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Mesoscopic magnetization fluctuations for metallic grains close to the Stoner instability

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This paper is devoted to the magnetic properties of isolated mesoscopic grains. We demonstrate that under very general conditions the electron-electron interactions in such grains can be taken into account by a simple interaction Hamiltonian. This Hamiltonian involves only three coupling constants, which correspond to charging, exchange interaction, and superconducting correlations. The most important condition for such a description is that Thouless conductance of each grain is large. Under this condition sample-to-sample fluctuations of the coupling constants can be neglected. However, the thermodynamic properties can still remain sample specific due to the one-electron part of the Hamiltonian. If the grain is made from a material that is close to the threshold of ferromagnetic instability, the mesoscopic fluctuations of the magnetization are especially strong. Moreover, the situation becomes multistable: free energy of each grain as a function of the magnetization is characterized by a large number of local minima. We analyze the statistics of these minima and show that it possesses simple scaling properties. Numerical simulations confirm this scaling.

I. INTRODUCTION

The simplest model of ferromagnetism in metallic systems was proposed by Stoner.[1] The magnetic ordering in this model takes place when the increase in the orbital energy due to the promotion of electrons to higher-energy states is smaller than the energy gain due to the exchange interaction. As soon as this happens, the system becomes unstable with respect to the transition to a state with a nonzero total spin S and, hence, broken $\mathcal{T}$ invariance. In a bulk system only macroscopically large S matters. Therefore, the onset of the instability is well determined—both the exchange and the orbital energies are self-averaging quantities.

This might not be the case for a small (mesoscopic) metallic grain since both orbital and exchange energies are sample specific. Therefore, one should expect strong mesoscopic fluctuations of the magnetization of the grain made from a material that is close to the Stoner instability. This paper is an attempt to develop a theoretical description of these mesoscopic fluctuations.

Consider a mesoscopic grain with an even number of electrons at zero temperature, $T=0$. Restricting ourselves to the Hartree-Fock approximation, we can speak about orbital states with energies $\mathcal{E}_\alpha$. For a weak exchange interaction all of the orbitals below the Fermi level E_F are double occupied (2-orbitals), while those with $\mathcal{E}_\alpha > E_F$ are empty (0-orbitals). This state is a singlet, $S=0$. Let $\alpha=0,1$ label correspondingly the highest 2-orbital and the lowest 0-orbital in the singlet ground state, see Fig. 1.

For the stronger exchange a state with $S_{tot}\neq 0$ can become a ground state. Indeed, let us compare the lowest energies $E_0(S)$ of the singlet $(S=0)$ and triplet $(S=1)$ states (see Fig. 1). The lowest triplet state has two single-occupied orbitals: $\alpha=0,1$ (1-orbitals), while $\alpha>1$ and $\alpha<0$ label 0-orbitals and 2-orbitals, respectively. For the ferromagnetic sign of the spin exchange the two electrons on the 1-orbitals have parallel spins. Assuming SU(2) symmetry in the spin space of the system, we can write the exchange energy of two electrons, which occupy the orbital states α and β, in the usual Heisenberg form

$$\epsilon^H_{\alpha\beta} = -2J_{\alpha\beta}\hat{\mathbf{s}}_1\hat{\mathbf{s}}_2, \tag{1.1}$$

where $\hat{\mathbf{s}}_{1,2}$ are the spin operators. From this point on, the superscript H indicates the quantities belonging to the systems with the Heisenberg form of the exchange interaction, Eq. (1.1). We can write the following expression for the energy difference between the lowest energy states with $S=0$ and $S=1$:

$$E^H_0(1) - E^H_0(0) = \mathcal{E}_1 - \mathcal{E}_0 - \frac{1}{2}J_{01} - \frac{3}{2}J_{00}. \tag{1.2}$$

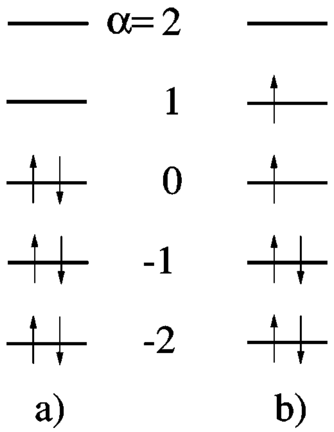

FIG. 1. Spin configuration for (a) the lowest energy $S=0$ state. $\alpha=0, -1, -2, \ldots,$ correspond to 2-orbitals. $\alpha=1,2,\ldots,$ correspond to 0-orbitals; (b) the lowest energy $S=1$ state. $\alpha=-1, -2, \ldots,$ correspond to 2-orbitals, $\alpha=0$, 1 correspond to 1-orbitals, and $\alpha=2, 3, \ldots,$ correspond to 0-orbitals.

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[In derivation of Eq. (1.2) we used the fact that $2\hat{\mathbf{s}}_1\hat{\mathbf{s}}_2=S(S+1)-3/2$, when we add spins of two-spin-1/2 particles.] Therefore, the triplet state becomes energetically more favorable than the singlet one, $E_0(1)<E_0(0)$, provided that $J_{01}+3J_{00}>2(\mathcal{E}_1-\mathcal{E}_0)$.

This is a sufficient rather than a necessary condition for S to be nonzero in the ground state. Even for $E_0(1)>E_0(0)$, the spin S of the ground state is not necessarily zero. For the lowest energy among the states with a total spin S we have

$$E_0^H(S)-E_0^H(0)=\sum_{\alpha=1}^{S}\left(\mathcal{E}_\alpha-\mathcal{E}_{1-\alpha}-\frac{3}{2}J_{1-\alpha,1-\alpha}\right)-\sum_{1-S\leqslant\alpha<\beta\leqslant S}\frac{1}{2}J_{\alpha\beta}. \tag{1.3}$$

Here $\alpha<1-S$ labels 2-orbitals, $1-S\leqslant\alpha\leqslant S$ labels 1-orbitals, and 0-orbitals have labels $\alpha>S$.

One can also consider the situation with strong spin anisotropy. Let it be the easy axes (Ising) anisotropy, so that the state of an electron is characterized by the z component s_z of its spin ($s_z=\pm 1/2$), and the exchange energy equals

$$\epsilon_{\alpha\beta}^I=-2J_{\alpha\beta}s_{z(1)}s_{z(2)}. \tag{1.4}$$

From this point on the superscript I indicates the quantities belonging to the systems with the Ising form of the exchange interaction [Eq. (1.4)]. The energy difference between states with zero and finite total spin in this Ising case is

$$E_0^I(S)-E_0^I(0)=\sum_{\alpha=1}^{S}\left(\mathcal{E}_\alpha-\mathcal{E}_{1-\alpha}-\frac{1}{2}J_{1-\alpha,1-\alpha}\right)-\sum_{1-S\leqslant\alpha,\beta\leqslant S}\frac{1}{2}J_{\alpha\beta}. \tag{1.5}$$

In a general case the orbital energies $\mathcal{E}_\alpha$ and the exchange energies $J_{\alpha\beta}$ are random. In the limit $S\to\infty$ summation in Eqs. (1.3) and (1.5) leads to the self-averaging. Calling $\delta_1=\langle\mathcal{E}_{\alpha+1}-\mathcal{E}_\alpha\rangle$ mean-level spacing and $J=\langle J_{\alpha\beta}\rangle$ mean-exchange coupling constant (here $\langle\cdots\rangle$ stands for the ensemble averaging), we obtain from Eqs. (1.3) and (1.5)

$$E_0^H(S)-E_0^H(0)=S^2\delta_1-\frac{1}{2}\left[3S+\frac{2S(2S-1)}{2}\right]J=S^2\delta_1-JS(S+1), \tag{1.6a}$$

$$E_0^I(S)-E_0^I(0)=S^2\delta_1-\frac{1}{2}\left[S+\frac{2S(2S-1)}{2}\right]J=S^2\delta_1-JS^2, \tag{1.6b}$$

where S is an integer.

Note that for a grain with an odd number of electrons Eqs. (1.6a) and (1.6b) are slightly modified. The lowest possible spin is now $S=1/2$ and the energy of a state with a spin S is given by

$$E_0^H(S)-E_0^H\left(\frac{1}{2}\right)=S^2\delta_1-JS(S+1)-\frac{1}{4}\delta_1+\frac{3}{4}J, \tag{1.7a}$$

$$E_0^I(S)-E_0^I\left(\frac{1}{2}\right)=S^2\delta_1-JS^2-\frac{1}{4}\delta_1+\frac{1}{4}J, \tag{1.7b}$$

where S is a half integer. One can see that for both Heisenberg and Ising exchange interactions, the system is unstable at

$$\delta_1<J. \tag{1.8}$$

Indeed, under this condition, $E(S)$ in Eq. (1.6b) tends to $-\infty$ as $S\to\infty$. Equation (1.8) is nothing but the familiar Stoner criterion of this instability. As soon as the parameters of the system surpass the instability threshold, the ground state acquires magnetization proportional to the volume of the system.

