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Disorder induced ferromagnetism

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Abstract. We study the influence of on-site disorder on the magnetic properties of the ground state for restricted geometries. We find that for two dimensional systems disorder enhances the spin polarization of the system . The tendency of disorder to enhance magnetism in the ground state may be relevant to recent experimental observations of spin polarized ground states in quantum dots.

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1 Introduction

The interplay between disorder and interactions[1] and the possibility that it leads to ground state ferromagnetism has been the subject of much interest[2]. In several new experiments in restricted geometries, such as zero temperature transport measurements of the conductance through semiconducting quantum dots[3] and carbon nanotubes[4], tantalizing hints of a weakly ferromagnetic ground state of small systems with a few hundreds of electrons have appeared. The ground state spin polarization may be directly measured by coupling the dot or tube to external leads and measuring the differential conductance. Also from a recent mean field treatment of electron-electron interactions in disordered electronic systems[5] as well as from a numerical study of such systems[6] a partially magnetized ground state seems probable. In this work, we suggest that the presence of disorder might enhance the possibility of magnetic ground state (GS).

The GS spin polarization of small clean clusters is known to be highly fluctuating as a function of the number of electrons, and boundary conditions [7]. We wish to show that in some sense the situation in the disordered case is simpler. Analysis of the competing effects which lead to the complex dependence of the GS spin polarization, shows that as disorder decreases the sensitivity to boundary conditions of the single-particle wave-functions suppress the singlet favoring effect, while the polarization favoring effect does not depend as much on disorder. Therefore, one might expect a transition from a singlet state to a polarized state, as a function of disorder. A numerical study of the $U = \infty$ Hubbard model with a nearly half-filled band supports the existence of such transition.

2 Analytical considerations

In the high-density limit, the GS is obtained by a consecutive filling of the lowest single-particle levels possible. Thus, the GS is a singlet. However, in the low density limit, where the Coulomb energy dominates the kinetic energy, the weight of doubly occupied states is reduced, and the possibility of a magnetic GS arises. We start by considering the simplest case of a hole in a full band. The spin comes to play since the hopping of the hole around the lattice induces permutations in the spin ordering. The hopping term is then effectively reduced by a factor proportional to the overlap of the permuted spin function with the original one, averaged over the different permutations. In order to maximize the hopping term, thus minimizing the kinetic energy, this overlap should be maximal. This is achieved in the fully polarized, symmetric, state. This consideration is not changed by the presence of disorder. An exact manifestation of this argument was given by Nagaoka [8], who showed that the GS of one hole in an otherwise half-filled band of the $U = \infty$ Hubbard model is a fully saturated ferromagnetic state, for any realization of the on-site disordered potential. The situation is more complicated when more than one hole exists. Although the above argument for preferring a ferromagnetic order equally applies for the case of several holes, it is known that Nagaoka's theorem can not be extended even to the case of two holes[9, 10]. In order to understand the reason for this complexity, we first describe the situation in 1D (one dimension).

It was shown [11] that the problem of m interacting electrons on a ring (at $U = \infty$) can be mapped onto a system of m non-interacting spinless fermions on a 1D ring, where the effect of the spin is replaced by a fictitious flux Φ_j, $\Phi_j/\Phi_0 = 2\pi j/m$ ($j = 0, 1 \cdots, m-1$), where the fully polarized state corresponds to the trivial case $\Phi_{j=0} = 0$. The GS energy is obtained by minimization of the GS energies with respect to the possible "flux" values j. It is well known that the flux value which minimizes the GS energy of a spinless particle on a ring is $\Phi = 0$. This is so even is the presence of disorder [11]. Therefore, the 1D one-holes GS is minimized by a trivial spin background. On the other hand, when a (real) flux π is applied to the ring, the GS is obtained by creating a spin background which forms a fictitious flux $-\pi$, which masks the real flux. In terms of this picture, we now suggest an explanation to the 2D behavior. In 2D particles can bypass each other, and change their ordering, in many ways. For each couple of two holes, the hopping of one hole around the other one is equivalent to a hopping of that hole around a flux π, since a phase π accompanies each winding of a fermion around another. Since it may be energetically favorable to screen these fluxes, a non-trivial spin background may be generated. In short, we can say that the spin background in the 2D GS is due to the need to optimally mask the fermionic BC (boundary conditions) between the holes. One should remember, however, that while in the 1D case, the Nagaoka's effect was not relevant, as explained above, in the 2D case there is a competition between these effects. In general, one obtains a complex dependence on the details of small clean clusters [7], due to these competing effects.

