Itinerant Ferromagnetism in Disordered Metals: A Mean-Field Theory

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We develop a mean-field approach to interacting disordered systems of itinerant electrons based on a statistical treatment of disorder enhanced Hartree-Fock interactions. We demonstrate that for $d \leq 2$ a disordered system may exhibit a finite temperature partial spin polarization even if its clean analog is paramagnetic. The disorder and temperature dependent magnetization and spin susceptibility are calculated. Possible relevance to recent experiments on quantum dots is discussed. [S0031-9007(98)07325-6]

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The study of thermodynamic and transport properties of disordered systems of interacting electrons has been the subject of extensive theoretical and experimental work (see Refs. [1,2] for a review). One of the most interesting aspects of the problem, which attracted much attention in the past [3–5], is the existence and the nature of the itinerant ferromagnetism in such systems.

In metals the long range part of the Coulomb interaction is screened. Its short range part, however, leads to strong correlations of the electron liquid, and is frequently studied within the framework of the Hubbard model with a short range pulsive interaction $U\delta(\vec{r} - \vec{r}')$. In clean metals that short range part of the interaction leads to ferromagnetic (Stoner) instability at sufficiently large values of the interaction strength (see, for example, Ref. [6]). The particular details depend on the band spectrum. In general, the instability with respect to a formation of a spin-polarized state occurs when the dimensionless interaction strength $V = \nu_d U \approx 1$ (the Stoner criterion), where ν_d is a density of states at the Fermi level. The physical mechanism behind the instability is analogous to the familiar from atomic physics Hund's rule. For strong interactions the energy gain due to the exchange interaction in a spin-polarized state exceeds the loss in the kinetic energy. The former is proportional to the interaction matrix element between two wave functions close to the Fermi surface $V^{\alpha\beta} \approx U \int d\vec{r} |\phi_\alpha(\vec{r})|^2 |\phi_\beta(\vec{r})|^2$, the latter to the mean level spacing, $\Delta \propto \nu_d^{-1}$. In a clean metal the wave functions are plane waves, which immediately leads to the Stoner criterion.

In disordered metals the interaction matrix element between wave functions which are close in energy is enhanced due to the increased return probability and may satisfy the instability criterion for a weaker bare interaction. This can be interpreted as an effective increase of the interaction strength due to the fact that the particles spend more time together if their motion is diffusive [1,2]. This effect is especially strong in low dimensions, $d \leq 2$, since the integrated return probability diverges in the long time (low frequency) limit. These infrared divergences are cut off either by the system size, L, or by the temperature, T, and lead to diverging perturbative corrections to various physical observables. For example, the first order interaction correction $\delta\chi_s$ to the Pauli spin susceptibility, χ_{s0}, for $d = 2$ is [1]

$$\frac{\delta\chi_s}{\chi_{s0}} = \frac{V}{4\pi^2 g} \ln\left(\frac{\min\{L, L_T\}}{l}\right). \tag{1}$$

Here $g = 2\nu_2 D > 1$ is the dimensionless conductance (in units $e^2/\hbar$), D is the diffusion constant, and l is the elastic mean-free path [7]. We denote $L_T = \sqrt{D/T}$. In $d < 2$ dimensions Eq. (1) takes the form $\delta\chi_s/\chi_s \sim L_T^{2-d}/\nu_d D$. Being perturbative, Eq. (1) cannot be trusted once $Vg^{-1} \ln L_T/l > 1$ and thus does not describe the susceptibility at a very low temperature. The renormalization group approach [8] shows the tendency towards a creation of a spin-polarized state.