The situation in finite systems is somewhat different. We start our discussion with a simple but instructive example of a grain with an even number of electrons without any disorder, i.e., $\mathcal{E}_{\alpha+1}-\mathcal{E}_\alpha=\delta_1$ and $J_{\alpha\beta}=J$. It turns out that for the Heisenberg case the spin of the ground state S_g is finite already at

$$\delta_1<2J, \tag{1.9}$$

as can be directly seen from Eq. (1.2). Therefore, S can be greater than zero even for the exchange, which is below the critical value given by the Stoner criterion (1.8) ($\delta_1/2=J_0<J<J_c=\delta_1$). In this parameter domain $S_g=J/(2\delta_1-2J)$. Because δ_1 and J are inversely proportional to the volume of the system, the spin of the ground state S_g does not scale with the volume. Equation (1.7a) implies that for an odd number of electrons the system spin $S_g>1/2$ (though finite) in the interval $2\delta_1/3=J_0<J<J_c=\delta_1$. On the contrary, in the case of Ising interaction, $S_g=0$ (1/2) for an even (odd) number of electrons as long as $\delta_1>J$.

In more realistic models, which take the randomness in both the level spacing and the exchange interaction into account, the magnetization at $0<J<\delta_1$ is *essentially random*. Situation far from Stoner instability was discussed in Refs. 2 and 3. In this paper we propose a theory of the magnetization near this critical point, $\delta_1-J\ll\delta_1$.

For finite S the functions $E_0(S)$ from Eqs. (1.6a) and (1.6b) are random. Their statistics are determined by the probability distributions of E_α and $J_{\alpha\beta}$. Below we derive the correlation function $\langle E_0(S_1)E_0(S_2)\rangle$ for large but finite $S_{1,2}$ in a realistic model of a weakly disordered or chaotic metallic grain. This correlation function is sufficient to describe the statistical mechanics of the grain. At high temperatures the randomness can be treated perturbatively in powers of $1/T$ (high-temperature expansion). The low-temperature behavior of those systems is determined by the position and the structure of the deepest minimum of the $E(S)$ function. Therefore, one has to develop a description of the spin S_g of the ground state: $E_0(S_g)=\min\{E_0(S)\}$. Since S_g is random, one might be interested in the statistics of S_g and of $E(S)$ for S close to S_g. The problem of evaluation of statistics of S_g is not trivial. In this paper we do not solve it completely. We restrict ourselves to scaling analysis and numerical simulation. Our attempt to construct an analytical description based on the replicas symmetry breaking paradigm[4] will be published elsewhere.[5]

The remainder of this paper is organized in the following way. In Sec. II we discuss a model of interacting electrons in a weakly disordered metallic grain and the statistics of E_α and $J_{\alpha\beta}$ that follow from this model. Section III is devoted to the derivation of the correlation function $\langle E_0(S_1)E_0(S_2)\rangle$. The scaling analysis of the structure of the minima of $E_0(S)$ is performed in Sec. IV. In Sec. V the results are compared with numerical simulations. Our findings are summarized in Sec. VI.

II. ELECTRON-ELECTRON INTERACTIONS IN ISOLATED METALLIC GRAINS

Let us discuss the energy scales that determine properties of a finite system of electrons. The single electron spectrum $\{\mathcal{E}_\alpha\}$ is characterized by the mean-level spacing

$$\delta_1=\langle\mathcal{E}_{\alpha+1}-\mathcal{E}_\alpha\rangle, \tag{2.1}$$

where $\langle\cdots\rangle$ stands for the ensemble averaging. Another relevant energy scale of the problem is the Thouless energy $E_T\approx\hbar/t_{erg}$, where t_{erg} is the time it takes for a classical counterpart of an electron to cover the energy shell in the single-particle phase space. For diffusive and ballistic systems t_{erg} equals L^2/D and L/v_F, respectively. Here L is the size of the system, v_F denotes the electronic Fermi velocity, and D is the diffusion coefficient.

The important characteristic of the system is the ratio of these two energy scales:

$$g=E_T/\delta_1, \tag{2.2}$$

which is known as the dimensionless conductance. Here we discuss only metallic grains where all single-electron states are extended, and thus the dimensionless conductance is large:

$$g\gg 1. \tag{2.3}$$

It is well known[6–8] that in this regime the statistics of the spectrum $\{\mathcal{E}_\alpha\}$ on the scales smaller than the Thouless energy E_T are well described by the random matrix theory (RMT).[9–11] RMT gives a quantitative description of the phenomenon of the level repulsion. For an ensemble of $N\times N, N\to\infty$ matrices with random and independent matrix elements the probability density of a realization of the spectrum $\{\mathcal{E}_\mu\}$ is given by[9,11]

$$P(\{\mathcal{E}_\mu\})\propto\exp\left[\frac{\beta}{2}\sum_{\mu\neq\nu}\ln\left(\frac{|\mathcal{E}_\mu-\mathcal{E}_\nu|}{\delta_1}\right)\right]. \tag{2.4}$$

The parameter β in Eq. (2.4) can be equal to 1, 2, or 4 for orthogonal, unitary, and simplectic ensembles, respectively. The orthogonal (unitary) RM ensemble corresponds to weakly disordered grains with preserved (violated) $\mathcal{T}$ invariance and negligible interaction between orbital and spin degrees of freedom. In what follows, we restrict ourselves by these two ensembles, i.e., do not consider grains with spin-orbit interaction. The latter would correspond to the simplectic ensemble, $\beta=4$.

Now let us take the effects of electron-electron interaction in the grain into consideration. It turns out that a large class of such effects in a *given* disordered closed metallic grain can, under very general conditions, be described by a remarkably simple Hamiltonian with only three system-dependent coupling constants. Let the dimensionless conductance g of the grain tend to infinity. We start with the simplest case when the electrons interact via a short-range potential:

$$\hat{H}_{int}(\vec{r})=\lambda\,\delta_1 V\delta(\vec{r}). \tag{2.5}$$

Here $V\propto L^d$ is the volume of the grain and λ is a dimensionless coupling constant. The matrix element of this interaction in the basis of eigenstates $\varphi_\alpha(\vec{r})$ of the noninteracting Hamiltonian is given by

$$M^{\alpha\gamma}_{\mu\nu}=\lambda\,\delta_1 V\int d\vec{r}\,\varphi^*_\alpha(\vec{r})\varphi^*_\gamma(\vec{r})\varphi_\mu(\vec{r})\varphi_\nu(\vec{r}). \tag{2.6}$$

We first consider the situation without magnetic field ($\mathcal{T}$-reversal invariance is preserved). Since no spatial symmetries are assumed, *the one-particle orbitals are not degenerate* and the eigenfunctions of one-particle Hamiltonian $\varphi_\mu(\vec{r})$ *can be chosen to be real*. The off-diagonal elements in Eq. (2.6) are small as $\delta_1/E_T=1/g$ because the integrand quickly oscillates. Thus they can be neglected. On the contrary, diagonal matrix elements (α, γ, μ, ν are equal pairwise) are much larger since the integrand in Eq. (2.6) is positive definite. Substituting the integrand by its mean value, e.g.,

$$\langle\varphi^2_\alpha(\vec{r})\varphi^2_\gamma(\vec{r})\rangle=V^{-2}, \tag{2.7}$$

we find

$$M^{\alpha\gamma}_{\alpha\gamma}=M^{\alpha\alpha}_{\gamma\gamma}=M^{\alpha\gamma}_{\gamma\alpha}=\lambda\,\delta_1. \tag{2.8}$$

Corrections to Eq. (2.8) are negligible for exactly the same reason as the off-diagonal matrix elements. As a result, in the limit $E_T\to\infty$, Eq. (2.8) becomes exact. [Equation (2.8) is valid for $\alpha\neq\gamma$; we discuss the significance of the ''double diagonal'' element $M^{\alpha\alpha}_{\alpha\alpha}$ later, see Eq. (2.21).]

For the following discussion it is convenient to introduce operators of the number of electrons $\hat{n}_\alpha$ on the orbital α and the spin $\vec{S}_\alpha$ on this orbital:

$$\hat{n}_\alpha=\sum_\sigma a^\dagger_{\alpha\sigma}a_{\alpha\sigma},\quad \vec{S}_\alpha=\frac{1}{2}\sum_{\sigma\sigma_1}a^\dagger_{\alpha\sigma}a_{\alpha\sigma_1}\vec{\sigma}_{\sigma\sigma_1}. \tag{2.9}$$

Here $a^\dagger_{\alpha\sigma}$ ($a_{\alpha\sigma}$) creates (annihilates) an electron with a spin σ on the orbital α and $\sigma^i_{\sigma\sigma_1}$ are the Pauli matrices. Neglecting the off-diagonal terms in the interaction Hamiltonian reduces it to the form

$$\begin{aligned}\hat{H}_{int}=\hat{H}^{(1)}+\hat{H}^{(2)}+\hat{H}^{(3)}=\sum_{\alpha\gamma\sigma\sigma_1}&[M^{\alpha\gamma}_{\alpha\gamma}a^\dagger_{\alpha\sigma}a_{\alpha\sigma}a^\dagger_{\gamma\sigma_1}a_{\gamma\sigma_1}\\&+M^{\alpha\gamma}_{\gamma\alpha}a^\dagger_{\alpha\sigma}a_{\alpha\sigma_1}a^\dagger_{\gamma\sigma_1}a_{\gamma\sigma}+M^{\alpha\alpha}_{\gamma\gamma}a^\dagger_{\alpha\sigma}a^\dagger_{\alpha\sigma_1}a_{\gamma\sigma}a_{\gamma\sigma_1}].\end{aligned} \tag{2.10}$$

