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SLAVE-BOSON APPROACHES TO STRONGLY CORRELATED SYSTEMS

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We give a general presentation of the different slave-boson representations introduced in the problem of strong correlations. Then, choosing one of this representation, we show how to set up a perturbation expansion providing the microscopic basis of a Fermi liquid theory.

The importance gained these last years by the study of strongly-correlated systems lead to the search of new methods of tackling the problem of correlations. We present here one of them, the slave-boson approach [1] which turned out to be extremely powerful in the study of heavy fermions [2] (Anderson lattice) and whose more recent adaptation to the Hubbard [3,4] (or related t-J) model appears to already give very encouraging results. For more clarity, we choose to present the method exclusively on a single example (Hubbard or t-J model). Indeed, there is not one possible slave-boson representation but rather a serie of them more or less connected. In a first part, we will review the different available choices with some emphasis on their similarities but also their differences. Then, keeping one of this representation, we will show in a second part how to set up a perturbation theory - saddle point plus gaussian fluctuations - adapted to the presence of constraints.

I. DIFFERENT SLAVE BOSON REPRESENTATIONS OF THE HUBBARD MODEL (OR RELATED t-J MODEL).

a) Kotliar-Ruckenstein[3] (KR) representation

To keep track of the local configurations (4 configurations : empty, singly-occupied of spin σ and doubly-occupied on each site), K.R. introduced some additional degrees of liberty represented by four fields e_i, $p_{i\sigma}$ and d_i. The corresponding occupation numbers $e_i^+ e_i$, $p_{i\sigma}^+ p_{i\sigma}$ and $d_i^+ d_i$ represent the projectors on the 4 possible states on site i. One can get the following correspondence between the initial representation of fermions $\{f_{i\sigma}\}$ and the new enlarged representation $\{c_{i\sigma}\} \otimes \{e_i, p_{i\sigma}, di\}$:

Initial representation		new representation
$\|0\rangle = \|vac\rangle$	$\longrightarrow$	$\|1\rangle = e_i^+\|vac\rangle$
$\|\uparrow\rangle_i = f_{i\uparrow}^+\|vac\rangle$	$\longrightarrow$	$\|2\rangle = p_{i\uparrow}^+ c_{i\uparrow}^+\|vac\rangle$
$\|\downarrow\rangle_i = f_{i\downarrow}^+\|vac\rangle$	$\longrightarrow$	$\|3\rangle = p_{i\downarrow}^+ c_{i\downarrow}^+\|vac\rangle$
$\|\uparrow\downarrow\rangle_i = f_{i\uparrow}^+ f_{i\downarrow}^+\|vac\rangle$	$\longrightarrow$	$\|4\rangle = d_i^+ c_{i\uparrow}^+ c_{i\downarrow}^+\|vac\rangle$

The two representations are equivalent provided that some constraints are satisfied which guarantee the physical interpretation of the fields :

$$P_i = e_i^+ e_i + \sum_\sigma p_{i\sigma}^+ p_{i\sigma} + d_i^+ d_i - 1 = 0 \qquad (1)$$

(completeness of the projectors)

$$Q_{i\sigma} = c_{i\sigma}^+ c_{i\sigma} - (p_{i\sigma}^+ p_{i\sigma} + d_i^+ d_i) = 0 \qquad \forall\sigma \qquad (2)$$

(redundancy between c_σ and p_σ , d degrees of liberty).

Note that there is an exact correspondence between $f_{i\sigma}^+ f_{i\sigma}$ and $c_{i\sigma}^+ c_{i\sigma}$ in each representation. The constraint (1) automatically implies that the operators $n_\alpha = \alpha^+\alpha$ (with α = e, p_σ or d) satisfy the algebra of projectors

$$n_\alpha n_\beta = \delta_{\alpha\beta} n_\alpha \qquad (3)$$

In order to obtain the expression of the Hubbard Hamiltonian in the new representation, let us establish the following correspondence (easy to proof matricially) :

$$f_{i\sigma}^+ f_{i\sigma} \longrightarrow \bar{z}_{i\sigma} \bar{z}_{j\sigma}^+ c_{i\sigma}^+ c_{j\sigma} \qquad \text{for } i \neq j$$

