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► To cite this version:

R Raimondi, M. Lavagna. Spin Fluctuations beyond the Gutzwiller Approximation : a Renormalised Paramagnon Theory. Journal of Low Temperature Physics, 1995, 99 (3-4), pp.355 - 357. 10.1007/BF00752308 . hal-01896235

HAL Id: hal-01896235

<https://hal.science/hal-01896235>

Submitted on 17 Oct 2018

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Spin Fluctuations beyond the Gutzwiller Approximation : a Renormalised Paramagnon Theory

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We analyze the spin fluctuations in the single-band lattice Hubbard model by using the slave-boson technique. It is shown that, at the Gaussian level beyond the saddle-point approximation, spin fluctuations obey a simple RPA-like form at all frequencies and wavevectors. Spin fluctuations, then, appear to give rise to an effective renormalized paramagnon theory opening new perspectives for the discussion of the effect of a magnetic field on Mott-Hubbard systems.

PACS numbers: 71.30+h, 75.30Kz, 71.28+d, 72.80 Ga

Spin fluctuations in a paramagnetic metal have been an intensive subject of research for many years. Stoner and paramagnon theories are among the most used in interpreting experiments in a large variety of circumstances because of their simplicity and direct physical interpretation. For example, the recently measured magnetization of liquid $^3\text{He}^1$ as a function of the magnetic field, bending downwards below the initial slope, appears to be explained, at least qualitatively, by a paramagnon model.² This should be contrasted with the Gutzwiller approximation for the single-band Hubbard model which predicts a metamagnetic transition at high fields³ above a critical value of the interaction. More recently, the infinite dimension approach⁴ brought new enlightenments on the question, confirming the Gutzwiller approximation for small enough value of the interaction, but predicting a smooth transition at large U from paramagnetic Mott insulator to fully-polarized insulator without any evidence for metamagnetism.

In this paper, we address the problem of accounting for spin fluctuations in the Hubbard model beyond the Gutzwiller approximation. The analysis is performed within the four slave-boson approach introduced by Kotliar and Ruckenstein.⁵ The slave-boson approach at its lowest level of approximation (saddle-point) is equivalent to the Gutzwiller approximation and allows for a systematic expansion. The first correction, i.e. Gaussian fluctuations about saddle-point, has been considered by a number of authors,⁶ although much of their analysis has been confined to the small

frequency and wavelength limit. Our main aim, here, is to extend this analysis for arbitrary wavevector and frequency. It will be shown that the expression for the spin fluctuation spectrum has a simple RPA form as in the paramagnon theory, with particle mass and local interaction suitably renormalized. This result suggests that the metamagnetic transition which has been seen as a consequence of the strong localized character of the quasiparticles close to a Mott metal-insulator transition, could be reduced by allowing spin fluctuations, as in the paramagnon theory.

Our starting point is the formulation of the single-band Hubbard model in the slave-boson language,⁵ whose Lagrangian reads :

$$\begin{aligned} \mathcal{L}(\tau) = & -t \sum_{i,j,\sigma} z_{i\sigma}^\dagger z_{j\sigma} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i,\sigma} c_{i\sigma}^\dagger (\partial/\partial\tau + \lambda_{i\sigma}^{(2)} - \mu) c_{i\sigma} \\ & + \sum_i d_i^\dagger (\partial/\partial\tau + \lambda_i^{(1)} + U - \sum_\sigma \lambda_{i\sigma}^{(2)}) d_i + \sum_i e_i^\dagger (\partial/\partial\tau + \lambda_i^{(1)}) e_i \\ & + \sum_{i,\sigma} p_{i\sigma}^\dagger (\partial/\partial\tau + \lambda_i^{(1)} - \lambda_{i\sigma}^{(2)}) p_{i\sigma} - \sum_i \lambda_i^{(1)}. \end{aligned} \quad (1)$$

The physical subspace is defined by the constraints : $e_i^\dagger e_i + d_i^\dagger d_i + \sum_\sigma p_{i\sigma}^\dagger p_{i\sigma} = 1$ and $d_i^\dagger d_i + p_{i\sigma}^\dagger p_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$. The $z_{i\sigma}$ are composite fields of the form $z_{i\sigma} = U_i (e_i^\dagger p_{i\sigma} + p_{i-\sigma}^\dagger d_i) V_i$ in which U_i and V_i are kept unspecified at that level. Because charge and spin fluctuations decouple at the Gaussian level, it is convenient to introduce the following symmetric and antisymmetric combinations $p_{qs(a)} = \frac{1}{\sqrt{2}} (p_{q\uparrow} \pm p_{q\downarrow})$. Considering spin fluctuations is equivalent to study the fluctuations of the field p_{qa} . The corresponding Lagrangian is given by $\mathcal{L} = \frac{1}{2} \sum_{q\nu} x_a^\dagger(q, \nu) \Gamma_{\alpha, \beta}(q, \nu) x_\beta(q, \nu)$ where $x_\alpha(q, \nu) = (p_{q\nu a}, p_{-q-\nu a}^\dagger)$ and :