To begin with, let us consider the first two terms in Eq. (2.10). Using Eq. (2.9) and the identity

$$\vec{\sigma}_{\sigma\sigma'}\vec{\sigma}_{\sigma_1\sigma_1'}=2\,\delta_{\sigma\sigma_1'}\delta_{\sigma'\sigma_1}-\delta_{\sigma\sigma'}\delta_{\sigma_1\sigma_1'},$$

one can present $\hat{H}^{(1)}+\hat{H}^{(2)}$ in a usual Hartree-Fock form:

$$\hat{H}^{(1)}+\hat{H}^{(2)}=\sum_{\alpha\gamma}\left[\left(M^{\alpha\gamma}_{\alpha\gamma}-\frac{1}{2}M^{\alpha\gamma}_{\gamma\alpha}\right)\hat{n}_\alpha\hat{n}_\gamma-2M^{\alpha\gamma}_{\gamma\alpha}\hat{\vec{S}}_\alpha\hat{\vec{S}}_\gamma\right]. \tag{2.11}$$

Now we can use the remarkable independence of the matrix elements of their indices, Eq. (2.8), and present Eq. (2.11) as

$$\hat{H}^{(1)}+\hat{H}^{(2)}=\lambda\,\delta_1\left[\frac{1}{2}\hat{n}^2-2\hat{\vec{S}}^2\right]. \tag{2.12}$$

Here $\hat{\vec{S}}$ and $\hat{n}$ are the operators of the total spin and the total number of electrons correspondingly,

$$\hat{\vec{S}}=\sum_\alpha\hat{\vec{S}}_\alpha,\quad \hat{n}=\sum_\alpha\hat{n}_\alpha. \tag{2.13}$$

The third term in Eq. (2.10) can be treated in a similar fashion. One can write it as

$$\hat{H}^{(3)}=\lambda\,\delta_1\hat{T}^\dagger\hat{T},\quad \hat{T}=\sum_\alpha\hat{a}_{\alpha\uparrow}\hat{a}_{\alpha\downarrow}. \tag{2.14}$$

It follows from Eqs. (2.12) and (2.14) that the Hamiltonian $\hat{H}_{int}$ can be presented in terms of three operators $\hat{n}$, $\hat{S}$, and $\hat{T}$ from Eqs. (2.13) and (2.14), rather than in terms of all the operators $\hat{n}_\alpha$, $\hat{S}_\alpha$, and $\hat{a}_{\alpha\uparrow}\hat{a}_{\alpha\downarrow}$ with different α. In fact, this feature is not specific to the particular short-range interaction Hamiltonian (2.5) and is determined by the chaoticity of the eigenfunctions $\varphi_\alpha(\vec{r})$. It turns out that $\varphi_\alpha(\vec{r})$ are Gaussian random variables that are not correlated with each other. This is correct for eigenvectors of $N\times N$, $N\to\infty$ random matrices:[11]

$$\langle\varphi^*_\mu(m)\varphi_\nu(n)\rangle=\frac{1}{N}\delta_{\mu\nu}\delta_{mn},$$
$$\langle\varphi_\mu(m)\varphi_\nu(n)\rangle=\frac{2-\beta}{N}\delta_{\mu\nu}\delta_{mn}, \tag{2.15a}$$

and $\langle\varphi_\mu(m)\rangle=0$. It is also correct for the Berry ansatz[12] for the wave functions in a chaotic grain

$$\langle\varphi^*_\mu(\vec{r}_1)\varphi_\nu(\vec{r}_2)\rangle=\frac{1}{V}\delta_{\mu\nu}h(\vec{r}_1-\vec{r}_2),$$
$$\langle\varphi_\mu(\vec{r}_1)\varphi_\nu(\vec{r}_2)\rangle=\frac{2-\beta}{V}\delta_{\mu\nu}h(\vec{r}_1-\vec{r}_2). \tag{2.15b}$$

Here $h(\vec{r})$ is the familiar Friedel function:

$$h(\vec{r})=\Gamma(d/2)\frac{J_{d/2-1}(x)}{x^{d/2-1}},\quad x=\frac{2\pi|\vec{r}|}{\lambda_F}, \tag{2.16}$$

where d is the spatial dimension of the grain, J is the Bessel function, and λ_F is the Fermi wavelength. The characteristic scale of the decay of this function is of the order of the electron wavelength, λ_F, and for the purposes of convolution with any smooth function can be substituted by $\lambda_F^3\delta(\vec{r})$. Equation (2.15b) becomes exact in the limit $g\to\infty$.

It is easy to see that the correlators of the eigenvectors (eigenfunctions) (2.15) are invariant with respect to an arbitrary orthogonal transformation performed over them:

$$\varphi_\mu(m)\to\sum_{\mu',m'}O^{\mu\mu'}_{mm'}\varphi_{\mu'}(m'),$$
$$\varphi_\mu(\vec{r})\to\sum_{\mu'}\int d\vec{r}_1O^{\mu\mu'}(\vec{r},\vec{r}_1)\varphi_\mu(\vec{r}_1), \tag{2.17a}$$

$$\sum_{\mu',m'}O^{\mu\mu'}_{mm'}O^{\mu'\nu}_{m'n}=\delta_{mn}\delta_{\mu\nu},$$
$$\int d\vec{r}\sum_{\mu'}O^{\mu\mu'}(\vec{r}_1,\vec{r})O^{\mu'\nu}(\vec{r},\vec{r}_2)=\delta_{\mu\nu}\delta(\vec{r}_1-\vec{r}_2). \tag{2.17b}$$

Therefore, the ensemble-averaged part of the interaction Hamiltonian must also be invariant with respect to such transformations. [As to mesoscopic fluctuations of $\hat{H}_{int}$, they disappear in the universal (RM) limit, $g\to\infty$ $(N\to\infty)$, and can be neglected under the condition (2.3).] There are only three operators, quadratic in the fermionic fields, that possess this invariance:

$$\hat{n}=\sum_{\alpha,\sigma}\hat{a}^\dagger_{\alpha,\sigma}\hat{a}_{\alpha\sigma},$$
$$\hat{\vec{S}}=\frac{1}{2}\sum_{\alpha,\sigma_1,\sigma_2}\hat{a}^\dagger_{\alpha\sigma_1}\vec{\sigma}_{\sigma_1,\sigma_2}\hat{a}_{\alpha,\sigma_2},$$
$$\hat{T}=\sum_\alpha\hat{a}_{\alpha\uparrow}\hat{a}_{\alpha\downarrow}, \tag{2.18}$$

and the quartic operators may be constructed only as second powers or products of these operators. Moreover, the Hamiltonian $\hat{H}_{int}$ should also be invariant with respect to SU(2) rotations in the spin space. Therefore, the spin may enter into the interaction Hamiltonian only through the combination $\hat{\vec{S}}^2$. Finally, $\hat{H}_{int}$ must be invariant with respect to U(1) gauge transformations. It means that $\hat{H}_{int}$ can include the operator $\hat{T}$ only as a product $\hat{T}^\dagger\hat{T}$. We conclude that in the general case the limit of the infinite conductance g corresponds to

$$\hat{H}_{int}=E_c\hat{n}^2-J(\hat{\vec{S}})^2+\lambda_{BCS}\hat{T}^\dagger\hat{T}. \tag{2.19}$$

(Linear in $\hat{n}$ term is allowed, but it can be included into the one-particle part of the Hamiltonian.) We introduced three coupling constants E_c, J, and λ_{BCS}, that correspond to the three operators permitted by the symmetries. In the simple model with the short-range interaction and preserved $\mathcal{T}$ invariance, $\beta=1$, the above coupling constants have the following form:

$$E_c=\frac{1}{2}\lambda\,\delta_1,\quad J=2\lambda\,\delta_1,\quad \lambda_{BCS}=\lambda\,\delta_1. \tag{2.20}$$

If the $\mathcal{T}$ invariance is broken, $\beta=2$, transformations (2.17) become unitary. The operator $\hat{T}$ from Eq. (2.18) is incompatible with such symmetry and thus $\lambda_{BCS}=0$, for $\beta=2$.

We would like to emphasize once again that Eq. (2.19) is the most general form of the Hamiltonian in the limit $g \to \infty$. For instance, one can check that it correctly takes into account interactions of the two electrons on the same orbital. Indeed, it follows from Eq. (2.6) and the Gaussian distribution of $\varphi_\alpha(\vec{r})$ [with correlation functions determined by Eqs. (2.15)] that the ‘‘double diagonal’’ matrix element $M^{\alpha\alpha}_{\alpha\alpha}$ is different from diagonal ones, given by Eq. (2.8):

$$M^{\alpha\alpha}_{\alpha\alpha}=(4-\beta)M^{\alpha\gamma}_{\alpha\gamma}=(4-\beta)\lambda\,\delta_1. \tag{2.21}$$

At first sight it appears that the Hamiltonian (2.19) has to be supplemented by an additional term proportional to $M^{\alpha\alpha}_{\alpha\alpha}$:[3]

$$\hat{H}_{?}\propto\lambda\,\delta\sum_{\alpha}\ \hat{a}^{\dagger}_{\alpha,\uparrow}\hat{a}_{\alpha,\uparrow}\hat{a}^{\dagger}_{\alpha,\downarrow}\hat{a}_{\alpha,\downarrow}. \tag{2.22}$$

However, one notices that for any two distinct labels $\alpha\neq\gamma$ there are three different off-diagonal elements $M^{\alpha\gamma}_{\alpha\gamma}$, $M^{\gamma\alpha}_{\alpha\gamma}$, and $M^{\gamma\gamma}_{\alpha\alpha}$, whereas double-diagonal term $M^{\alpha\alpha}_{\alpha\alpha}$ should be taken into account only once. As a result, the relationship (2.21) is exactly what is needed for Eq. (2.10) to be valid, provided that the sum in the right-hand side involves terms with $\alpha=\gamma$ as well as those with $\alpha\neq\gamma$. Therefore, the interaction between electrons on the same orbital *does not violate the invariance under the rotation of the basis*, which becomes exact in the $g\to\infty$ limit. On the other hand, *an additional term of the form Eq.* (2.22) *explicitly violates this symmetry*. For this reason we think that taking such a term into account, as it was done in Ref. 3 is incorrect.