$$\text{with } \bar{z}_{i\sigma} = e_i^+ p_{i\sigma} + p_{i-\sigma}^+ d_i$$

$$f^+_{i\sigma} f_{i\sigma} \longrightarrow c^+_{i\sigma} c_{i\sigma}$$

$$n_{i\uparrow} n_{i\downarrow} \longrightarrow d^+_i d_i$$

Then the expression of the Hubbard hamiltonian in the new representation can be written

$$H = -\sum_{ij\sigma} t_{ij}\, \bar{z}^+_{i\sigma}\, \bar{z}_{j\sigma}\, c^+_{i\sigma}\, c_{j\sigma} + U \sum_i d^+_i d_i \tag{4}$$

(within the constraints).

Let us make two remarks :

(i) To guarantee the fermionic character of the physical particle, the operators which represent it in second quantification must respect the usual anticommutation rules. This is automatically insured if $c_{i\sigma}$ obey Fermi statistics, and e_i $p_{i\sigma}$, d_i Bose statistics (hence the term of "slave-boson"). We will see in the following that this is not the only choice.

(ii) Indeed, the choice $\bar{z}_{i\sigma}$ is not unique but one can replace $\bar{z}_{i\sigma}$ by any combination $U_{i\sigma}\bar{z}_{i\sigma}V_{i\sigma}$ where $U_{i\sigma}$ and $V_{i\sigma}$ are diagonal matrix whose only non-zero term (equal to 1) appears respectively on $|0\rangle$, $|-\sigma\rangle$ and $|\sigma\rangle$, $|\uparrow\downarrow\rangle$ lines. One can in particular choose as K.R.

$$z_{i\sigma} = (1 - d^+_i d_i - p^+_{i\sigma} p_{i\sigma})^{-1/2}\ \ \bar{z}_{i\sigma}(1 - e^+_i e_i - p^+_{i-\sigma} p_{i-\sigma})^{-1/2} \tag{5}$$

All the choices are formally equivalent as far as the constraints are exactly satisfied. This is no longer true when one makes approximations. Typically, the mean-field approximation satisfies the constraint on average, and leads to different results depending on the special choice of $z_{i\sigma}$. These discrepancies are supposed to disappear if one could include quantum fluctuations at all orders. When stopping at mean-field, the choice (5) is more sensible since it renormalizes $\bar{z}_{i\sigma}$ by its value in the uncorrelated case and gives back the free electron gas in the limit $U = 0$. It is this choice that will be retained in part II.

b) Zou-Anderson and Schwinger-boson representation

Many other representations have been proposed such as :

$$f_{i\sigma} \longrightarrow e_i^+ c_{i\sigma} + \sigma c_{i-\sigma}^+ d_i \tag{6}$$

The same rules stand as before : this transformation acts for any intersite hopping term, but not for intrasite term where $f_{i\sigma}^+ f_{i\sigma}$ simply transforms as $c_{i\sigma}^+ c_{i\sigma}$, and $n_{i\uparrow} n_{i\downarrow}$ as $d_i^+ d_i$. This transformation has the advantage to require the introduction of only one constraint :

$$e_i^+ e_i + \sum_\sigma c_{i\sigma}^+ c_{i\sigma} + d_i^+ d_i = 1 \tag{7}$$

There are at least two choices which guarantee the Fermi statistics of the particles : $c_{i\sigma}$ may be taken as fermions, implying e_i, d_i bosons [5]. Another choice which seems to be even more interesting consists in taking $c_{i\sigma}$ as bosons (Schwinger-bosons) and e_i, d_i as fermions [6].

c) Large U limit of the Hubbard model

In the large U limit, the Hubbard model can be projected on the Hilbert subspace of states which do not contain any double-occupied sites. This leads to the t-J model which can be derived within a canonical transformation. This comes down in the slave-boson representation, to truncate the second part of the expression containing d.