Let us now consider the effect of disorder on the tendency towards a complex spin background. As disorder increases, the single particle functions become less sensitive to the boundary conditions, and thus the fermionic BC constraint becomes less important. Therefore, one may expect that the incentive for re-ordering of the spin

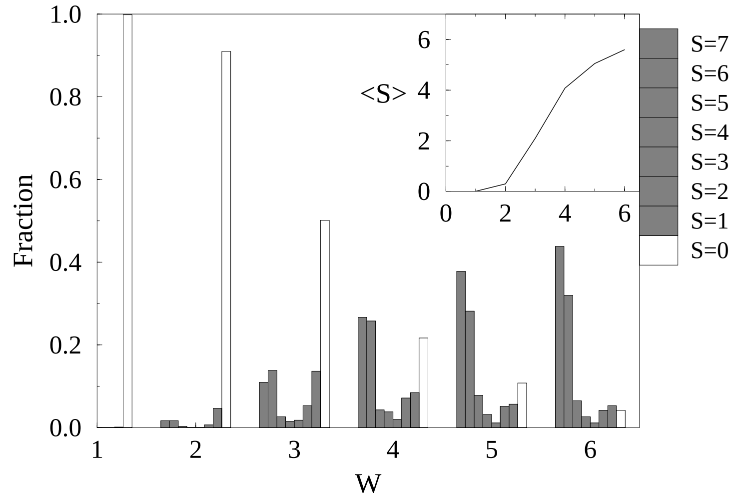

Fig. 1 The spin distributions as a function of disorder W for 600 realizations of a 4×4 lattice with 14 electrons. For each W, the bar chart represents the probability of finding the GS of the system at a particular value of S. The inset presents the average spin $\langle S \rangle$ as a function of W.

background decreases, while, as in the one hole case, there still is a contribution from the hopping amplitude leading to a Nagaoka state.

3 Numerical results

A numerical study of this effect was done in the framework of the $U = \infty$ Hubbard model, a canonical model for the study of itinerant ferromagnetism [12]. The on-site energies were drawn randomly according to a box distribution between $-W/2$ and $W/2$. Note that the infinite U limit has the attractive feature of suppressing antiferromagnetic correlations which are clearly not relevant to quantum dots, even in the clean limit [13]. Exact diagonalization for the full many-particle Hamiltonian was used to test the above arguments. We have used up to 14 electrons on up to 4×4 lattices. In the ordered case, the GS was a singlet, in accordance with [9, 10]. Figure 1 presents the GS-spin distributions as a function of W, for 14 electrons on a hard-wall 4×4 lattice. The average spin $\langle S \rangle$ is also plotted against W, and one can see that it increases significantly with W. In the presence of disorder, one gets a distribution of GS-spin values. For weak disorder, the main effect is smearing the peak at $S = 0$ to low S values. Thus, a tendency towards weak ferromagnetism is clearly demonstrated even for weak disorder ($W = 3t$) which corresponds to a ballistic (mean free path larger than the system size) regime. Moreover, as disorder increases, high S values dominate the distribution. For $W = 6t$ corresponding to a diffusive regime a clear dominance of the high spin state appears. Similar behavior was obtained for smaller lattices and periodic BC. One sees that, in contrast with the situation in the ordered case, our results are not sensitive to the lattice size or the BC. This manifests the chaotic nature of the dot, which suppress dependencies on the details of the system. Exact diagonalization also confirms the tendency towards non-zero ground state spin values even for a higher number of holes. We have studied the spin distribution for 12 electrons on a hard-wall 5×3 lattice (3 holes). The GS-spin is significantly enhanced as function of disorder, although the most probable spin state is not fully ferromagnetic. Similar results were obtained for higher hole ratios. A simple variational treatment shows that the tendency towards ferromagnetism persists for larger systems.

In conclusion, the influence of disorder on the magnetic properties of the GS was studied. For an ordered system, large magnetic moments are generally suppressed, and the spin structure of the GS, if any, is very complicated. On the other hand, we have shown that disorder plays an important role in determining the spin polarization of 2D systems described by the infinite U Hubbard model. Weak disorder tends to create a partially polarized ground state, while stronger disorder tends to stabilize a fully ferromagnetic GS. This behavior clearly indicates that there is a basis to expect that for more realistic descriptions of the experimental systems ($U \neq \infty$) disorder will play an important role in creating a spin polarized ground state.

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