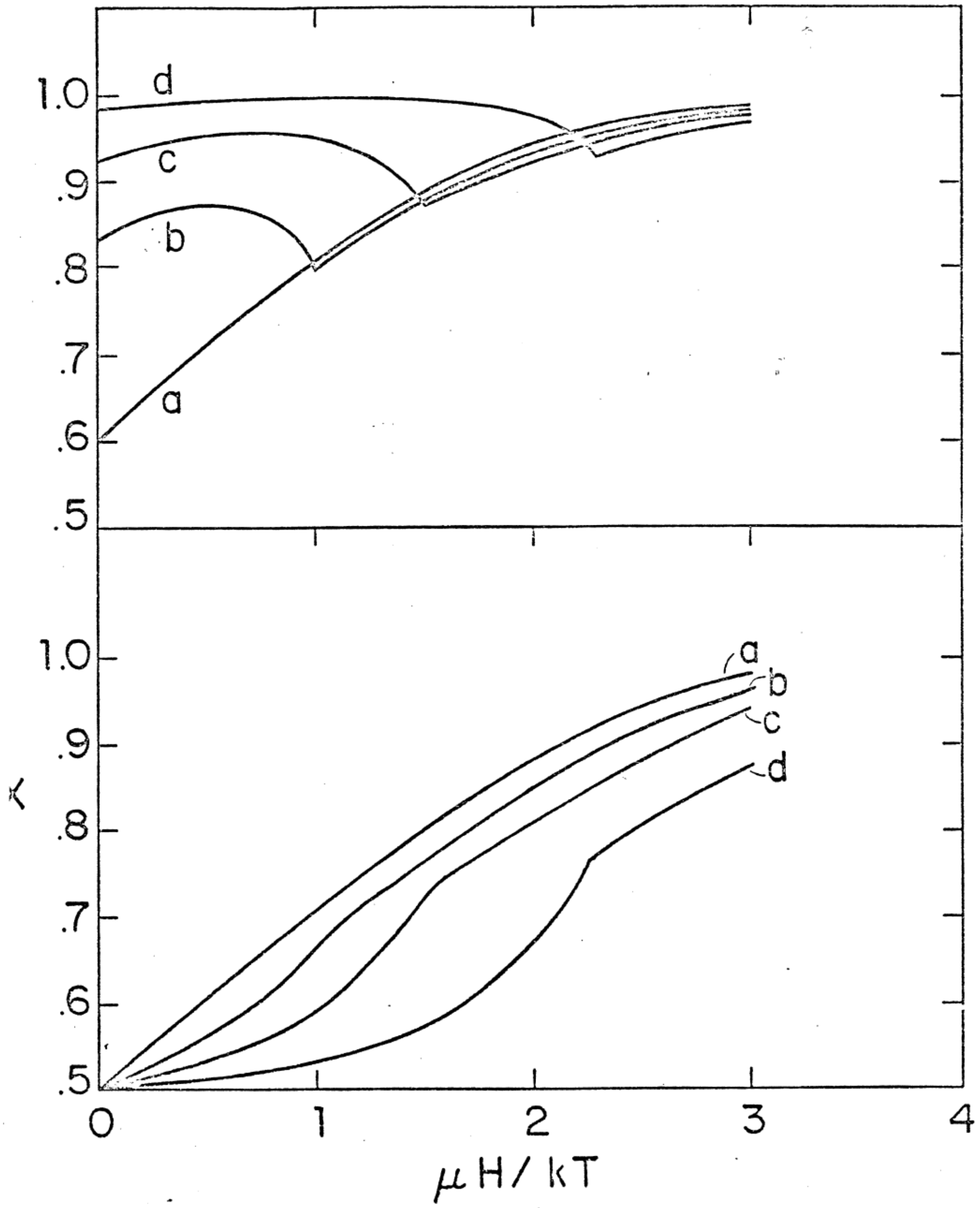

Figure 10

