Quantum topological transitions and spinons in metallic ferro- and antiferromagnets

V. Yu. Irkhin
M. N. Mikheev Institute of Metal Physics, 620108 Ekaterinburg, Russia

Abstract
An effective Hamiltonian describing fluctuation effects in the magnetic phases of the Hubbard model in terms of spinon excitations is derived. A comparison of spin-rotational Kotliar-Ruckenstein slave boson and Ribeiro-Wen dopon representations is performed. The quantum transition into the half-metallic ferromagnetic state with vanishing of spin-down Fermi surface is treated as the topological Lifshitz transition in the quasimomentum space. The itinerant-localized magnetism transitions and Mott transition in antiferromagnetic state are considered in the topological context. Related metal-insulator transitions in Heusler alloys are discussed.

Keywords: Slave boson; Lifshitz transitions; Hubbard model; Half-metallic magnetism

1. Introduction

Exotic quantum phase transitions (QPT) in topological materials have recently been extensively investigated [1]. Besides the simplest one-electron Lifshitz transitions, there is a more complicated quantum scenario: vanishing of quasiparticle residue, accompanied by spin-charge separation, and occurrence of incoherent states and spinon Fermi surface [2]. QPT are treated in both usual paramagnetic and (in the presence of frustrations) exotic spin-liquid states [3]. However, concepts of exotic QPT can be applied to ferromagnetic (FM) and antiferromagnetic (AFM) phases too. Here belong also problems of magnetism in high-Tc cuprates [2] and Kondo lattices [3, 4].

An important class of ferromagnets are half-metallic ferromagnets (HMF) which possess unusual electronic properties connected with the presence of states with only one spin projection at the Fermi surface and by energy gap for another spin projection [5]. In such a situation, incoherent (non-quasiparticle) contributions play an important role. Vanishing of the partial Fermi surface in the HMF state can be treated as a topological transition in the quasimomentum space; a similar transition can be considered in an antiferromagnet. We shall demonstrate that these systems have quite non-trivial topological properties from the microscopic point of view (within the many-electron models). To this end we develop the concept of spinons in the magnetic phases by using the slave-particle representations.

2. Slave-particle representations

We study the problem both in the Hubbard and s-d exchange (Kondo lattice) models. The Hamiltonian of the former model reads

$$\mathcal{H}_H = \sum_{i\sigma} t_i c_i^\dagger \sigma c_i^\sigma + U \sum_i n_i \hat{n}_i \ (1)$$

where $c_i^\sigma$ are electron creation operators.

First we treat the strong correlation limit. Here it is convenient to use auxiliary (“slave”) boson and fermion representations. Anderson’s [6] representation exploiting the idea of the separation of the spin and charge degrees of freedom of electron ($\sigma = \pm 1$) reads

$$c_{i\sigma} = X_i(0, \sigma) + \sigma X_i(-\sigma, 2) = e_i f_{i\sigma} + \sigma d_i f_{i\sigma}^\dagger \ (2)$$

where $X$ are the Hubbard operators, $f_{i\sigma}$ are the annihilation operators for neutral fermions (spinons), and $e_i$, $d_i$ for charged spinless bosons (holons and doublons). For large $U$ and for hole doping (where electron concentration $n < 1$), we have to retain only the term with holon operators. The choice of the Fermi statistics for spinons and Bose one for holons is not unique and depends on the physical picture (e.g., presence or absence of magnetic ordering, see also [7]).

A more complicated representation was proposed by Kotliar and Ruckenstein [8]. We use a rotationally invariant version [9, 10] [11]. This is suitable for magnetically ordered phases to take into account spin fluctuation corrections and non-quasiparticle states treated in Refs. [12, 5]. We have

$$c_{i\sigma} = \sum_{i'\sigma'} f_{i\sigma} z_{i\sigma'\sigma} \ z_i = e_i^{\dagger} \hat{L}_\sigma \hat{R}_\sigma \hat{P}_i + \sigma d_i^{\dagger} \hat{L}_\sigma \hat{R}_\sigma \hat{d}_i \ (3)$$

where

$$\hat{L}_\sigma = [(1 - d_i^{\dagger} d_i) \sigma_0 - 2 \hat{P}_i \hat{P}_i]^{1/2} \ (4)$$

$$\hat{R}_\sigma = [(1 - e_i^{\dagger} e_i) \sigma_0 - 2 \hat{P}_i \hat{P}_i]^{1/2} \ (5)$$

$$M_i = (1 + e_i^{\dagger} e_i + \sum_{\mu=0}^3 p_{i\mu} p_{i\mu} + d_i^{\dagger} d_i)^{1/2} \ (6)$$