Let us briefly discuss the physical meaning of the three terms in the Hamiltonian Eq. (2.19). The last one exists only in the orthogonal case ($\beta=1$) and leads to the superconducting instability provided that $\lambda_{BCS}<0$, i.e., there is an attraction in the Cooper channel. Superconducting correlations are suppressed by the magnetic field, and thus do not exist at $\beta=2$. Here we are not interested in the effects of superconductivity and assume that the grain is a normal metal at $T=0$. It means that $\lambda_{BCS}>0$. It is well known that the very same renormalization that leads to superconductivity at $\lambda_{BCS}<0$ renormalizes the repulsive effective coupling constant in the Cooper channel to zero (see, e.g., Ref. 13). This fact enables us to simply neglect this interaction.

The first two terms in Eq. (2.19) represent the dependence of the energy of the grain on the total number of the electrons inside and on the total spin, respectively. They commute with each other and with the single-particle part of the Hamiltonian $\Sigma\mathcal{E}_\alpha\hat{a}^{\dagger}_{\alpha,\sigma}\hat{a}_{\alpha,\sigma}$ provided the grain is isolated. Therefore, all states of the grain can be classified by n and S.

As long as we are interested in spin structure of the system with a *fixed number of electrons*, we can disregard the first term in Eq. (2.19). As a result we arrive at a simple Hamiltonian

$$H=\sum_{\alpha,\sigma}\ \mathcal{E}_{\alpha}\hat{a}^{\dagger}_{\alpha,\sigma}\hat{a}_{\alpha,\sigma}-J(\hat{S})^2. \tag{2.23}$$

Note that the only random component of the problem is the single-particle spectrum $\{\mathcal{E}_\alpha\}$, while the exchange J does not fluctuate.

It should be noted though that the RM theory is just an approximation. It becomes exact only in the limit $g\to\infty$. For finite g there are corrections to Eq. (2.19), which sometimes are of importance. However, these corrections at $g\gg 1$ do not bring essentially new physics to the problem of the small grain magnetization. For this reason we restrict ourselves to the Hamiltonian Eq. (2.19).

Choosing the direction of the total spin of the system to coincide with the z axis, we can express the energy of the system through the occupation numbers $n_{\alpha,\sigma}$:

$$E^{H}=\sum_{\alpha,\sigma}\ \mathcal{E}_{\alpha}n_{\alpha,\sigma}-JS(S+1), \tag{2.24}$$

where

$$S=\frac{1}{2}\left|\sum_{\alpha}\ (n_{\alpha,\uparrow}-n_{\alpha,\downarrow})\right|=|S_z|, \tag{2.25}$$

and $\Sigma n_{\alpha,\sigma}=N$.

Throughout this section we assumed that the metallic grain possesses rotational symmetry in the spin space. In addition, it is worthwhile to discuss a case in which this symmetry is broken and the interaction as only along one easy axes. To make connection with the energy $E^{I}_{0}(S)$ that has been defined in Eq. (1.6b), we adopt the following Hamiltonian:

$$H=\sum_{\alpha,\sigma}\ \mathcal{E}_{\alpha}\hat{a}^{\dagger}_{\alpha,\sigma}\hat{a}_{\alpha,\sigma}-J(\hat{S}_z)^2. \tag{2.26}$$

Using the notation of Eq. (2.25), we express the energy for the Ising case as

$$E^{I}=\sum_{\alpha,\sigma}\ \mathcal{E}_{\alpha}n_{\alpha,\sigma}-JS^2. \tag{2.27}$$

The energy $E_0(S)$ that was introduced in the previous section can be obtained by minimizing E at fixed S with respect to the occupation numbers $n_{\alpha,\sigma}$. In spite of the simple form of Eqs. (2.24), (2.27), and (2.25) the problem remains nontrivial, since the spectrum $\{\mathcal{E}_\alpha\}$ is random. In the following sections we consider the effect of this randomness on the properties of the ground state.

III. THE EFFECTIVE HAMILTONIAN

We are interested in the spontaneous magnetization of the system at low temperatures. Therefore, in the following discussion we only compare the energies of the lowest lying states with a given spin. Hence, the state labeled by the total spin S is the state for which the first $N/2+S$ single electron states are occupied by spin-up and the first $N/2-S$ by spin-down electrons. We ignore the excited states with the same total spin in the following discussion. (It can be shown that taking these states into account introduces a nonessential addition to the free energy.) This enables us [based on the Hamiltonian (2.24)] to write the following energy functional:

$$E(S,\xi)=\int_{0}^{\mathcal{E}_>}\epsilon\rho(\epsilon)d\epsilon-\int_{\mathcal{E}_<}^{0}\epsilon\rho(\epsilon)d\epsilon-JS(S+\xi-1), \tag{3.1}$$

where $\rho(\epsilon)=\Sigma_\alpha \delta(\epsilon-\mathcal{E}_\alpha)$ is the one-electron density of states and J is the strength of the exchange interaction, and parameter $\xi=1,2$ characterizes two limiting cases of spin anisotropy: $\xi=2$ corresponds to the isotropic spin orientation (Heisenberg model) with the degeneracy of the state $2S+1$, while $\xi=1$ describes the easy axes (Ising) model where states are only double degenerate. We have 2-orbitals at $\mathcal{E}_\alpha<\mathcal{E}_<$, 1-orbitals at $\mathcal{E}_<<\mathcal{E}_\alpha<\mathcal{E}_>$, and empty 0-orbitals at $\mathcal{E}_\alpha>\mathcal{E}_>$. From the conservation of the total number of particles we obtain the following equations for $\mathcal{E}_>$ and $\mathcal{E}_<$:

$$S=\int_0^{\mathcal{E}_>}\rho(\epsilon)d\epsilon=\int_{\mathcal{E}_<}^0\rho(\epsilon)d\epsilon. \tag{3.2}$$

The minimum of the energy functional (3.1) is the same as the ground state of the original system. The density of states can be represented as

$$\rho(\epsilon)=1/\delta_1+\delta\rho(\epsilon). \tag{3.3}$$

We are interested in the value of the spin $S\gg 1$, which translates into the scale of orbital energies that is much larger than δ_1. The fluctuations of the density of states averaged over such an energy scale are much smaller than its mean value $1/\delta_1$, and it is sufficient to keep only the terms linear in $\delta\rho$. Thus we obtain from Eq. (3.2),

$$\mathcal{E}_>/\delta_1=S-\int_0^{S\delta_1}d\epsilon\,\delta\rho(\epsilon),$$

$$\mathcal{E}_</\delta_1=-S+\int_{-S\delta_1}^0 d\epsilon\,\delta\rho(\epsilon). \tag{3.4}$$

In what follows we adopt the notation

$$\mu=2\delta_1-2J\ll\delta_1. \tag{3.5}$$

According to Eq. (1.8), the bulk Stoner instability emerges at $\mu=0$, so that the parameter μ characterizes how close the system is to the criticality threshold.

Substituting Eqs. (3.4) into Eq. (3.1), we obtain

$$E(S,\xi)=\frac{\mu}{2}S^2-(\xi-1)(\delta_1-\mu/2)S-\delta_1 S\int_{-S\delta_1}^{S\delta_1}\delta\rho(\epsilon)d\epsilon$$
$$+\int_0^{S\delta_1}[\delta\rho(\epsilon)+\delta\rho(-\epsilon)]\epsilon d\epsilon. \tag{3.6}$$

Integrating Eq. (3.6) by parts and using Eq. (3.5) to neglect μ as compared to δ_1, we obtain

$$E(S,\xi)=\frac{\mu}{2}S^2-(\xi-1)\delta_1 S-\int_0^{S\delta_1}d\epsilon\int_0^{\epsilon}d\epsilon_1$$
$$\times[\delta\rho(\epsilon_1)+\delta\rho(-\epsilon_1)]. \tag{3.7}$$

Thus we reduced the original problem to finding the minima of the random function

$$E(S,\xi)=\frac{\mu}{2}S^2-(\xi-1)\delta_1 S+V(S), \tag{3.8}$$

where μ is fixed (and small compared to δ_1), and $V(S)$ is a random potential which is determined by the fluctuations of the density of states $\delta\rho(\epsilon)$:

$$V(S)=-\int_0^{\delta_1 S}d\epsilon\int_0^{\epsilon}d\epsilon_1[\delta\rho(\epsilon_1)+\delta\rho(-\epsilon_1)]. \tag{3.9}$$

Below, we refer to this problem as a random potential problem (RPP). Such a problem is well defined provided that the correlation function for random potential $V(S)$ is given. One can evaluate the statistics of the potential $V(S)$, Eq. (3.9), using RMT.

