Ground-State Magnetization in Disordered Systems:
Exchange vs. Off-Diagonal Interaction Fluctuations

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Abstract

In a Hartree-Fock picture, itinerant ferromagnetism results from a competition between kinetic and exchange energy, with the magnetized state being favored at large interaction strength. In a recent paper we showed that in contrast to this average effect, fluctuations of off-diagonal interaction matrix elements systematically reduce the ground-state magnetization. When the interaction dominates, the occurrence of a non-zero ground-state magnetization depends on the ratio $\lambda$ between average exchange energy and the fluctuation amplitude of the off-diagonal matrix elements, and a nonzero critical value $\lambda_c$ is necessary to magnetize the ground-state. We extend these results by numerical studies of $\lambda$ for standard tight-binding models which indicate a regime of intermediate disorder where off-diagonal fluctuations should play an important role for ground-state magnetization. We also emphasize the presence of strong correlations between minimal eigenvalues of different magnetization blocks which further reduce the probability of a nonzero ground-state spin.

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Itinerant ferromagnetism results from the interplay between the Pauli principle and the electronic interactions. The exchange energy can be minimized when the fermionic antisymmetry is supported by the spatial wavefunction and when the resulting energy gain exceeds the corresponding loss in kinetic energy; this implies spin alignment and a nonzero ground-state magnetization. Because of the locality of the Pauli principle, ferromagnetism is often studied in the framework of the Hubbard model for which a simple Hartree-Fock picture predicts ferromagnetism to occur when the Stoner criterion \[ U_c \rho(\epsilon_F) = 1, \]\[ \rho(\epsilon_F) \] is the one-particle density of states at the Fermi energy. Within perturbation theory, the effective interaction strength is enhanced by the presence of disorder \[ \] and this had led to recent predictions of the occurrence of a ferromagnetic instability already below the Stoner threshold \[ \]. However as we recently pointed out, there is a competing effect of the interaction manifested through the fluctuations of off-diagonal interaction matrix elements which suppresses magnetization \[ \]. Indeed as is known from studies of models in nuclear physics, strong off-diagonal fluctuations can determine the variance of the Many-Body Density of States (MBDOS) \[ \]. When one includes the spin degree of freedom within such models, the Hamiltonian splits into blocks of different total magnetization \( \sigma_z \) and one finds that these fluctuations result in a broader MBDOS for the block with smallest magnetization, increasing thereby the probability of finding a non magnetized ground-state; therefore the average exchange effect must compete not just with the kinetic energy but with off-diagonal fluctuations.

To shortly summarize the results presented in \[ \], we start from a Hamiltonian for \( n \) spin-1/2 particles distributed over \( m/2 \) one-particle orbitals \( \epsilon_\alpha \in [-m/2; m/2] \) (the mean level spacing is then fixed as \( \Delta \equiv 1 \) with spin degeneracy)

\[
H = H_0 + H_U + H_S = \sum \epsilon_\alpha c_\alpha^\dagger c_\alpha + \sum U_{\alpha,\beta}^\gamma c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta + \lambda U \sum |s_\alpha s_\beta| \quad (1)
\]

This Hamiltonian is a generic model of interacting fermions expressed in the basis of Slater determinants constructed from the eigenstates \( \psi_\alpha \) of the corresponding free fermions model \( H_0 \). The interaction matrix elements are given by \( U_{\alpha,\beta}^\gamma = \int d\vec{r} d\vec{r'} U(\vec{r} - \vec{r'}) \)
\( \vec{r} \psi_\alpha^*(\vec{r}) \psi_\beta^*(\vec{r}') \psi_\gamma(\vec{r}') \psi_\delta(\vec{r}) \), where \( U(\vec{r} - \vec{r}') \) is the interaction potential. Disorder results in a random character of the \( \psi_\alpha \)’s, leading to fluctuations in \( U_{\alpha,\beta}^{\gamma,\delta} \) around their average value. Only diagonal matrix elements have a nonzero average leading to mean-field charge-charge and spin-spin diagonal interactions. We neglect in (1) the mean-field charge-charge contribution since it has no influence on the magnetization and assume gaussian-distributed \( U_{\alpha,\beta}^{\gamma,\delta} \): 

\[
P(U_{\alpha,\beta}^{\gamma,\delta}) \propto e^{-(U_{\alpha,\beta}^{\gamma,\delta})^2/2U^2}.
\]

