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PHASE TRANSITIONS IN THE HUBBARD HAMILTONIAN

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ABSTRACT

We study phase transition in the isotropic non-degenerate Hubbard Hamiltonian within the renormalization group techniques, using the $\varepsilon = 4 - d$ expansion to first order in ε. The functional obtained from the Hubbard hamiltonian displays full rotation symmetry and describes two coupled fields : a vector spin field, with n components and a non-soft scalar charge field. This coupling is pure imaginary, which has interesting consequences on the critical properties of this coupled field system. The effect of simple constraints imposed on the charge field is considered. The relevance of the coupling between the fields in producing Fisher renormalization of the critical exponents is discussed. The possible singularities introduced in the charge-charge correlation function by the coupling are also discussed.

INTRODUCTION

In this paper we shall consider the effects of the spin-charge coupling on the magnetic transition of the electron gas, described by the non degenerate Hubbard Hamiltonian[1]. The latter has been studied with the use of functional integral techniques[2,3] by several authors in recent years[4,5]. This formulation exhibits a coupling between spin fluctuations and charge fluctuations, which has usually been disregarded in the literature, as is understandable when one realizes that charge fluctuations cannot be unstable at any temperature or space dimension within the non degenerate Hubbard Hamiltonian.

Recently, two of us[5] have undertaken the study of the consequences of this spin-charge coupling on the thermodynamic properties of the electron gas, in particular on its critical properties. In reference (5) the first part discusses some difficulties related with the functional integral technique : one can derive various exact formulations for the partition function of the electron gas ; some of these, once they are approximated by Landau-Ginzburg like free energy functionals, exhibit spin fields with only one component (Ising-like fields) while others have spin fields with $n = 3$ components (Heisenberg-like fields). Given the importance of symmetry in the critical properties of the magnetic phase transition, and given the spin rotational invariance of the original hamiltonian, it was argued in (5) that the correct formulation must explicitly exhibit the vector nature of the spin field. However, in the second part of (5) the effect of spin-charge coupling was studied with the aid of renormalization group results[6], within a theory with Ising-like spin fields. The reason was that the renormalization group had been used previously in the study of a phenomenological free energy functional[6], quite similar to the one derived from the Hubbard Hamiltonian, describing the critical properties of a coupled field system, with a non soft scalar field and a soft Ising-like one. The study of the Hubbard Hamiltonian in reference (5) relied on the results of that theory. It was shown that the spin-charge coupling restricts the domain of existence of first order transitions with respect to that predicted by a spin-only theory.

In this paper we study a general free-energy functional, with a n-component spin field, the Hubbard model corresponding to $n = 3$.

The question of what happens to a usual second order transition when the order parameter is coupled to some other (non-soft) degrees of freedom, has received considerable theoretical attention in the past few years, essentially in connection with the spin-phonon problem, when the magnetic exchange interactions depend on separation between ionic spins. This is due to the fact that real systems have finite elastic constants and the modulation of the couplings, e.g. the exchange interactions, by the lattice vibrations may lead to qualitative effects on the phase transition[7]. Fisher[8] formulated a theory based on thermodynamic assumptions, of renormalization of critical exponents describing the second-order exponents by constrained "hidden variables". An example is the constraint of constant volume. If one assumes that the specific heat at constant pressure, C_p, diverges, i.e., $C_p \sim |T - T_c(p)|^{-\alpha_I}$, where $\alpha_I > 0$ (as is the case for the Ising model) and $T_c(p)$ is a well behaved function, one can then show that the specific heat at constant volume, C_v, must be finite at the transition, except when $\frac{dT_c}{dp} = 0$. More precisely, one can show that, close to T_c, C_V is given by

$$C_V = \text{const.} + \text{const.}\ |T-T_c(v)|^{-\alpha_R}$$

where

$$\alpha_R = -\alpha_I/(1-\alpha_I) < 0$$

is the Fisher-renormalized critical exponent. When $\alpha_I < 0$, as is the case for the Heisenberg model, no such renormalization can occur.

Sak used renormalization group recursion relations for the effective spin hamiltonian obtained after integrating out the elastic modes. This Hamiltonian has an additional coupling term, which was also considered by Rudnick, Bergman and Imry[9].

Starting from a completely different microscopic hamiltonian, suitable to describe a metamagnet in the presence of an external magnetic field, Nelson and Fisher[10] derived a free energy density which also exhibits two coupled order parameters, which reflects the existence of alternate planes of spins, coupled ferromagnetically within a plane and antiferromagnetically between adjacent planes. Instead of integrating out the non soft modes Nelson and Fisher[10] carry out the renormalization group procedure for both fields, and verify the gaussian like nature of the critical exponents for space dimension d = 3 at the tricritical point. In their case, due to the different exchange interactions, intra and inter-planes, the two fields are not simultaneously soft and consequently, a scaling consistent with that is adopted.

Achiam and Imry[6] study a phenomenological free energy functional describing two coupled fields, a (soft) Ising-like spin field and a (non-soft) scalar field, the coefficient of the coupling term in their theory is real.

They investigate the role of constraints imposed on the (non-soft) scalar field, and they discuss the weak singularities of the non-soft field at the critical point, when constraints are present or not, and also when the coupling between the soft and the non-soft field changes its form. A result of special interest obtained by Achiam and Imry is that the constraint imposed on the non-soft field results in stabilizing the renormalized-Ising critical point, which in Sak's treatment, was not physically allowed, due to the impossibility of negative bulk modulus[7]. The parameter space they use is richer, since it contains the zero wave-vector coupling between fields, as well. Therefore the chart of fixed-points they obtain is richer as compared to other treatments. Four groups of fixed points are obtained, i.e. Gaussian, Ising, renormalized Ising and spherical. Some fixed points differ only by the relevance of the coupling between the two fields.

Two questions arise about the work of Achiam and Imry. Firstly the validity of the results they obtained when the number n of components of the soft field is greater than $n = 1$. Since the specific heat exponent α changes sign when n goes from 1 to 3, one expects the chart of fixed points to be altered and the stability of the Fisher renormalized fixed points to be exchanged with that of the usual unrenormalized fixed point. Secondly, the consequences of the spin charge coupling coefficient being pure imaginary, which turns out to be the case for the Hubbard model, have to be investigated in detail.

In part I, we derive the free energy functional corresponding to the (isotropic) Hubbard Hamiltonian, introducing explicitly spin rotational invariance.

Part II is divided in three subparagraphs. The first one is the group renormalization study of the free energy functional obtained in part

I, keeping explicitly both fields and imposing a simple constraint. The second one is a thermodynamic study of the crossover exponents describing the Hamiltonian flow between the renormalized critical point and the conventional one. The third subparagraph deals with the charge-charge correlation function and its possible singularities at the critical point.

