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FERROMAGNETIC PHASE TRANSITIONS IN THE HUBBARD MODEL

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Abstract. We show that the coupling of charge and spin density fluctuations in the three-dimensional Hubbard model with total charge fixed severely restricts the occurrence of a continuous ferromagnetic transition.

This work focuses in one of a series of long-standing problems related to the one-band Hubbard model [1], namely the existence and nature of a finite-temperature ferromagnetic phase transition in three dimensions. The solution of this problem is of special interest since it can shed some light on the mechanism underlying the ferromagnetism of itinerant electron systems, such as the transition metals and their alloys. Despite the great effort [2] to overcome the difficulties encountered by the Stoner (mean-field) theory of itinerant-electron ferromagnetism to explain the finite-temperature properties of these systems, a satisfactory theory of critical phenomena [3] is still not available. On the other hand, numerical [4] and rigorous [5] results are in their initial stages. Here, we shall address ourselves to two fundamental questions within this context: first, what extra conditions, besides a Stoner-type criterion, must the system fulfill to undergo a continuous transition to a ferromagnetic state? Second, is the coupling between spin and charge density fluctuations, which is not considered in most magnetic studies [3], of any relevance?

Mean-field (MF) theory [2, 3] predicts that if Stoner’s criterion is satisfied, namely $U N_T(E_F) = 1$, where $N_T(E_F)$ is the density of states near the Fermi level, averaged over an energy range of order $kT$ through the factor $(\partial f / \partial E)$, with $f(E)$ the Fermi distribution function and $U$ is the local Coulomb repulsion [1], then the system undergoes a second-order ferromagnetic phase transition if

$$
\frac{3N''_T(E_F)^2}{2N_T(E_F)} > N''_T(E_F), \quad (1)
$$

whereas a first-order transition occurs for the reverse inequality and prime means differentiation. At this level of approximation, the coupling between the spin and charge degrees of freedom tends to enhance continuous transitions [2, 3], which otherwise would occur for $N''_T(E_F) < 0$.

How does this picture stand when charge and spin density fluctuations are allowed in the theory? We answer this question using a functional integral representation [6] for the partition function of the Hubbard Hamiltonian – in the regime where the Coulomb term can be treated perturbatively as well as field-theoretic and renormalization-group techniques [7]. Based on an $\epsilon = (4 - d)$ expansion calculation, the flux diagrams of the fixed points (FPs) are studied according to the boundary conditions imposed on the system, namely fixed charge or constant chemical potential. We find that condition (1) is true only when the system is controlled by a constant chemical potential. In contrast, if the total charge is held fixed, the basin of attraction of the Heisenberg FP, the most stable one, is not given by (1) but rather by the much more restricted condition

$$
\frac{3N''_T(E_F)^2}{2N_T(E_F)} < \frac{(6\alpha/\nu\nu)}{(\lambda^*_H + (6\alpha/\nu\nu))} N''_T(E_F), \quad (2)
$$

where $n = 3$ is the number of components of the spin field representing the magnetic degrees of freedom, $\lambda^*_H$ is the value of the coupling constant of a $\phi^4$ theory [7] at the Heisenberg FP and $\alpha, \nu$ are critical exponents, $(6\alpha/\nu\nu)/[(\lambda^*_H + (6\alpha/\nu\nu))] \approx -0.3$. At the Heisenberg FP $N''_T(E_F) < 0$ and $N''_T(E_F) = 0$.

Equation (2) is the main result of this paper. It predicts, for example, that a system with parabolic-type density of states [$N_T(E) \propto E^{1/2}$] cannot achieve criticality, in contradiction with equation (1). These severe restrictions are a consequence of the coupling between charge and spin density fluctuations and are not manifest in the MF theory. If the spin-charge coupling is too strong, violating condition (2), ferromagnetic criticality fails to occur and the system is compelled to undergo a first-order phase transition [8].