\( s_\alpha \equiv \sum_{s,t} c_{\alpha,s}^\dagger \sigma_{s,t} c_{\alpha,t} \) are spin operators and the parameter \( \lambda > 0 \) is given by 

\[
\lambda \equiv \langle U_{\alpha,\beta}^{\beta,\alpha} \rangle / (2 \text{RMS} \left[ U_{\alpha,\beta}^{\gamma,\delta} \right]),
\]

i.e. it is half the ratio of the average exchange interaction to the root mean square value of the off-diagonal matrix elements. Finally, the interaction commutes with the total magnetization so that the second sum on the right-hand side of (1) is restricted to spin indices satisfying \( s + s' = t + t' \). The Hamiltonian acquires a block structure where blocks are labelled by their total magnetization. Each block’s size is given in term of binomial coefficients as \( N(\sigma_z) = \binom{m/2}{n/2-\sigma_z} \binom{m/2}{n/2+\sigma_z} \). Most importantly, the two-body interaction we consider connects only Slater determinants which differ by at most two one-particle indices and each magnetization block’s connectivity (the number of nonzero matrix elements per row) \( K(\sigma_z) \) is a monotonously decreasing function of \( \sigma_z \).

Similarly as in [5] we estimate the variance of each magnetization block’s MBDOS as

\[
\frac{1}{N(\sigma_z)} \sum_{I,J} H_{I,J}^2 \delta(\sigma_I - \sigma_Z) \approx K(\sigma_z)U^2
\]

where \( H_{I,J} = \langle I | H | J \rangle \) and \( |I\rangle \) is a Slater determinant. Hence each block’s bandwidth goes as \( \sqrt{K(\sigma_z)U} \). Moreover, earlier work tells us that in such models as (1), the MBDOS is approximately gaussian with vanishing corrections in the dilute limit \( 1 \ll n \ll m \) [5]. We can therefore conclude that the full MBDOS is a sum of approximately gaussian contributions from each spin block with a variance proportional to the corresponding connectivity. The latter is a monotonously decreasing function of \( \sigma_z \), hence the broadest MBDOS corresponds to the minimally magnetized block and the ground state will be found in this block with increased probability. For approximately gaussian distributions one may assume that the tail of each block’s MBDOS scales with its variance (up to a numerical factor \( \beta \)). Neglecting contributions from \( H_0 \), the typical spin gap can be estimated (for \( \lambda = 0 \) as
\[ \Delta_s^U \approx \beta U \left[ \sqrt{K(|\sigma_{\min}|)} - \sqrt{K(|\sigma_{\min}| + 1)} \right] \]  

(3)

Switching on the mean-field spin-spin interaction \( H_S \) induces shifts of the block’s MBDOS by energies of at most \(-\lambda U \sigma_z^2\) and the spin gap becomes on average

\[ \langle \Delta_s \rangle = \Delta_s^U - \tilde{\lambda} U \]  

(4)

Results presented in [1] indicate only a very weak \( m \)-dependence of \( \Delta_s^U \). It has however a strong even-odd dependence : \( \Delta_s^U \approx 4U \ (8U) \) for even (odd) number \( n \) of electrons. This effect is nevertheless compensated by a twice larger antiferromagnetic shift between the two lowest magnetized blocks for odd \( n \) (\( \sigma_z = 1/2 \) and 3/2) than for even \( n \) (\( \sigma_z = 0 \) and 1). Hence we introduced \( \tilde{\lambda} = (3 - (-1)^n)\lambda/2 \) in (4) which results in a parity independent behavior of \( \lambda \). Numerically we found a critical value of \( \lambda_c \approx 2 \) to have a non-negligible probability of magnetizing the ground-state. A larger value \( \approx 4 \) is then necessary to have \( \langle \Delta_s \rangle = 0 \) resulting in a 50\% probability of nonvanishing magnetization.

