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COUPLED CHARGE AND SPIN FIELDS IN ITINERANT-ELECTRON PARAMAGNETS

A.A. Gomes*, P. Lederer and C.M. Chaves**

Laboratoire de Physique des Solides, Université Paris-Sud, Centre d'Orsay

91405 Orsay, France

ABSTRACT

Consideration is given to the combined effect of charge and spin fluctuations on the thermodynamic properties of the Hubbard Hamiltonian. As a consequence of the existence of a spin charge coupling term, the occurence of first order magnetic transitions in metals is quite less common than a spin only theory predicts. We also discuss briefly the critical properties.

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*Permanent address: C.B.P.F., Rio de Janeiro, BRAZIL

**Permanent address: P.U.C., Dept. of Physics, Rio de Janeiro, BRAZIL

1. Introduction

This paper summarises some of our recent work in attempting to elucidate certain properties of the non-degenerate Hubbard Hamiltonian. A review of the general setting of the problem is given by Cyrot [1] in these proceedings.

The non-degenerate Hubbard Hamiltonian has been studied in recent years [2,3] using, among others, the functional integral technique. This formulation relies on the Hubbard-Stratonovich transformation, which carries the original many-body Hamiltonian into an effective free energy density from which the thermodynamic quantities may be evaluated. Two fluctuating effective fields, coupled respectively to the spin and charge densities, are introduced. However, charge fluctuations have been disregarded in past work. In what follows, charge fluctuation effects are taken into account in the derivation of the free energy density. The resulting functional exhibits spin-charge coupling terms. We compare this two field problem to others studied in the literature [4] , concentrating on the consequences of spin-charge coupling for the critical behaviour of an itinerant-electron system.

2. Symmetry Considerations

The Hubbard model exhibits spin-rotation invariance. Consequently, in the construction of a functional adequate to describe the model, this requirement should be taken into account.

Various procedures have been proposed to transform the Coulomb term [5] . For example, one may use the identity [2b] :

$$n_\uparrow n_\downarrow = \frac{1}{4}(n_\uparrow + n_\downarrow)^2 - \frac{1}{4}(n_\uparrow - n_\downarrow)^2 \qquad (1)$$

and apply the Hubbard-Stratonovich transformation to each square term, i.e.

$$e^{\alpha A^2} = \frac{\pi}{\alpha} \int_{-\infty}^{+\infty} e^{-\alpha x^2 + 2\alpha A x} dx \qquad (2)$$

where A is either $(n_\uparrow + n_\downarrow)$ or $(n_\uparrow - n_\downarrow)$. When use is made of equ. (2) in the partition function Z = Trace $e^{-\beta H}$ for the Hubbard hamiltonian, one transforms the original many body problem into a gaussian average over the partition functions of a single particle interacting with two external fields X_1 and X_2 coupled respectively to $(n_\uparrow + n_\downarrow)$ and $(n_\uparrow - n_\downarrow)$.

However, the spin field which results from the use of (1) and (2) is Ising-like, thus violating the rotational invariance of the original Hamiltonian. This point is discussed further below.

Schrieffer [2a] used the identity $n_\sigma^2 = n_\sigma$ to write:

$$n_\uparrow n_\downarrow = \frac{1}{2}(n_\uparrow + n_\downarrow) - \frac{1}{2}(n_\uparrow - n_\downarrow)^2 \qquad (3)$$

the term $\frac{1}{2}(n_\uparrow + n_\downarrow)$ is incorporated in the one-electron part of the Hamiltonian and the squared operator $-\frac{1}{2}(n_\uparrow - n_\downarrow)^2$ is transformed using (2). The representation (3) was discussed in detail by Keiter [2c] . It introduces a spurious interaction among equal spins. Furthermore the original rotational invariance is lost in the remaining term: $(n_\uparrow - n_\downarrow)^2 = S_Z^2$.

Equ. (3) together with the transformation (2) necessitates the introduction of a single auxiliary field ξ coupled to the Z-component of the spin density and ζ which is coupled to the charge density $(n_\uparrow + n_\downarrow)$.

Yet another identity can be used:

$$n_\uparrow n_\downarrow = \frac{1}{4}(n_\uparrow + n_\downarrow) + \frac{1}{8}(n_\uparrow + n_\downarrow)^2 - \frac{1}{2}\vec{S} \cdot \vec{S} \qquad (4)$$

Contrasting with equ. (1) and (3) which only deal with S_z (Ising-like fields) equ. (4) has Heisenberg like character i.e., the rotational invariance of the spin term is explicitely included. It yields a functional with two coupled fields-one, $\vec{\xi}$ is a vector, with n = 3, coupled to $\vec{S}$, while ζ is a scalar, coupled to the charge density.