$$H^{proj} = - \sum t_{ij}\, e_i c_{i\sigma}^+ e_j^+ c_{j\sigma} + J(\vec{S}_i . \vec{S}_j - \frac{n_i \cdot n_j}{4}) \tag{8a}$$

with $\vec{S}_i = \sum_{\alpha,\beta} c_{i\alpha}^+ (\tilde{\tau})_{\alpha\beta}\, c_{i\beta}$

where $\tilde{\tau}$ represent the Pauli matrix, $J = 4t^2/u$ and the constraint becomes :

$$e_i^+ e_i + \sum c_{i\sigma}^+ c_{i\sigma} = 1 \tag{9}$$

As before, one can choose as well the fermionic or the bosonic representation. The Schwinger bosons $c_{i\sigma}$ can be viewed as hard-core bosons. It is worth noting that the fermionic representation $(e_i^+ c_i)$ coïncide with K.R's at the saddle point level in the limit of infinite U and infinite spin degeneracy N. However, while the saddle-point approximation is exact at infinite N and the gaussian fluctuations at the order 1/N, the fermionic representation requires much higher orders in the expansion to describe the magnetism at half-filling which manifestly occurs in the physical systems closer to the situation N = 2. From this point of view, K.R's representation seems to be more suitable since, as we will see below, the exchange interaction is already taken into account at the level of gaussian fluctuations. It is this representation that we will retain in the rest of the paper where we will set up a systematic perturbation theory.

II. PERTURBATION THEORY IN KOTLIAR-RUCKENSTEIN REPRESENTATION

Since the time evolution generated by H preserves the constraints $([H, P_i] = [H, Q_{i\sigma}] = 0)$, it is only necessary to enforce the constraints at one particular time : this is done by introducing time-independent Lagrange multipliers $\lambda_i^{(1)}$ and $\lambda_{i\sigma}^{(2)}$. The partition function can thus be written as a functional integral over the fermion and boson fields :

$$Z = \int \mathcal{D}c\,\mathcal{D}e\,\mathcal{D}p_\sigma\,\mathcal{D}d \prod_{i\sigma} d\lambda_i^{(1)}\, d\lambda_{i\sigma}^{(2)} \exp\left[-\int_0^\beta \mathcal{L}(\tau)d\tau\right] \tag{10a}$$

where the Lagrangian $\mathcal{L}(\tau)$ is :

$$\begin{aligned}\mathcal{L}(\tau) = &\sum_{ij\sigma} c_{i\sigma}^+[(\partial\tau + \lambda_{i\sigma}^{(2)})\, \delta_{ij} + z_{i\sigma}^+ z_{j\sigma}\, t_{ij}]c_{j\sigma} \\ &+ e_i^+(\partial_\tau + \lambda_i^{(1)})\, e_i + p_{i\sigma}^+(\partial_\tau + \lambda_i^{(1)} - \lambda_{i\sigma}^{(2)})p_{i\sigma} \\ &+ \sum_i d_i^+(\partial_\tau + \lambda_i^{(1)} - \sum_\sigma \lambda_{i\sigma}^{(2)} + U)d_i \end{aligned} \tag{10b}$$

a) Saddle-point

The idea is to start from the simplest saddle-point approximation where is considered uniform and static distribution of boson fields. One can then integrate over the Grassman variables and obtain for the free energy :

$$F_o = f_o + Ud_o^2 + \lambda_o^{(1)} \left[e_o^2 + \sum_\sigma p_{o\sigma}^2 + d_o^2 - 1 \right]$$

$$+ \sum_\sigma \lambda_{o\sigma}^{(2)} (n_{o\sigma} - p_{o\sigma}^2 - d_o^2) \tag{11a}$$

$$\text{where } f_o = -\frac{1}{\beta} \sum_{k,i\omega_n,\sigma} \ln(-i\omega_n + q_{o\sigma}\varepsilon_k) \tag{11b}$$