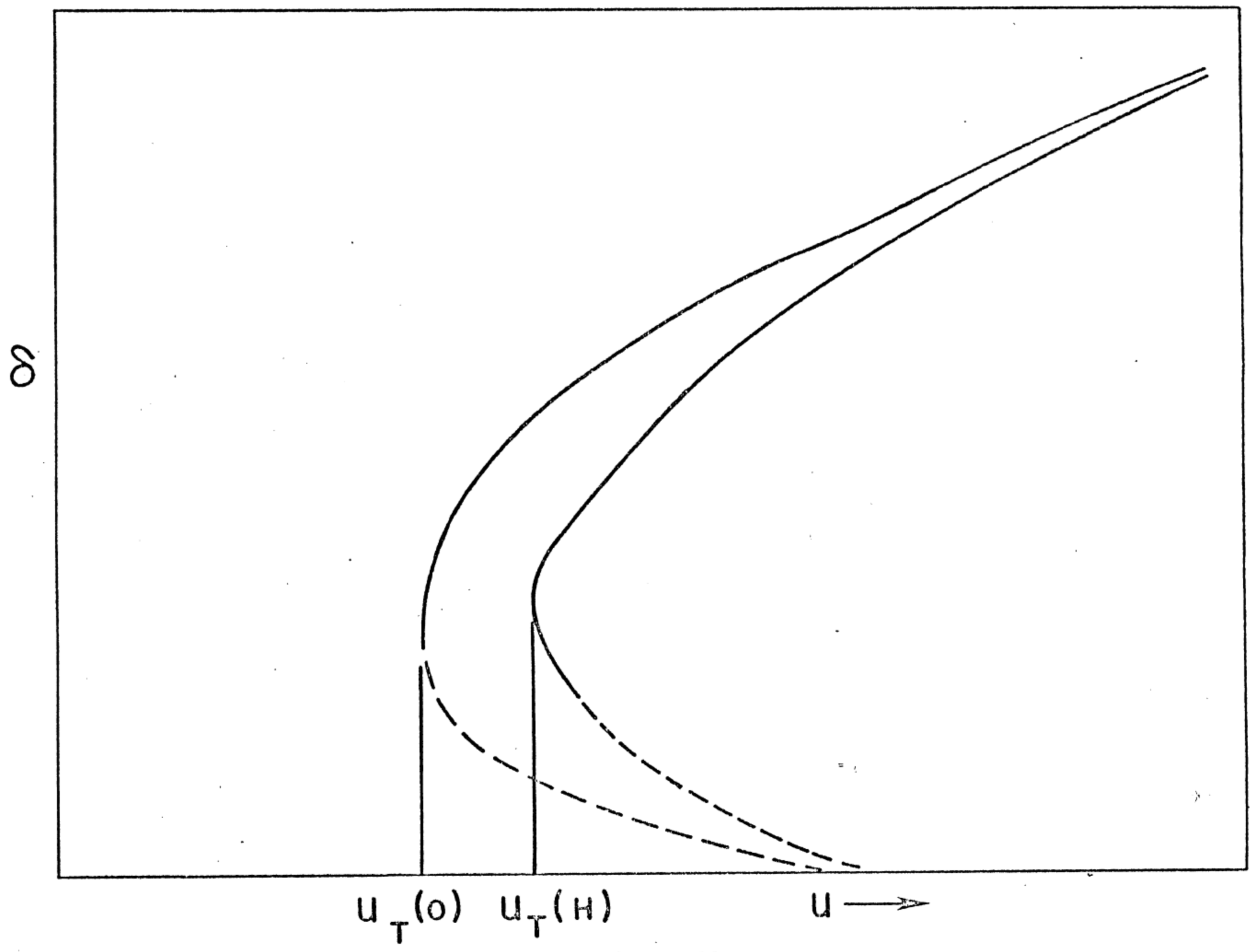

Figure 11