Below, we develop a simple mean-field theory which demonstrates that a low dimensional disordered system may develop a finite temperature spin polarization for substantially weaker interaction strength than its clean counterpart. This implies divergence of the spin susceptibility, χ_s, at a disorder-dependent temperature, T_c, below which the system is ferromagnetic. The key ingredient of our approach is utilization of the exactly known (apart from the Anderson localization corrections) statistical properties of the interaction matrix elements, $V^{\alpha\beta}$. Similarly to $\delta\chi_s$ [Eq. (1)] they contain factors $g^{-1} \ln L/l$ at $d = 2$ (or $L^{2-d}/\nu_d D$ at $d < 2$). However, in the case of the matrix elements these factors may be trusted even if they are not small. This statement originates from the relation between the matrix elements and the integrated return probability. The latter may be indeed essentially large in $d \leq 2$ if the waiting time is long enough. Let us emphasize that we deliberately restrict ourselves to a treatment of the finite size systems. Therefore we do not discuss a true thermodynamic phase transition. The limitation stems from the fact that we disregard the onset of the Anderson localization. As a result, the possible system size is limited by the localization length (in $d = 2$, this is not actually a strong limitation, if the

unitary case is considered). We also disregard fluctuation effects since for the system size, considered here, they do not destroy the mean field solution. The role of localization and fluctuations in establishing the nature of the true thermodynamic low-temperature phase is beyond the scope of this paper. Nevertheless, the discussed "transition" gives definite predictions for the experimental samples, such as large chaotic quantum dots [9].

Consider a system of interacting electrons in a random disorder potential. One can expand the electron field operator in terms of exact single electron eigenfunctions for a given disorder configurations, $\phi_\alpha(\vec{r})$, as $\Psi_\sigma(\vec{r}) = \sum_\alpha a_{\alpha\sigma}\phi_\alpha(\vec{r})$, here $\sigma = \uparrow, \downarrow$ is the electron spin. For convenience we measure all energies in units of Δ. If we neglect the electron-phonon interaction the Hamiltonian of such a system may be written as (cf. Ref. [10])

$$H = \sum_{\alpha\sigma} \epsilon_\alpha a^\dagger_{\alpha\sigma} a_{\alpha\sigma} + \frac{1}{2} \sum V^{\alpha\beta}_{\gamma\delta} a^\dagger_{\alpha\sigma} a^\dagger_{\beta\sigma'} a_{\gamma\sigma'} a_{\delta\sigma}\,, \tag{2}$$

where the summation in the second term runs over all repeated indices. Both the interaction matrix elements, $V^{\alpha\beta}_{\gamma\delta} = \Delta^{-1} \int d\vec{r} d\vec{r}\,' V(\vec{r} - \vec{r}\,')\phi^*_\alpha(\vec{r})\phi^*_\beta(\vec{r}\,')\phi_\gamma(\vec{r}\,')\phi_\delta(\vec{r})$, and the single electron energies, ϵ_α, are random. To characterize the system one needs to know their statistics. Employing the powerful tools of treating noninteracting disordered systems, one may demonstrate that the following statistical properties of the interaction matrix elements are true [10–12]: (i) The probability distribution function of the random quantity $V^{\alpha\beta}_{\gamma\delta}$ is sharply peaked near its average value. The relative width of the distribution is $1/g \ll 1$. (ii) The only matrix elements which have nonzero mean value are $V^{\alpha\beta}_{\alpha\beta}$ and $V^{\alpha\beta}_{\beta\alpha}$. Their mean (disorder-averaged) values are [11]

$$\langle V^{\alpha\beta}_{\alpha\beta} \rangle = V(0) + V(k_F) \mathrm{Re}\,\mathrm{Tr}\,\hat{D}(\epsilon_\alpha - \epsilon_\beta)\,, \tag{3a}$$

$$\langle V^{\alpha\beta}_{\beta\alpha} \rangle = V(k_F) + V(0) \mathrm{Re}\,\mathrm{Tr}\,\hat{D}(\epsilon_\alpha - \epsilon_\beta)\,, \tag{3b}$$

where $V(0)$ and $V(k_F)$ are slow and fast components of the screened interaction potential, correspondingly. We shall assume that $V(0) > V(k_F)$. The trace of the diffusion propagator represents the classical return probability and is given by