The fluctuations of the density of states, $\delta\rho$, averaged over energy intervals larger than δ_1 in the ensembles of RM are Gaussian random variables. Therefore, using Eq. (3.9), we conclude that $V(S)$ is a Gaussian random variable as well. The correlation function $\langle V(S)V(S')\rangle$ can be expressed through the correlator of the density of states. The correlation function of the Fourier components of $\delta\rho(\epsilon)$ is given by[10]

$$\langle\delta\rho_k\delta\rho_p\rangle=\frac{2|k|}{\beta}\delta(p+k), \tag{3.10}$$

where β is 1 or 2 depending on whether the Hamiltonian belongs to an orthogonal or a unitary ensemble. Averaging the product $V(S_1)V(S_2)$ with the help of Eqs. (3.9) and Eq. (3.10), we obtain the correlation function:

$$\langle V(S_1)V(S_2)\rangle=\frac{\delta_1^2}{\pi^2\beta}\biggl[-S_1^2\ln S_1^2-S_2^2\ln S_2^2+\frac{(S_1+S_2)^2}{2}$$
$$\times\ln(S_1+S_2)^2+\frac{(S_1-S_2)^2}{2}\ln(S_1-S_2)^2\biggr]. \tag{3.11}$$

Equations (3.8) and (3.11) define the random potential problem. In the next section we will show that the statistical description of this function possesses simple scaling properties.

IV. SCALING ANALYSIS

It follows from Eq. (3.11) that the correlation function of the random potential is a homogeneous function of degree two:

$$\langle V(\gamma S_1)V(\gamma S_2)\rangle=\gamma^2\langle V(S_1)V(S_2)\rangle. \tag{4.1}$$

Equation (4.1) means that the probability of the potential realization $V(S)$ is the same as the probability of the potential $\gamma V(\gamma^{-1}S)$, and by no means expresses the scaling for the potential of a given realization.

Our goal now is to demonstrate that this property of the Gaussian random potential dictates a particular scaling form for all the moments of the free energy F of the system:

$$F(T,\mu;\{V(S)\})=-T\ln\left\{\sum_{S\geqslant 0}2\left(S+\frac{1}{2}\right)^{\xi-1}\times\exp\left(-\frac{E(S,\xi)}{T}\right)\right\}$$
$$=-T\ln\left\{2\int_0^\infty dSS^{\xi}\exp\left(-\frac{E(S,\xi)}{T}\right)\right\},\tag{4.2}$$

where energy $E(S)$ is given by Eq. (3.8). Note that in Eq. (4.2), which is valid in the continuous limit, we neglected unity in comparison with $2S$. This is because we have already used several times the fact that $S\gg 1$, and keeping this unity in the pre-exponential factor would be beyond the accuracy of the calculation.

It follows from Eqs. (4.2) and (3.8) that for any given realization of the random potential $V(S)$, the following identity holds:

$$F(\gamma T,\gamma^{-1}\mu;\{\gamma V(\gamma^{-1}S)\})+\gamma T\ln 2+\gamma\xi T\ln\gamma$$
$$=\gamma F(T,\mu;\{V(S)\})+T\ln 2.\tag{4.3}$$

According to Eq. (4.1) the probability of the potential realization $V(S)$ is the same as the probability of the potential $\gamma V(\gamma^{-1}S)$. Therefore, the moments of the free energy possess the following scaling property:

$$\langle F(\gamma T,\gamma^{-1}\mu)\rangle+\gamma T\ln 2+\gamma\xi T\ln\gamma$$
$$=\gamma\langle F(T,\mu)\rangle+T\ln 2\langle F^n(\gamma T,\gamma^{-1}\mu)\rangle_c$$
$$=\gamma^n\langle F^n(T,\mu)\rangle_c,\quad n=2,3,4,\ldots,\tag{4.4}$$

where $\langle\cdots\rangle$ stands for the ensemble averaging and subscript c means the irreducible average (cumulant).

We can use the fact that the only available variable with the dimensionality of energy is $\delta_1/\sqrt{\beta}$, see Eq. (3.11), and conclude that the moments of the free energy should be of the following scaling form:

$$\langle F(T,\mu)\rangle=-T\left[\frac{\xi}{2}\ln\left(\frac{T}{\mu}\right)+\ln 2+\frac{2-\xi}{2}\ln\frac{\pi}{2}\right]-\frac{\delta_1^2}{\beta\mu}f_\xi^{(1)}(\theta,\beta),$$
$$\langle[F(T,\mu)]^n\rangle_c=\left(\frac{\delta_1^2}{\beta\mu}\right)^n f_\xi^{(n)}(\theta,\beta),\quad n=2,3,\ldots.\tag{4.5}$$

Here we introduced scaling variable

$$\theta=\frac{\beta\mu T}{\delta_1^2},\tag{4.6}$$

which has the meaning of a dimensionless temperature. In Eq. (4.5), $f_\xi^{(n)}$ are dimensionless functions that cannot be found from the scaling arguments alone.

The statistics of the magnetization can be calculated with the help of the identity that follows straightforwardly from Eqs. (3.8) and (4.2):

$$\overline{S^2}=2\frac{\partial F}{\partial\mu}.\tag{4.7}$$

The overbar in Eq. (4.7) and below stands for the thermodynamic average within a given realization of $V(S)$. In a complete analogy with the derivation of Eq. (4.5), we obtain the following scaling behavior of the magnetization:

$$\langle\overline{S^2}\rangle=\frac{\xi T}{\mu}+\frac{\delta_1^2}{\beta\mu^2}G_\xi^{(1)}(\theta,\beta),$$
$$\langle[\overline{S^2}]^n\rangle_c=\left(\frac{\delta_1^2}{\beta\mu^2}\right)^n G_\xi^{(n)}(\theta,\beta),\quad n=2,3,\ldots.\tag{4.8}$$

For $n=1$ one finds from Eq. (4.7) that

$$G_\xi^{(1)}(\theta,\beta)=-2\theta^2\frac{d}{d\theta}[\theta^{-1}f_\xi^{(1)}(\theta,\beta)].\tag{4.9}$$

There is no straightforward relation between $G^{(n)}$ and $f^{(n)}$ functions for $n>1$. It is noteworthy that for the easy axis (Ising) case ($\xi=1$) the scaling functions $f_1^{(n)}$ (θ,β) and $G_1^{(n)}$ (θ,β) do not depend on β.

Let us discuss the asymptotic behavior of functions $f_\xi^{(1,2)}$ from Eq. (4.5). We begin with the high-temperature regime, $\theta\to\infty$. One can expand Eq. (4.2) up to second order in the potential $U(S)$, where

$$U(S)=-(\xi-1)S+V(S),\tag{4.10}$$

to obtain

$$F\approx -T\frac{\xi}{2}\ln\left(\frac{T}{\mu}\right)-T\ln 2-T\frac{2-\xi}{2}\ln\frac{\pi}{2}+\overline{U(S)|_0}$$
$$-\frac{\overline{U(S)^2|_0}-\overline{U(S)|_0}^2}{2T}.\tag{4.11}$$

Here we introduced the following notation:

$$\overline{\cdots|_0}\equiv\frac{\int_0^\infty dSS^{\xi-1}e^{-\mu S^2/2T}\cdots}{\int_0^\infty dSS^{\xi-1}e^{-\mu S^2/2T}}.\tag{4.12}$$

The fourth and fifth terms in the expansion (4.11) are random quantities. Averaging them with the help of Eq. (3.11), we obtain

$$f_1^{(1)}(\theta)=\frac{\ln 2}{\pi^2}+O(1/\theta),\quad f_1^{(2)}(\theta)=\theta\frac{2\ln 2}{\pi^2}+O(1),\tag{4.13a}$$

$$f_2^{(1)}(\theta,\beta)=\sqrt{\theta}\sqrt{\frac{\beta\pi}{2}}+\beta\left(2-\frac{\pi}{2}\right)+\frac{4\ln 2}{\pi^2}-\frac{C_2}{2}+O\left(\frac{1}{\sqrt{\theta}}\right),\tag{4.13b}$$

$$f_2^{(2)}(\theta,\beta)=\theta C_2+2\sqrt{\theta\beta}\left[D_2-\sqrt{\frac{\pi}{2}}C_2\right]+O(1).$$

The numerical coefficients C_2 and D_2 have the following meaning:

$$C_2=\frac{\beta\mu}{T\delta_1^2}\langle\overline{V(S)|_0}^2\rangle,$$
$$D_2=\beta\left(\frac{\mu}{T\delta_1^2}\right)^{3/2}\langle(\overline{V(S)|_0})\cdot(\overline{S\cdot V(S)|_0})\rangle. \tag{4.14}$$

Their numerical values are

$$C_2=\frac{2}{\pi^2}\left(\int_0^1\frac{dx}{\sqrt{x}}\frac{(1-x)^2}{(1+x)^3}\ln\frac{1}{x}-1\right)$$
$$=\frac{1}{4\pi^2}[\Psi'(1/4)-\Psi'(3/4)]\approx 0.3712,$$
$$D_2=\pi^{-3/2}[6\ln(\sqrt{2}+1)-2\sqrt{2}\ln 2]\approx 0.5976,$$

where $\Psi'(z)=(d^2/dz^2)\ln\Gamma(z)$ is the second logarithmic derivative of the Γ function. Substituting Eqs. (4.13a) and (4.13b) into Eq. (4.9), we find

$$G_1^{(1)}(\theta)=\frac{2\ln 2}{\pi^2}+O\left(\frac{1}{\theta}\right),$$
$$G_2^{(1)}(\theta)=2f_2^{(1)}(\theta,\beta)-\sqrt{\theta}\sqrt{\frac{\beta\pi}{2}}+O\left(\frac{1}{\sqrt{\theta}}\right). \tag{4.15}$$

Equations (4.13a), (4.13b), and (4.15) are valid in the high-temperature regime where the disorder only weakly affects the temperature fluctuations of the spin. There is no parametrically justified theoretical approach to analyze the situation at low temperatures. The popular approach to the RPP is the replica symmetry breaking ansatz.[4,14–16] The results of such a calculation will be published elsewhere.[5] Here we restrict ourselves to a qualitative consideration, which yields the answers up to numerical coefficients.

