Spin-Fermion model of \textit{U}Ge$_2$

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It is assumed that \textit{U} atoms in \textit{U}Ge$_2$ have a number of \textit{f} electrons appropriate to give them each a spin $s = 1$ as well as one extra itinerant electron which may equally well be on one or other \textit{U} atom. The dynamical degrees of freedom are spin-$s$ operators of localized spins and spin-$1/2$ fermi operators of itinerant electrons. Applying hydrostatic pressure changes the bandwidths of spin-up and spin-down itinerant electrons in different way, which leads to decreasing of the contribution of the fermions to the magnetization keeping the spin-fermion interaction unchanged. In turn the local spin-fermion interaction leads to ferromagnetic superconductivity. The model accounts, in a quantitative and natural way, for the characteristics of the coexistence of superconductivity and ferromagnetism in \textit{U}Ge$_2$, including many of the key experimental results: metamagnetic transitions, quantum transition from ferromagnetism to ferromagnetic superconductivity, the position of the highest superconducting critical temperature etc.

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\textit{U}Ge$_2$ is the first example where ferromagnetism and superconductivity coexist\textsuperscript{1, 2}. The superconductivity is found experimentally only in ferromagnetic phase, and only in a limited pressure range($p_x, p_c$). There are two successive quantum phase transition, from ferromagnetism to ferromagnetic superconductivity at $p_x$, and at higher pressure $p_c$ to paramagnetism (fig1a).

As the pressure is increased there is an abrupt decrease of the ordered moment at $p_x$ ($p_x < p < p_c$) and another at $p_c$ (fig1b). The ferromagnetic state below $p_x$ is referred to as FM2 and the high pressure ferromagnetic state as FM1\textsuperscript{3}. It has been suggested that a spin and charge density wave might be formed in the FM2 state, due to the nesting of the Fermi surface, and they are responsible for the transition at $p_x$\textsuperscript{4}. However, neutron diffraction studies have not detected any static order due to a spin and charge density wave. Another possibility is that the transition at $p_x$ is a result of a novel tuning of the Fermi surface topology by the magnetization\textsuperscript{5}.

The temperature dependence of the magnetization in \textit{U}Ge$_2$ is quite different from that found in weak itinerant ferromagnets. At zero pressure, above and well away from $p_x$ the low temperature dependence of the magnetization has the form $M(T) = M(0) \sim [1 - (T/T_c)^{3}]^{1/2}$\textsuperscript{6}. Strictly speaking, \textit{U}Ge$_2$ is not a weak itinerant ferromagnet, and the point where ferromagnetism and superconductivity disappear simultaneously is not a quantum critical point at all. The Curie temperature $T_c$ decreases while the magnetization remains unchanged. For conventional weak ferromagnets the Curie temperature scales with magnetization. \textit{U}Ge$_2$ differs mainly in having a stronger spin orbit interaction that leads to an unusually large magneto-crystalline anisotropy with easy magnetization axis along shortest crystallographic axis. The differential susceptibility has been measured, since it gives a measure of the spectrum of the magnetic excitations. The main conclusion is that the differential susceptibility is strongly anisotropic in the high pressure FM1 and paramagnetic phases but weakly anisotropic in the low pressure FM2 phase\textsuperscript{7}. It is plausible that increasing the pressure, one changes the anisotropy, which in turn shifts the system from itinerant behaviour to a higher pressure phase which is dominated by localized spins.

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{fig1.png}
\caption{(a)The $p$-$T$ phase diagram of \textit{U}Ge$_2$. $T_c$ is Curie temperature, $T_s$ is the superconducting transition temperature.(b) Pressure dependence of the dimensionless magnetization per lattice site.}
\end{figure}

So far, there are no theoretical considerations of these complicated phenomena. The calculations have considered the superconductivity to appear from completely itinerant ferromagnet state\textsuperscript{7, 8, 9, 10}, or have been based on the physics of local moments\textsuperscript{2, 11}. Motivated by the experimental findings, one assumes that \textit{U} atoms in \textit{U}Ge$_2$ have a number of \textit{f} electrons appropriate to give them each a spin $s = 1$ as well as one extra itinerant electron which may equally well be on one or other \textit{U} atom. The dynamical degrees of freedom are spin-$s$ spin operators $S_i$ of localized spins and spin-$1/2$ fermi operators $c_{i\sigma}$ of itinerant electrons, where $i$ denotes the sites of a three dimensional lattice. The dimensionless magnetization $M = \mu/\mu_B$ of the system per lattice site at zero temperature is $M = s + m$ where $m$ is the contribution of mobile electrons. The parameter $m$ de-
pends on the microscopic parameters of the theory and characterizes the vacuum. If, in the vacuum state, every lattice site is occupied by one electron with spin up, then $m = 1/2$, and the electrons are highly localized as in the uranium compounds known as "heavy-fermion systems". When, in the vacuum state, some of the sites are doubly occupied or empty, then $m < 1/2$ and the electrons are itinerant. The system approaches the internal point (IP) when $m \to 0$ ($M = s$). It corresponds to the point $p_x$ of the phase diagram of $UGe_2$ (fig1).