The additional square-root factors in (4)-(6) can be treated in spirit of mean-field approximation. In particular, the factor $M$ (missed in earlier work [9]) is equal to $\sqrt{2}$ due to sum rule (8) and enables one to obtain an agreement with the small-$U$ limit...
and with the FM case. The scalar and vector bosons $p_{0\alpha}$ and $p_\sigma$ are introduced as

$$\hat{p}_\sigma = \frac{1}{2}(p_{0\alpha}r_\alpha + p_\sigma q)$$(7)

with $q$ being Pauli matrices and $\hat{p}_{\alpha} = (1/2)(p_{0\alpha}r_\alpha - p_\alpha q)$ the time reverse of operator $\hat{p}_\sigma$. The constraints read

$$e^*_i e_j + \sum_{\mu=0}^3 p_\mu^* p_\mu + d^*_i d_j = 1,$$(8)

$$2d^*_i d_i + \sum_{\mu=0}^3 p_\mu^* p_\mu = \sum_{\ell} e^*_i e_{i\ell}.$$ (9)

Eq. (8) can be simplified in the case of magnetic ordering near half-filling (the electron concentration $n < 1$) where, in the mean-field approach, $p_{0\alpha} = p' = p = 1/\sqrt{2}$ in the FM state (and correspondingly in the AFM state in the local coordinate system, $e = (e') = (1 - n)^{1/2}$. Probably, this simplification in the local coordinate system can work also in the systems with strong spin fluctuations and short-range order (e.g., in the single RVB state), but not in the usual paramagnetic state.

We work with the projected electron operator

$$\tilde{c}_{i\sigma} = X_i(0|\sigma) = c_{i\sigma}(1 - n_{i\sigma})$$ (10)

We perform the transformation by using the sum rule (8) and taking into account the eigenvalues of the denominators in (4), (5) (cf. Ref. [16]). Further on, we express again the numerator in terms of the Pauli matrices using explicitly their matrix elements. Neglecting the terms proportional to holon operators we derive

$$\tilde{c}_{i\sigma} = \hat{1} \sqrt{2} f_i (p_{0\alpha} + \tilde{p}_{\alpha})$$

Since the terms proportional to $f_i$ and $p_{0\alpha}$ are small (note that in the magnetic ordering case $p_{0\alpha}$ is not related to spin operators, see below Eq. (14)) we can restore rotational invariance and write down approximately

$$\tilde{c}_{i\sigma} = \sqrt{2} \sum_{\alpha'} \tilde{p}_{i\sigma'\alpha'} f_{i\alpha'} = \frac{1}{\sqrt{2}} \sqrt{2} \sum_{\alpha'} f_{i\alpha'}[\delta_{\sigma\sigma'} p_{0\alpha} + (p_{0\alpha} q)]$$ (11)

This representation satisfies exactly commutation relations for Hubbard’s operators.

We see that the factor $e^*_i$ in the numerator of (3) is canceled and the system has only spin degrees of freedom. On the other hand, in the paramagnetic case (in particular, in the problem of the metal-insulator transition), the charge fluctuations connected with $e$ are important (see, e.g., [13, 14]). The situation is similar to Weng’s consideration of confinement in cuprates [15]. According to this, in the underdoped regime the antiferromagnetic and superconducting phases are dual: in the former, holons are confined while spinons are defocused, and vice versa, and the gauge field, radiated by the holons (spinons), interacts with spinons (holons) through minimal coupling.

Defining spinor operators $\tilde{c}_i = (\tilde{c}_{i\uparrow}, \tilde{c}_{i\downarrow})$ etc. we derive the beautiful representation

$$\tilde{c} = f \hat{p}$$ (12)

The vector gapless boson $p$ restores the rotational invariance and describes spin degrees of freedom since

$$S = \frac{1}{2} \sum_{\alpha} \sigma_{\alpha\alpha'} \sigma_{\alpha\alpha'}^+ + \frac{1}{2} \sum_{\alpha=0}^3 (p_{0\alpha}^2 + p_{0\alpha}^2 - i [\hat{p}_{0\alpha}^2 + \hat{p}_{0\alpha}^2])$$ (13)

with $p = (p'^\alpha, -p'^\alpha, p^-)$. The corresponding spectrum $\omega_q$ is determined by effective intersite exchange interaction or by additional Heisenberg interaction

$$\mathcal{H}_d = \sum_q J_q S_{-q} S_q$$

in the $t - J$ model and has essentially spin-wave form. In the FM case we obtain $S_+^i = p_+^i$, so that

$$\mathcal{H}_d = \sum_q \omega_q (p_{q-++}^i + p_{q-+}^i)$$ (14)

with $p^\pm = 2^{-1/2}(p^+ \pm ip^-)$. It should be stressed that the vector product in (13) has to be retained to derive this result (otherwise the bosons $p$ and $p'$ are mixed), unlike the consideration in Ref. [10].