Part III is devoted to a physical discussion of the results obtained in part II.

I - The Free Energy Functional for the Isotropic Hubbard Hamiltonian.

We start with the non-degenerate Hubbard Hamiltonian[1]

$$H = \sum_{i,j,\sigma} T_{ij}\, C^{+}_{i\sigma}\, C_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{1-a}$$

where, as usual, T_{ij} is the hopping integral between sites i and j , $C^{+}_{i\sigma}$ and $C_{j\sigma}$ are the creation and destruction operator for electrons in the sites i and j, with spin σ , respectively. U is the Coulomb interaction, supposed to exist only between electrons in the same site and $n_{i\sigma} = C^{+}_{i\sigma}\, C_{i\sigma}$, with $\sigma = +1$ or $\uparrow$ and -1 or $\downarrow$.

With the aid of the identity[5]

$$U\, n_{i\uparrow}\, n_{i\downarrow} = \frac{U}{4}\,(n_{i\uparrow} + n_{i\downarrow}) + \frac{U}{8}\,(n_{i\uparrow} + n_{i\downarrow})^2 - \frac{U}{2}\, \vec{S}_i \cdot \vec{S}_i$$

We rewrite (1) as

$$H = \sum_{i,j,\sigma} \tilde{T}_{ij}\, C^{+}_{i\sigma}\, C_{j\sigma} + \frac{U}{8} \sum_i (n_{i\uparrow} + n_{i\downarrow})^2 - \frac{U}{2} \sum_i \vec{S}_i \cdot \vec{S}_i \tag{1-b}$$

where $\tilde{T}_{ij} = T_{ij} + \frac{U}{4}\delta_{ij}$. A number of identities used to transform the interaction term in the Hubbard Hamiltonian exists in the literature[2,4,5]. However, as discussed in reference 5, the identity used here is the appropriate one if rotation invariance is to be preserved, as it should, and if, in addition we want to take into account the "vector" nature of the spin, without introducing spurious many-body interaction[13].

Now we use the Hubbard Stratonovich identity[2] in its vector form

$$e^{\vec{A}^2} = T\int_{-\infty}^{+\infty} D\vec{\xi}\; e^{\int_0^1\left[-\pi\,\vec{\xi}^2(\tau) + 2\sqrt{\pi}\,\vec{A}(\tau)\,\vec{\xi}(\tau)\right]d\tau} \tag{2}$$

for the last term in (1-a) and its scalar version for the second term in (1a). In (2) T is the time-ordering operator needed to preserve the non-commutativity of the operators, which are now (imaginary) time-dependent. After some manipulation (see for example reference 2) one gets for the partition function Z

$$Z = Z_o \int D\vec{\xi}\, Dy\; e^{-H(\vec{\xi}_i,\, y_i)} \tag{3-a}$$

with

$$H(\vec{\xi}_i, y_i) = \sum_i \int_0^{\beta} d\tau\; \pi\left[\vec{\xi}_i^{\,2}(\tau) + y_i^2(\tau)\right] - \sum_{\sigma}\operatorname*{Trace}_{i,\tau}\log(1-VG^o) \tag{3-b}$$

where the potential V has matrix elements given by

$$_{i\sigma}V_{j\sigma'} = -\delta_{ij}\sqrt{\frac{\pi U}{2}}\,\{(i\,y_i + \sigma\,\xi_i^z)\,\delta_{\sigma\sigma'} + \xi_i^{-\sigma}\,\delta_{\sigma',-\sigma}\} \tag{4}$$

Z_o and G^o are the partition function and the Green function, respectively, for the noninteracting system. It is seen from (4) that the use of the

Hubbard-Stratonovich identity enables us to change from a two-body hamiltonian to a one-body problem, but the potential is now complex and depends on time, spin and the site, as well. The first term in the diagonal contribution $\delta_{\sigma\sigma'}$, in (4) is the electric potential with pure imaginary coupling $i\sqrt{\frac{U}{2}}$, y_i being the charge field at site i, while the remaining terms represent the vector magnetic field. In addition a gaussian weight factor appears in the functional integral (3).

Expanding the Tr Log $(1 - VG^o)$ up to fourth order in V (second order in U) and using the Fourier transform representation with $q_i \equiv (q_i, \omega_i)$ to include both the momentum q_i and the Matsubara fermion frequency ω_i, we get

$$H(\vec{\xi},y) = \frac{1}{2}\sum_{q,\alpha}(1-U\,\chi_o(q))\,\xi^{\alpha}_{q}\,\xi^{\alpha}_{-q} + \sum_{\substack{q_1q_2q_3\\ \alpha,\beta}}\mu(q_1,q_2,q_3)\,\xi^{\alpha}_{q_1}\xi^{\alpha}_{q_2}\xi^{\beta}_{q_3}\xi^{\beta}_{-(q_1+q_2+q_3)}$$

$$+ \frac{1}{2}\sum_{q}(1+U\,\chi_o(q))y_q\,y_{-q} + \sum_{q_1q_2}V_3(q_1,q_2)\,y_{q_1}y_{q_2}y_{-(q_1+q_2)} + \qquad (5)$$

$$+ \sum_{q_1q_2q_3}V_4(q_1,q_2,q_3)\,y_{q_1}\,y_{q_2}y_{q_3}\,y_{-(q_1+q_2+q_3)} +$$

$$+ \sum_{\substack{q_1,q_2\\ \alpha}}\mu(q_1,q_2)y_{q_1}\xi^{\alpha}_{q_2}\,\xi^{\alpha}_{-(q_1+q_2)} + \sum_{q_1q_2q_3}I^{sc}_{2}(q_1q_2q_3)\,\xi^{\alpha}_{q_1}\,\xi^{\alpha}_{q_2}\,y_{q_3}y_{-(q_1+q_2+q_3)}$$

where the sum over α runs from 1 to n. The function $\chi_o(q)$ is the non-enhanced susceptibility of the electron gas; the coupling constants are function of the interaction energy U and of the bare fermion loops[3]. Some versions of the transformations of the Hubbard Hamiltonian through equ.(2) exhibit incorrect RPA spin correlation function (2). Equ. (5) has the correct RPA spin- or charge-correlation function, along with spin-rotational invariance and spin-charge coupling. Note that μ and V_3 are pure imaginary. The factor $(1 + U\chi_o(q))$ in the gaussian charge term implies the impossibility of a charge instability, as is well known for the Hubbard model. That is the reason why the charge terms are usually neglected; we conserve them since we are interested in studying their possible effects on the magnetic transition through the two last coupling terms in (5). Nevertheless, if an appropriate scaling of the field is made, the last term in (5), the V_3 and V_4 terms, as well the q^2 dependence of the Gaussian term in the charge field, which appears when we expand the susceptibility (see below), are irrelevant in the renormalization group sense[6,10], so we neglect them. The choice of that scaling is dictated by the fact that the charge field is not soft within the pure Hubbard model, as stated above.

