Ferromagnetic Quantum critical behavior in three-dimensional Hubbard model with transverse anisotropy

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One-band Hubbard model with transverse anisotropy is considered at density of electrons \( n = 0.4 \). It is shown that when the anisotropy is appropriately chosen, the ground state is ferromagnetic with magnetic order perpendicular to the anisotropy. The increasing of the ratio \( \frac{t}{U} \), where \( t \) is the hopping parameter and \( U \) is the Coulomb repulsion, decreases the Curie temperature, and the system arrives at the quantum critical point \( (T_C = 0) \). The result is obtained introducing Schwinger bosons and slave Fermions representation of the electron operators. Integrating out the spin-singlet Fermi fields an effective Heisenberg model with ferromagnetic exchange constant is obtained for vectors which identifies the local orientation of the spin of the itinerant electrons. The amplitude of the spin vectors is an effective spin of the itinerant electrons accounting for the fact that some sites, in the ground state, are doubly occupied or empty. Owing to the anisotropy, the magnon fluctuations drive the system to quantum criticality and when the effective spin is critically small these fluctuations suppress the magnetic order.

Quantum phase transitions (QPT) arise in many-body systems because of competing interactions that support different ground states. At quantum critical point (QCP) the matter undergoes a transition from one phase to another at zero temperature. A nonthermal control parameter, such as pressure, doping or magnetic field, drives the system to QCP. Quantum phase transitions are a subject of great interest \([1–5]\). At this point, the quantum critical fluctuations give rise to unconventional temperature dependence of magnetic, thermal, and transport parameters \([1–6]\).

Quantum phase transition can be induced in a wide range of materials. Most prominent experimental realization of ferromagnetic quantum phase transition is found in magnetic properties of \( \text{LiHoF}_4 \). At low temperature the magnetic degrees of freedom in this material are the spins of the holmium atoms. They have an easy axis, and below \( T_C = 1.53K \) the compound is ferromagnetic. In \([7]\) the authors measured the magnetic order as a function of temperature and a magnetic field applied perpendicular to the easy axis. The increasing of the magnetic field reduces Curie temperature monotonically. When it is larger than some critical field (about 50kOe) the long-range order in the material is destroyed even at zero temperature. The spin flip operators are the quantum fluctuations which drive the system to the quantum critical point \([2, 3, 6]\). Another examples of field-induced quantum phase transitions are discussed in the review articles \([2, 3, 6]\).

Pressure driven transformation of \( \text{CeRu}_4\text{Ge}_2 \) from ferromagnet into paramagnet, at zero temperature, is studied in \([8]\). The suppression of magnetic order at the critical pressure \( p_{cr} = 67kbar \) is accompanied by non-Fermi-liquid behavior.

The magnetic properties of \( \text{URh}_{1-x}\text{Ru}_x\text{Ge} \) alloys are investigated in \([8]\). The Curie temperature vanishes linearly with \( x \) and the ordered moment is suppressed in a continuous way at \( x_{cr} = 0.38 \). The thermal, transport, and magnetic properties of \( \text{URh}_{1-x}\text{Ru}_x\text{Ge} \) near the critical concentration are investigated. The data provide evidence for continuous ferromagnetic quantum phase transition.

The earliest theory of a ferromagnetic quantum phase transition was the Stoner theory \([10]\). In later paper \([11]\) Hertz derived an effective Ginzburg-Landau-Wilson theory starting from a microscopic theory of itinerant electrons with four-fermion interaction. He concluded that in the dimensions \( d = 2 \) and \( d = 3 \) the quantum phase transition from paramagnet to ferromagnet in isotropic system is a second-order transition with mean-field critical behavior. In contrast to this it was shown \([11, 12]\) that the quantum phase transition from a metallic paramagnet to an itinerant ferromagnet in \( d = 2 \) and \( d = 3 \) is discontinuous. It was proved that this conclusion is true and for anisotropic systems with magnetic order parallel to anisotropy axis \([14]\).

