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DESTRUCTION OF ANTIFERROMAGNETISM BY VACANCIES FOR THE HUBBARD AND ANDERSON LATTICE MODELS

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Abstract. – We study the itinerant antiferromagnetism of fermions with hard-core repulsion, like in the weak hopping Anderson lattice or the strong U Hubbard Hamiltonian. It is found that the critical temperature T_N decreases very quickly when vacancies are injected. The effect of the dynamic three-sites magnetic interaction is studied.

We study the depression of the Néel temperature for fermions with hard-core repulsion when the electronic density deviates from half-filling. Such strong local repulsions are believed to play an important role both in the heavy fermions compounds and in the high- T_c cuprate materials. The strong- U single band Hubbard model and the weak hopping Anderson lattice model [1] can both be described by an effective hamiltonian involving only one kind of particles with infinite on-site repulsion and nearest-neighbour two and three-sites second-order interactions. We will keep only the magnetic interactions:

$$H_{\text{eff}} = \sum_{ij\sigma} t b_{i\sigma}^+ b_{j\sigma} - \frac{1}{2} \sum_{ij} I S_i \cdot S_j - \sum_{ijl} I' S_{il} \cdot S_j \quad (1)$$

where $b_{i\sigma} = (1 - a_{i-\sigma}^+ a_{i-\sigma}) a_{i\sigma}$, S_i and S_{il} are expressed with the $b_{i\sigma}$ as usual, ij and jl are nearest neighbours sites.

We will estimate the Neel temperature for antiferromagnetism by the difference of energy at zero temperature between the non-magnetic state and the one with a staggered magnetization m . The value of this antiferromagnetic magnetization will be found by minimizing the energy $\langle H_{\text{eff}} \rangle$ with respect to m .

We consider a lattice with no frustration. We approximate the energy coming from the two last terms of (1) by:

$$-\frac{1}{2} \sum_{ij} I \langle S_i^z \rangle \langle S_j^z \rangle - \sum_{ijl} I' \langle S_{il}^z \rangle \langle S_j^z \rangle \quad (2)$$

which is supposed to be the main contribution to the m -dependent part, and where nearest neighbour magnetic correlations are neglected. This approximation which gives the mean-field result in the localized limit is hoped to be valid at least in three dimensions.

We describe the motion of the particles by a method which gives the good variation of the kinetic energy as a function of the staggered magnetization. Some

works are related to this question [2], but we use here a very simple description: The Hubbard's I approximation [3] contains the main point necessary to our purpose which is the reduction of the bandwidth with increasing magnetization. The equation of motion for the Green's function $G_{im\sigma} = \langle \langle b_{i\sigma}, b_{m\sigma}^+ \rangle \rangle$ is in this approximation:

$$\omega G_{im\sigma} = \langle 1 - n_{i-\sigma} \rangle + \langle 1 - n_{i-\sigma} \rangle \sum_l t_{il} G_{lm\sigma}. \quad (3)$$

We impose a given magnetization $m = \sum_{\sigma} \sigma \alpha \langle b_{i\alpha\sigma}^+ b_{i\alpha\sigma} \rangle$ where $\alpha = \pm 1$ is an index for the two sublattices. Note that we have not included the effect of the interactions I and I' in the equation of motion (3) because we just want to calculate $\langle b_{i\sigma}^+ b_{j\sigma} \rangle$ (and $\langle b_{i\sigma}^+ b_{l\sigma} \rangle$) for the kinetic magnetization $\langle S_{il}^z \rangle$ which is governed by the first term of H_{eff} - the hopping amplitude t - which is at least an order of magnitude larger than I and I' . These second order interactions nevertheless come into play indirectly through the imposed magnetization m . The equation (3) is easily solved introducing two propagators (intra- and inter-sublattice):

$$G_{k\sigma}^{\alpha\alpha} = \left(1 - \frac{n}{2} + \sigma \alpha \frac{m}{2} \right) \frac{\omega}{\omega^2 - E_k^2} \quad (4)$$

$$G_{k\sigma}^{-\alpha\alpha} = \left(\left(1 - \frac{n}{2} \right)^2 - \frac{m^2}{4} \right) \frac{\varepsilon_k}{\omega^2 - E_k^2}$$

where n is the number of effective particles per site in the effective Hamiltonian (1), and:

$$E_k = \varepsilon_k \sqrt{\left(1 - \frac{n}{2} \right)^2 - \frac{m^2}{4}}. \quad (5)$$