Now we are interested in studying the system close to its ferromagnetic instability, possibly at low temperatures but not very close to $T = 0$. This means that it is enough to consider the dependence on q of the coupling constants and fields, for small $\vec{q}$ and $\omega \approx 0$. But in such case we can neglect all dependence on $\vec{q}$ of the coupling constants[14] and we can write χ_o as[15]

$$\chi_o(\vec{q}) \equiv \chi_o(\vec{q}) \equiv N(E_F)\left[1 - \frac{1}{3}\left(\frac{q}{2k_F}\right)^2\right]$$

where $N(E_F)$ is the density of states at the Fermi level E_F. A word of caution about this expansion should be said, for $d \neq 3$. We assume its validity around $d = 4$, including $d = 3$. In fact, it has been shown[16], for a free electron band, in the $q = 0$ limit, that $\chi_o(q) \approx \chi_o(0)\{1 - \frac{d-2}{3}\left(\frac{q}{2k_F}\right)^2\}$

the d-dependence appearing only in the multiplicative factor $\frac{d-2}{3}$. (The $d = 2$ case shows a peculiarity which need not concern us here).

So the Hamiltonian becomes

$$H = \frac{1}{2} \sum_\alpha \int_q (r+q^2)\, \xi^\alpha_q \, \xi^\alpha_{-q} + u \sum_{\alpha\beta} \int_{q_1 q_2 q_3} \xi^\alpha_{q_1} \, \xi^\alpha_{q_2} \, \xi^\beta_{q_3} \, \xi^\beta_{-(q_1+q_2+q_3)} +$$

$$\frac{1}{2}\beta \int_q y_q y_{-q} + \mu \sum_\alpha \int_{q_1 q_2} y_{q_1} \, \xi^\alpha_{q_2} \, \xi^\alpha_{-(q_1+q_2)} \qquad (6)$$

where

$$r \simeq 1 - UN(E_F) \qquad \text{and} \qquad \beta \simeq 1 + UN(E_F).$$

We recall that the couplings u and μ are connected to the band structure through $N(E_F)$ and its derivatives:

$$u = -(kT_c)\, U^2 \left.\frac{d^2N(E)}{dE^2}\right|_{E_F} \qquad \mu = i(kT_c)^{1/2} U^{3/2} \left.\frac{dN(E)}{dE}\right|_{E_F}$$

This constrasts with reference 10 where the coupling between the fields depends on the external magnetic field.

In (6) appropriate units were chosen in order to get rid of some constant factors(*). The Hamiltonian now looks quite similar to two Landau-Ginzburg-Wilson Hamiltonians plus a rotation invariant coupling between the two fields, the first of which is vectorial and may become soft and the other, a non-soft scalar field. The passage to the continuous limit was made $\int_q = \frac{1}{(2\pi)^d}\int d^d q$, $\underline{d}$ being the space dimension.

As stated above we also want to consider the effect of cons - traints imposed on the charge field. Following Achiam and Imry[6] we res trict our attention to the q = 0 component of y_q, that is, on the uniform total charge and we correspondingly single out that component, allowing different coupling constants for them

$$
\begin{aligned}
H = {} & \frac{1}{2}\sum_{\alpha}\int_q (r+q^2) S_q^{\alpha} S_{-q}^{\alpha} + u \sum_{\alpha,\beta}\int_{q_1 q_2 q_3} S_{q_1}^{\alpha} S_{q_2}^{\alpha} S_{q_3}^{\beta} S_{-(q_1+q_2+q_3)}^{\beta} \\
& + \frac{\beta_o}{2\Omega} y_o^2 + \frac{1}{2}\beta \int_q' y_q y_{-q} + \frac{\mu_o}{\Omega} y_o \sum_{\alpha}\int_q S_q^{\alpha} S_{-q}^{\alpha} \\
& + \mu \sum_{\alpha}\int_{q_1}' \int_{q_2} y_{q_1} S_{q_2}^{\alpha} S_{-(q_1+q_2)}^{\alpha}
\end{aligned}
\tag{7}
$$

where we have changed the notation, putting $\vec{\xi} = \vec{S}$. The prime in the integral means that the origin is excluded from the domain of integration. The terms involving the q = 0 component were divided by Ω , the volume of the system, in order to keep their dimensionality equal to that of the corresponding $q \neq 0$ terms. The hamiltonian has now its final form; in the next sections we study the phase transition in systems governed by it.

Note that (7) coincides, for n = 1, with the phenomenological hamiltonian of Achiam and Imry[6] when μ is real. We have shown that, for n = d = 3 it can be quite generally derived from the Hubbard hamiltonian. Now we extend it to arbitrary $\underline{n}$ and $\underline{d}$. In what follows we will discuss the Hamiltonian (7) for general μ (that is real or pure imaginary). It should be borne in mind however, that for the Hubbard Hamiltonian μ is pure imaginary. This modifies in a non-trivial way the results corresponding to the real coupling situation.

II - a) The Renormalization Group Approach

We now proceed to study (7) within the renormalization group techniques to first order in $\varepsilon = 4 - d$; we first integrate out all the variables y_q and s_q with momenta greater than $1/b$, where $b > 1$; we then rescale the momenta variables by $\underline{b}$ and the fields y_o, y_q and S_q by c_o, c and ζ, respectively[10,6]. ζ is determined by imposing that the coefficient of the q^2 term in the transformed hamiltonian is equal to unity, and from this we get $\zeta = b^{3-\varepsilon/2}$. On the other hand, we choose[6,10] c and c_o such that $\beta' = \beta$ and $\beta_o' = \beta_o$ where the prime denotes the corresponding parameter in the transformed hamiltonian. We have already pointed out that this choice is convenient since the charge field cannot become soft. Using the recursion relations for β and β_o

$$\beta' = \beta\, c^2\, b^{-d}(1 - 2ZnA_2) \quad \text{and} \quad \beta_o' = \beta_o\, c^2\, b^{-d}(1-2\omega n A_2)$$

where

$$Z = \mu^2/\beta \qquad \omega = \mu_o^2/\beta_o \qquad \text{and} \qquad A_\ell = \int_{|q|>\frac{1}{b}} \frac{1}{(r+q^2)^\ell}$$

We find

$$c = b^{2-\varepsilon/2}(1+ZnA_2) \quad \text{and} \quad c_o = b^{2-\varepsilon/2}(1+\omega n A_2) \qquad (8)$$

Clearly, under the renormalization group operations, the terms V_3, V_4 and I_2^{sc} in (5) transform like $b^{-2+\varepsilon/2}$, $b^{-4+\varepsilon}$ and $b^{-2+\varepsilon}$, respectively, being for that reason, irrelevant after many iterations. The same argument applies to the q^2 term in the charge field, as well.