In the present paper the three-dimensional Hubbard model with transverse anisotropy is investigated. The experimental observations in \( \text{LiHoF}_4 \) inspire that the anisotropy could be of great importance for the existence of a quantum critical behavior in the system. It is shown that when the anisotropy is appropriately chosen, the ground state is ferromagnetic with magnetic order perpendicular to the anisotropy. The increasing of the ratio \( \frac{t}{U} \), where \( t \) is the hopping parameter and \( U \) is the Coulomb repulsion, decreases the Curie temperature. Owing to the anisotropy, the spin flip fluctuations (magnons) drive the system to quantum criticality and when the effective spin is critically small these fluctuations suppress the magnetic order. Critically high double occupancy is phenomena of basic relevance to second-order quantum phase transition in itinerant magnets.

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We consider a theory with Hamiltonian
\[ h = -t \sum_{\langle ij \rangle} (c_{i\uparrow}^+ c_{j\downarrow} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_i n_i \\
- J' \sum_{\langle ij \rangle} (S_i^x S_j^x + \kappa S_i^y S_j^y + S_i^z S_j^z) \] (1)

where \( c_{i\sigma}^+ \) and \( c_{i\sigma} \) (\( \sigma = \uparrow, \downarrow \)) are creation and annihilation operators for spin-1/2 Fermi operators of itinerant electrons, \( n_{i\sigma} = c_{i\sigma}^+ c_{i\sigma} \), \( n_i = n_{i\uparrow} + n_{i\downarrow}, \) \( t > 0 \) is the hopping parameter, \( U > 0 \) is the the Coulomb repulsion, and \( \mu \) is the chemical potential. The exchange constant in the Heisenberg term is ferromagnetic \( J' > 0, \) \( \kappa \) is a parameter of anisotropy, and the spin of the itinerant electron is
\[ S_i^\alpha = \frac{1}{2} \sum_{\sigma, \sigma'} c_{i\sigma}^+ \tau^\alpha \tau_{\sigma\sigma'} c_{i\sigma'} \] (2)

where \( \tau^x, \tau^y, \tau^z \) are the Pauli matrices. The sums in Eq.(1) are over all sites of a three-dimensional cubic lattice, and \( \langle i, j \rangle \) denotes the sum over the nearest neighbors.

We represent the Fermi operators, the spin of the itinerant electrons and the density operators \( n_{i\sigma} \) in terms of the Schwinger bosons \( (\varphi_{i\sigma}, \varphi_{i\sigma}^+ \) and slave Fermions \( (h_i, h_i^+, d_i, d_i^+) \). The Bose fields are doublets (\( \sigma = 1, 2 \)) without charge, while Fermions are spinless with charges 1 \( (d_i) \) and -1 \( (h_i) \).

\[ c_{i\uparrow} = h_i^\uparrow \varphi_{i\uparrow} + \varphi_{i\uparrow}^+ d_i, \quad c_{i\downarrow} = h_i^\downarrow \varphi_{i\downarrow} - \varphi_{i\downarrow}^+ d_i, \quad n_i = 1 - h_i^\uparrow h_i^\downarrow + d_i^+ d_i, \quad S_i^\sigma = \frac{1}{2} \sum_{\sigma'} \varphi_{i\sigma} \tau_{\sigma\sigma'} \varphi_{i\sigma'}, \] (3)

\[ c_{i\uparrow}^+ c_{i\uparrow} + c_{i\downarrow}^+ c_{i\downarrow} = d_i^+ d_i \]

To solve the constraint (Eq. 3), which entangles the Fermi and Bose operators, one makes a change of variables, introducing Bose doublets \( \zeta_{i\sigma} (c_{i\sigma}^+) \) [15]
\[ \varphi_{i\sigma} = \zeta_{i\sigma} (1 - h_i^\sigma h_i - d_i^+ d_i)^{1/2}, \]
\[ \varphi_{i\sigma}^+ = \zeta_{i\sigma}^+ (1 - h_i^\sigma h_i - d_i^+ d_i)^{1/2}. \] (5)