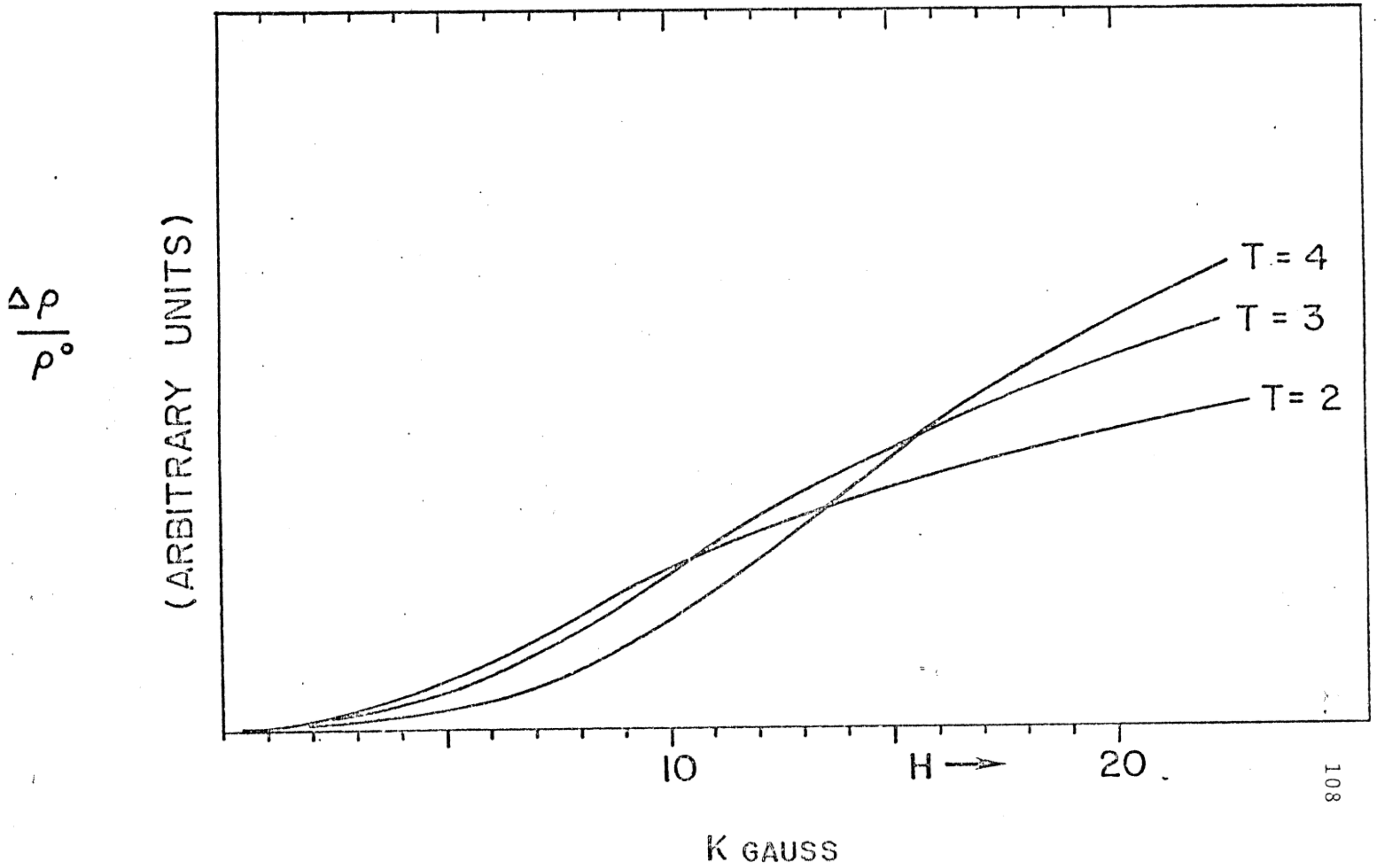

Figure 12