We are thus faced with the following problem: equ. (1),(3) and (4) provide exact transformations of the Hubbard hamiltonian into various free energy functionals which apparently do not have the same physical properties. This problem is discussed in details in ref. [5]. To summarize, if one is interested in deriving a Landau-Ginsburg-Wilson free energy functional for the Hubbard model (see below eq.(5)), the best choice among equ. (1),(3) and (4) is provided by equ. (4), the latter allows an expansion in terms of powers of auxiliary fields $\vec{\xi}$ and ζ which exhibit rotation invariance term by term.

3. The free energy functional

Following the procedure used by Schrieffer |2| and Hertz |3|, but keeping both the charge and the spin terms, one obtains a free energy density which exhibits coupled order parameters:

$$H(\vec{\xi},\zeta) = \frac{1}{2}\sum_{\underset{\sim}{q},\alpha}\left(1 - U\chi^{o}(\underset{\sim}{q})\right)\xi^{\alpha}_{\underset{\sim}{q}}\ \xi^{\alpha}_{-\underset{\sim}{q}}$$

$$+ \sum_{\substack{q_1,q_2,q_3 \\ \alpha,\beta}} \mu_4(q_1,q_2,q_3)\,\xi^{\alpha}_{q_1}\,\xi^{\alpha}_{q_2}\,\xi^{\beta}_{q_3}\,\xi^{\beta}_{-(q_1+q_2+q_3)}$$

$$+ \frac{1}{2} \sum_{q} \left(1 + U\chi_o(q)\right) \zeta_q\,\zeta_{-q}$$

$$+ \sum_{q_1,q_2} I^{sc}_1(q_1, q_2)\,\zeta_{q_1}\,\xi^{\alpha}_{q_2}\,\xi^{\alpha}_{-(q_1+q_2)} \tag{5}$$

$$+ \sum_{\substack{q_1,q_2,q_3 \\ \alpha}} I^{sc}_2(q_1,q_2,q_3)\,\xi^{\alpha}_{q_1}\,\xi^{\alpha}_{q_2}\,\zeta_{q_3}\,\zeta_{-(q_1+q_2+q_3)}$$

The notation $q_i \equiv (\vec{q}_i, \omega_i)$ takes account of both the momentum and frequency dependence. $\chi_o(q)$ is the usual non-enhanced susceptibility. The term $1 + U\chi_o(q)$ in the Gaussian charge term of eq. (5) is a characteristic feature of the Hubbard Hamiltonian. The coupling constants for the $(\vec{\xi}^{\,2})(\vec{\xi}^{\,2})$ term is μ_4, I^{sc}_1 and I^{sc}_2 are likewise the spin charge couplings.

Eq. (5) shows no possibility of a charge instability, as expected. If one considers finite temperatures (only $\omega_i = 0$ frequencies are retained) and neglects the q_i dependence of the interaction vertices, the first two terms in (5) give a Wilson-type free energy for Heisenberg spins ($n = 3$).

The lowest order spin-charge coupling term is

$$I_1^{sc} \approx i\,(k_B T_c)^{1/2}\, U^{3/2} \left.\frac{dn(\varepsilon)}{d\varepsilon}\right|_{\varepsilon_F}$$

where $n(\varepsilon)$ is the density of states and ε_F is the Fermi level. It is pure imaginary. The coefficients of the $\vec{\xi}^2 \zeta^2$ and $\zeta^2 \zeta^2$ terms are respectively

$$I_2^{sc} = -\mu_4 = k_B T_c U^2 \left.\frac{d^2 n(\varepsilon)}{d\varepsilon^2}\right|_{\varepsilon_F}$$

(We restrict the discussion to the vicinity of the critical temperature T_c).

The terms involving only the fields ζ_q describe a system of charge fluctuations which do not become critical at any temperature. This is why terms in ζ^3 and ζ^4 are omitted in equ. (5). The latter exhibits coupling terms between the magnetic modes ξ_q which become soft at T_c and the charge modes which do not.

Note that I_1^{sc} vanishes when the Fermi level lies at an extremum of the density of states. When such is the case, one has a second order phase transition when the extremum is a maximum ($n''(\varepsilon_F) < 0$) and a first order transition when the extremum is a minimum ($n''(\varepsilon_F) > 0$); see fig. 1. (In the latter case, terms in ξ^6 have to be introduced in the free energy functional.)

4. Analogy with other coupled-field problems. The role of constraints

Various authors have recently studied coupled-field problems, starting either from a microscopic Hamiltonian (for a metamagnet or spin phonon system) or from a phenomenological free energy density (see ref. [5] for a more detailed review). A renormalization group procedure shows the irrelevance of the fourth order cross term (corresponding to I_2^{sc} in (4)) and of the third and fourth order coupling terms between fluctuations in the "non-ordering" field; these results have been obtained with an Ising-like order parameter (n = 1). We have studied the extension to arbitrary n [6] .