Now, only the new Bose fields are constrained \( c_{i\sigma}^+ \zeta_{i\sigma} = 1 \). In terms of the new fields the spin vectors of the itinerant electrons have the form
\[ S_i^\alpha = \frac{1}{2} \sum_{\sigma, \sigma'} \zeta_{i\sigma} \tau^\alpha \tau_{\sigma\sigma'} \zeta_{i\sigma'} [1 - h_i^\sigma h_i - d_i^+ d_i] \] (6)

When, in the ground state, the lattice site is empty, the operator identity \( h_i^\sigma h_i = 1 \) is true. When the lattice site is doubly occupied, \( d_i^+ d_i = 1 \). Hence, when the lattice site is empty or doubly occupied the spin on this site is zero. When the lattice site is neither empty nor doubly occupied \( (h_i^\sigma h_i = d_i^+ d_i = 0) \), the spin equals \( s_i = 1/2 n_i \), where the unit vector
\[ n_i^\sigma = \sum_{\sigma'} \zeta_{i\sigma}^\sigma \zeta_{i\sigma'} \] (7)

identifies the local orientation of the spin of the itinerant electron.

The Hamiltonian Eq.(1), rewritten in terms of Bose fields Eq.(5) and slave Fermions, adopts the form
\[ h = -t \sum_{\langle ij \rangle} [(d_j^+ d_i - h_i^+ h_j) \zeta_{i\sigma}^\sigma \zeta_{j\sigma} \\
+ (d_j^+ h_i^+ - d_i^+ h_j^+) (\zeta_{i\sigma} \zeta_{j\sigma} - \zeta_{i\sigma} \zeta_{j\sigma}) + h.c.] \\
\times (1 - h_i^\sigma h_i + d_i^+ d_i)^{1/2} (1 - h_j^\sigma h_j - d_j^+ d_j)^{1/2} \\
+ U \sum_i d_i^+ d_i - \mu \sum_i (1 - h_i^\sigma h_i + d_i^+ d_i) \\
- J' \sum_{\langle ij \rangle} [n_i^\sigma n_j^\sigma + \kappa n_i^\sigma n_j^\sigma + n_i^\sigma n_j^\sigma] \\
\times (1 - h_i^\sigma h_i - d_i^+ d_i) (1 - h_j^\sigma h_j - d_j^+ d_j). \] (8)

An important advantage of working with Schwinger bosons and slave Fermions is the fact that Hubbard term is in a diagonal form. The fermion-fermion and fermion-boson interactions are included in the hopping and spin exchange Heisenberg terms. To proceed we approximate the hopping term of the Hamiltonian Eq.(8) setting \( (1 - h_i^\sigma h_i - d_i^+ d_i)^{1/2} \sim 1 \) and keep only the quadratic, with respect to Fermions, terms. This means that the averaging in the subspace of the Fermions is performed in one fermion-loop approximation. Further, we represent the resulting Hamiltonian as a sum of two terms
\[ h = h_0 + h_{int}, \] (9)

where
\[ h_0 = -t \sum_{\langle ij \rangle} (d_j^+ d_i - h_i^+ h_j + h.c.) + U \sum_i d_i^+ d_i \\
- \mu \sum_i (1 - h_i^\sigma h_i + d_i^+ d_i), \] (10)

is the Hamiltonian of the free \( d \) and \( h \) fermions, and
\[ h_{int} = -t \sum_{\langle ij \rangle} [(d_j^+ d_i - h_j^+ h_j) (\zeta_{i\sigma} \zeta_{j\sigma} - 1) \\
+ (d_j^+ h_i^+ - d_i^+ h_j^+) (\zeta_{i\sigma} \zeta_{j\sigma} - \zeta_{i\sigma} \zeta_{j\sigma}) + h.c.] \\
- J' \sum_{\langle ij \rangle} [n_i^\sigma n_j^\sigma + \kappa n_i^\sigma n_j^\sigma + n_i^\sigma n_j^\sigma] \\
\times (1 - h_i^\sigma h_i - d_i^+ d_i) (1 - h_j^\sigma h_j - d_j^+ d_j). \] (12)

is the Hamiltonian of boson-fermion interaction.