The reductive factor (5) for the bandwidth is easily understood: The Hubbard's approximation means the effective hopping of a σ -electron to site i is reduced by

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the factor $\langle 1 - n_{i-\sigma} \rangle$ which is alternatively $1 - n/2 - m/2$ and $1 - n/2 + m/2$ when the σ -electron moves through the lattice. So the mean effective hopping must verify:

$$t_{\text{eff}}^2 = \left(1 - \frac{n}{2} - \frac{m}{2}\right) t \left(1 - \frac{n}{2} + \frac{m}{2}\right) t \quad (6)$$

which gives the same reductive factor (5).

The electronic density is easily calculated from (4) where f is the Fermi-Dirac function:

$$\frac{n}{2-n} = \frac{1}{N} \sum_k f(E_k) \quad f(x) = (e^{\beta(x-\mu)} + 1)^{-1}. \quad (7)$$

The kinetic energy (first term of (1)) is easily obtained from the Green's function:

$$K = K_0 \sqrt{1 - \frac{m^2}{(2-n)^2}} \quad (8)$$

where K_0 is the kinetic energy of the non-magnetic state. Similarly, the kinetic magnetization $\langle S_{it}^z \rangle$ is derived, and then the contribution of I' to the energy per site:

$$\frac{I'}{4} m^2 \left[-z \frac{n}{2-n} + \frac{1}{N} \sum_k \left(\frac{\varepsilon_k}{t} \right)^2 f(E_k) \right] \quad (9)$$

where z is the number of nearest neighbour. One can show that the expression (9) changes of sign at $n = 2/3$. A positive I' favors antiferromagnetism for $n > 2/3$ and favors ferromagnetism for $n < 2/3$. This is due to the sign of $\langle b_{i\sigma}^\dagger b_{i\sigma} \rangle$ which depends upon the electronic density. When $\delta \ll 1$, the energy (9) can be written:

$$-\frac{1}{2} z (z-1) \delta I' m^2 \quad (10)$$

and the total energy per site is:

$$E = K_0 \sqrt{1 - \frac{m^2}{(1+\delta)^2}} + \frac{z}{8} (I - 4(z-1)\delta I') m^2. \quad (11)$$

By minimizing E with respect to m , we find the critical value δ_c for the number of vacancies at which antiferromagnetism disappears:

$$\delta_c = -\frac{I/4}{2|t| - (z-1)I'}. \quad (12)$$

We recall that both in the Anderson lattice and in the Hubbard model, I is negative. A negative I' like in the Hubbard model reduces δ_c . But in the validity domain of the perturbation expansion in t which leads to (1), the second order interactions I and I' are far smaller than t , and the effect of I' is very small and can be neglected. The magnetization as a function of δ is:

$$m = \sqrt{1 - 64\delta^2 \frac{t^2}{I^2}} \quad (13)$$

and the difference of energy between the antiferromagnetic and non-magnetic state is:

$$\Delta E = -\frac{8zt^2}{I} \left(\delta + \frac{I}{8|t|} \right)^2. \quad (14)$$

These two quantities are shown in figure 1. The critical temperature T_N is expected to have the same shape as ΔE and one can notice the upward curvature of $\Delta E(\delta)$ and the difference of shape with $m(\delta)$. δ_c is a small value; for example in the Hubbard model where $I = -4t^2/U$:

$$\delta_c \simeq -I/8|t| = |t|/2U. \quad (15)$$

This quick destruction of the antiferromagnetic phase is due to the kinetic energy of the vacancies which is larger in the non-magnetic state than in the magnetic one. Yokoyama and Shiba [4] have obtained with a Gutzwiller variational technique a smaller decrease by a factor of two (a larger δ_c than (15)). The three-sites magnetic interaction which needs a sufficient amount of vacancies, do not play an important role for such electronic densities, this being very different from the work of Inui, Doniach and Gabay [5].

For the Anderson lattice, using the parameters calculated in [1], antiferromagnetism is then found only in the vicinity of $n = 1$, and leaves the superconductivity appear for $n > 1$ [6].

Fig. 1. - Destruction of the antiferromagnetic phase as a function of the number of vacancies $\delta = 1 - n$. The staggered magnetization m goes from 1 to zero.

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