To describe doped cuprates, also a representation of the Fermi dopons $d_{i\sigma}$ was proposed [16, 17, 18].

$$\tilde{c}_{i\sigma} = -\frac{\sigma}{\sqrt{2}} \sum_{\alpha'} d_{i\sigma}^+ (1 - n_{i\sigma'}) [S_\delta_{\sigma\sigma'} - (S_\sigma S_{\sigma'})]$$ (15)

where $\sigma = \pm$, $n_{i\sigma} = d_{i\sigma}^+ d_{i\sigma}$, and both Fermi spinon (Abrikosov) and Schwinger boson representations can be used for localized $S = 1/2$ spins. In the magnetic case the structure of (15) is identical to the spin-rotation invariant representation (3), except for the factor of $M = \sqrt{2}$. To incorporate such a correction in the dopon representation, we note that one can include into (15) an additional square root factor in terms of spinon and dopon operators,

$$\tilde{c}_{i\sigma} = -\frac{\sigma}{\sqrt{2}} \sum_{\alpha'} [1 + \sum_{\alpha'} (f_{i\alpha'}^+, f_{i\alpha'}) = d_{i\sigma}^+, d_{i\sigma})]^{1/2}$$

$$\alpha d_{i\sigma}^+ (1 - n_{i\sigma'} - [S_\delta_{\sigma\sigma'} - (S_\sigma S_{\sigma'})]^2$$ (16)

This factor has also eigenvalue of 1 on the physical space, but in the mean-field approach its average yields $\sqrt{2}$, which cancels the corresponding prefactor in (15).

The discrepancy is also removed in the classical limit of the s-d model (with arbitrary large $S$ in [15]), cf. Ref. [18]. It is interesting to note that spinons $f_{i\sigma}$ and dopons $d_{i\sigma}$ are exchanged in the representations [11] and [15].

The representation [16] can connect physics of the Kondo lattices and cuprates. Such an approach was developed also in Ref. [19] to describe the formation of spin liquid state in terms of frustrations in localized-spin subsystems, the Schwinger boson representation being used for the latter. One can see that according to [15] the distribution functions of dopons and physical electrons are simply related as

$$\langle \tilde{c}^+_{i\sigma} \tilde{c}_{i\sigma} \rangle = \frac{1}{2} + \sigma (\mathcal{S})^2 \langle d_{i\sigma}^+ d_{i\sigma} \rangle$$

+ smooth function of $k$. (17)
which differs from the consideration in Ref. [19] by the absence of the factor 1/2. The result (17) is in agreement with those for the saturated FM case (Nagaoka state) where the Green’s function residue for spin-up states equals unity, and spin-down states demonstrate purely non-quasiparticle (incoherent) behavior with zero residue [12].

At small doping the operator (16) can be rewritten as
\[ \tilde{c}_{i\sigma} = (d_{i\uparrow}^\dagger f_i^\dagger - d_{i\downarrow}^\dagger f_i^\dagger) f_{i\sigma} \] (18)
Introducing the Bose holon operator \( \tilde{c}_i = f_i^\dagger d_i^\dagger - f_i d_i \) we return to Anderson’s representation (2). We see again that the absence of the factor \( 2^{-1/2} \) is needed.

