MICROSCOPIC THEORY OF STRONGLY CORRELATED FERMI SYSTEMS

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INTRODUCTION

We present here a new approach to a purely lattice (Hubbard) model for correlated Fermi systems. We first motivate the model, and describe its features in physical terms. We then show how a many body theory can be developed, illustrating it with the example of a very strongly correlated Hubbard model with a low density of holes, for which we show that a hole density expansion exists.

In most strongly correlated electronic systems of interest, one has two kinds of states, one a broad sp band or spd band, and the other d or f configurations (eg., f^{n-1}, f^n and f^{n+1} at each lattice site) with hybridization between the two. In one common approach, the f electron degrees of freedom are integrated out, leading to an interacting spd Fermi liquid. This is done in two stages. If one of the f electron configurations is noticeably more stable than the others, e.g., $E_f n-1$ and $E_f n+1$ are much greater than $E_f n$, the high lying states f^{n-1} and f^{n+1} are virtual, and are eliminated to yield an (spd)spin (f)spin or Kondo interaction in which real f charge fluctuations are absent. At low temperatures, the f spin is quenched, but there is strong local self interaction among the strongly renormalized spd electrons, i.e., local spin fluctutions. The heavy fermion system is assumed to be a lattice version of this.

Now charge fluctuations are absent only if the situation is absolutely symmetric with respect to the configurations f^n and f^{n-1}, i.e., if $E_f n - E_f n-1 = E_f n - E_f n+1$ and the hybridization matrix elements are the same. Otherwise, the f charge can leak out; in a lattice there is an intersite transfer term of the sort $|V|^2 \; f^+_{i\sigma} f_{j\sigma} \langle a^+_{j\sigma} a_{i\sigma}\rangle$ where $f^+_{i\sigma}$ and $a^+_{j\sigma}$ create f and conduction electron excitations at sites i and j respectively (with spin index σ). In general therefore, one has both f charge excitations (and spin fluctuations) as well as strongly renormalised spd electrons, i.e., a two component Fermi liquid.

The essential physics is presumably in the strongly correlated f electron system. If so, instead of eliminating the f electron degrees of freedom, one should do exactly the reverse, namely eliminate the fast conduction (spd) electron variables; this leads to a Hubbard like model for the f electrons, with bare parameters possibly dependent on the conduction electrons.

We thus consider a Hubbard model, with two configurations per site, namely a doubly degenerate or magnetic configuration $|\sigma\rangle$ (electron, for f^n) and a nondegenerate nonmagnetic hole configuration $|0\rangle$ (for f^{n-1}). The operators in this atomic representation[1] are $|i\sigma\rangle\langle i0| = X^i_{\sigma 0}$ and $|i0\rangle\langle i\sigma| = X^i_{0\sigma}$ etc., . The Hamiltonian has the form

$$H = \sum_{i,\sigma} E\left(X^i_{\sigma\sigma} - X^i_{00}\right) + \sum_{i,j,\sigma} t_{ij} X^i_{\sigma 0} X^j_{0\sigma} + \sum_{i,j,\sigma,\sigma'} (t^2_{ij}/U)\, X^i_{\sigma\sigma'} X^j_{\sigma'\sigma} \qquad (1)$$

The states $|i\sigma\rangle$ and $|i0\rangle$ differ in energy by E. The matrix element for hopping from site i to site j is t_{ij}. The last term is an antiferomagentic coupling between electrons at sites i and j due to a virtual process involving the high lying nonmagnetic two electron f^{n+1} state with Hubbard repulsion energy U. The model is characterized by a bare kinetic energy scale zt, band filling or electron number $N^{-1}\langle\sum_{i,\sigma} X^i_{\sigma\sigma}\rangle = 1 - \delta$, and an antiferromagnetic energy $(t^2_{ij}/U) = E_A$.

As is well known, the regime of small δ and E_A is one with strong correlation, antiferromagnetic coupling and low effective Fermi energy. We discuss this region qualitatively and outline a quantitative approach for $U = \infty$, so that δ is the only relevant parameter. The general Hubbard model has, in addition, very low characteristic energies near the Mott transition, i.e., near $U \simeq U_c \simeq zt$ and for $\delta = 0$.

PHYSICAL DESCRIPTION

(i) $U = \infty$. Consider the infinitely correlated limit with a low density of holes. At temperatures much higher than $T^*_F = \delta T_F = \delta(zt)$, the system is best described as a collection of disordered spins. In the $U = \infty$ limit, the system is very degenerate as all spin configurations have the same energy. The motion of a single hole ($\delta = 1/N$) in such a medium has been discussed by Brinkman and Rice[2] and by Ohata and Kubo[3]. Because of the strong spin disorder, the hole mean free path is short, of order interatomic spacing. A single (or independent) hole theory describes the high temperature behaviour well.