In the following we briefly outline the main steps to derive the above-mentioned findings. The grand partition function can be written [6] as a functional integral over the fluctuations of the fields $S$ and $\phi$ conjugate to the charge and spin operators, respectively, where an expansion around the paramagnetic uniform-static saddle point value is made. It represents a field theory involving a critical three-component vector spin field coupled to a noncritical scalar charge field. To describe the critical behavior of the system, the spin-charge free-energy functional can be cast in the form

$$
\beta F\{\phi_q, S_q\} = \frac{1}{2} \sum_q \left( r_2 + g^2 \right) S_q S_{-q} +
+ \lambda_s \sum_{q_1, q_2, q_3} S_{q_1} S_{q_2} S_{q_3} S_{-(q_1 + q_2 + q_3)}
+ \frac{r_c}{2} \sum_q \phi_q \phi_{-q} + \lambda_c \sum_{q, k} S_k S_{-q} \phi_{-q}, \quad (3)
$$

where $r_2$ is the exchange interaction and $g$ is the spin-charge coupling constant.
where \( r_s = \left( 1 - \frac{U}{2N} \right) N_T(E_f) \), \( r_c = \left( 1 + \frac{U}{2N} \right) N_T(E_f) \), \( \lambda_s = -\left( \frac{U^2}{192\beta N} \right) N_T(E_f) \) and \( \lambda_{sc} = -i \left( \frac{U^3}{64\beta N} \right)^{1/2} N_T(E_f) \).

Notice that the cubic spin-charge coupling in (3) is pure imaginary. If the charge field is integrated out the result is a \( \phi^4 \) theory with an effective quartic spin coupling \( \lambda = \lambda_s - \lambda_c = \frac{\lambda_i^2}{2rc} \), where \( \lambda_c \) is always negative for \( U > 0 \). A MF solution of this problem would imply a line of instability \( \lambda_s - \lambda_c = 0 \) dividing the first- and second-order portions of the \((\lambda_c, \lambda_s)\) phase diagram (Fig. 1). Equation (1) would follow with a Stoner-type criterion [6] \( UN_T(E_f) = 1 \). However, to allow renormalization of the quartic spin coupling induced by the spin-charge interaction, and different boundary conditions, we break the symmetry of this coupling in momentum space in the form \( \lambda_c \sum_q (S^2)_q (S^2)_{-q} \). In this way, if the total charge is held fixed by imposing \( \phi_q = 0 \), the coupling of the cubic spin-charge interaction corresponding to \( q = 0 \) in equation (3) will vanish, i.e., \( \lambda_c^{(0)} = 0 \). In this case the MF line of instability is \( \lambda_s = 0 \) (Fig. 1) because only the \( q = 0 \) mode contributes in the MF approximation. On the other hand, if the system is controlled by a constant chemical potential the total charge fluctuates and \( \lambda_c^{(0)} = \lambda_c^{(1)} = \lambda_c \).

The renormalization group programme that follows is a generalization of that used in a \( \phi^4 \) theory [6]. Though the calculation is performed in the one-loop- and first-order \( \varepsilon \)-expansion approximations, careful inspection of the results allow one to discover relations between the fixed point values (and eigenvalues) and their critical exponents. We find eight fixed points and the flow diagrams are studied according to the boundary conditions imposed on the system (Fig. 1). For constant chemical potential one selects FP solutions satisfying \( \lambda_c^{(0)*} = \lambda_c^{(1)*} = \lambda_c^* \), whereas if the total charge is held fixed the FP solutions satisfy \( \lambda_c^{(0)*} = 0 \).

In figure 1 the runaway lines beyond the line \( \lambda_s - \lambda_c = 0 \) correspond to the expected MF instability [Eq. (1)]. The interesting aspect though are those runaway lines attracted to the extension of the invariant line joining FPs (3) and (4) or FPs (3) and (6). These lines do not cross the line \( \lambda_s - \lambda_c = 0 \) and therefore it is not at all clear whether the system undergoes a first-order ferromagnetic transition if the system is controlled by a constant chemical potential. However, an one-loop calculation of the renormalized free energy can show [8] that this transition is still second order, the line joining FPs (3) and (4) being a Heisenberg critical line. Condition (1) thus remains true. In contrast, if the total charge is held fixed, the Fisher-renormalized Heisenberg FP (6) is a tricritical point and condition (2) is the new condition in order for the system to undergo a continuous transition to a ferromagnetic state. It implies a dramatic change compared with condition (1), where charge effects enlarge the second-order portion of the phase diagram.

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