Ground-state spin structure of strongly interacting disordered 1D Hubbard model

1999 J. Phys. A: Math. Gen. 32 3599

(http://iopscience.iop.org/0305-4470/32/19/310)

J. Phys. A: Math. Gen. **32** (1999) 3599–3602. Printed in the UK PII: S0305-4470(99)01615-7

Ground-state spin structure of strongly interacting disordered 1D Hubbard model

E Eisenberg and R Berkovits

The Minerva Centre for the Physics of Mesoscopics, Fractals and Neural Networks, Department of Physics, Bar-Ilan University, Ramat-Gan 52900, Israel

Received 4 February 1999

Abstract. We study the influence of on-site disorder on the magnetic properties of the ground state of the infinite-U one-dimensional (1D) Hubbard model. We find that the ground state is not ferromagnetic. This is analysed in terms of the algebraic structure of the spin dependence of the Hamiltonian. A simple explanation is derived for the $1/N$ periodicity in the persistent current for this model.

The Hubbard model is the simplest model one can study to examine the effects of correlations between electrons in narrow energy bands. The Hamiltonian consists of a nearest neighbour hopping term and an electron–electron repulsion, U, which acts only when two electrons are on the same site. The Hubbard model is also the canonical model for the study of itinerant ferromagnetism. The strong coupling regime is of special importance for the study of ferromagnetism, since a theorem by Nagaoka [1] states that in the $U = \infty$ limit, the ground state (GS) is ferromagnetic given some connectivity property of the lattice (which holds in most cases for $d > 1$). The model is solvable in one dimension and it was shown [2] that for open boundary conditions (BCs) the GS for finite U is a singlet, i.e. there can be no ferromagnetism unless one postulates explicitly spin- or velocity-dependent forces. For infinite U, the GS of all spin sectors are degenerate.

The problem of the interplay between disorder and interactions in systems of electrons is challenging and has a long history [3]. It is of interest to study the influence of disorder on the possibility of forming a ferromagnetic GS. In this work we study the spin structure of the GS of a disordered $U = \infty$ Hubbard model in one dimension. We find that for periodic BCs as well as for open BCs, for any realization of on-site disorder, the GS is degenerate, where all spin sectors have the same lowest energy, except for the fully polarized one which has a higher energy. As a by-product of our proof we find that the GS of an even (odd) number of spinless fermions, on a one-dimensional (1D) ring threaded by flux, is minimal when the dimensionless flux Φ/Φ_0 equals π (0). This might be of interest for the study of persistent currents in disordered interacting 1D rings [4].

Lieb and Mattis [2] have considered the 1D clean Hubbard model for any $U < \infty$ given hard wall (or open) BCs. They found that the GS is always a singlet (for an even number of spins). When $U = \infty$ the GS in all the different spin sectors become degenerate. Here we present an analysis of $U = \infty$ with periodic BCs, in the presence of on-site disorder. As will become clear later, the different BCs change the character of the problem and the periodic BC case gives us an insight into the higher dimensional variants of the problem. Some of the

0305-4470/99/193599+04$19.50

following results, and related ones, were obtained by several different approaches in [5–7]. The Hamiltonian we consider is thus given by

$$H = \sum_{i\sigma} \varepsilon_i n_{i\sigma} - t \sum_{i\sigma} a^\dagger_{i\sigma} a_{(i+1)\sigma} + \mathrm{CC} + U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{1}$$

where $a^\dagger_{i\sigma}$ is the fermionic creation operator on site i with spin σ, $n_{i\uparrow} = a^\dagger_{i\uparrow} a_{i\uparrow}$, and the on-site energies ε_i are drawn uniformly between $-W/2$ and $W/2$.

The Hilbert space is composed of a direct product of the spatial wavefunctions, described by a basis composed of all the different possibilities of positioning N particles on N out of the M different sites. This space is isomorphic to the Hilbert space of N non-interacting spinless fermions on M sites. For finite U, the Hilbert space consists of functions with double occupancy as well and these exists only if the two particles on the same site are in singlet configurations. Thus, coupling between the spatial functions and spin functions is formed. However, in the $U = \infty$ case the spin Hilbert space is decomposed from the spatial Hilbert space and its natural basis is given by 2^N orderings of N spins.

The action of the hopping terms in the Hamiltonian on a wavefunction changes the spatial distribution of the particles, through moving one particle at a time to one of its neighbouring sites. Since double occupancy is restricted, particles cannot interchange their order via hopping. One gets another invariant of the Hamiltonian, namely, the order of the particles, the importance of which will become clear later. This holds in the hard wall BC case. However, the periodic BCs allow particles to 'bypass' through the boundaries and breaks this symmetry. Had the ordering of the spins been conserved, the GS would have been independent on the entire spin structure of the states. Consequently, in the hard wall BC case, all spin configurations GS are degenerate. However, the change in the spin ordering due to hopping through the boundaries, couples the spin part to the spatial part of the wavefunction. Each hopping term in the spatial part of the Hamiltonian is replaced by a matrix (in principle, $2^N \times 2^N$) which characterizes the re-ordering of the spins. Most of these matrices, namely, these which are not related to the boundary terms, are identity matrices. However, some describe the re-ordering due to hopping from site 1 to site N, and *vice versa*, and are not trivial.