4.a First order versus second order phase transitions - Effect of spin charge coupling.

The above mentioned works show that the condition for the occurence of a first order phase transition is

$$\mu_4^{eff} = \mu_4 - \frac{{I_1^{sc}}^2}{2\beta_o} \leq 0 \qquad (6)$$

where β_o is the coefficient of the $|\zeta_{q=0}|^2$ term in the L.G.W. functional (In our case $\beta_o = 1 + U\, n\,(\varepsilon_F)$). Tricritical behaviour obtains when the equality holds. Equation (6) is generally valid for coupled field systems (with one soft field only) and can be derived within the molecular field approximation.

A specific feature of the Hubbard model is that I_1^{sc} is pure imaginary. Thus equ. (6) becomes

$$\frac{3}{2}\,\frac{U}{1+U\,n(\varepsilon_F)}\left(\frac{dn(\varepsilon)}{d\varepsilon}\right)^2\Bigg|_{\varepsilon_F} \leq \frac{d^2n(\varepsilon)}{d\varepsilon^2}\Bigg|_{\varepsilon_F} \qquad (6')$$

If spin charge coupling is ignored, we have only

$$0 \leq \frac{d^2n(\varepsilon)}{d\varepsilon^2}\Bigg|_{\varepsilon_F} \qquad (6'')$$

which is the usual result (neglecting temperature corrections of the order of $(k_B T_C/\varepsilon_F)^2$).

Equation (6') shows that the existence of the spin-charge coupling reduces the domain of possible occurrence of first order transitions as shown schematically in fig. (1). It expresses the fact that, in order for μ_4^{eff} to be negative, $n''(\varepsilon_F)$ has to be negative enough to overcome the positive term $-(J_1^{sc})^2/2\beta_0$.

Only regions in energy near dips of the density of states allow for first-order magnetic phase transitions in metals. In the absence of spin-charge coupling, the occurrence of first order phase transitions in magnetic metals and alloys would be more frequent given the peaky nature of the density of states in transition metals.

4.b Renormalization group results for coupled systems: connection with the Hubbard model

Achiam and Imry [4] discussed a free energy functional which shows close similarity to eq. (5). They consider the role of constraints in affecting the stability of the various fixed points. Fisher renormalization of critical exponents is obtained (i.e. the renormalized Ising fixed point is the most stable one) when constraints are imposed. For example: one may set $\zeta_{q=0}$ = constant in the functional integral defining the partition function. In the Hubbard model, constraints must be imposed on the charge field, to ensure particle number conservation, or charge neutrality if one describes a charged Fermi liquid. Thus the discussion of the coupled field problem in ref [4] is especially relevant to the Hubbard model. An important difference however arises in this case, due to the fact that J_1^{sc} is pure imaginary.

The map of fixed points is different when the spin field is Ising-like ($n = 1$) or when it is Heisenberg-like ($n = 3$). The reason is that there is a change in the stability of various points when the coefficient α changes sign, as happens when n changes from 1 to 3. In order to work this out, one must generalize the investigation of Achiam and Imry [4] ; in their study, the spin order parameter has $n = 1$, while the (isotropic) Hubbard model has $n = 3$. This generalization is carried through in ref. [6] to first order in $\varepsilon = 4 - d$. To that order, the exchange of stability of fixed points occurs for $n = 4$, so that it would seem that the isotropic Hubbard model has the same map of fixed points, with the same stability as the anisotropic ($n = 1$) case.

However, one can show [6] that the exchange of stability between fixed points really occurs with the change of sign of α ; the coefficient of the specific heat. Since α for $n = 3$ and $d = 3$ is negative, the most stable fixed points do not exhibit Fisher renormalized critical exponents, contrary to what happens for $n = 1$. Again one must keep in mind that the physical requirement that I_1^{SC} is pure imaginary in the Hubbard model. The consequence of this is that a number of fixed points which are found in the general coupled field problem are not physically acceptable for the Hubbard model.

This situation is discussed at more length in reference [6] together with the observability of a possible weak singularity in the charge-charge correlation function.

6. Summary

We have derived a generalized Landau-Ginzburg-Wilson functional for the non-degenerate Hubbard model. Rotation invariance is preserved, and as a consequence, couplings are generated among the charge and the spin fields.

Within the derived free energy, no charge instability is possible. This is a feature of the Hubbard Hamiltonian; and other mechanisms should be invoked (e.g. phonons or multi-band effects) if charge instabilities are to be produced.