The renormalization of (7) generates a term $\mu_o\, c_o\, A_1\, y_o n$, which appears when the two spin fields are contracted in the $y_o S^2$-like term. Following references 6 and 10 we have made a shift in y_o in order to eliminate it. This shift, on the other hand, introduces a term $-2\, b^2 A_1\, n\omega$ in r' recursion relation; this recursion relation, together with the corresponding for u', z' and ω' read then

$$u' = b^{\varepsilon}\{u - 4(n+8)\, u^2 A_2 + 24\, u\, Z\, A_2 - 4\, Z^2 A_2\}$$

$$Z' = b^{\varepsilon}\, Z\, \{1 - 8(n+2)\, u\, A_2 + 2(n+4)\, Z\, A_2\}$$

$$\omega' = b^{\varepsilon}\, \omega\, \{1 - 8(n+2)\, u\, A_2 + 8\, Z\, A_2 + 2\, \omega\, n\, A_2\}$$

$$r' = b^2\, \{r + 4(n+2)\, u\, A_1 - 4\, Z\, A_1 - 2\omega\, n\, A_1\} \qquad (9)$$

Equations (9) have eight fixed points. (In ref. (6), sixteen fixed points exist, since their parameter space has an additional coordinate corresponding to an energy-energy coupling).

The fixed-point parameters values, the eigenvalues and the eigenvector obtained by linearizing (9) (see reference 14, for example) together with the exponents ν (correlation length) and α (specific heat) are shown in table 1. It is seen from table 1 that the eight fixed points may be grouped in four groups each one specifying a given critical behaviour.

The n = 4 case is the border line for the exchange of stability between the fixed points; in what follows we shall limit the discussion for n in the interval $0 < n < 4$. The points labelled with 1 are then the most stable in each group.

The unconstrained Hamiltonian is such that $z = \omega$; this corresponds to H 1, once stable. If one integrates out the y_q - both for $q = 0$ and $q \neq 0$ - he gets an Hamiltonian analogous to (7) but with $\omega = z = 0$ and an effective u given by $u_{eff} = u - z/2$, the right hand side of the last equation refering to the situation where the integration has not yet been carried out. It is seen from table 1 that this corresponds to H 2, the integration decreasing by one its stability. The Gaussian point G 1 is analogous to H 1 but with the further condition $u = z/2$, thus decreasing by one its stability. If, again, we integrate out the y_q we will get $\omega = z = u = 0$, the fixed-point G 2, totally unstable.

RH 1 is obtained by imposing the constraint $y_o = \theta$ in (7), where θ is a constant. The $y_o S^2$ term in (7) may then be added to the first one, thus giving a shift in r and $\omega = 0$. The constraint increases its stability by one, RH 1 being the most stable fixed point, supposed to govern the critical behaviour of the system. RH 2 is obtained[6] by imposing a constraint in (7) of the form $\delta(y_o - \theta)$ and integrating out the $y_q \neq 0$ fields ($z = 0$ and $u_{eff} = u - z/2$). RH 2 has thus the same degree of stability as H 1.

The spherical fixed-points are obtained by the same procedure as described for the RH points, but with the additional restriction $u = z/2$, thus decreasing by one their stability. It is seen from Table 1 that the critical exponents of RH and S are those of H and G, but renormalized[8], as expected. The integration of the y_q in (7) introduces an effective u given by $u_{eff} = u - z/2$, as stated above. Thus the gaussian and the spherical fixed points correspond to tricritical points of the uncronstrained and constrained system, respectively.

II - b) The Hubbard model

First let us discuss the occurrence of first order transitions. In the absence of spin-charge coupling, the condition for a first order transition to occur is

$$\mu < 0 \quad \text{i.e.} \quad \left.\frac{d^2N}{dE^2}\right|_{E_F} > 0$$

This is never satisfied for a free fermion gas where $N(E) \sim \sqrt{E}$. However in a transition metal with a rapidly varying density of states, the regions in energy for which $d^2N/dE^2 > 0$ and those for which $d^2N/dE^2 < 0$ should alternate and be comparable in size.

In the presence of the spin charge coupling, the effective S^4 term becomes negative when

$$\left.\frac{d^2N}{dE^2}\right|_{E_F} > \frac{3}{2} \; \frac{U\left(\frac{dN}{dE}\right)^2\Big|_{E_F}}{1 + U\,N\,(E_F)}$$

Thus, a first order transition tends to be inhibited. In a free fermion gas, it will never occur; in a transition metal the energy ranges favouring a first order transition are shrunk towards the extrema with $\frac{d^2N}{dE^2} > 0$, i.e. the dips in the density of states. The latter are unfavourable for magnetism (Stoner's criterion). Thus we can understand why most ferromagnetic metals exhibit second order phase transitions.

II - c) Discussion of the critical properties of the Hubbard model

In paragraph (II-a) we have presented the renormalization group analysis of the Hamiltonian (7), thus extending the work of Achiam and Imry[6] for arbitrary n. In that paragraph we have followed strictly the procedure of (6), and no emphasis was made in the peculiar form of the coupling constants in (7) for the Hubbard model. Now we need to discuss the effective stability of the fixed points for n = d = 3; furthermore, the various fixed points obtained above do not necessarily pertain to the parameter space of the Hubbard Hamiltonian. We divide this paragraph in several parts: the region of parameter space describing the Hubbard model, the results for a first order calculation, the connection with the specific heat, a thermodynamic analysis of the anomalous dimensions and finally the correlation function for the non-critical field.

i) The spin-charge coupling is purely imaginary. This implies that the parameters $Z = \mu^2/\beta$ and $\omega = \mu_o^2/\beta_o$ are negative. So, if one is to describe the critical properties of the Hubbard model, only trajectories on the parameter space which correspond to Z and ω negative or zero are allowed. The fixed points consequently should satisfy this requirement also. This differs from the results of Achiam and Imry[6] for whom no restriction on the parameters were imposed. It is to be noted that the allowed region (allowed fixed points) according to table 1 (which is a first order calculation) should be carefully discussed.

ii) We discuss the allowed region within the first order approximation in ε of table 1. First of all we note that the Gaussian fixed points G1 and G2 are respectively forbidden and allowed for all values of n. Similarly the spherical points S1 and S2 are respectively forbidden and allowed (for all n). The Heisenberg and renormalized Heisenberg fixed points H1 and RH1 are both forbidden for $n < 4$ thus contrasting with H2 and RH2 which are allowed ($n < 4$). Clearly (cf. table 1) for $n > 4$ the points indexed by 1 are allowed and those by 2 forbidden. The border line $n = 4$ is a typical feature of the first order approximation in ε and does not correspond to physical reality (cf. below for a further analysis).

iii) Concerning the anomalous dimensions of Z and ω table 1 shows for Heisenberg and constrained Heisenberg fixed points a n-dependence of these dimensions. Again, $n = 4$ is the border line of stability. This is a typical feature of the first order calculation.