The local spin-fermion interaction leads to an effective four-fermion interaction which in turn leads to p-type magnon-induced ferromagnetic superconductivity (FM-superconductivity)\[8\]. The order parameter is a spin anti-parallel component of a spin-1 triplet with zero spin superconductivity. It splits the spin-up and spin-down Fermi surfaces and leads to a nonzero contribution of itinerant electrons to the magnetization. Driving the system to the internal point (IP) one has to compensate this overall shift in the relative position of the energy bands keeping the spin-fermion interaction unchanged. In this paper a mechanism of compensation by means of different changes in bandwidths of spin-up and spin-down electrons is considered. The Hamiltonian of the spin-fermion model is

$$\hat{H} = -J \sum_{<i,j>} \hat{S}_i \cdot \hat{S}_j - J' \sum_{<i,j>} \hat{S}_z^i \hat{S}_z^j - J_l \sum_i \hat{S}_i \cdot \hat{s}_i - t \sum_{<i,j>,\sigma} \left( \hat{c}_{i\sigma}^+ \hat{c}_{j\sigma} + \text{h.c.} \right) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \mu \sum_i \hat{n}_i + F \sum_{<i,j>} \left( \hat{c}_{i\uparrow}^+ \hat{c}_{i\downarrow}^+ \hat{c}_{j\uparrow} \hat{c}_{j\downarrow} + \text{h.c.} \right) \quad (1)$$

Here $\hat{c}_{i\sigma}^+$ and $\hat{c}_{i\sigma}$ are creation and annihilation operators for itinerant electrons, $\hat{n}_{i\sigma} = \hat{c}_{i\sigma}^+ \hat{c}_{i\sigma}$ are density operators, $\hat{s}_i = 1/2 \sum_{\sigma\sigma'} \hat{c}_{i\sigma}^+ \hat{c}_{i\sigma'}$, where $\sigma$ denotes the vector of Pauli matrices, are the spin operators of itinerant electrons, and $\hat{S}_i$ are spin-s operators of localized spins. The sums are over all sites of a three-dimensional lattice, $<i,j>$ denotes the sum over the nearest neighbors, and $\mu$ is the chemical potential. In (1) the $J$-term corresponds to a direct Heisenberg exchange of localized spins which is ferromagnetic ($J > 0$). The magnitude of the magnetocrystalline anisotropy is given by $J'$. Here I focus on uniaxial anisotropy, $J' > 0$, with the easy axis of magnetization along the $z$ axis. The local spin-fermion interaction is ferromagnetic, too ($J_l > 0$), and the $F$-term describes the hopping of local pairs consisting of spin-up and spin-down electrons ($F > 0$)\[1\].

Still, the question remains whether the off-diagonal hopping parameters in the Hamiltonian, which involve orbital overlaps between neighbouring sites, would be sufficiently large in view of the fact that $U - f$ orbitals are well localized. One expects that hybridization between Ge electrons and $U - f$ electrons which gives an itinerant character to the $f$-electrons, leads to larger overlaps than pure $f$ orbitals.

I introduce Schwinger representation for the localized spin operators $\hat{S}_i = 1/2 \sum_{\sigma\sigma'} f_{i\sigma\sigma'}^+ f_{i\sigma\sigma'}$, where the boson operators satisfy the condition $f_{i\sigma\sigma'}^+ f_{i\sigma\sigma'} = 2s$. The partition function can be written as a path integral over the complex functions of the Matsubara time $\tau$, $f_{\sigma\sigma}^\dagger(\tau)$, $f_{\sigma\sigma}(\tau)$ and Grassmann functions $c_{\sigma\uparrow}(\tau)$ and $c_{\sigma\downarrow}(\tau)$ replacing the operators in the Hamiltonian Eqs\[1\] with the functions\[12\]. In terms of Schwinger bosons the theory is $U(1)$ gauge invariant, where the boson fields have a charge 1, with respect to gauge transformations, while the fermi fields are gauge invariants.