The ground state of the system, without accounting for the spin fluctuations, is determined by the free-fermion Hamiltonian \( h_0 \) and is labeled by the density of electrons
\[ n = 1 - h_i^\sigma h_i + d_i^+ d_i > \] (13)
(see equation (3)) and the "effective spin" of the electron
\[ m = \frac{1}{2} \left( 1 - < h_i^+ h_i > - < d_i^+ d_i > \right). \tag{14} \]

At density of electrons \( n = 0.4 \) one calculates the chemical potential \( \mu \) as a function of \( t/U \) and utilizes the result to calculate the effective spin of the itinerant electron "m" as a function of the control parameter \( t/U \). The result is depicted in Fig. (1)-black triangles-left scale.

Let us introduce the vector,
\[ M_i^\nu = m \sum_{\sigma \sigma'} \xi_{i \sigma}^\nu \sigma' \sigma \xi_{i \sigma'} \quad M_i^2 = m^2. \tag{15} \]

Then, the spin-vector of itinerant electrons Eq. (14) can be written in the form
\[ S_i = \frac{1}{2m} M_i \left( 1 - h_i^+ h_i - d_i^+ d_i \right), \tag{16} \]
where the vector \( M_i \) identifies the local orientation of the spin of the itinerant electrons. The contribution of itinerant electrons to the total magnetization is \( < S_i^z > \). Accounting for the definition of \( m \) (see Eq. (14)), one obtains \( < S_i^z > = < M_i^z > \).

The Hamiltonian is quadratic with respect to the Fermions \( d_i, d_i^\dagger \) and \( h_i, h_i^\dagger \), and one can average in the subspace of these Fermions (to integrate them out in the path integral approach). As a result, one obtains an effective model for vectors \( M_i \) with Hamiltonian
\[ h_{eff} = - J'' \sum_{\langle ij \rangle} M_i \cdot M_j \tag{17} \]
\[ - J'' \sum_{\langle ij \rangle} \left[ M_i^x M_j^x + \kappa M_i^y M_j^y + M_i^z M_j^z \right]. \tag{18} \]
The effective exchange constant \( J'' \) is calculated in the one fermion-loop approximation, in the limit when the frequency and the wave vector are small. At zero temperature, one obtains
\[ J'' = \frac{t}{6m^2 N} \sum_k \left( \sum_{\nu=1}^3 \cos k_{\nu} \right) \left[ \theta(-\varepsilon_k^d) - \theta(-\varepsilon_k^h) \right] \tag{19} \]
\[ - \frac{2t^2}{3m^2 U N} \sum_k \left( \sum_{\nu=1}^3 \sin^2 k_{\nu} \right) \left[ 1 - \theta(-\varepsilon_k^h) - \theta(-\varepsilon_k^d) \right], \]
where \( N \) is the number of lattice’s sites, \( \varepsilon_k^h \) and \( \varepsilon_k^d \) are Fermions’ dispersions,
\[ \varepsilon_k^h = 2t(\cos k_x + \cos k_y + \cos k_z) + \mu \tag{19} \]
\[ \varepsilon_k^d = -2t(\cos k_x + \cos k_y + \cos k_z) + U - \mu, \]
and the wave vector \( k \) runs over the first Brillouin zone of a cubic lattice. The "m" dependence of \( J'' \) is a consequence of the definition of the vector \( M_i \) Eq. (15), and \( J''m^2 \) doesn’t depend on "m".

It is convenient to rewrite the effective hamiltonian in the form
\[ h_{eff} = - J \sum_{\langle ij \rangle} \left[ M_i^x M_j^x + r M_i^y M_j^y + M_i^z M_j^z \right], \tag{20} \]
with exchange constant \( J = J'' + J' \) and effective parameter of anisotropy \( r = (J'' + \kappa J')/(J'' + J') \).

The exchange constant \( J \), the effective spin \( m \) and the effective anisotropy parameter \( r \) are functions of the ratio \( t/U \). They are calculated at density of itinerant electrons \( n = 0.4 \), for anisotropy parameter \( \kappa = -0.83 \) and \( J'/t = 10 \). The functions are depicted in Fig. (1).