These points have been studied in details in [1]. Here we first address the fact that equation (4) gives the average value of the spin gap, based on the assumption that the lowest levels \( E_0 \) and \( E_1 \) in the two blocks with lowest magnetization (they define the spin gap \( \Delta_s \equiv E_1 - E_0 \)) have uncorrelated distributions. To check this we study the following cross-correlation function

\[ R(E_0, E_1) = \frac{\langle (E_0 - \langle E_0 \rangle)(E_1 - \langle E_1 \rangle) \rangle}{\sqrt{\langle (E_0 - \langle E_0 \rangle)^2 \rangle \langle (E_1 - \langle E_1 \rangle)^2 \rangle}} \]  

(5)

It is easily seen that if \( E_0 \) and \( E_1 \) fluctuate independently around their disorder averages \( \langle E_0 \rangle \) and \( \langle E_1 \rangle \), \( R(E_0, E_1) \rightarrow 0 \) whereas strong correlations between \( E_0 - \langle E_0 \rangle \) and \( E_1 - \langle E_1 \rangle \) - i.e. if a large (small) value of one of them corresponds to a large (small) value of the other - implies \( R(E_0, E_1) \approx 1 \). Fig.1 shows the \( U \)-dependence of \( R(E_0, E_1) \) for the Hamiltonian (1) and \( n=4, 5 \) and 6 electrons on \( m = 10 \) orbitals (the function is independent on \( \lambda \)). The numerical data show indeed strong correlations between extremal levels of the two lowest magnetized blocks. Even though \( R(E_0, E_1) \) is somehow reduced by \( H_U \), correlations still remain quite
strong $R(E_0, E_1) > 0.8$ up to very large $U = 10$. This is understandable if we remember that all blocks, having $K(\sigma_2)N(\sigma_2)$ nonzero matrix elements, are constructed out of the same set of only $(m(m-1)/2)^2$ different two-body interaction matrix elements. Extremal eigenvalues in the distribution are then due to special realizations of the latter inside the blocks. These realizations are presumably not very different in blocks with consecutive magnetization which results in strong eigenvalues correlations. The existence of these strong correlations is confirmed by the gap distribution $P(\Delta_U^s)$ for $H_U$ plotted on Fig. 2. Indeed the probability to find a zero or negative gap is vanishingly small ($\int_{-\infty}^{0} P(\Delta_U^s) d(\Delta_U^s) = 0$ for $n = 5$ and $< 0.002$ for $n = 4$ and 6), whereas even at large average gap, it would not vanish in the case of two independent distributions for $E_0$ and $E_1$. Fig. 2 indicates an effective repulsion between extremal eigenvalues of different random matrices, built however from the same (small) set of matrix elements. This repulsion results in a further decrease of the probability for a magnetized ground-state. Note that the even-odd dependence of the average of these distributions is removed due to the horizontal scaling $\Delta_U^s / \langle \Delta_U^s \rangle$.

We now turn our attention to the microscopic computation of the magnetization parameter $\lambda$ for realistic solid-state models. Specifically, we concentrate on the two-dimensional Anderson lattice

$$H = V \sum_{\langle i,j \rangle} c_{i,s}^\dagger c_{j,s} + \sum_i W_i c_{i,s}^\dagger c_{i,s} \quad (6)$$

where $\langle i; j \rangle$ restricts the sum to nearest neighbors, $W_i \in [-W/2; W/2]$ and $W$ is the disorder strength. Also we consider different interaction potentials of the form

$$U(\vec{r} - \vec{r'}) = U_0 \delta(\vec{r} - \vec{r'}) + U_1 / |\vec{r} - \vec{r'}| \quad (7)$$

Fig. 3 shows the disorder dependence of $\lambda$, for the Hubbard interaction case $U_1 = 0$ and different linear system size $L=10, 20, 50$ and 80. The data have been obtained from averages over 30 wavefunctions in the middle of the band $E = 0$ and for $10 \ (L = 80)$ to $200 \ (L = 10)$ disorder realizations. Clearly, three regimes are distinguishable. (I) At low disorder, the one-electron dynamics undergoes a crossover from ballistic to diffusive regime as the linear
system size is increased beyond the elastic mean-free path $l_e \sim 50(V/W)^2$. In the ballistic regime $l_e \gg L$, wavefunctions are plane-waves. In this case, a Hubbard interaction gives $\lambda \sim L^2$, since the RMS $\left[U^{\gamma,\delta}_{\alpha,\beta}\right] \sim L^{-4}$ and $\langle U^{\beta,\alpha}_{\alpha,\beta}\rangle \sim L^{-2}$, whereas once the diffusive regime is reached, one expects $\lambda \sim \Delta/(\Delta/g) \sim g$ ($g$ is the conductance) [3,7]. (II) In the regime of intermediate disorder, both off-diagonal fluctuations and exchange are increased by disorder, and apparently they compensate each other, resulting in a $L$-independent $\lambda \approx 4$, i.e. close to the critical value to have a vanishing average gap [4]. Therefore we can expect that in this regime, and even for very strong interaction, the probability for finite ground-state magnetization does not exceed 50%. Note that for $W/V = 5$, the localization length is slightly below the largest system size considered and one can expect finite-size effects to play only a minor role. (III) In the regime of strong disorder, one-particle wavefunctions are strongly localized on fewer and fewer sites, so that many of the interaction matrix elements are much smaller than $U$, the off-diagonal fluctuations are sharply reduced and again exchange dominates. Note that eventually, the latter disappears also, but at a lower rate than the fluctuations.