We employ arguments similar to those of Larkin[17] for the collective pinning of the vortex lattice, and of Imry and Ma[18] for the random spin systems. Let us first discuss the Ising, $\xi=1$, case. At the point S_g of the global minimum of the energy $E(S)$, Eq. (3.8), $\min\{E(S)\}=E(S_g)$, the random potential $V(S_g)$ is of the same order of magnitude as the quadratic term $\mu S_g^2/2$ and has the opposite sign. This condition can be written as

$$\frac{\mu}{2}S_g^2\simeq\sqrt{\langle V^2(S_g)\rangle}. \tag{4.16}$$

At $T=0$ the entropy term is not important. Hence the spin at zero temperature is equal to S_g and does not depend on the degeneracy of the state. Using Eq. (3.11), we find that

$$\langle\overline{S^2}\rangle^I\simeq\frac{\delta_1^2}{\beta\mu^2}. \tag{4.17}$$

Therefore, the function $G_1^{(1)}$ tends to a constant independent of β as $\theta\to 0$.

The estimate of the position of the minimum, S_g, for the Heisenberg case, $\xi=2$, differs from Eq. (4.16) only slightly. It follows from Eq. (3.8) that

$$\mu S_g-1\approx\sqrt{\langle V^2(S_g)\rangle}. \tag{4.18}$$

As a result,

$$\langle\overline{S^2}\rangle^H=\frac{\delta_1^2}{\mu^2}\left(1+\frac{a}{\beta}\right). \tag{4.19}$$

Here a is a numerical constant of order unity, which cannot be determined within scaling considerations only. Therefore, the function $G_2^{(1)}$ tends to a constant as $\theta\to 0$ but in the Heisenberg case this constant depends on β.

According to Eq. (4.9), this means that $f^{(1)}$ also has a finite limit at $T=0$. Moreover, the squared spin of the ground state fluctuates from sample to sample and the fluctuations are of the order of its average value $\langle S_g^2\rangle$. As a result, all of the functions $f^{(n)}$, $\mathcal{G}^{(n)}$ must reach finite limits for both Heisenberg and Ising cases.

Let us discuss the physical meaning of the low-temperature expansion using

$$G_\xi^{(1)}(\theta)=G_\xi^{(1)}(0)+\theta\frac{dG_\xi^{(1)}}{d\theta}+O(\theta^2) \tag{4.20}$$

as an example. Both the constant term and the derivative have a simple interpretation in terms of the characteristics of the absolute minima of the random potential $V(S)$.

Consider a realization of the random potential $V(S)$. The energy of the system (3.8) has only a finite number of minima and there are no symmetry reasons for degeneracies. Therefore, at low enough temperatures, only the vicinity of the ground-state spin S_g determines all of the thermodynamic properties of the system. Close to the minimum the Hamiltonian can be approximated as

$$E(S)\approx E(S_g)+\frac{\mu_r}{2}(S-S_g)^2. \tag{4.21}$$

The corresponding value of the square of the magnetization is

$$\overline{S^2}=S_g^2+3^{\xi-1}\frac{T}{\mu_r}. \tag{4.22}$$

Naturally, $\overline{S^2}$ is a sample-dependent quantity as well as μ_r and S_g. Averaging Eq. (4.22) over the realization and comparing the result with Eqs. (4.8) and (4.20), we find

$$\langle S_g^2\rangle=\frac{\delta_1^2}{\beta\mu^2}G_\xi^{(1)}(0),$$
$$3^{\xi-1}\mu\left\langle\frac{1}{\mu_r}\right\rangle=\frac{dG_\xi^{(1)}}{d\theta}+\xi. \tag{4.23}$$

This means that the low-temperature expansion determines the averaged location of the absolute minima and the curvature in this minima.

V. NUMERICAL SIMULATIONS

The RPP (3.8) with the Gaussian random potential $V(S)$, characterized by its correlator (3.11), is easily accessible for numerical simulations. Indeed, instead of generating the ensemble of potentials $V(S)$ with the given correlator, one can use the connection of $V(S)$ with the spectra of random matrices (see Sec. III).

We carried out numerical simulations for both the orthogonal $(\beta=1)$ and unitary $(\beta=2)$ ensembles. In the former case we generated 1200×1200 symmetric $(H_{\alpha\gamma}=H_{\gamma\alpha})$ matrices with real matrix elements $H_{\alpha\gamma}$. These matrix elements were independent Gaussian random numbers with the following moments:

$$\langle H_{\alpha\gamma}\rangle=0, \quad \langle (H_{\alpha\gamma})^2\rangle=1. \tag{5.1}$$

To obtain a matrix from the unitary ensemble we generated simultaneously a symmetric $\mathrm{Re}\, H_{\alpha\gamma}$ and an antisymmetric $\mathrm{Im}\, H_{\alpha\gamma}$ real matrices $(\mathrm{Re}\, H_{\alpha\gamma}=\mathrm{Re}\, H_{\gamma\alpha};\ \mathrm{Im}\, H_{\alpha\gamma}=-\mathrm{Im}\, H_{\gamma\alpha})$ with the same dispersion as above (Eq. (5.1)). The combination $\mathrm{Re}\, H_{\alpha\gamma}+i\,\mathrm{Im}\, H_{\alpha\gamma}$ is a matrix element of the Hamiltonian from the unitary ensemble.

In our analytic calculations we assumed that the mean-level spacing δ_1 does not depend on the location of the energy strip where δ_1 is calculated. Strictly speaking, this is not the case for the Gaussian ensembles of random matrices. It is well known[11] that the density of the random matrix eigenvalues is distributed according to the Wigner semicircle law: This density is larger in the middle of the band (ϵ close to zero) and vanishes at the band edges $\pm\epsilon_0$ as $\sqrt{\epsilon_0^2-\epsilon^2}$. Accordingly the mean-level spacing depends on the energy:

$$\delta_1(\epsilon)=\delta_1(0)\sqrt{\frac{\epsilon_0^2}{\epsilon_0^2-\epsilon^2}}. \tag{5.2}$$

It is also well known that Eq. (5.2) is just an asymptotic law, which becomes exact in the limit $N\rightarrow\infty$, where N is the rank of the matrices; $\epsilon_0\propto\sqrt{N}$. At finite N there are corrections to Eq. (5.2), which become most pronounced close to the edges.[11]

Taking all of this into account, we first discarded the lowest and the highest 100 states in the spectrum of each random matrix. After that, we unfolded the rest of the spectrum according to Eq. (5.2) and obtained for each matrix 1000 eigenstates that obey local Wigner-Dyson statistics and have uniform density. We also scaled out $\delta_1(0)$ and ended up with the mean-level spacing equal to unity.

To evaluate the realization of $V(S)$, which corresponds to a given random matrix, one can simply sum up energies of the lowest $500+S$ states (filled by electrons with spin up) and the lowest $500-S$ states (spins down). Subtracting S^2 from the resulting sum, we obtain the random potential $V(S)$ in units of δ_1. Some particular realization of the random potential for different β is presented in Fig. 2.

Using the generated potential $V(S)$, we calculated the free energy, $F(\mu,T)$, Eq. (4.2), and the thermodynamic magnetization

$$\overline{S^2}=\frac{1}{Z}\sum_{S\geqslant 0} S^2(2S+1)^{\xi-1}\exp\left(-\frac{E(S)}{T}\right), \tag{5.3}$$

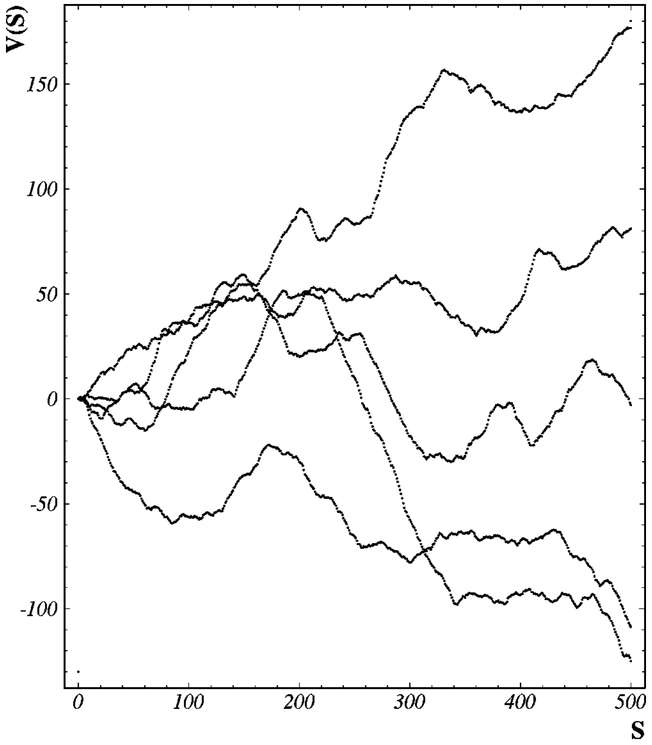

FIG. 2. Several realizations of the random potential $V(S)$ for $\beta=2$.

$$Z=\sum_{S\geqslant 0}(2S+1)^{\xi-1}\exp\left(-\frac{E(S)}{T}\right) \tag{5.4}$$

for a given realization and then evaluated the ensemble average of different moments of random $F(\mu,T)$ and $\overline{S^2}$. All of the data presented below are results of averaging over 12 000 realizations of random matrices.