$$\mathrm{Re}\,\mathrm{Tr}\,\hat{D}(\omega) = \frac{1}{\pi\nu_D} \mathrm{Re} \int \frac{d^d q}{(2\pi)^d} \frac{1}{Dq^2 - i\omega} = \frac{1}{\pi^2 g} \ln L_\omega / l\,, \tag{4}$$

where $L_\omega = \sqrt{D/|\omega|}$ [7]. In $d < 2$ the corresponding expression is $L_\omega^{2-d}/(\nu_d D)$. We stress again that the validity of Eqs. (3) and (4) is *not* restricted to the frequency range where $g^{-1} \ln L_\omega / l < 1$, but is extended even to much smaller frequencies. For a finite size system the increase of the matrix elements is eventually saturated at $\omega \approx E_c = D/L^2$.

Based on the above mentioned statistics of the matrix elements, we shall adopt the following approximations: we disregard all matrix elements except $V^{\alpha\beta}_{\alpha\beta}$ and $V^{\alpha\beta}_{\beta\alpha}$, which we shall treat as nonrandom (deterministic) given by their mean values [Eq. (3)]. As a result, one obtains the following truncated Hamiltonian:

$$\tilde{H} = \sum_\alpha (\epsilon_\alpha \hat{n}_\alpha - \vec{H}^0 \hat{\vec{s}}_\alpha) + \frac{1}{2} \sum_{\alpha\beta} (V_s^{\alpha\beta} \hat{n}_\alpha \hat{n}_\beta - V_t^{\alpha\beta} \hat{\vec{s}}_\alpha \hat{\vec{s}}_\beta)\,, \tag{5}$$

which is written in terms of the charge, $\hat{n}_\alpha = \sum_\sigma a^\dagger_{\alpha\sigma} a_{\alpha\sigma}$, and spin, $\hat{\vec{s}}_\alpha = \sum_{\sigma\sigma'} a^\dagger_{\alpha\sigma} \vec{\sigma}_{\sigma\sigma'} a_{\alpha\sigma'}$, operators of a state α. The singlet and triplet interaction matrix elements are defined as $V_s^{\alpha\beta} = \langle V^{\alpha\beta}_{\alpha\beta} \rangle - 1/2 \langle V^{\alpha\beta}_{\beta\alpha} \rangle$ and $V_t^{\alpha\beta} = 1/2 \langle V^{\alpha\beta}_{\beta\alpha} \rangle$, correspondingly. Finally, $\vec{H}^0$ is an external magnetic field (in units of the Bohr magneton times the Lande factor). The truncated Hamiltonian [Eq. (5)] fully accounts for the disorder-enhanced interactions on the Hartree-Fock level. It is sufficient for developing a mean-field theory of the ferromagnetic transition. The subsequent calculations do not contain any essential approximations.

To calculate the grand canonical partition function $Z(\beta, H^0) = \mathrm{Tr} \exp\{-\beta(\tilde{H} - \mu\hat{N})\}$ (here Tr denotes trace over the Hilbert space of the system, and β is the inverse temperature), one may write it as an imaginary time fermionic path integral [13]. We then decouple the singlet and triplet interaction terms by means of the Hubbard-Stratonovich transformation introducing the auxiliary boson fields Φ_α and $\vec{H}_\alpha$. These fields have the clear physical meaning of the effective scalar potential and the exchange magnetic field, correspondingly. Aiming to develop an effective mean-field theory of the finite temperature transition, we concentrate on the zero Matsubara component of these fields only. After this transformation the fermionic integrals for different states α may be performed separately. As a result one obtains

$$Z(\beta, H^0) = \int D\vec{H} D\Phi \exp\{-S[\vec{H}, \Phi]\}\,, \tag{6}$$

where the effective bosonic action is given by

$$S[\vec{H}, \Phi] = \frac{\beta}{2} \sum_{\alpha,\beta} \{\Phi_\alpha (\tilde{V}_s^{-1})^{\alpha\beta} \Phi_\beta + \vec{H}_\alpha (V_t^{-1})^{\alpha\beta} \vec{H}_\beta\} - \sum_\alpha \{\ln[1 + \exp(-\beta\xi_{\alpha\uparrow})] + \ln[1 + \exp(-\beta\xi_{\alpha\downarrow})]\}\,. \tag{7}$$