$$\Gamma(q, \nu) = \begin{pmatrix} i\nu + \lambda_0^{(1)} - \lambda_0^{(2)} - \Sigma_{11}(q, \nu) & -\Sigma_{12}(q, \nu) \\ -\Sigma_{21}(q, \nu) & -i\nu + \lambda_0^{(1)} - \lambda_0^{(2)} - \Sigma_{22}(q, \nu) \end{pmatrix} \quad (2)$$

having indicated with $\Sigma_{\alpha\beta}(q, \nu)$ the matrix of the self-energies written as :

$$\begin{aligned} \Sigma_{\alpha\beta}(q, \nu) = & -4 \left[(\alpha, \beta) + \frac{1}{2} (\alpha)(\beta)^\dagger + \frac{1}{2} (\alpha)^\dagger(\beta) \right] S_0 + 2(\alpha)(\beta)^\dagger i\nu P(q, \nu) \\ & - 2(\alpha)^\dagger(\beta) i\nu P(-q, -\nu) + 2 \left[(\alpha)^\dagger(\beta)^\dagger + (\alpha)(\beta) + (\alpha)^\dagger(\beta) + (\alpha)(\beta)^\dagger \right] \Pi(q, \nu) \end{aligned} \quad (3)$$

where we have adopted the convenient notation $(\alpha) \equiv \frac{\partial z_\alpha}{\partial x_\alpha}$, $(\alpha)^\dagger \equiv \frac{\partial z_\alpha^\dagger}{\partial x_\alpha}$, $(\alpha, \beta) \equiv \frac{1}{2} z_0 \frac{\partial^2}{\partial x_\alpha \partial x_\beta} (z_\sigma + z_\sigma^\dagger)$. The various quantities appearing in Eq.(3) are given by $S_0 = \sum_k (-2t\epsilon_k) f(-2tz_0^2\epsilon_k)$, $\Pi(q, \nu) = (2tz_0)^2 \sum_{k,n} \epsilon_{k+q} \epsilon_k G(k, n) G(k+q, n+\nu)$, and $P(q, \nu) = 2t \sum_{k,n} \epsilon_k G(k, n) G(k+q, n+\nu)$ with $G(k, n)$ being the Green function of the saddle-point paramagnetic solution $G(k, n) = (i\omega_n + 2tz_0^2\epsilon_k)^{-1}$. To analyse

the spin fluctuations, we take the determinant of the fluctuation matrix $\Gamma(q, \nu)$:

$$\det\Gamma(q, \nu) = \nu^2 + \left(\lambda_0^{(1)} - \lambda_0^{(2)} - 4 \left[(p_a^\dagger, p_a) + (p_a, p_a) \right] S_0 \right) \left(\lambda_0^{(1)} - \lambda_0^{(2)} - 4 \left[(p_a^\dagger, p_a) - (p_a, p_a) + 2(p_a)^2 \right] S_0 - 4(p_a)^2 \frac{\nu^2}{z_0^2} \chi(q, \nu) \right) \quad (4)$$

having used the fact that $i\nu [P(q, \nu) - P(-q, -\nu)] = -\nu^2/z_0^2 \chi(q, \nu)$, χ being the Lindhardt function for the quasi-particles. The expressions derived up to this point are general. Let us now specify them to the cases of Regime I ($\delta = 0$ and $U < U_c$) and Regime II ($\delta \ll 1$ and $U > U_c$) as defined in Ref.⁶ We use at that step the fields $z_{i\sigma}$ corresponding to the Kotliar-Ruckenstein choice⁵ which allows to recover the uncorrelated limit ($U = 0$) at saddle-point level. It is easy, but tedious, to see that Eq.(4) can be rewritten in the final more transparent form :

$$\det\Gamma(q, \nu) = \nu^2 \{ 1 - F_0^a(z_0^2/\rho_F^0) \chi(q, \nu) \} \quad (5)$$

with $\lim_{\nu \rightarrow 0, q \rightarrow 0} \chi = -\rho_F^0/z_0^2$, ρ_F^0 being the free particle density of states. F_0^a is the Landau parameter, as obtained in Refs.^{3,6} playing the role of the local effective interaction whatever the value of the coupling is, and equalling $-U$ in the weak-coupling limit giving back the paramagnon theory.

Eq.(5) is now essential for our discussion of the effect of a magnetic field on Mott-Hubbard systems. It means that the free energy of the system is given by the sum of two contributions : first, the saddle-point term totally equivalent to the Gutzwiller approximation, and second the spin-fluctuation term exactly as in the paramagnon theory but with renormalized values of the parameters $\frac{m^*}{m}$ and F_0^a . It reconciliates the "almost-localized" picture provided by the G.A. and the "almost-magnetic" one given by the paramagnon theory. By allowing self-consistent effects in presence of an external magnetic field, it appears extremely interesting to examine to what extent spin-fluctuations will draw the system away from the metamagnetic transition predicted by the Gutwiller approximation. Such study is presently under investigation.

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ACKNOWLEDGMENTS

This work was supported by E.U. contract number ERB 4050 PL920925.

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