Figure 3 demonstrates the scaling properties for the mean free energy derived in the preceding section, Eq. (4.5). We evaluated $f^{(1)}$ for different values of T, μ, and β, and plotted it as a function of the scaling variable θ, Eq. (4.6). One can see that for the Ising case the data for different values of μ and for both $\beta=1$ and $\beta=2$ collapse on a single curve in accord with Eq. (4.5). The scaling function $f_1^{(1)}(\theta)$ at $\theta\gg 1$ approaches its high-temperature asymptotic value of $\pi^{-2}\ln 2\approx 0.070$ [Eq. (4.13a)] within statistical errors.

For the Heisenberg case the high-temperature expansion predicts that $f_2^{(1)}$ behaves at $\theta\gg 1$ as [compare with Eq. (4.13b)]

$$f_2^{(1)}(\theta,\beta)\approx 1.25\sqrt{\theta\beta}+0.429\beta+0.095. \tag{5.5}$$

The best-fit lines obtained for the numerical data are described by

$$\begin{aligned} f_2^{(1)}(\theta,\beta)\approx{}&(1.182\pm 0.002)\\ &\times\sqrt{\theta\beta}+(0.31\pm 0.02)\beta+0.12\pm 0.03. \end{aligned} \tag{5.6}$$

This is in a good agreement with Eq. (5.5), taking into account the fact that there should be corrections to Eq. (4.13b) of order $1/\sqrt{\theta}$ and μ [since we neglected μ as compared to δ_1 using the condition in Eq. (3.5)].

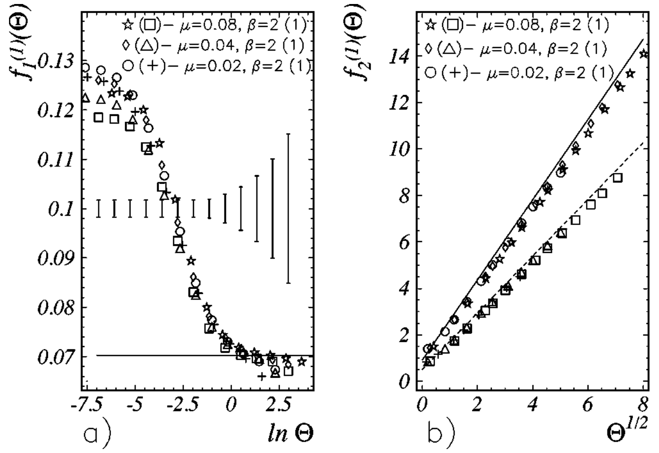

FIG. 3. (a) The contribution to the free energy from disorder [function $f_1^{(1)}$, Eq. (4.5)] in the Ising ($\xi=1$) case. The logarithmic scale is chosen to demonstrate the fact that the scaling function goes to a constant in both low- and high-temperature regimes. The solid line is the result of the high-temperature expansion. The statistical errors depend on θ only and are plotted in the center of the figure. (b) Function $f_2^{(1)}$ in the Heisenberg case ($\xi=2$). The scaling functions are different for the unitary ($\beta=2$) and orthogonal ($\beta=1$) ensembles. The $\sqrt{\theta}$ scale was chosen to illustrate the agreement with the high-temperature expansion obtained in Eq. (4.13b). Solid (dotted) line represents the predicted high-θ behavior for the unitary (orthogonal) case. At low temperature the functions tend to constants larger than the ones predicted by the high-θ expansion.

Figure 4 illustrates the behavior of the mesoscopic fluctuations of the free energy, see Eq. (4.4),

$$f_\xi^{(2)}(\theta)=\frac{(\beta\mu)^2}{\delta_1^4}\{\langle[F(T,\mu)]^2\rangle-\langle F(T,\mu)\rangle^2\}.$$

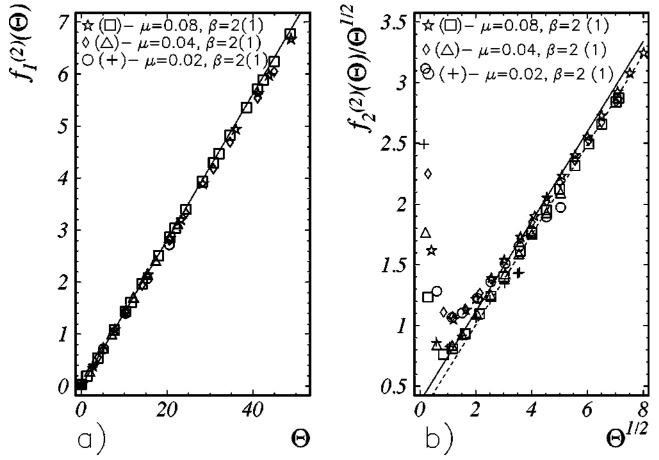

FIG. 4. (a) The averaged fluctuations of the free energy of the grain in the Ising case ($\xi=1$) rescaled according to Eq. (4.5). At $\theta\to 0$ the scaling function approaches a positive constant. The solid line is the high-θ asymptotic behavior described by Eq. (4.13a). (b) The averaged fluctuations of the free energy in the Heisenberg case rescaled as in (a). We divided the scaling function $f_2^{(2)}$ by $\sqrt{\theta}$ and plotted the ratio as a function of $\sqrt{\theta}$ to demonstrate the agreement with the high-temperature expansion [Eqs. (4.13b)]. The solid (dotted) line represents high-θ asymptotic behavior for the unitary (orthogonal) case $\beta=2$ (1).

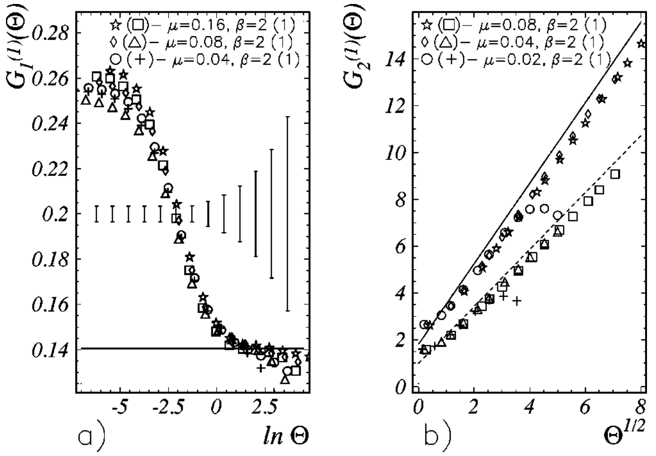

FIG. 5. (a) The contribution from disorder to the averaged magnetization squared in Ising case ($\xi=1$) scaled by $\beta\mu^2$ [see Eq. (4.8) for the definition]. One can see that the scaling function $G_1^{(1)}$ has constant limits in both low- and high-temperature regimes. The solid line is a high-temperature expansion [Eq. (4.15)]. The statistical errors depend on θ only and are plotted in the center of the figure. (b) The contribution from disorder and $-JS$ term to the averaged magnetization squared in the Heisenberg case ($\xi=2$) scaled as in (a). The scaling functions are different for the unitary ($\beta=2$) and orthogonal ($\beta=1$) ensembles. The $\sqrt{\theta}$ scale was chosen to illustrate the agreement with the high-temperature expansion obtained in Eq. (4.15). Solid (dotted) line represents result of high-θ expansions for the unitary (orthogonal) case. At low temperature the functions go to constants higher than the ones predicted by the high-θ expansions.

For the Ising case at $\theta\gg 1$ according to Eq. (4.13a) $f_1^{(2)}\approx 0.1405\theta$. The numerical simulations give the slope of the best-fit line equal to 0.1358 ± 0.0002. Therefore, the results agree well. We can rewrite Eq. (4.13b) for the Heisenberg case as

$$\frac{f_2^{(2)}(\theta,\beta)}{\sqrt{\theta}}\approx 0.371\sqrt{\theta}+2\times 0.132\sqrt{\beta}+O(1/\sqrt{\theta}), \quad (5.7)$$

i.e., $f_2^{(2)}(\theta,\beta)/\sqrt{\theta}$ is a linear function of $\sqrt{\theta}$. The numerics indeed demonstrates such a linear dependence which can be best fitted by

$$\frac{f_2^{(2)}(\theta,\beta)}{\sqrt{\theta}}\approx(0.353\pm 0.006)\sqrt{\theta}+2(0.160\pm 0.003)\sqrt{\beta}+O(1/\sqrt{\theta}). \quad (5.8)$$

Once again, the agreement is quite reasonable since there are corrections $O(\mu)$ to the coefficients.