Here the effective quasiparticle energies are introduced as

$$\xi_{\alpha\uparrow,\downarrow} \equiv \epsilon_\alpha - \mu + \Phi_\alpha \mp |\vec{H}_0 + \vec{H}_\alpha|\,. \tag{8}$$

In what follows we substitute energy summations by integration and neglect fluctuations of the single particle density of states, $\Delta^{-1}(\epsilon) = \sum_\alpha \delta(\epsilon - \epsilon_\alpha)$. This is justified, since all of the important effects take place on a scale much larger than Δ. The interaction matrix elements are functions of energy differences only, given by Eqs. (3) and (4). Since the total charge is a conserved quantity, the constant part of $V_s^{\alpha\beta}$ can be omitted. We have thus introduced $\tilde{V}_s(\epsilon) \equiv V_s(\infty) - V_s(\epsilon)$. Then the operators $\tilde{V}_s$ and V_t are both positively defined, which validates the use of the Hubbard-Stratonovich transformation.

The long range (in the energy direction) coupling of the bosonic Φ and $\vec{H}$ fields allows us to evaluate the functional integral in Eq. (6), by a saddle point approximation. Expanding the second term on the right-hand side (r.h.s.) of Eq. (7) up to the second order in the bosonic fields, one finds that the resulting quadratic form in $\vec{H}_\alpha$ has negative eigenvalues at sufficiently low temperatures [14]. Thus, the trivial extremum, $\Phi_\alpha = \vec{H}_\alpha = 0$, is unstable and one should search for another minimum. We look for the minimum of the action [Eq. (7)] of the form $H_{\alpha,x} = H_{\alpha,y} = 0$; $H_{\alpha,z}$, $\Phi_\alpha \neq 0$. The saddle point equations read as

$$\Phi(\epsilon) = -\int_{-\infty}^{\infty} d\epsilon' \tilde{V}_s(\epsilon - \epsilon')[f_T(\xi_\uparrow(\epsilon')) + f_T(\xi_\downarrow(\epsilon'))], \tag{9a}$$

$$H_z(\epsilon) = \int_{-\infty}^{\infty} d\epsilon' V_t(\epsilon - \epsilon')[f_T(\xi_\uparrow(\epsilon')) - f_T(\xi_\downarrow(\epsilon'))]. \tag{9b}$$

Here $f_T(z) = [1 + \exp(\beta z)]^{-1}$ is the Fermi function. For the ground state solution of Eqs. (8) and (9), $\xi_{\uparrow/\downarrow}(\epsilon)$ are monotonically increasing functions of energy. We denote the points where quasiparticle energies cross zero as $\mu_{\uparrow/\downarrow}$; correspondingly, $\xi_{\uparrow/\downarrow}(\mu_{\uparrow/\downarrow}) = 0$. These quantities play the role of Fermi energies of spin up and down electrons, correspondingly. The difference between them, $\delta\mu \equiv \mu_\uparrow - \mu_\downarrow$, is the width of the magnetized energy strip, which plays a role of the order parameter. Employing Eq. (8) one obtains the following self-consistency conditions:

$$\delta\mu + \Phi(\mu_\uparrow) - \Phi(\mu_\downarrow) = 2H^0 + H_z(\mu_\uparrow) + H_z(\mu_\downarrow). \tag{10}$$