3. Electron Green’s functions in the HMF state

Consider the electron Green’s functions for a saturated ferromagnet in the representation \( |11 \rangle \). The spin-up states propagate freely on the background of the FM ordering, but the situation is quite non-trivial for spin-down states. Spin-down state is a complex of spinon \( f_i^\dagger \) and boson \( (p^-)^\dagger \) (generally speaking, coupled by gauge field):
\[ G_{k\downarrow}(E) = \sum_{qI} \langle p^I_k f_{k-q}^\dagger f^\dagger_{k-q}(p^I_q)^\dagger \rangle E \] (19)
The simplest decoupling in the equation of motion for the Green’s function in the right-hand side of (19) yields
\[ G_{k\downarrow}^0(E) = \sum_q \frac{1 + N(\omega_q) - n(k_{-q})}{E - k_{-q} - \omega_q} \] (20)
with \( N(\omega) \) and \( n(E) \) being the Bose and Fermi functions. A more advanced decoupling yields the result
\[ G_{k\downarrow}(E) \sim \frac{1}{E - \mu + \left[G_{k\downarrow}^0(E)\right]^{-1}} \] (21)
These results were obtained earlier by treating the Hubbard ferromagnet in the many-electron representation of Hubbard’s operators \( |20 [12] \). The analogy with Anderson’s spinons (which are also described by the Green’s function with zero residue) being mentioned. The Green’s function \( |20 \) has a purely non-quasiparticle nature. Because of the weak \( k \)-dependence of the corresponding distribution function the non-quasiparticle (incoherent) states possess a small mobility and do not carry current.

At small doping \( 1 - n \), the Green’s function \( |21 \) has no poles above the Fermi level, so that the above conclusions are not changed. However, with increasing \( 1 - n \), it acquires a spin-polaron pole above \( E_F \), and the saturated ferromagnetism is destroyed.

The description of the transition to the saturated state (vanishing of the quasiparticle residue) is similar to that of the Mott transition in the paramagnetic Hubbard model \( |21 \). Thus the situation is somewhat analogous to a partial Mott transition in the spin-down subband, see the discussion of the orbital-selective Mott transition in the review \( |3 \).

Now we pass to the case of finite coupling which can be treated both in the Hubbard and s-d models \( |22 [12] \). The Hamiltonian of the latter model reads
\[ \mathcal{H} = \sum_k \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \mathcal{H}_d - \sum_{\omega, \sigma'} (S, t\sigma\sigma') c_{\omega\sigma'}^\dagger f_{\sigma'} \] (22)
Note that magnetic ordering in this model as a rule does not vanish owing to existence of local moments and intersite exchange interactions (except for the Kondo effect situation which can occur at \( I < 0 \)). Thus we have only one phase transition – from saturated to non-saturated state. Consistent solution for \( I > 0 \) in the HMF state yields \( |23 [24] \)
\[ G_{k\downarrow}(E) = \frac{1}{E - \mu + IS} \] (23)
\[ G_{k\downarrow}(E) = \left( E - \mu + IS - \frac{2IS}{1 - 4IR_k(E)} \right)^{-1} \] (24)
\[ R_{k\downarrow}(E) = \frac{1}{n(k_{-q})} G_{k\downarrow-q\downarrow}(E - \omega_q) \] (25)
The result for the Hubbard model differs from \( |25 \) by the replacement \( I \rightarrow U [12] \). The incoherent states occur above the Fermi level.
For \( I < 0 \), \( G_{k\downarrow}(E) \) has the same form, and we can write down an approximate solution
\[ G_{k\downarrow}(E) = \left( E - \mu - IS + \frac{2IS}{1 + 4IR_k(E)} \right)^{-1} \] (26)
\[ R_{k\downarrow}(E) = \frac{1}{n(k_{-q})} G_{k\downarrow-q\downarrow}(E + \omega_q) \] (27)
so that the incoherent states occur below the Fermi level. The cases \( I > 0 \) and \( I < 0 \) are not simply related by the particle-hole transformation because of the Kondo divergence of the denominator in \( |25 \) in the latter case, which indicates a quantum phase transition with increasing electron concentration or \( |U| \). A consistent treatment of this case in the large-\( |U| \) case where the incoherent states predominate is given in Ref. \( |24 \). For \( I \rightarrow -\infty \) we have
\[ G_k^0(E) \sim \frac{2S}{2S + 1} (\epsilon - \mu)^{-1} \] (26)
\[ G_k^0(E) \sim \frac{2S}{2S + 1} \left( \epsilon - \mu + \frac{2S}{R_k^\downarrow} \right)^{-1} \] (27)
\[ R_k^\downarrow(\epsilon) \sim \sum_{q} \frac{n(k_{-q})}{\epsilon - \mu} \] (28)
with \( \epsilon = E - IS + 1, \mu = [2S/(2S + 1)] \mu_k \). For \( S = 1/2 \) this case is equivalent to the Hubbard model with the replacement \( \mu_k \rightarrow \mu_k/2 \).