**FIG. 1:** (Colour on-line) The effective spin of the itinerant electrons \( m \) as a function of the control parameter \( t/U \)-black triangles(left scale) The exchange constant \( J/t \) as a function of \( t/U \)-red rhombuses(right scale). Inset: The effective anisotropy constant \( r \) as a function of \( t/U \). The functions are calculated at density of itinerant electrons \( n = 0.4 \), for anisotropy parameter \( \kappa = -0.83 \) and \( J'/t = 10 \).

For chosen parameters the exchange constant is positive \( J > 0 \) and a ferromagnetic order along \( z \) axis, perpendicular to the anisotropy, is stable. To study this phase one introduces the Holstein-Primakoff representation of the spin vectors \( M_j(a_j^+, a_j) \)
\[ M_j^+ = M_j^x + i M_j^y = \sqrt{2m - a_j^+ a_j} a_j \]
\[ M_j^- = M_j^x - i M_j^y = a_j^+ \sqrt{2m - a_j^+ a_j} \]
\[ M_j^z = m - a_j^+ a_j, \tag{21} \]
where \( a_j^+, a_j \) are Bose fields and \( m \) is the effective spin of itinerant electrons. In spin-wave approximation, in momentum space representation the effective Hamiltonian (Eq. (20) adopts the form
\[ h_{eff} = \sum_k \left[ \varepsilon_k a_k^+ a_k - \gamma_k \left( a_k^+ a_{-k} + a_{k} a_{-k} \right) \right] \]
\[ \varepsilon_k = Jm \left[ 6 - (1 + r) (\cos k_x + \cos k_y + \cos k_z) \right] \]

\[ \gamma_k = Jm \frac{(1 - r)}{2} (\cos k_x + \cos k_y + \cos k_z). \] (22)

To diagonalize the Hamiltonian one introduces new Bose field \( \alpha_k, \alpha_k^+ \): \( \alpha_k = u_k \alpha_k + v_k \alpha_k^+ \), where the coefficients \( u_k \) and \( v_k \) are real functions of the wave vector. The transformed Hamiltonian adopts the form

\[ h_{\text{eff}} = \sum_k \left( E_k \alpha_k^+ \alpha_k + E_k^0 \right), \] (23)

with dispersion

\[ E_k = 2Jm \sqrt{(3 - \delta_k)(3 - r\delta_k)}, \]

\[ \delta_k = \cos k_x + \cos k_y + \cos k_z \] (24)

and vacuum energy \( E_k^0 = \frac{1}{2} |E_k - \varepsilon_k| \).

The dispersion Eq. (24) shows that the ferromagnetism with magnetic order perpendicular to the anisotropy axis is stable if the effective anisotropy constant satisfies the condition \(-1 < r < 1\). The inset in Fig. (1) shows that all calculated values of the effective anisotropy constant satisfy the above condition.

The dispersion is equal to zero at \( k = (0, 0, 0) \). Therefore, \( \alpha_k \)-Boson describes long-range excitation (magnon) in the system. Near the zero vector the dispersion adopts the form \( E_k \propto c_s |k| \) with spin-wave velocity

\[ c_s = Jm \sqrt{6(1 - r)}. \] (25)

The unusual, for ferromagnetism, dispersion is in consequence of anisotropy. When the isotropy is restored \((r = 1)\) one obtains the well known ferromagnetic dispersion.

The magnetization is defined by the equation \( m = \int d^3 r \rho \). At Curie temperature \( T_C \), the magnetization is zero and one calculates the critical temperature solving the equation

\[ 2m + 1 = \frac{1}{N} \sum_k \frac{\varepsilon_k}{E_k} \left[ 1 + \frac{2}{e^{\varepsilon_k/T_C} - 1} \right]. \] (26)

When the parameter of anisotropy \( r \) is fixed, the critical temperature decreases, decreasing the effective spin \( m \). At quantum critical point \((T_C = 0)\) one obtains a dependence of the critical value of the effective spin \( m_{cr} \) on the anisotropy parameter. The relation is given by the equation

\[ 2m_{cr} + 1 = \frac{1}{2N} \sum_k \frac{6 - (1 + r)\delta_k}{\sqrt{(3 - \delta_k)(3 - r\delta_k)}} \] (27)

with \( \delta_k \) from Eq. (21), and is depicted in Fig. [2].