It is convenient to introduce two spin-singlet fermi
fields
\[
\Psi_i^A(\tau) = \frac{1}{\sqrt{2s}}[f_{i1}(\tau)c_{i2}(\tau) - f_{i2}(\tau)c_{i1}(\tau)]
\]
\[
\Psi_i^B(\tau) = \frac{1}{\sqrt{2s}}f_{i\sigma}^+(\tau)c_{i\sigma}(\tau)
\]
which are gauge variant with charge 1 and -1 with respect to gauge transformations. Equations (2) can be regarded as a SU(2) transformation and the Fermi measure is invariant under the change of variables. An important advantage is the fact that in terms of the spin-singlet fields the spin-fermion interaction is diagonalized for it exactly. The total spin of the system \(S_i^{tot} = S_i + s_i\) can be rewritten in the form
\[
S_i^{tot} = \frac{1}{s} \left[ s + \frac{1}{2} (\Psi_i^B \Psi_i^B - \Psi_i^A \Psi_i^A) \right] S_i + \frac{1}{2} \Psi_i^A \Psi_i^B T_i + \frac{1}{2} \Psi_i^B \Psi_i^A T_i^\dagger
\]
where \(S_i\) is the spin vector of localized spins \(S_i^2 = s^2\), and \(T_i\) and \(T_i^\dagger\) are complex vectors which depend on Schwinger’s bosons. They are orthogonal to the spin vector \(S_i\). \(T_i^2 = T_i^{\dagger 2} = 0, T_i\cdot T_i^\dagger = 2\). The gauge invariance imposes the conditions \(\Psi_i^A \Psi_i^B = (\Psi_i^B \Psi_i^B - \Psi_i^A \Psi_i^A) = 0\). As a result, the dimensionless magnetization per lattice site \(M = <S_i^{tot}\rangle^2\) reads
\[
M = \frac{1}{8} \left[ s + \frac{1}{2} <(\Psi_i^B \Psi_i^B - \Psi_i^A \Psi_i^A)\rangle > <S_i\rangle^2
\]
At zero temperature \(<S_i\rangle = s\) and \(M = s + m\), where \(m = 1/2 <(\Psi_i^B \Psi_i^B - \Psi_i^A \Psi_i^A)\rangle >\) is the contribution of the itinerant electrons.

Rewriting the Hamiltonian in terms of A and B fields, one obtains the following representations for Hubbard and pair-hopping terms
\[
\sum_{<ij>} n_i^+ n_j = -\frac{1}{2} \sum_i (\Psi_i^B \Psi_i^B - \Psi_i^A \Psi_i^A)^2,
\]
\[
\sum_{<ij>} c_i^+ c_j c_j^+ c_i^+ = \sum_{<ij>} \Psi_i^B \Psi_j^B \Psi_i^A \Psi_j^A.
\]
One can decouple these terms by means of the Hubbard-Stratanovich transformation, introducing a real field \(m_i(\tau)\) associated with the composite field \(1/2(\Psi_i^B \Psi_i^B - \Psi_i^A \Psi_i^A)\), and complex fields \(a_i^I(\tau)\) associated with \(\Psi_i^B \Psi_i^B\), where \(R\) stands for \(A\) or \(B\). Then, the action is quadratic with respect to the fermions and one can integrate them out. The obtained free energy is a function of the composite fields and the integral over them can be performed approximately by means of the steepest descendent method. To this end one sets the first derivatives of the free energy with respect to composite fields equal to zero. These are the mean-field equations.

The solutions of the mean-field equations are assumed to be constants independent of the lattice sites and bonds \(m_i(\tau) = m, u_i^R(\tau) = u_R\), where \(m\) is the itinerant electron contribution to the magnetization (see Eq. (3)). The equations for \(m, u\) and the number of itinerant electrons \(n\) are
\[
m = \frac{1}{2} \int \frac{d\epsilon}{2} \left( \epsilon - \epsilon_f^A + m \right) N(\epsilon) e^{\epsilon_f^B(\epsilon) - \epsilon_f^A(\epsilon) - \epsilon + \frac{m^2}{2}}
\]
\[
u_R = \frac{1}{2} \int \frac{d\epsilon}{2} \left( \epsilon - \epsilon_f^B + m \right) N(\epsilon) e^{\epsilon_f^R(\epsilon) - \epsilon_f^B(\epsilon) - \epsilon + \frac{m^2}{2}}
\]
\[
n = \frac{1}{2} \int \frac{d\epsilon}{2} \left( \epsilon - \epsilon_f^B + m \right) N(\epsilon) e^{\epsilon_f^B(\epsilon) - \epsilon_f^A(\epsilon) - \epsilon + \frac{m^2}{2}}
\]
where \(\epsilon_f^R(\epsilon)\) is the Fermi function, \(N(\epsilon)\) is the density of state for band energy \(\epsilon_k = -t \sum \delta|\mathbf{k} + \mathbf{x}|D\) with \(\delta / 2\) a vector connecting a site to its nearest neighbors and \(z\) the number of nearest neighbors. In equations (6) the fermion dispersions are
\[
\epsilon^A(\epsilon_k) = \left( 1 - \frac{F}{t} u \right) \epsilon_k + 2mU + \frac{sJ_1}{2} - \mu,
\]
\[
\epsilon^B(\epsilon_k) = \left( 1 - \frac{F}{t} u \right) \epsilon_k - 2mU - \frac{sJ_1}{2} - \mu.
\]
I assume for simplicity a flat density of states: \(N(\epsilon) = 1/D, -D/2 < \epsilon < D/2\). Unlike in the Stoner model, the model with pair-hopping term does not depend strongly on energy variation of the density of states. Now the system can be analytically solved at zero temperature.

