HIGHT-Tc SUPERCONDUCTORS AS ALMOST-LOCALIZED SYSTEMS: RESONANCE AND FLUCTUATIONS

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HIGHT-T_c SUPERCONDUCTORS AS ALMOST-LOCALIZED SYSTEMS: RESONANCE AND FLUCTUATIONS

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Abstract. – Many experimental results seem to relate the superconducting oxides to the phenomenon of Mott localization in strongly correlated systems. We will give a brief review of the different theories developed until then to treat the Mott localization in the Hubbard model: variational Ansatz of Gutzwiller or RVB Ansatz, leading to fundamentally different ground states. In this context, we propose a new approach which consists to take account of the quantum fluctuations around the mean-field solution provided by the Gutzwiller approximation. We show how to understand the ground state in terms of a resonance (split by the Mott gap in the almost-localized regime) in complete analogy with the Abrikosov-Suhl resonance of the Kondo problem – heavy fermions. Superconductivity appears as induced by the constrained intersite correlations developed by quantum fluctuations around this resonant state.

There has been a recent resurgence of interest in the problem of localization induced by correlations (Mott localization) since it appears that it probably plays a major role in the onset of high-T_c in the new superconducting pxides. By the simplicity of its formulation, the Hubbard model is particularly attractive since it already contains the essental physics of the phenomenon. In the strong coupling regime, the effect of the large Coulomb repulsion is to reduce the probability of double-occupancy, and gives rise to a Mott transition at half-filling ($n = 1$) upper a critical value of U. The more successful approach consists to introduce a variational wavefunction $|\psi_G\rangle$ – Gutzwiller Ansatz [1] – wich explicitly accounts for the reduction of probability of states with doubly-occupied sites:

$$|\psi_G\rangle = g^D\,|\text{P.S.}\rangle \underset{U\to\infty}{\rightarrow} P_G\,|\text{P.S.}\rangle \qquad (1)$$

where the "parent state" $|\text{P.S.}\rangle$ is the ideal Fermi gas, D is the number of doubly-occupied sites, g is a variational parameter ($g < 1$), and P_G is the operator which projects out the states with doubly-occupied sites.

Many very "physical" results are predicted by this Ansatz which takes a particularly simple form when one introduces the additional Gutzwiller approximation. In particular, it gives an antiferromagnetic Mott insulating phase for $n = 1$ and $U > U_c$ at 3-dimension. Besides its success [2], this approach presents some weaknesses since it fails in describing any exchange interactions. This is to be imputed to the fact that it is essentially a mean-field approach wich misses any fluctuation effects.

More recently, it has been postulated that in some situations, the insulating ground state is not antiferromagnetic, but rather resonant among all the dimers of singlet pairs [3]: this is the resonant valence bond (RVB) state. A new Ansatz has been proposed to account for this, taking another choice of the parent state in equation (1):

$$|\text{P.S.}\rangle = \left[\sum_\tau a_i(\tau)\, c_{i\uparrow}^+ c_{i+\tau\downarrow}^+\right]^{N/2} |0\rangle \qquad (2)$$

corresponding to the formation of $N/2$ singlet pairs.

We develop here another point of view and propose that, as the Stoner theory in the weak coupling regime, the Gutzwiller approximation (G.A.) is a good starting point which should be improved by adding quantum fluctuations. We present a new approach which allows to account for the fluctuations around the Gutzwiller ground state and shows how this describes the intersite correlations in presence of strong on-site constraints.

Let us start from the formulation [4] of the $N = 2$ Hubbard model in terms of the 4 projectors α_i (e_i, $p_{i\sigma}$ and d_i boson operators) on the empty, singly-occupied σ and doubly-occupied i site. The partition function Z is written in terms of the Lagrangian:

$$Z = \int [Dc]\,De]\,[DP_{\pm\sigma}]\,[Dd] \prod_{i\sigma} d\lambda_i^{(1)} d\lambda_{i\sigma}^{(2)} \times \times \exp\left[-\int_0^\beta d\tau L(\tau)\right] \qquad (3a)$$

$$L(\tau) = \sum_o e_i^+ \left(\partial_\tau + \lambda_i^{(1)}\right) e_i + + \sum_{i\sigma} p_{i\sigma}^+ \left(\partial_\tau + \lambda_i^{(1)} - \lambda_{i\sigma}^{(2)}\right) p_{i\sigma} + \sum_i d_i^+ \left(\partial_\tau + \lambda_i^{(1)} - \sum_\sigma \lambda_{i\sigma}^{(2)} + U\right) d_i + \sum_{ij\sigma} c_{i\sigma}^+ \left[\left(\partial_\tau + \lambda_{i\sigma}^{(2)}\right) \times \quad \delta_{ij} + t_{ij} z_{i\sigma}^+ z_{j\sigma}\right] c_{i\sigma} \qquad (3b)$$

with

$$z_{i\sigma} = e_i^+ p_{i\sigma} + p_{i-\sigma}^+ d_i \qquad (4)$$

$\lambda_i^{(1)}$ and $\lambda_{i\sigma}^{(2)}$ are Lagrange multipliers to enforce the constraints:

$$e_i^2 + \sum_\sigma p_{i\sigma}^2 + d_i^2 = 1$$

and $n_{i\sigma} = p_{i\sigma}^2 + d_{i'}^2$ and μ is the chemical potential. (3) is strictly equivalent to the Hubbard model with $z_{i\sigma}$ specified by (4). However, the choice of $z_{i\sigma}$ is not unique, and one can replace $z_{i\sigma}$ by any combination $U_i z_{i\sigma} V_i$ where U_i and V_i are diagonal operators such as $U_i = 1$ in the (0) and $(-\sigma)$ configurations, and $V_i = 1$ in $(+\sigma)$ and $(\uparrow\downarrow)$. Taking advantage of this, it has been shown that, for a sensible choice, the saddle-point approximation on the boson-fields is equivalent to the Gutzwiller approximation. The merit of the slave-boson formulation is to transform the variational procedure into a standard field theory problem and so to open the way to further developments.