In principle precise conclusions can be drawn only by extending the calculation to higher order in ε. We argue, however that thermodynamic arguments suggest a way to discuss the exchange of stabilities among the fixed points for arbitrary order in ε. In fact, it is shown below that, to any order in ε, ϕ_z - the anomalous dimension of the coupling $z = \mu^2/\beta$ - is equal to $\phi_z = \alpha/\nu$, where α is the specific heat exponent and ν the correlation length exponent. Now, from the proportionality of ϕ_z and α we expect a change in sign of ϕ_z close to $n = 2$, due to the corresponding[14] one in α. (For $d = 3$ and $n > 2$, α is negative.)

We demonstrate now the relation $\phi_z = \alpha/\nu$. This follows from the use of the fluctuation-dissipation theorem as applied to the specific-heat: $c \sim \int d\vec{x}\,\{\langle E(\vec{x})E(o)\rangle - \langle E(\vec{x})\rangle\langle E(o)\rangle\}$ where $E(\vec{x})$ is the energy density with anomalous dimension ϕ_E. From $c \sim t^{-\alpha}$ and $\xi \sim t^{-\nu}$, where ξ is the correlation length, one obtains $2\phi_E = -\alpha/\nu + d$. Clearly from this relation, one gets, for a coupling of the form vS^4, $\phi_v = \alpha/\nu$ where ϕ_v is the anomalous dimension of the coupling v. This is precisely Sak's result[7]. In our case we have to consider the coupling $\mu y S^2$ and βy^2, so $\phi_\mu + \phi_y + \phi_E = d$ and $\phi_\beta + 2\phi_y = d$, where again we have used the fact that the anomalous dimension of the free energy density is d. So the anomalous dimension of z is $\phi_z \equiv 2\phi_\mu - \phi_\beta = d - 2\phi_E = \alpha/\nu$. The same argument applies to ϕ_ω and one has $\phi_\omega = \phi_z$.

iv) The thermodynamic discussion above, together with the first order results of table I suggest a relation between the specific heat behaviour as a function of n and the allowed parameter space regions for the Hubbard model. From table 1 one verifies that the fixed points H1, RH1 and RH2 have z^* and ω^* values which are proportional to the specific heat exponent α. We will make the hypothesis that, to all orders in ε the fixed point values for z^* and ω^* change sign with α. We emphasize that we have no rigorous proof of this, which is only indicated by the anomalous dimension analysis and by the first order calculation. Once this hypothesis is made and recalling that the specific heat exponent changes sign from positive to negative around n = 2 one can draw figures 1 and 2. The chart of allowed fixed points is then different for n = 1 and n = 3. From fig. 2 one sees that the Heisenberg fixed point is the most stable one and corresponds to vanishing spin-charge coupling. The renormalized fixed point for n = 3 is then less stable than the Heisenberg one and this strongly contrasts with the n = 1 case for which the most stable fixed point is the renormalized Heisenberg with non zero spin-charge coupling. The number of allowed fixed points (as contrasted with the results in first order in ε) changes with n; 5 fixed points for n = 3 and 4 fixed points for n = 1.

Since the Gaussian and spherical fixed point coordinates along the z and ω axis do not change in sign with n to first order in ε, and are assumed to do so for all orders, they are common to both figures. Their stability is however low. Note that for n = 3 (usual case), since the most stable fixed point has vanishing spin-charge coupling, interesting effects should be observed through crossover effects as indicated in fig. 2. There exists a particular surface in parameter space such that Hubbard hamiltonians represented by points belonging to this surface have critical properties governed by a fixed point HI with non zero spin-charge coupling.

II - c) Correlation function for the non-soft field

As pointed out by Achiam and Imry[6], the existence of a coupling between the two fields may introduce a weak singularity in the correlation function of the charge field .

To see this we define:

$$\chi_y(q) = < y_q \, y_{-q} > = \frac{1}{Z} \int e^{-H} \, y_q \, y_{-q}$$

where $Z = \int e^{-H}$ and H is given by (7).

Introducing an external field term in (7) given by $\int_q h_{-q} \, y_q$ where at the end we let $h_{-q} \to 0$, transforming the new hamiltonian by eliminating the linear term in y_q [6] one obtains:

$$< y_q \, y_{-q} > = \frac{1}{\beta} + \left(\frac{\mu}{\beta}\right)^2 \sum_{\alpha,\alpha'} < (S^{(\alpha)})^2_q \, (S^{\alpha'})^2_{-q} >$$

$$= \frac{1}{\beta} + \left(\frac{\mu}{\beta}\right)^2 < (\vec{S})^2_q \, (\vec{S})^2_{-q} > \qquad (10)$$

Equation (10) is a typical feature of the coupling yS^2 among the soft and non-soft field. In (10) we have conserved the regular term $1/\beta = 1/(1+U\,\chi(q))$, contrary to Achiam and Imry. This is necessary since the second term is negative for the Hubbard model. From the preceeding thermodynamic arguments this clearly implies, for q = 0, that the critical exponent for $\chi_y(o) = <y_o \, y_o>$ is precisely that of the specific heat of the magnetic system, namely α. Since α is small and negative, one expects $\chi_y(0,T)$ to exhibit a small cusp at T_c when the critical behaviour is governed by a fixed point with non vanishing spin charge coupling. This cusp is subtracted out from the regular part $1/\beta$ (eq. 10).

Since spatial correlations between the y's are transmitted via the coupling to the soft field, one expects that the unique independent length of the problem is the spin-spin correlation length ξ . The exponent η_y defined by $< y_q\, y_{-q} > \sim q^{-2+\eta_y}$ at T_c can be found[6] by comparing the behaviour of the two members in the above definition under rescaling. The right hand side and the left hand side scale like $b^{2-\eta_y}$ and $c^2 b^{-d}$, respectively, where c is given by (8). Consequently we find:

$$2 - \eta_y = \frac{2z^* \eta\, A_2}{\log b} \qquad (11)$$

Usually (one soft field) the critical exponent η is $O(\varepsilon^2)$; in the particular case of a fixed point with <u>non-vanishing coupling to the non-soft field</u>, we get a first order correction to η . The non corrected value $\eta_y = 2$ reflects the fact that y_q is not critical, thus suppressing the long range behaviour of the correlation function.