4. The case of antiferromagnets and discussion

Now we consider the antiferromagnetic case. The slave boson representation in the local coordinate system (cf. \( |11 \)) yields the same spinon form \( |11 \).
Mott transition in antiferromagnets usually goes in two steps: first from the AFM insulator to AFM metal (the energy gap between AFM subbands vanishes), and then from AFM metal to paramagnetic metal [25]. Thus the situation is similar to half-metallic ferromagnetism, but even more distinct: here we have the true insulator gap for both spin directions. In the situation of doping, we have again the transition between two types of AFM metals which can be denoted as saturated (localized-moment) and non-saturated (itinerant). These types correspond to classification of Ref. [26]: type A (when the Fermi surface does not cross the magnetic zone boundary) and type B (when the Fermi surface crosses the magnetic zone boundary). Although in the weak-coupling case this is a simply geometrical difference, in the case of strong correlations (in particular, in the Hubbard model with large $U$) the gap has essentially a Mott-Hubbard nature. Note that, unlike FM case, the band splitting in the saturated AFM state can be very small.

Delocalization transitions from local-moment to itinerant magnetism take place also in the Kondo systems [3]. Such a delocalization phase diagram can be considered for both ferromagnetic and antiferromagnetic Kondo lattices [27].

The numerical calculations in the large-$U$ Hubbard model within the slave-boson approach were performed in Ref. [28]. For the two-dimensional (2D) square lattice with finite next-nearest-neighbor transfer integral $t'$ they demonstrate the first-order transition from HMF to paramagnetic (PM) state with increasing hole doping and second-order transition from saturated AFM to PM state with electron doping. At the same time, for the 3D cubic lattice the intermediate non-saturated FM phase occurs. The difference is due to strong Van Hove singularities in the electron spectrum of the square lattice which favor saturated state; this circumstance has also a topological nature.

According to Ref. [29], a breakdown in the composite nature of the heavy electron can take place at the quantum critical point between AFM and Kondo heavy Fermi-liquid states.

The paramagnetic Mott insulator state can be related to deconfinement of spinons and holons [21]. The deconfinement magnetically ordered spin-density-wave state SDW* with a reduced moment can be also considered [30,31].

Unlike 2D systems, where monopoles prevent deconfinement, in the 3D systems the U(1) gauge theory admits a deconfined phase where the spinons potentially survive as good excitations. This deconfined phase has a Fermi surface of spinons coupled minimally to a gapless “photon” (U(1) gauge field), whereas monopoles are gapped [32]. Transitions to SDW* in 3D situation are more probable too.

The situation with deconfinement can be treated in different ways. According to [33], there is no true spin-charge separation in the ordered phases, but the spin-charge separation (or deconfinement) can be treated as a driving force in the unconventional phase transitions.

Since one-magnon scattering processes are forbidden in the half-metallic ferromagnets and saturated antiferromagnets, usual and half-metallic systems demonstrate different temperature dependences of electronic and magnetic properties and characteristics, e.g., of resistivity, spin-wave damping etc. [34].

Let us discuss some experimental examples of topological transitions in magnetic systems. The compound Co$_2$TiSn, which is supposed to be HMF, demonstrates transition from semiconducting to metallic state as the system undergoes the paramagnetic to ferromagnetic transformation [33]. CoFeTiSn shows the same feature; on the other hand, CoFeVGa demonstrates a semiconducting behaviour down to 90 K, below which it shows a window of metallic region and antiferromagnetism [34]. First principle calculations yield nearly half-metallic electronic structure for CoFeTiSn and CoFeVGa (see discussion in Ref. [35]), which may indicate topological instabilities of the Fermi surface. Note that the saturated HMF state is most stable in the mean-field theory of Kondo lattices [35]; inclusion of additional field is required to obtain more exotic states [36]. In Ref. [36] the HMF state was rediscovered in the Kondo model within the framework of the DMFT method and called “spin-selective Kondo insulator” (remember again the analogy with the orbital-selective Mott state [3]).

The compound UNiSn turns out to be an antiferromagnet, although the band structure calculations yield a HMF structure (see references in [37]). An unusual transition from metallic AFM state to small-gap semiconductor PM state with increasing $T$ takes place at 47 K. Most simple explanation is that the emergence of the sublattice magnetization results in a shift of the Fermi level outside the energy gap, but the Kondo origin of the gap seems to be more probable. Then the possible explanation of the metal-insulator transition observed is that the AFM exchange interaction suppresses the Kondo order parameter $V \sim (c^\dagger f)$ and, consequently, the gap [32]. This transition can be treated as a topological transition from large to small Fermi surface [30].

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