in the notation $q_{o\sigma} = z_{o\sigma}^2$

$$\varepsilon_k = \sum_{ij} t_{ij} \exp^{i\vec{k}(\vec{R}_i - \vec{R}_j)}$$

The physical picture provided at the saddle-point level is that of a gaz of quasiparticles (represented by the operator $c_{i\sigma}$) of enhanced mass $m^* = m/q_o$. The saddle-point equation (minimization of the free energy) allows to determine the values of the boson fields and Lagrange muiltipliers. It is particularly interesting to remark, that, thanks to $U_{i\sigma}$ and $V_{i\sigma}$, one finds exactly the results of the Gutzwiller approximation[7)] for q_o. One recovers at half-filling the Brinkman-Rice transition (Mott localization due to correlations) above a critical edge of localizatin $U_c = 16 \int \omega\rho_o(\omega)d\omega$ (proportional to the averaged energy per site in the uncorrelated case). We put here the results for the two interesting regimes close to half-filling.

Regime I (metallic regime) : $U = U/U_c < 1$ and $n = 1$

$$q_o = 1 - u^2$$

Regime II (vacancy regime) : $u > 1$ and $1 - n = \delta << 1$.

$$q_o = \frac{2\delta}{\sqrt{1 - U_c/U}}$$

Regime I ($U < U_c$) is believed to provide a "lattice" description of normal ^3He, and the Copper oxides (high T_c) in the normal phase are supposed to be good candidates for regime II.

There is an additional information contained in the slave-boson formulation which is the determination of the Lagrange multipliers at the saddle-point : their evolution as a function of U is reported on figure 1. It is very interesting to remark the existence of a gap delimited by the values of $\lambda_o^{(2)}$ in the vacancy regime ($n \leq 1$) and the electronic regime ($n \geq 1$). This gap of width $\Delta = U\sqrt{1 - U_c/U}$ can be interpreted as a Mott gap.

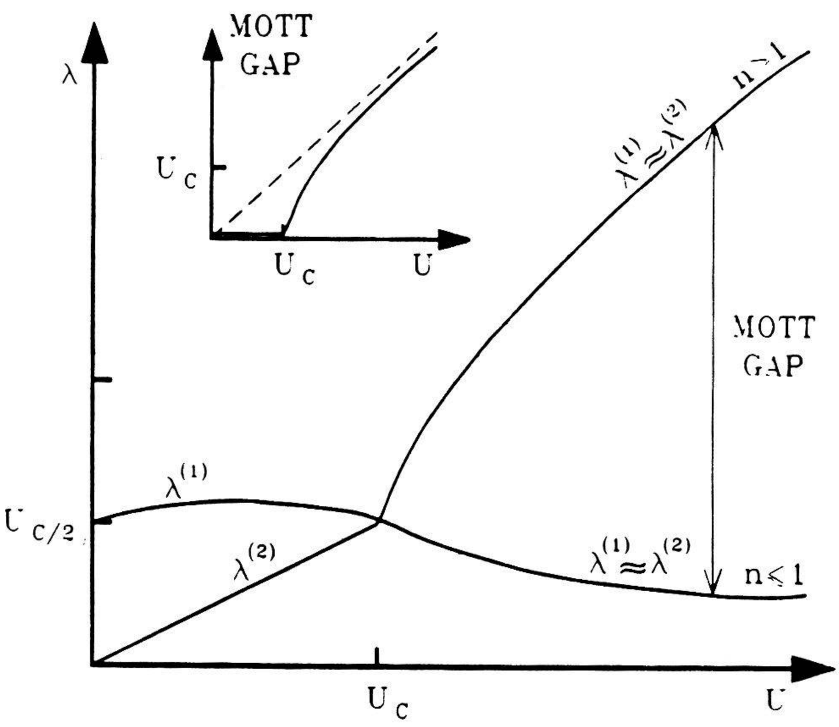

Fig. 1 Saddle-point values of the Lagrange multipliers Notice the opening of a Mott gap for $U > U_c$. In the insert, U dependence of the Mott gap.