Let T be the permutation in spin ordering due to hopping of a particle at site 1, to site N. The minimal subgroup of the permutation group which contains T (and T^{-1}, which corresponds to hopping in the inverse direction) is the cyclic group generated by T. The different spin orderings induce a representation of this cyclic group. Since the cyclic group is commutative, its irreducible representations are 1D. Thus, we will find the decomposition of the induced representation in irreducible parts, and then diagonalize the spatial Hamiltonian for each of the irreducible representations. The GS is the lowest of the eigenvalues obtained for each representation. Our goal is to determine to which S value the irreducible representation corresponds with the lowest eigenvalue.

We note that since $T^N = I$, all the representations must be of the form $\chi_j(T^k) = \exp(2\pi \mathrm{i} jk/N)$. Thus, different representations correspond to assigning a phase $\chi_j(T) = 2\pi j/N$ to the transition through the boundaries. This is equivalent to adding a flux $\Phi = 2\pi j/N$ through the ring to the N spinless fermions problem. We now prove the following

Theorem 1. *Let $\epsilon(\Phi)$ be the GS of N non-interacting spinless particles on a (disordered) ring, as a function of the flux Φ. $\epsilon(\Phi)$ has a minimum at $\Phi = \pi$ for even numbers of particles (and at $\Phi = 0$ for odd N).*

Proof. The energy as a function of the flux $\epsilon(\Phi)$, is symmetric in the parameter Φ with respect to the points $\Phi = 0, \pi$. Therefore, the first derivative $\epsilon'(\Phi)$ vanishes in these points. We now calculate the second derivative at these points in order to find which is the maximum and which is the minimum. Expansion of $\epsilon(\Phi)$ in the vicinity of $\Phi = \pi$ is given by perturbation theory. The flux dependence of the matrix elements is always through the expression $e^{i\Phi}$, and therefore, one obtains

$$\epsilon(\Phi) - \epsilon(\pi) = \sum_n a_n (1 - e^{i(\Phi-\pi)})^n. \tag{2}$$

The curvature, i.e. the second derivative at $\Phi = \pi$ is thus given by

$$\left.\frac{\partial^2 \epsilon}{\partial \Phi^2}\right|_{\Phi=\pi} = a_1 - 2a_2. \tag{3}$$

At the point $\Phi = \pi$, all the off-diagonal elements in the Hamiltonian are negative, since the -1 factor of the flux which multiplies the boundary hopping matrix elements cancels with the $(-1)^{N-1}$ factor from the interchange of the fermionic operators. Thus, the GS eigenvector v_0 has no nodes, i.e. all its elements are of the same sign. Now, let us write explicitly a_1 and a_2

$$a_1 = \langle v_0 | \Delta H | v_0 \rangle = \sum_{[ij]} g_i g_j > 0 \tag{4}$$

$$a_2 = \sum \frac{|\langle v_n | \Delta H | v_0 \rangle|^2}{E_0 - E_n} < 0. \tag{5}$$

The sum over $[ij]$ is restricted to states i and j which are coupled by boundary hopping terms.

It then follows that the curvature at $\Phi = \pi$ is positive and, therefore, it is a local minimum point. Unless there is an additional accidental point of the vanishing derivative, this is also the global minimum. Similar arguments apply to the point $\Phi = 0$ for odd N. □

Note that this theorem holds for off-diagonal disorder as well, as long as all the hopping integrals are of the same sign.

One concludes that for even-N, the irreducible representation which yields the GS is $\chi_{N/2}$ and $\chi_{N/2}(T) = \chi_{N/2}(T^{-1}) = -1$. We now have to find out for which S values the induced representation includes $\chi_{N/2}$ in its decomposition. There is only one state with $S = S_z = S_{\max}$, and thus the induced representation is 1D and irreducible. It is easy to see that it is χ_0 (which corresponds to the maximum energy). It will now be shown that the representation induced by $S = 0$ always include $\chi_{N/2}$.