The renormalization group techniques applied to the functional (5) give a set of four fixed points, each one, depending on its stability, governing the behaviour of the system near the critical point. The most stable fixed point exhibits Fisher renormalization only for $n \leq 2$, which corresponds to an anisotropic Hubbard model. In all cases the possibility remains of tricritical points or first-order transitions. As stated above, this possibility depends on the strength of the intraatomic Coulomb interaction and on the density of states and its derivatives at the Fermi level.

The imaginary coupling between spin and charge fields makes more difficult the occurrence of first order magnetic transitions in metals.

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FIGURE CAPTION

Fig. 1 - If spin-charge coupling is neglected, a magnetic metal exhibits a first order transition if the Fermi level falls between A and A' ($n''(\varepsilon) > 0$) . When the spin charge coupling is taken into account, the region for first order transition shrinks to the segment BB'.

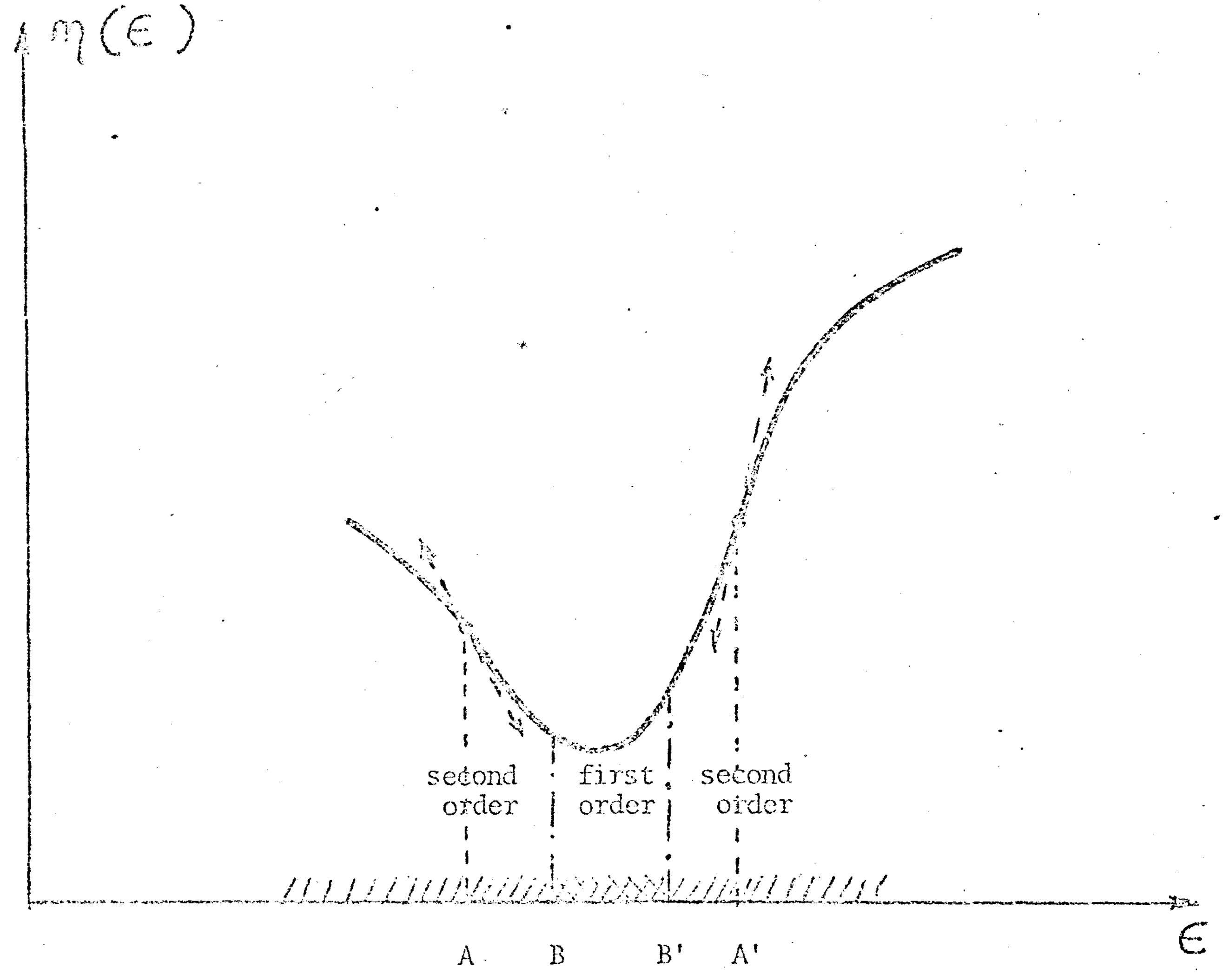

FIG. 1