b) Gaussian fluctuations

For the consideration of quantum fluctuations, it is useful to remark that $\mathcal{L}(\tau)$ obeys a local gauge invariance :

$$e_i \longrightarrow \exp[i\,\theta_i]e_i'$$

$$d_i \longrightarrow \exp[i(\theta_i - \sum_\sigma \chi_{i\sigma})]d_i'$$

$$p_{i\sigma} \longrightarrow \exp[i(\theta_i - \chi_{i\sigma}]p_{i\sigma}'$$

$$c_{i\sigma} \longrightarrow \exp[i\chi_{i\sigma}]c_{i\sigma}'$$

$$\lambda_i^{(1)} \longrightarrow \lambda_i^{(1)'} + i\dot{\theta}_i$$

$$\lambda_{i\sigma}^{(2)} \longrightarrow \lambda_{i\sigma}^{(2)'} + i\dot{\chi}_{i\sigma}.$$

It is often more convenient to absorb the phases of the boson fields into the Lagrange multipliers which turn out to also be fields. This defines the "radial" gauge that will be retained in the following since it introduces only real fields. We are then left with the problem of two fermion fields ($c_{i\sigma}$) in interaction with 7 boson fields which can be classified into symmetric and antisymmetric channels :

$$\left\{ e,\ d,\ p_o = \frac{p_\uparrow + p_\downarrow}{2},\ \lambda^{(1)},\ \lambda_o^{(2)} = \frac{\lambda_\uparrow^{(2)} + \lambda_\downarrow^{(2)}}{2} \right\} \quad \text{and}$$

$$\left\{ p_z = \frac{p_\uparrow - p_\downarrow}{2},\ \lambda_z^{(2)} = \frac{\lambda_\uparrow^{(2)} - \lambda_\downarrow^{(2)}}{2} \right\}.$$ In fact this formulation obviously breaks the spin-rotation invariance which can be restored by introducing 2 x 2 spinor fields :

$$\tilde{P}_i = p_{io}\,.\,\tilde{1} + \sum_{\alpha=1}^{3} \vec{P}_{i\alpha}\,.\,\tilde{\tau}^\alpha \qquad \text{(where } \tilde{\tau} \text{ are Pauli matrix)}$$

The generalized basis of 11 boson-fields has the advantage of making the unperturbated boson propagators $\tilde{D}_o^{-1}$ block-diagonal

$$\tilde{D}_o^{-1} = \begin{bmatrix} \tilde{D}_{os}^{-1} & 0 & 0 & 0 \\ 0 & \tilde{D}_{oa}^{-1} & 0 & 0 \\ 0 & 0 & \tilde{D}_{oa}^{-1} & 0 \\ 0 & 0 & 0 & \tilde{D}_{oa}^{-1} \end{bmatrix} \tag{12a}$$

where $$\tilde{D}_{os}^{-1} = \begin{bmatrix} \lambda_o^{(1)} & 0 & 0 & e_o & 0 \\ 0 & U+\lambda_o^{(1)}-\lambda_o^{(2)} & 0 & d_o & -2d_o \\ 0 & 0 & 2(\lambda_o^{(1)}-\lambda_o^{(2)}) & 2p_o & -2p_o \\ e_o & d_o & 2p_o & 0 & 0 \\ 0 & -2d_o & -2p_o & 0 & 0 \end{bmatrix} \tag{12b}$$

and $$\tilde{D}_{oa}^{-1} = \begin{bmatrix} 2(\lambda_o^{(1)}-\lambda_o^{(2)}) & -4p_o \\ -4p_o & 0 \end{bmatrix} \tag{12c}$$

The effects of the quantum fluctuations can be carried out in the functional integral formalism[4)]. The role of the correlations is to introduce some effective interactions (mediated by the slave-bosons) among the quasiparticles defined at the saddle point level. Coming from the structure of the boson fields, there is a complete separation between symmetric and antisymmetric channels as represented in the energy diagrams of figure 2.

Within the approximation where one can neglect the $\vec{k}$-dependence of the vertex, this defined effective interactions $F^{s(a)}(\vec{q})$ which can be expanded into Legendre polynomial (or cubic) if the symmetry is spherical (or cubic). We are left with a Fermi liquid picture with quasiparticles interacting through a set of Landau parameters F_l^s , F_l^a.