Since the explicit construction of states with definite S and S_z is non-trivial, let us look at the representations induced by the sets of states with definite S_z only. The irreducible representations induced by $S_z = M$, which are not induced by $S_z = M + 1$ correspond to $S = M$. According to character theory, the number of times an irreducible representation with character χ exists in the decomposition of a representation ϕ is given by $(1/K)\sum_k \phi(k)\chi^*(k)$, where the index k runs through all the group elements, and K is the group order. The character of a representation is just the trace of the representing matrices. The character of the representation induced by a set of states is given by the sum over k of the number of states in the relevant set which are invariant under the kth element of the group. Accordingly, one obtains that the number of occurrences of $\chi_{N/2}$ in the representation induced by $S = 1$ is given by

$$k_1 = \begin{cases} \dfrac{(N-1)!}{(N/2+1)!(N/2-1)!} & N/2 \text{ even} \\ \dfrac{(N-1)!}{(N/2+1)!(N/2-1)!} - \dfrac{(N/2)!}{N((N+2)/2)!((N-2)/2)!} & N/2 \text{ odd} \end{cases} \tag{6}$$

and the number of occurrences in the representation induced by $S = 0$ is bounded by

$$k_0 \leqslant \frac{(N-1)!}{(N/2)!(N/2)!}. \tag{7}$$

It then follows that $k_0 > k_1$, i.e. there exists at least one occurrence of $\chi_{N/2}$ induced by $S = 0$ states. Therefore, the GS is obtained in the $S = 0$ sector.

We have shown that for each (even) N, the GS is obtained at the $S = 0$ sector, while the lowest energy in the $S_{\max}$ sector is higher.

This solution is based on the fact that the permutations induced by the 1D boundary hopping terms spans only the cyclic group, which is commutative. The representation induced by the spin states is highly reducible with respect to this subgroup. In higher dimensions, reordering of spins is not only generated by boundary terms, and the whole (non-commutative) permutation group is needed to characterize the spin dependence. It can be shown that the representation induced is irreducible with respect to the full non-commutative group. Thus, the spin dependence of the Hamiltonian is not equivalent to a trivial flux-like correction.

It is now very easy to consider the effect of magnetic flux added to the Hamiltonian. As we have seen, for an even number of electrons, the optimal total flux (physical flux + flux added by spin configuration) is (in dimensionless units) π. This indeed is the fictitious flux generated by the spins in the GS of the Hamiltonian without an external flux. Now, when we turn on the magnetic flux, the GS energy will increase. It is, therefore, favourable for the system to produce an inverse fictitious flux to cancel out the influence of the magnetic flux. However, as we have seen, this fictitious flux comes in quanta of $2\pi\Phi_0/N$, where N is the number of particles. Thus, magnetic flux of integer multiples of $2\pi\Phi_0/N$ can be completely cancelled out by the spin ordering, such that the GS energy is exactly as it were in the absence of flux. Therefore, as one increases the magnetic flux, the GS energy rises, up to the point $\Phi = \pi\Phi_0/N$, where it is favourable for the system to produce a negative fictitious flux such that the total flux is (in absolute value) less than the magnetic flux. We thus have a simple and transparent explanation for the flux dependence of the GS energy which is periodic with period $2\pi/N$ instead of the usual 2π period [8].

In conclusion, we have shown in this work that the GS of spin $1/2$ fermions on a 1D ring is not polarized in the $U = \infty$ limit, for any realization of disorder. This is accounted for by mapping the spin background of the 1D problem onto a fictitious flux. In two dimensions the influence of the spin background is non-commutative and therefore much more complex. This leads to ferromagnetic GS for one hole [1] and to disorder-induced ferromagnetism for higher hole concentration [9]. It was also shown that the energy of spinless fermions is minimized when the applied magnetic flux is half the flux period, again, for any realization of disorder. This fact is relevant for persistent current calculations.

References

[1] Nagaoka Y 1966 *Phys. Rev.* **147** 392
[2] Lieb E H and Mattis D C 1962 *Phys. Rev.* **125** 164
[3] See, for example, Altshuler B L and Aronov A G 1985 *Electron–Electron Interactions in Disordered Systems* ed A J Efros and M Pollak (Amsterdam: North-Holland) pp 1–153
Fukuyama H 1985 *Electron–Electron Interactions in Disordered Systems* ed A J Efros and M Pollak (Amsterdam: North-Holland) pp 153–230
[4] Gogolin A O and Prokof'ev N V 1994 *Phys. Rev.* B **50** 4921
Giamarchi T and Shastry B S 1995 *Phys. Rev.* B **51** 10 915
Kamal M, Musslimani Z H and Auerbach A 1995 *J. Physique* **5** 1487
[5] Herring C 1975 *Phys. Rev.* **11** 2056
[6] Aizenman M and Lieb E H 1990 *Phys. Rev. Lett.* **65** 1470
[7] Mielke A 1991 *J. Stat. Phys.* **62** 509
[8] Kusmartsev F V 1991 *J. Phys.: Condens. Matter* **3** 3199
Yu N and Fowler M 1992 *Phys. Rev.* B **45** 11 795
Häusler W 1996 *Physica* B **222** 43
[9] Eisenberg E and Berkovits R *Preprint* cond-mat/9812264