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At the saddle-point, one can integrate over the Grassmann variables and obtain the following action S_0 (and free energy F_0) :

$$F_0 = k_B T (S_0) = k_B T \sum_{k, i\omega_n, \sigma} \times \mathrm{Ln}\left(-i\omega_n + q_{0\sigma}\varepsilon_k\right) + U d_0^2 \quad (5)$$

where $q_{0\sigma} = z_{0\sigma}^2$ is a factor of band renormalization. Minimizing the free energy allows to determine the value of q_0, and also of the Lagrange multipliers $\lambda_0^{(1)}$ and $\lambda_{0\sigma}^{(2)}$. In principle, the resolution of the saddle-point equations can be done at any point (U, n). However, we give here the results only for the two interesting regimes I and II. Noting

$$\left\langle \sum_{ij} t_{ij} c_{i\sigma}^{+} c_{j\sigma} \right\rangle = \bar{\varepsilon}_\sigma = \bar{\varepsilon}_0 / 2 = -U_c / 16$$

in the paramagnetic half-filled band case, we get:
Regime I: $(u = U / U_c < 1$ and $n = 1)$
$d_0^2 = (1-u) / 4$ and $q_0 = 1 - u^2$
$\lambda_0^{(1)} = U_c (1+u)(2-u) / 4$ and $\lambda_0^{(2)} = U / 2$.

The Mott transition $(q_0 \to 0)$ naturally arises for $U > U_c$.
Regime II: $(u = U / U_c > 1$ and $(1-n) = \delta \ll 1)$
$d_0^2 = \delta (1-z)^2 / 4\zeta$ and $q_0 = 2\delta / \zeta$
within the notation $\zeta = \sqrt{1 - 1/u}$

$$\lambda_0^{(1)} = \lambda_0^{(2)} = U \left(1 \pm \sqrt{1 - 1/u}\right) / 2$$

(+ and − for $n > 1$ and $n < 1$, respectively).

These results take all their physical meaning if remark that $\left(\lambda_0^{(2)}\right)$ represents the chemical potential of the quasiparticles. It fixes the position of the narrow band and gives rise to a gap (Mott gap) for $U > U_c$ of width $U\sqrt{1 - U_c / U}$. By analogy with the Abrikosov-Suhl resonance of the Kondo problem, we interpret the renormalization of the band as a resonance pinned at the fermi level, and cut by a gap for $U > U_c$.

Compared to the standard large degeneracy expansion, the particularity here is an additional enhancement of the density of longitudinal spin susceptibility $\kappa_G(q,\omega)$ and transverse spin susceptibility $\chi_G(q,\omega)$ coming from the implicit dependence of q_σ with the magnetization M and doping δ, leading to an antiferromagnetic instability close to the Mott transition.

The effect of the Gaussian fluctuations around the saddle-point turns out to dress the bare boson propagators $\overline{\overline{D}}_0(\mathbf{q},\omega)$ into:

$$\overline{\overline{D}}^{-1}(\mathbf{q},\omega) = \overline{\overline{D}}_0^{-1}(\mathbf{q},\omega) - \overline{\overline{\varepsilon}} q_0 \chi_0(q,\omega) \qquad (8)$$

where the propagators are matricially expressed in the e, p_σ, d basis, and $\overline{\overline{\varepsilon}}$ is the vertex matrix connecting boson to fermion lines. The bare boson propagators $\overline{\overline{D}}_0^{-1}(\mathbf{q},\omega)$ are defined from equation (3b) and reflect the sets of exchange couplings:

$$J_{ec} = t^2 / \lambda_0^{(2)}, J_{p\sigma p\sigma} = t^2 / \left(\lambda_0^{(1)} - \lambda_{0\sigma}^{(2)}\right)$$

and

$$J_{dd} = t^2 / \left(U + \lambda_0^{(1)} - \sum_\sigma \lambda_{0\sigma}^{(2)}\right)$$

(reducing to the usual exchange coupling t^2 / U in the $U = \infty$ limit). In other words, the consideration of quantum fluctuations around the G.A. is equivalent to develop a constrained perturbation theory as a function of these exchange coupling interactions. The permits to treat in a self-consistent way the almost localized character of the ground state, and the exchange couplings. There is no need here to use an extra-canonical transformation: both effects naturally arises at the different steps of the expansion.

We have looked at the pairing of quasiparticles introduced by these quantum fluctuations. The pairing is found to be repulsive in s and p channels, but attractive in the d channels close to the Mott transition. The physical origin of this superconducting pairing is due to intersite exchange couplings combined with large on-site constraints. It is close to the situation found in the $1 / N$ expansion of the Anderson model [6]. The largeness of the cut-off energy scales qW, is a factor which can explain the high T_c observed in the new oxides.

In conclusion, we have sketched here a new kind of study of the Mott transition in the strong-coupling regime of the Hubbard model. This gives an insight into the deep similitude between these systems and heavy fermions. The approach to the localization which is inherent to both situations is described in a very paralle way:

– mean-field broken symmetry asociated to a resonant state,

– effect of quantum fluctuations azssociated to exchange correlations combined with large on-site constraints.

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