A further simplication stems from the fact that the Fermi function at low temperatures rapidly changes from zero to unity in the narrow region of $\xi_{\uparrow/\downarrow}$ around zero. Therefore in the region of interest one can approximate $\xi_{\uparrow/\downarrow}(\epsilon) \approx (\epsilon - \mu_{\uparrow/\downarrow})\partial\xi_{\uparrow/\downarrow}/\partial\epsilon|_{\mu_{\uparrow/\downarrow}}$ leading to

$$f_T(\xi_{\uparrow/\downarrow}(\epsilon)) \approx f_{T^*}(\epsilon - \mu_{\uparrow/\downarrow}), \tag{11}$$

where the effective temperature, T^* [15], is defined as $T/T^* \equiv \partial\xi_{\uparrow/\downarrow}/\partial\epsilon|_{\mu_{\uparrow/\downarrow}}$, and is to be determined self-consistently from Eqs. (8), (9), and (11). The effective temperature accounts for the interaction induced increase of the mean level spacing near the Fermi surface [1,2]. Substituting Eqs. (9) into Eq. (10) one finally obtains the self-consistency equation for the order parameter, $\delta\mu(T)$:

$$\delta\mu - 2H^0 = \int_{-\infty}^{\infty} d\omega[V_t(\omega) - \tilde{V}_s(\omega)] \times [f_{T^*}(\omega - \delta\mu) - f_{T^*}(\omega + \delta\mu)], \tag{12}$$

According to Eqs. (3), $V_t - \tilde{V}_s = V(k_F)[1/2 + \mathrm{Re}\,\mathrm{Tr}\,\hat{D}(\omega)]$. As may be expected, only the fast component of the interaction potential, $V(k_F)$, is relevant. Employing Eq. (4) [7], one finds for zero temperature (and zero external field) magnetization in $d = 2$

$$\delta\mu(T = 0) = \epsilon_F \exp\{-\pi^2 g[V^{-1}(k_F) - 1]\}. \tag{13}$$

This result means that even below the Stoner criterion, $V(k_F) < 1$, the ground state is spin polarized. The condition $\delta\mu(T = 0) > E_c$ dictates the minimum system size to have this effect. For $d < 2$ one obtains $\delta\mu(T = 0) \approx \Delta_\xi[1/V(k_F) - 1]^{2/(d-2)}$, where $\Delta_\xi = (\nu_d \xi^d)^{-1}$ and $\xi^{2-d} = \nu_d D$.

To determine the susceptibility above the critical temperature we expand the Fermi functions on the r.h.s. of Eq. (12) to the first order in $\delta\mu$ to obtain a linear dependence of the order parameter $\delta\mu$ on H^0, $\delta\mu = \chi_s(T^*)H^0$ with

$$\chi_s(T^*) = 2\left(1 - V(k_F) - \frac{V(k_F)}{\pi^2 g} \ln\frac{\tilde{\epsilon}_F}{T^*}\right)^{-1}, \tag{14}$$

where $\tilde{\epsilon}_F = \epsilon_F 2e^C/\pi$, C is the Euler constant. One thus obtains the mean-field exponent: $\chi_s \sim (T^* - T_c^*)^{-1}$, where the critical temperature, $T_c^* \approx 1.13 \times \delta\mu(T = 0)$. At high temperature, $T \gg T_c$, one can expand Eq. (14) to the first order in $1/g$ to obtain the well-known logarithmic correction to the Pauli susceptibility [cf. Eq. (1)]. Below T_c the system develops a spontaneous magnetization. Expanding the r.h.s. of Eq. (12) to the third order in $\delta\mu$, one obtains, for $T_c - T \ll T_c$,

$$\delta\mu(T^* < T_c^*) = \sqrt{12\pi^2 T_c^*(T_c^* - T^*)/[7\zeta(3)]}. \tag{15}$$

Finally, using Eqs. (8), (9), and (11) one can find the relation between T^* and T. This expression in the vicinity of the critical temperature and at low temperature can be written in a unified way as

$$T = T^*\left(1 + \frac{V(0) - \alpha V(k_F)}{4\pi^2 g} \ln\frac{\tilde{\epsilon}_F}{\pi T^*}\right), \tag{16}$$

where $\alpha = 1$ for $T \ll T_c$ and $\alpha = 2$ for $T \geq T_c$.