A solution with \(m = 0\) exists if \(u^A\) and \(u^B\) are nonzero and have opposite signs, which in turn requires \(g = F/t > 4\). Then the equation for the contribution of itinerant electrons to the magnetization \(m\) is
\[
m^2 + \left( \frac{2U}{Dg} - \frac{(n - 1)^2}{4} - \frac{1}{4} \right) m - \left( \frac{n - 1}{2g} - \frac{sJ_1}{2gD} \right) = 0.
\]

The equation (8) has a solution \(m = 0\) if \(D = D_x\), where \(D_x = sJ_1/|n - 1|\). The Coulomb parameter \(U\) is large parameter in the theory, so one can choose it to satisfy \(2U/Dg > (n - 1/2)/4 + 1/4\). Then, the equation (8) has only one real solution.

To match the experimental results it is most adequate to keep the parameters of the local interactions \(U\) and \(J_1\), and the number of the itinerant electrons \(n\) fixed. I assume that hydrostatic pressure increases the pair-hopping at the expense of the single-electron hopping. This means, that the pair-hopping parameter \(F\) increases, while the hopping parameter \(t\) decreases when the pressure increases. At pressure \(p = p_c\) \(D = D_x\) and \(F = F_z\), where \(F_z = 4U/zn((n - 1)^2 + 1)\). The first
condition is necessary to have a zero \( m \) solution, the second one ensures an abrupt decrease of magnetization at \( p_x \). The last assumption is that when the pressure increases the parameter \( F \) scales like \( 1/D \), more exactly \( F/F_x = D_x/D \). Above \( p_x \) the parameters of the itinerant electrons remain unchanged. One can find justification of this assumption in the experimental fact that above \( p_x \) the physics of the system is dominated by the localized spins. It is important to stress that the transition, the paramagnetism of this assumption in the experimental fact that above \( p_x \) the magnetization results from the local-
of the itinerant electrons to the magnetization \( m \) as a function of the pair-hopping parameter \( F/F_x \) is depicted in fig.2 for \((n-1)^2 = 0.2\), and \( 1.6U = 3s_J \).

The graph (fig.2) as well as the expressions for \( F_x \) and \( D_x \) are an artifact of the approximate treatment of the density of states \( N(\epsilon) \). More accurate account for the energy dependence of \( N(\epsilon) \) will give us different conditions for the parameters and more realistic dependence of the magnetization on the parameters.

The proposed model of \( UGe_2 \) differs from the models discussed in [1, 3, 9, 10] in many aspects. First, degrees of freedom associated with localized spins and itinerant electrons are introduced, which enables one to describe two different ferromagnetic phases \( FM1 \) and \( FM2 \). The resistivity measurements reveal[2] the presence of an additional phase line that lies entirely within the ferromagnetic phase. It is suggested by a strong anomaly seen in the resistivity[2, 14]. The characteristic temperature of this transition, \( T_x(p) \), decreases with pressure and disappears at a pressure \( p_x \) (IP) at which the superconductivity is strongest. For pressures below \( p_x \) the itinerant electrons contribute to the magnetization, while for pressures above \( p_x \) the ferromagnetism is dominated by localized spins. This suggests to define \( T_x \) by the equation \( m(T_x) = 0 \). Above \( T_x \) the itinerant electrons do not contribute to the magnetization, and the ferromagnetism is entirely dominated by the spin fluctuations of the localized spins, while below \( T_x \) the itinerant electrons take part in the formation of the spin fluctuations. In particular, the itinerant electron mass renormalization is different below \( T_x \) and above this temperature. As a result, the slope in the \( d\rho/dT \) versus \( T \) diagram is different above \( T_x \) and well below \( T_x \). Increasing the temperature from below \( T_x \) the slope changes smoothly from its value well below \( T_x \) to its value above \( T_x \) This means a non-Fermi-liquid temperature dependence of the resistivity within a temperature interval around \( T_x \). The present description of the ferromagnetism above and below \( T_x \) is in very good agreement with the experimental finding that the high pressure ferromagnetic phase might have the more localized character[6].

Second, the model explains in a unified way the superconductivity and \( T_x \) transition near \( p_x \) point. At \( p_x \) the contribution of the itinerant electron to the magnetization \( m \) becomes equal to zero and hence it is the end of the \( T_x \) line, as follows from the definition above. On the other side, it was explained that when \( m = 0 \) the superconducting critical temperature is highest.

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