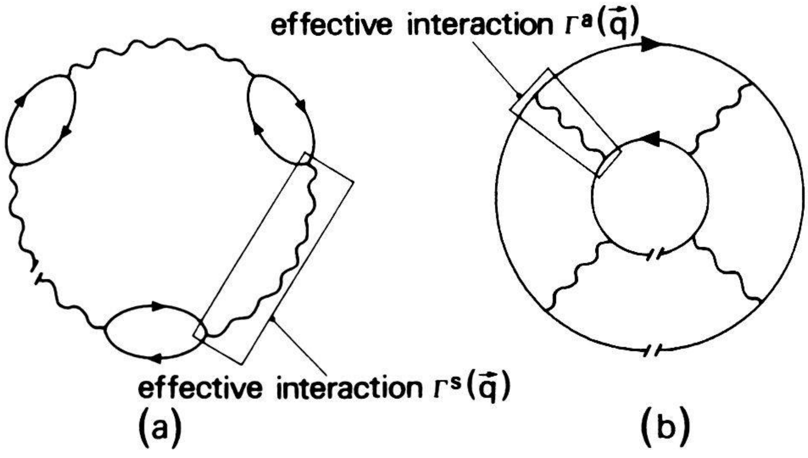

Fig. 2 Diagrammatic representation of the free energy
(2a) Bubble diagrams; (2b) Ladder diagrams.

We have explicitely calculated these parameters in the channel l = 0. It is remarkable that the values that we draw from the calculation of gaussian fluctuations, cöincide exactly with those obtained in the Gutzwiller approximation. This is a very sensible result since in our language here the Gutzwiller approximation corresponds to a self-consistent saddle-point with an implicit dependence of the boson-fields with the external excitations (electromagnetic fields). We found :

$$F_o^a = -1 + \frac{ed}{(e+d)^2} \frac{1}{(2p^2)^2} \quad \text{in regime I or II} \tag{13a}$$

Explicitely : $F_o^a = [-1 + 1/(1 + u)^2]$ in regime I

and $F_o^a = [-1 + 1/4u)$ in regime II

$$F_o^s = -1 + \frac{1}{(1-u)^2} \quad \text{in regime I} \tag{13b}$$

$$F_o^s = -1 + \frac{2u-1}{2\delta\sqrt{u(u-1)}} \quad \text{in regime II} \tag{13c}$$

In the weak U limit, we recover the standard RPA results of weak coupling ($F_o^s = 2U$ and $F_o^a = -2U$). In regime II, we find $F_o^s \sim 1/\delta$ and the compressibility is enhanced as expected for an incompressible Fermi liquid. This approach seems to be very powerful since it provides a unique interpolation between the weak-coupling regime (paramagnon theory) and the strong-coupling regime (incorporating the dynamic effects which were missing in the Gutzwiller approximation).

The discussion of the eventual instabilities (magnetic, flux phase, superconducting...) essentially depends on the structure of the correlation function χ_o considered in the unperturbated case. For a spherical symmetry, χ_o is given by the Lindhard functions, and one finds a ferromagnetic instability at large U but no antiferromagnetic instability. The situation is rather different in the case of an alternated structure (e.g. cubic) where the nesting property of the paramagnetic Fermi surface at half filling gives an AF instability at $n = 1$ for infinitesimal small value of U. The ferromagnetic instability occurs above $U_F = 1/[4(1-\alpha)]$ at $n = 1$. The F-AF boundary is asymptotic to the line $n = 1$ at $U = \infty$ as required by Nagaoka's theorem.

From a general point of view, the Fermi surface of the perturbated system is identical to that of the unperturbated system. Then, the eventuality of a superconducting or flux phase might be examined by already breaking the symmetry at the unperturbated level (through χ_o). In that sense, we think that the above calculation may be useful since it may be adapted to any "unperturbated" structure. It constitutes a frame in which a set of parameters $q_o = m/m^*$, F_o^s, F_o^a, $\lambda_{(o)}^{(1)}$, $\lambda_o^{(2)}$ are defined independently of the structure. It would be interesting to apply it to some more complex situations (flux phase, superconductivity...) perhaps in closer connection to the physics of high-T_c superconductors.

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