Figure 5 presents the numerical results for the spontaneous magnetization (5.3). We plot the difference between $\langle S^2\rangle$ and its high-temperature asymptotic:

$$G^{(1)}=\mu^2\beta\left[\overline{\langle S^2\rangle}-\frac{\xi T}{\mu}\right] \quad (5.9)$$

as the function of the scaling variable θ. Once again, all the curves collapse in accordance with Eq. (4.8). The function $G_1^{(1)}$ approaches the asymptotic value within statistical errors. The collapse of the data at $\theta\to 0$ justifies the order-of-magnitude estimate that led to Eq. (4.17). For the Heisenberg case Eq. (4.15) predicts the following high-θ behavior:

$$G_2^{(1)}(\theta)=1.25\sqrt{\theta\beta}+0.858\beta+0.190+O\left(\frac{1}{\sqrt{\theta}}\right). \tag{5.10}$$

The best-fit lines are described by

$$G_2^{(1)}(\theta)=(1.171\pm 0.006)\sqrt{\theta\beta}+(0.54\pm 0.01)\beta +(0.29\pm 0.03). \tag{5.11}$$

Again the results agree up to $O(\mu)$ in the slope and $O(1/\sqrt{\theta})$ in the intercept. There are downward deviations for the smallest μ at high temperature. They are likely due to the finite-size effects (the magnetization becomes too close to its maximal value $S=500$ determined by the size of the RM). As a result the scaling is violated.

As a matter of fact, the scaling is violated when μ is too small or too large. At large μ the typical ground-state spin becomes of the order of unity and the condition $S\gg 1$, used throughout this paper, no longer holds. As μ decreases, the magnetization becomes of the order of the system size, $S\approx 500$, whereas in making arguments about scaling we assumed no upper bound on the value of S. Therefore, in obtaining the numerical values for the scaling functions at $\theta\to 0$, we used the values of μ that correspond to the ground-state magnetization S_g from ~ 15 to ~ 150 hundreds. The linear interpolation of the numerical curves at $\theta\to 0$ results in the following values for the low-temperature asymptotics of the scaling functions $G^{(1)}$, Eq. (4.8):

$$G_1^{(1)}(0)=0.256\pm 0.005,\quad G_2^{(1)}(0,\beta=1)=1.60\pm 0.01, \quad G_2^{(1)}(0,\beta=2)=2.65\pm 0.01. \tag{5.12}$$

In the Ising case the slope of this function can be determined rather well:

$$\frac{dG_1^{(1)}}{d\theta}=-0.7\pm 0.1, \tag{5.13a}$$

whereas evaluation of this slope in the Heisenberg case requires much better statistics. From what we had it follows that

$$\frac{dG_2^{(1)}(\beta=1)}{d\theta}=0.1\pm 0.2,\quad \frac{dG_2^{(1)}(\beta=2)}{d\theta}=0.2\pm 0.3. \tag{5.13b}$$

Even though the values of the slope are smaller than the statistical errors, we do know the behavior of S^2 at low temperature. The smallness of the slope just means that the change of magnetization squared with temperature is only slightly different from the one predicted by the high-T expansion. Using Eqs. (5.13a), (5.13b), and Eqs. (4.23), we conclude that

$$\langle S_g^2\rangle^I=(0.256\pm 0.005)\frac{\delta_1^2}{\beta\mu^2}, \tag{5.14a}$$

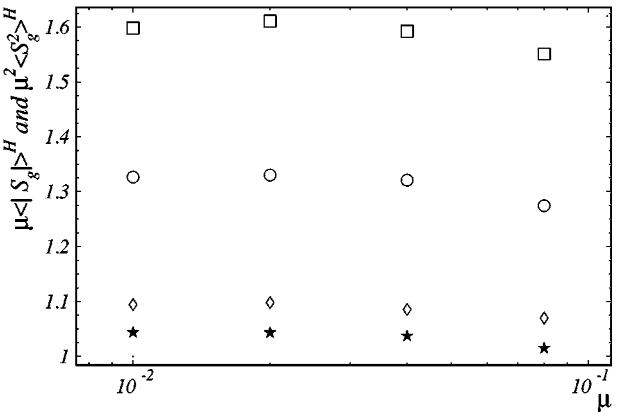

FIG. 6. □ (○) represents $\langle\mu^2 S_g^2\rangle^H$ for $\beta=1$ (2). ◇ (★) represents $\langle\mu|S_g|\rangle^H$ for $\beta=1$ (2). All data are for the Heisenberg ($\xi=2$) case. Without disorder the relation $\langle\mu^2 S_g^2\rangle=\langle\mu|S_g|\rangle=1$ holds (δ_1 is set to 1).

$$\langle S_g^2\rangle^H_{\beta=1}=(1.60\pm 0.01)\frac{\delta_1^2}{\mu^2},\quad \langle S_g^2\rangle^H_{\beta=2}=(1.33\pm 0.01)\frac{\delta_1^2}{\mu^2}, \tag{5.14b}$$

and

$$\left\langle\frac{1}{\mu_r}\right\rangle=\frac{1}{\mu}\begin{cases}0.3\pm 0.1, & \xi=1\\ 0.7\pm 0.1, & \xi=2.\end{cases} \tag{5.15}$$

Figure 6 illustrates the behavior of the averaged and rescaled zero-temperature magnetization $\mu\langle|S_g|\rangle^H$ and its square $\mu^2\langle S_g^2\rangle^H$ in the Heisenberg case. The magnetization squared $\langle S_g^2\rangle^H$ is well described by Eq. (4.19) with the numerical constant $a\approx 0.6$. The contribution from disorder to the averaged magnetization $\langle|S_g|\rangle^H$ is an order of magnitude smaller than the magnetization itself. Without disorder $[V(S)=0]$ the magnetization is the same for all grains $S_g=1/\mu$ [Eq. (3.8)]. The correction due to randomness is around 9% in the orthogonal $\beta=1$ and 4% in the unitary $\beta=2$ case.

VI. CONCLUSIONS

We considered manifestations of electron-electron interactions in the properties of isolated metallic grains with large Thouless conductance, $g\gg 1$. It turned out that the interaction effects can be taken into account by a rather simple interaction Hamiltonian (2.19). We then applied this description to study the mesoscopic spontaneous magnetization of the metallic grains whose bulk counterparts are only slightly below the point of Stoner instability. In this case the problem maps onto the random potential problem, Eq. (3.8), where the total spin of the system plays the role of the coordinate. The randomness is manifested by the potential $V(S)$ and is entirely due to the fact that *the one-electron spectrum* in such a grain is sample specific. At the same time, the fluctuations of the exchange interaction constant can be neglected provided that $g\gg 1$.

The correlation function (3.11) of the random potential $V(S)$ follows directly from the Wigner-Dyson spectral statistics and possesses a specific invariance (4.1) under scaling transformations. This invariance dictates a particular scaling of the ensemble averaged thermodynamic properties of the grains as well as of the higher moments of their mesoscopic fluctuations. Dependence of all these quantities on temperature T and on the distance from the point of Stoner instability μ can be determined, see Eqs. (4.5), (4.8), and (4.9), up to some functions of the dimensionless effective temperature $\theta=\beta\mu T$, where $\beta=1$ (2) corresponds to the orthogonal (unitary) Dyson ensemble.

According to Eq. (4.8), in the Ising case the zero-temperature magnetization typically gets reduced by a factor of $\sqrt{2}$ when the system is driven from $\beta=1$ to $\beta=2$. In the Heisenberg case the average zero-temperature magnetization is largely determined by the nonrandom part of the Hamiltonian (3.8) (without disorder $S_g=1/\mu$). The fluctuations of the magnetization become suppressed by a factor of $\sqrt{2}$ as the system goes from the orthogonal to the unitary ensemble. If the grains are large enough, the transition between these ensembles can be completed in magnetic fields, which produce still negligible Zeeman splitting. As a result, an anomalously weak magnetic field would substantially *reduce* the spontaneous magnetization in the Ising case or suppress its fluctuations in the Heisenberg one. This is due to the well-known fact that the unitary spectra are more rigid than orthogonal ones. However, the difference between the average magnetization with and without disorder is about 9% for orthogonal ($\beta=1$) and 4% for unitary ($\beta=2$) ensembles (see Fig. 6) in the Heisenberg case. Therefore, in the Heisenberg case a small magnetic field should suppress the average magnetization by only 5%. This is a much smaller effect than the one predicted in Ref. 3. The discrepancy is due to erroneous choice of the model Hamiltonian in that reference [see the discussion in Sec. II after Eq. (2.21)].

Of course, the evaluation of the scaling functions lies beyond the simple analysis. In the high-temperature regime it is possible to develop a regular perturbative expansion. At low temperature an analytic technique based on the replica symmetry breaking paradigm can be used. The corresponding calculation will be reported elsewhere.[5]

In the present paper, we analyzed the low-temperature asymptotic behavior numerically. We have shown that these asymptotics are determined by a single absolute minimum of a random potential (not accessible by a regular perturbation theory). Using those numerical results, we were able to determine the average position and curvature for such minima, see Eqs. (5.12) and (5.13b).

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