At low temperatures $T \ll T^*_F$, the effect of hole motion is crucial. The holes move around and homogenize the system which is thus a Fermi liquid. A spin at any site loses its memory once a hole passes through, so that there are spin fluctuations with a low energy scale T^*_F. The valence at each site also fluctuates with the same energy scale. Since the Fermi energy is also T^*_F, we have a Fermi liquid in which the kinetic energy and interactions are both comparable.

The obvious question concerns the ground state. Nagaoka[4] pointed out that for one hole, the lowest energy state occurs when all spins are parallel. This does not prove that the ground state for a finite hole density is ferromagnetic. The method of static spin configurations used in Refs. 2-4 is a high temperature approach which does not access the Fermi liquid regime. We shall see that the system is paramagnetic to lowest order in hole density. There are interactions between electrons in this Fermi liquid which favour non s-wave pairing or anisotropic superconductivity.

(ii) Finite U :- For large but finite U, and say $\delta = 0$, the ground state is an antiferromagnetic insulator. Even for a small density of holes and in the absence of disorder effects the sytems is metallic. Is it antiferromagenetically ordered? If so, is it incommensurate or commensurate? If not, what is the range of antiferromagnetic correlations? There is a strong coupling between hole motion and antiferromagnetic order; as the hole moves through it leaves behind a wake of broken bonds. Thus either the hole does not move singly (a correlated pair motion[7] leaves the spin order undisturbed) or it does and long range AF order is destroyed leaving only antiferromagnetic correlations. These could promote attractive interaction between electrons, the most interesting regime being $\delta(zt) \simeq (zt^2/U)$ where the hole depinning or kinetic energy and the Neel energy are comparable.

MANY BODY THEORY

In the regime of strong correlations, conventional methods fail. We use a formalism developed for spin systems by Vaks, Larkin and Pikin[5] and applied to the Hubbard model by Zaitsev[6]. In standard many body perturbation theory, the amplitude for a complicated process, i.e. the expectation value of a product of fermion operators can be written as a sum of products of all possible pairs (Wick's theorem). This is ultimately based on the anticommutators of two fermions being c numbers. In a system such as that described by Eq.1, operators are defined with respect to specific initial and final states, so that their anticommutators are not c numbers, eg., $[X^i_{\sigma 0}, X^i_{0\sigma'}]_+ = X^i_{\sigma\sigma'} + \delta_{\sigma\sigma'} X^i_{00}$ somewhat like spin operators. However a generalized Wick's theorem is possible, based on the fact that the number of operators on the right side of the above relation is one less that on the left. There are now diagrammatic terms describing on site correlation effects, of relative order (1/z) in an expansion based on intersite hopping (t_{ij}) to z nearest neighbours. Such an inverse range expansion developed by Vaks, Larkin and Pikin[5] fails for spin systems near a critical point. But since in the Hubbard model correlations generally have a finite range the (1/z) expansion is likely to converge.

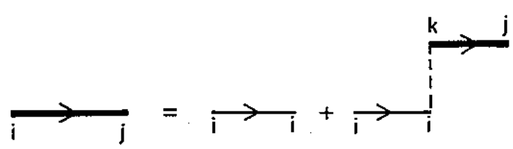

Fig.1. The thick line donotes the true propagator, and the thin line the bare propagator, with hopping (dotted line) as perturbation.

Let us consider, as an example, a calculation of the single particle Green functions G_{ij}. To zero order in δ and 1/z, the self energy, Σ_{ik} is just the hopping matrix element t_{ik}, and the Dyson equation can be represented as in Fig.1. This self energy corresponds to a bare bandwidth of zt. To next order in z^{-1}, but still to order δ^{o}, one has terms which correspond to spin disorder scattering[2,3].

However, there are novel terms to the self energy, to first order in the hole density. These are shown in Figs.2a and 2b. They describe scattering of an electron by spin and charge fluctuations respectively. Spin and charge fluctuate because of hole motion; this is seen in their propagators D, which are shown schematically in Fig.3, which describes them as repeated propagation of electron hole pairs.