The figure (2) demonstrates very well the nature of the quantum criticality in itinerant ferromagnets with anisotropy. At quantum critical point the effective spin, which is the fermion contribution to the magnetization without accounting for the spin fluctuations, is nonzero. Magnon fluctuations suppress this magnetization to zero.

Hence, the magnon (spin flip) fluctuations drive the system to quantum critical point. This is a second order quantum phase transition from ferromagnetic phase with long-range magnon fluctuations to paramagnetic phase with gapped magnons.

This is in contrast to quantum phase transition in isotropic itinerant ferromagnets \((r = 1)\). For this systems the quantum phase transition is from ferromagnetic phase with long-range magnon fluctuations to paramagnetic phase without spin-flip fluctuations \((m_{cr} = 0)\). This explains the non-second order nature of the transition.

Utilizing the dependence of the effective spin \( m \) and the exchange constant \( J/t \) on the control parameter \( t/U \), see Fig. [1], one can obtain the dependence of the dimensionless temperature \( T_C/t \) on the ration \( t/U \). The phase diagram in the plane of temperature \( T_C/t \) and control parameter \( t/U \) is depicted in figure [3]. At density of electrons \( n = 0.4 \), anisotropy parameter \( \kappa = -0.83 \) and \( J'/t = 10 \) the quantum critical value of the ratio is \( t/U = 2 \).

In the present paper the Hubbard model of itinerant ferromagnetism with transverse anisotropy was studied. Increasing the ratio \( t/U \) decreases the effective spin of itinerant electron which in turn decreases the Curie temperature. The equations (23) and (24) show that at fixes density of electrons \( n = 0.4 \) the decreasing of the effective spin increases the density of doubly occupied states. The result shows that the quantum critical ground state state is a state with high concentration of doubly occupied states.

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FIG. 3: (Colour on-line) The phase diagram in the plane of temperature $T_C/t$ and control parameter $t/U$. At density of electrons $n = 0.4$, anisotropy parameter $\kappa = -0.83$ and $J'/t = 10$ the quantum critical value of the ratio is $t/U = 2$.

[1] J. Hertz, Phys. Rev. B 14, 1165 (1976).
[2] S. Sachdev, Quantum Phase Transition (Cambridge University Press, Cambridge 1999).
[3] Matthias Vojta, Rep. Prog. Phys. 66 2069 (2003).
[4] Hilbert v. Löhneysen, Achim Rosch, Matthias Vojta, and Peter Wölfle, Rev. Mod. Phys., 79, 1015 (2007).
[5] Philipp Gegenwart, Qimiao Si, and Frank. Steglich, Nature Phys. 4 186 (2008).
[6] A. J. Millis, Phys. Rev. B 48, 7183 (1993).
[7] D. Bitko, T. F. Rosenbaum, and G. Aeppli, Phys. Rev. Lett. 77, 940 (1996).
[8] S. Süllov, M. C. Aronson, B. D. Rainford, and P. Haen, Phy. Rev. Lett. 82, 2963 (1999).
[9] N. T. Huy, A. Gasparini, J. C. P. Klaasse, A. de Visser, S. Sakarya, and N. H. van Dijk, Phys.Rev. B 75, 212405 (2007).
[10] E. C. Stoner, Proc.Roy.Soc.London A165, 372 (1938).
[11] D. Belitz, T. R. Kirkpatrick, and T. Vojta, Phys. Rev. Lett. 82, 4707 (1999).
[12] T. R. Kirkpatrick and D. Belitz, Phys. Rev. B 67, 024419 (2003).
[13] Andrey V. Chubukov, Catherine Pépin, and Jerome Rech, Phys. Rev. Lett. 92, 147003 (2004).
[14] T. R. Kirkpatrick and D. Belitz, Phys. Rev. B 85, 134451 (2012).
[15] D. Schmeltzer, Phys. Rev. B 43, 8650 (1991).