The fixed-points with $z^* = 0$ correspond to uncoupled fields and we have already pointed out that it is precisely the coupling that transmits some degree of criticality to the y_q field.

A final remark concerning the Hubbard model. The allowed fixed points should satisfy $z^* \leq 0$. Consequently in contrast with Achiam and Imry, the correlation function varies with q with a positive slope near criticality (eq. 11).

III - Summary and conclusions

We derived a free energy functional from the Hubbard Hamiltonian which explicitly takes into account the three-dimensional vector nature of the spin field, i.e., the spin rotational invariance of the original Hamiltonian. In this respect, we generalized the work of references (5) and (6).

We have found that the stability of the fixed points is significantly altered, as compared to the results of ref. (6), because of the change of sign of the specific heat exponent between $n = 1$ and $n = 3$. Furthermore, because spin-charge coupling is pure imaginary, some fixed points are not physically attainable. The main change is that the most stable exhibits unrenormalized exponents and zero spin-charge coupling. A fixed point with non-zero spin charge coupling is once unstable and governs the critical behaviour of a restricted class of Hamiltonians. The singularities of the charge field correlation function, in general, obey a crossover regime to regular behaviour at the most stable fixed point. The singularity in χ_y is weak, since the corresponding critical index is α. In particular α being negative and small ($\alpha = -0.1$) for the most stable fixed point and for $n = d = 3$, the charge correlation function may at most exhibit a weak negative cusp at T_c, which may not be easily observed. However the spin charge coupling in any case restricts the possibility of occurrence of first order transition, since these can occur only if the Fermi level of the paramagnetic metal is near a dip in the density of states. Since the condition for the existence of a tricritical point is given in terms of the density of states and its derivatives at ϵ_F, an external variable controlling these quantities is necessary. Alloying techniques may be a suitable tool.

Our work sets the stage for a treatment of systems where both the spin field and the charge field may become soft simultaneously. There exists several experimental examples[17] of charge instabilities in metallic systems; however, one should invoke other mechanisms than those contained in the simple Hubbard model in order to explain those experiments. In particular, phonon softening at a given wave vector q_o due to nesting in the Fermi surface found in two-dimensional systems, for example - may be conjectured to produce charge softening. It is tempting to start with a phenomenological free energy like (7), where the coefficients of the gaussian terms are replaced by $1 - U_i\ _o(q)$, $i = 1,2$ where $U_i > 0$ for both spin and charge terms. In systems having two or more soft fields the renormalization group treatment is qualitatively different from that of this work, since the scaling of the charge field must insure that the coefficient of the q^2 term in the quadratic part is constant. (In particular it can be easily shown that the critical dimension in that case is $d_c = 6$ and that the term ν^3 is now relevant).

In a recent work, Ashkenazi and Weger[19] suggested that various thermodynamic states in Ti_2O_3 and V_2O_3 such as spin ordered state and charge density waves have almost the same free energy around the transition temperature. In their case the existence of a diverse range of nearly degenerate instabilities is due to orbital degeneracy. This calls for further study of coupled spin and charge fluctuation systems. In our case, also, the degeneracy of the d-band has been disregarded. Again, the Hubbard-Stratonovich approach, in a rotational invariant form, can be performed in this case.

In the text we have considered only the situation where the n-component vector field is soft, the one-component field being kept non-soft. The inverse situation could also be imagined and one proceeds as in the above case, except that now the q^2 term of the n-component field is imposed to be irrelevant. Experimental situations where this might happen, concern phase transitions with the occurrence of quadrupolar ordering, together with a crystallographic transition. It has been pointed out[18] that the n vector model with $n > 4$ may be used to describe such phase transition.

We have considered the electron-electron interaction to be local As briefly discussed in reference (5), a q-independent Coulomb term in (1) can be justified in terms of s-electron screening in a transition metal described in terms of s-d bands. For pure d-like bands, one expects that screening is less effective and the interactions tend to be long-range. This particular case should be considered separately since the scaling must now be different.

Finally a comment should be made on the approximation made in eq. (5) which consisted in disregarding the q-dependence of the higher-order fermion loops. If we expand these functions in powers of q (for $\omega = 0$), it can easily be shown that, with the adopted scaling, the new terms will be irrelevant. This contrasts with the results of Moura et al.[12]. Their couplings, after the elimination of the phonon degrees of freedom, depend only on angle variables but not on the magnitude of the wave vectors.

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REFERENCES

(*) Permanent address: P.U.C., Department of Physics, Rio de Janeiro, Brazil.

(**) Permanent address: C.B.P.F., Rio de Janeiro, Brazil

1 - J. Hubbard, Proc. Roy. Soc. A 276, 238 (1963)

2 - J.R. Schrieffer, unpublished lecture notes, CAP summer school, Banff (1969)

3 - J.A. Hertz and M.A. Klenin, Phys. Rev. B 10, 1084 (1974)

4 - J.A. Hertz, A.I.P. Conference Proceedings 24, 298 (1975)

5 - A.A. Gomes and P. Lederer, to be published

6 - Y. Achiam and Y. Imry, Phys. Rev. B 12, 2768 (1975)

7 - J. Sak, Phys. Rev. B 10, 3957 (1974)

8 - M.E. Fisher, Phys. Rev. 176, 257 (1968)

9 - J. Rudnick, D.J. Bergman and Y. Imry, Phys. Lett. A 46, 449 (1974)

10 - D.R. Nelson and M.E. Fisher, Phys. Rev. B 11, 1030 (1974)

See also J. Kosterlitz, D. Nelson and M. Fisher, Phys. Rev. B 13, 412 (1976) where uniaxially anisotropic antiferromagnets are discussed in the context of bicritical and tetracritical points. In that case also, the existence of two interpenetrating sub-lattice implies couplings among fields.

11 - D.J. Bergman and B.I. Halperin, Phys. Rev. B 13, 2145 (1976)

12 - M.A. Moura, T.C. Lubensky, Y. Imry and A. Aharony, Phys. Rev. B 13, 2176 (1976)

13 - H. Keiter, Phys. Rev. B 2, 3777 (1970)

14 - K.G. Wilson and J. Kogut, Phys. Reports 12 C, 75 (1974)

15 - S. Doniach and S. Engelsberg, Phys. Rev. Lett. 17, 750 (1966)

16 - M.T. Béal-Monod, Phys. Lett. 54 A, 197 (1975) and M. Gabay and M.T. Béal-Monod, to be published

17 - Proceedings of the conference on Metal-non metal transitions, Au - trans, France, 1976

18 - D. Mukamel, Phys. Rev. Lett. 34, 481 (1975); D. Mukamel and S. Krinsky, Phys. Rev. B 13, 5065 and 5078, (1976) and D. Bak and D. Mukamel, Phys. Rev. B 13, 5086 (1976).