We thus find that

$$D_q(z_m) = 2\pi_q(z_m)\ [\ z_m - \pi_q^2(z_m)]^{-1} \tag{2a}$$

with

$$\pi_q(z_m) = t^2 \frac{1}{\beta} \sum_{k,\nu_\ell} G_k\ (\nu_\ell)\ G_{k+q}(\nu_\ell + z_m) \tag{2b}$$

A spectral density analysis of π shows that it is proportional to hole density , as expected physically. Thus $D_q(z_m) \sim (1/\delta)$ for frequencies $|z_m| \lesssim \delta t$, and has a total strength of order unity since, e.g.,

$\langle X^i_{+-}\ X^i_{-+} \rangle = \langle X^i_{++} \rangle \simeq 1/2$. Consequently the single particle self energy $\Sigma_k(\nu_\ell)$ has a part of order unity which varies on an energy scale $\nu \simeq \delta t$;

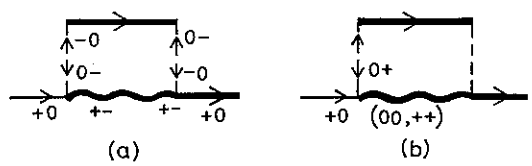

Fig.2. Fluctuation terms in the self energy. The thick wavy line stands for transverse spin (a) and charge (b) fluctuation propagators.

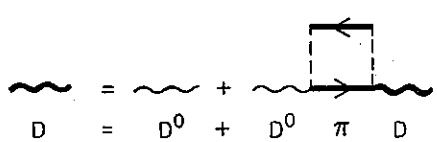

Fig.3. Fluctuation propagator D in terms of bare propagator D^{o} and polarisation π .

$(\partial\Sigma / \partial\nu) \simeq 1/\delta$. This is the cause of heaviness in the fermi system. the spatial scale of $D_q(z_m)$ and hence of $\Sigma_k(\nu)$ is unrenormalised, and thus a z^{-1} expansion for them is convergent.

It is instructive to compare this system where heaviness is due to coupling with diffusive low energy fluctuations, and the electron phonon system. In the latter, the fluctuation scale is $\langle x^2\rangle \simeq (m/M)^{1/2}$ i.e., small, so that $\Sigma \sim (m/M)^{1/2}\epsilon_F$. But since the energy scale over which Σ varies is also of order $(m/M)^{1/2}\epsilon_F$, $(\partial\Sigma / \partial\nu) \sim 1$. In the present case, fluctuation scale is of order unity, so that $\Sigma(\nu) \sim t$, but the energy scale is low (δ t) and thus $(\partial\Sigma / \partial\nu) \sim (1/\delta)$.

Counting the number of hole lines in any diagram enables one to make a hole density expansion, i.e., to schematically write

$\Pi(0,0) = A\,\delta + B\,\delta^2$, where A has a z^{-1} expansion, i.e.,

$A = A_o + A_1 z^{-1} + A_2 z^{-2}$ etc.. From this kind of form it follows that the spin susceptibility $\chi(0,0)$ which is proportional to $\Pi(0,0)^{-1}$ goes as $(A_o\,\delta)^{-1}$ to leading order in hole density i.e.,it is finite and positive. This result of a systematic expansion argues against a ferromagnetic instability of a Nagaoka type. The large value of susceptibility is due not to incipient ferromagnetism but to large renormalization effects of local spin, caused by hole motion. The quasiparticle-quasiparticle interaction due to these local fluctuations seems to be attractive; this is being investigated.

To conclude, the low hole density Hubbard band (correlated f system) is a heavy fermion system with a crossover from a disordered spins, low density of independent holes, and short mean free path regime at high temperatures to mobile holes, a Fermi liquid with well defined quasiparticles, and spin and charge fluctuations at low temperatures $(T \ll T_F^* = \delta t)$.

The Fermi liquid has a low energy scale, not exactly because of a static blockage of sites, i.e., not because $t^{eff}_{ij} \simeq \langle X_{oo}\rangle t_{ij}$ but because excitations scatter off lowlying fluctuations. It is an intrinsically many body system without a good one body narrow band limit. For low hole densities (or in general if there is a low energy scale, e.g., even for large δ if (t/U) is very small) a systematic small parameter expansion of physical properties is possible in powers of δ [or(t/U)] and the inverse range z^{-1} of the intersite hopping [in typical three dimensional systems, $z^{-1} \simeq (1/12)$].

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REFERENCES

1. J. Hubbard, Proc. Roy, Soc. A 285, 542 (1965)
2. W.F. Brinkman and T.M. Rice, Phys. Rev. B 2, 1324 (1970).
3. N. Ohata and R. Kubo, J. Phys. Soc. Japan, 28, 1402 (1970).
4. Y. Nagaoka, Phys. Rev. 147, 392 (1966)
5. V.G. Vaks, A.I. Larkin and S.A. Pikin, Soviet Physics JETP 37, 176 (1967).
6. R. Zaitsev. Soviet Phys JETP 43 576 (1977); Sov. Phys. Solid State 19, 1874 (1978).
7. We thank B. Sutherland for this remark.