We finally evaluate the influence of the interaction range by considering $U_1 \neq 0$. The average exchange interaction term is explicitly given by

$$\langle \int d\vec{r} d\vec{r}' U(\vec{r} - \vec{r}') \psi^*_\alpha(\vec{r}) \psi^*_\beta(\vec{r}') \psi_\beta(\vec{r}) \psi_\alpha(\vec{r}') \rangle_{\alpha,\beta}$$

(8)

$\langle...\rangle_{\alpha,\beta}$ is an average taken over one-particle wavefunctions close to the Fermi level. Due to their orthogonality, taking this average over the full set of wavefunctions gives a $\delta$-function so that only the on-site term contributes. This last procedure is exact if the one-body dynamics is described by Random Matrix Theory (RMT) for which the structure of the eigenstates is homogeneous all through the spectrum. In this case - which is relevant for irregular quantum dots with chaotic scattering at the boundary [6] - only the on-site part of the interaction contributes to the exchange, whereas it is expectable that increasing the strength $U_1$ of the long-range terms leads to stronger off-diagonal fluctuations, and a reduction of $\lambda$. For the Anderson model however, one-particle wave-functions are different from RMT so that
the average over wavefunctions close to the Fermi level leads only to a more or less sharply
peaked function of $\langle \vec{r} - \vec{r}' \rangle$: there are also contributions to the exchange from the long-range
terms, but still we expect that the average damps them with respect to their contribution
to off-diagonal fluctuations (This damping of course depends on the disorder strength.) so
that $\lambda$ should decrease with increasing interaction range. The validity of this reasoning is
illustrated on Fig. 4 where we plot the evolution of $\lambda$ for different disorders as the long-range
part of the interaction becomes more and more important. Clearly, $\lambda$ is increased by the
screening of the electron-electron interaction, and therefore the Hubbard results presented
on Fig. 3 give an upper boundary for $\lambda$. One thus expects the demagnetizing effect described
here and in [1] to be more efficient at low filling when the screening length exceeds the elastic
mean free path.

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FIG. 1. Cross-correlation function (5) between the lowest energy levels in the two blocks with lowest magnetization for 1000 realisations of the Hamiltonian (1) with $n=4$ (circles), 5 (squares) and 6 (diamonds) particles on $m=10$ orbitals.
FIG. 2. Distribution of the spin gap $\Delta_s^U$ for $n=4$ (full circles), 5 (empty squares) and 6 (diamonds) particles on $m=10$ orbitals. The distributions have been constructed from 20000 realisations of the Hamiltonian $H_U$. 
FIG. 3. Magnetization parameter $\lambda$ vs. disorder strength $W/V$, for a Hubbard interaction and a two-dimensional $10 \times 10$ (full circles), $20 \times 20$ (empty squares), $50 \times 50$ (full diamonds) and $80 \times 80$ (empty triangles) Anderson lattice. One clearly differentiates three regimes: (I) At small disorder, $\lambda$ increases due to a crossover from ballistic to diffusive behaviour (see text). (II) At intermediate disorder, exchange and fluctuations compensate each other so that $\lambda$ is size-independent. (III) At large disorder one-body states are strongly localized over very few sites, which kills the off-diagonal fluctuations faster than the exchange and the latter dominates again.
FIG. 4. Effect of the interaction range on the magnetization parameter $\lambda$ for a two-dimensional $15 \times 15$ Anderson lattice and ratio $U_0/U_1 = 1$ (full circles), 4 (empty squares), 9 (full diamonds) and $\infty$ (Hubbard interaction - empty triangles). As expected, an increase in the interaction range leads to a stronger increase of the fluctuations than of the exchange, resulting in a lowering of $\lambda$. 