19 - J. Ashkenazi and M. Weger, to be published.

(*) The momentum integrals run over the Brillouin zone but for pratical purposes the zone may be approximated by a sphere in q-space. In this process the original coupling constants change a little, so that the values given above are only approximate.

TABLE CAPTION

Table 1 : Fixed points, eigenvalues ϕ_i and eigenvectors $\vec{\phi}_i$ and the exponents ν and α for the hamiltonian (7).

$$\bar{\varepsilon} = \frac{\ln b}{\Lambda_2}\,\varepsilon \quad ; \quad \rho = \frac{\Lambda_1 b^2}{b^2-1}\,\bar{\varepsilon} \qquad \vec{\phi}_i = (u,\ z,\ \omega)$$

TABLE 1

(Unconstrained) (H) $\nu = \frac{1}{2} + \frac{(n+2)}{4(n+8)}$ $r^* = -\frac{(n+2)}{n+8}\rho$ $\alpha = \frac{4-n}{2(n+8)}$

	u^*	z^*	ω^*	ϕ_1	$\vec{\phi}_1$	ϕ_2	$\vec{\phi}_2$	ϕ_3	$\vec{\phi}_3$
H1	$\frac{\bar{\varepsilon}}{n(n+8)}$	$\frac{4-n}{2n(n+8)}\bar{\varepsilon}$	$\frac{4-n}{2n(n+8)}\bar{\varepsilon}$	$-\varepsilon$	$(2,4-n,4-n)$	$\frac{n-4}{n+8}\varepsilon$	$(1,2,2)$	$\frac{4-n}{n+8}\varepsilon$	$(0,0,1)$
H2	$\frac{\bar{\varepsilon}}{4(n+8)}$	0	0	$-\varepsilon$	$(1,0,0)$	$\frac{4-n}{n+8}\varepsilon$	$(1,2,2)$	$\frac{4-n}{n+8}\varepsilon$	$(1,2,1)$

(Constrained) (RH) $\nu = \frac{1}{2} + \frac{3}{2(n+8)}\varepsilon$ $r^* = \frac{-6}{n+8}\rho$ $\alpha = \frac{n-4}{2(n+8)}\varepsilon$

	u^*	z^*	ω^*	ϕ_1	$\vec{\phi}_1$	ϕ_2	$\vec{\phi}_2$	ϕ_3	$\vec{\phi}_3$
RH1	$\frac{\bar{\varepsilon}}{n(n+8)}$	$\frac{(4-n)\bar{\varepsilon}}{2n(n+8)}$	0	$-\varepsilon$	$(2,4-n,0)$	$\frac{n-4}{n+8}\varepsilon$	$(1,2,0)$	$\frac{n-4}{n+8}\varepsilon$	$(0,0,1)$
RH2	$\frac{\bar{\varepsilon}}{4(n+8)}$	0	$\frac{n-4}{2n(n+8)}\bar{\varepsilon}$	$-\varepsilon$	$(n,0,2(n-4)$	$\frac{n-4}{n+8}\varepsilon$	$(0,0,1)$	$\frac{4-n}{n+8}\varepsilon$	$(1,2,2)$

(Unconstrained) (G) $\nu = \frac{1}{2}$ $r^* = 0$ $\alpha = \frac{\varepsilon}{2}$

	u^*	z^*	ω^*	ϕ_1	$\vec{\phi}_1$	ϕ_2	$\vec{\phi}_2$	ϕ_3	$\vec{\phi}_3$
G1	$\frac{\bar{\varepsilon}}{4n}$	$\frac{\bar{\varepsilon}}{2n}$	$\frac{\bar{\varepsilon}}{2n}$	$-\varepsilon$	$(1,2,2)$	ε	$(1,n+2,0)$	ε	$(0,0,1)$
G2	0	0	0	ε	$(1,0,0)$	ε	$(0,0,1)$	ε	$(0,1,0)$

(Constrained) (S) $\nu = \frac{1}{2} + \frac{\varepsilon}{4}$ $r^* = -\rho$ $\alpha = -\frac{\varepsilon}{2}$

	u^*	z^*	ω^*	ϕ_1	$\vec{\phi}_1$	ϕ_2	$\vec{\phi}_2$	ϕ_3	$\vec{\phi}_3$
S1	$\frac{\bar{\varepsilon}}{4n}$	$\frac{\bar{\varepsilon}}{2n}$	0	$-\varepsilon$	$(1,2,0)$	$-\varepsilon$	$(0,0,1)$	ε	$(1,n+2,0)$
S2	0	0	$-\frac{\bar{\varepsilon}}{2n}$	$-\varepsilon$	$(0,0,1)$	ε	$(n,3n,-2+2n)$	ε	$(0,n,-2)$

Figure Caption

Fig. 1 - Fixed points physically attainable within the Hubbard model (n = 1). The coordinates of the fixed points are:

	u^*	z^*	ω^*
H2	$\bar{\varepsilon}/36$	0	0
RH2	$\bar{\varepsilon}/36$	0	$-\bar{\varepsilon}/6$
G2	0	0	0
S2	0	0	$-\bar{\varepsilon}/2$

The arrows indicate the relevance of the various parameters along the local axis (see table 1).

Fig. 2 - Fixed points physically attainable within the Hubbard model (n = 3). The coordinates of the fixed points are:

	u^*	z^*	ω^*
H1	$\bar{\varepsilon}/33$	$\alpha/3$	$\alpha/3$
H2	$\bar{\varepsilon}/44$	0	0
RH1	$\bar{\varepsilon}/33$	$\alpha/3$	0
G2	0	0	0
S2	0	0	$-\bar{\varepsilon}/6$

The arrows indicate the relevance of the various parameters along the local axis (see table 3).