In summary, we have presented a mean-field theory of the ferromagnetic instability in disordered low dimensional ($d \leq 2$) metals. Our approach is based on the statistical treatment of interaction matrix elements between disordered wave functions. The Stoner instability for a disordered metal develops at a finite temperature even if the clean counterpart remains paramagnetic. This tendency towards the formation of the ferromagnetic

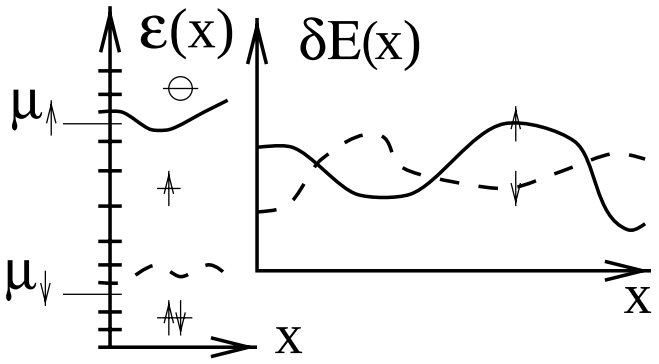

FIG. 1. Schematic drawing of electron energy levels ϵ_i in a dot as a function of magnetic field or gate voltage. For clarity, only the lowest unoccupied (solid line) and singly occupied (dashed line) states are drawn fully. Inset: Addition energies $\delta E(x)$ for spin up and spin down electrons (the position of the Coulomb blockade peak always corresponds to the lower of the two energies).

state originates from the effective enhancement of interactions due to diffusive dynamics of electrons. Let us emphasize that the electrons contributing to the spin polarization are described by typical metallic wave functions which are extended throughout the sample. This should be contrasted with the Griffiths instability scenario [4], in which local moments are attributed to electrons in localized states, and the global magnetization is formed because of interactions between them. The treatment of spin-wave and quantum fluctuations requires the analysis of the neglected off-diagonal interaction matrix elements and is beyond the scope of this paper. We want to point out, however, that for a finite system fluctuations should not invalidate the mean-field results as in the case of the Mermin-Wagner theorem, and our approach is a useful starting point. If the spin-orbit interaction promotes an easy axis ferromagnetic state, then the Goldstone modes acquire a finite gap, and their influence on thermodynamic quantities is further diminished.

The predicted effect may have implications for the experiments on the Coulomb blockade in large chaotic quantum dots [9]. Depending on the proximity to the Stoner criterion and the size of the dot, the ground state may have a certain strip ($\delta\mu \geq E_c$) of spin-polarized states (Fig. 1). In that case the addition spectrum of the dot is formed by two practically uncorrelated (since $\delta\mu \gg \Delta$) Wigner-Dyson sequences of levels. In particular, one should not expect to observe any spin degeneracy (bimodal distribution of Coulomb peak spacings) in the addition spectra—in agreement with the experiment [9]. Indeed, subsequent electrons tunneling into the dot with up and down spin are to occupy distinct states separated by $\delta\mu$. Since the lowest available states for up and down electrons are essentially distinct, they exhibit different dependences on an external parameter (e.g., flux). Thus, the actual trajectory of the Coulomb peak appears to be composed of two or more intersecting single-particle states (see the inset of Fig. 1). As a result, two subsequent Coulomb peaks, upon subtraction of the charging energy (Ref. [9]) are expected to have actual (not avoided) crossings in approximately half of the events. This also modifies the peak position correlation function in a qualitative agreement with experiment [9]. The direct measurement of the dot magnetization may verify our suggestion. The proposed effect could be also observed in thin films or wires of materials which are incipient Stoner ferromagnets in the clean case.

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