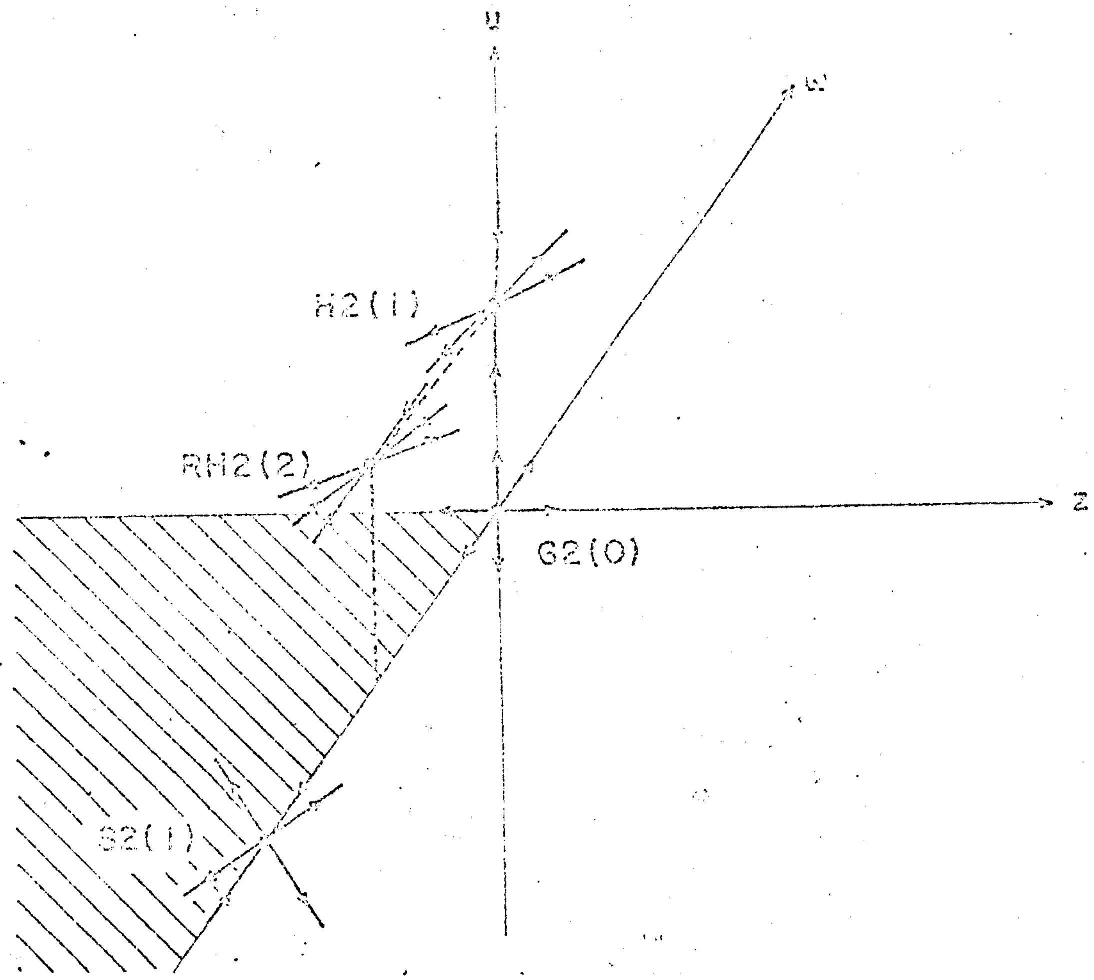

FIG. 1

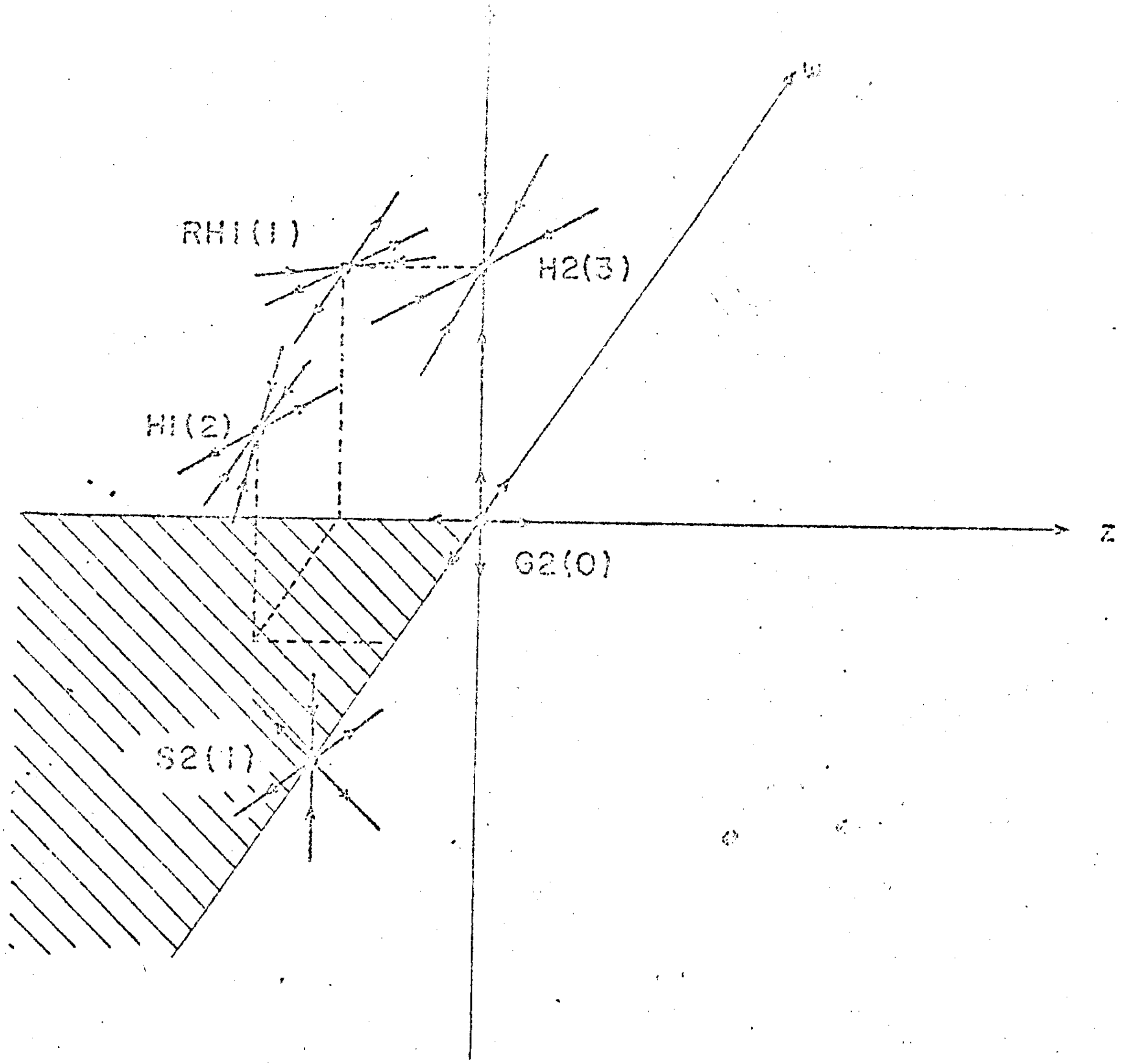

FIG. 2