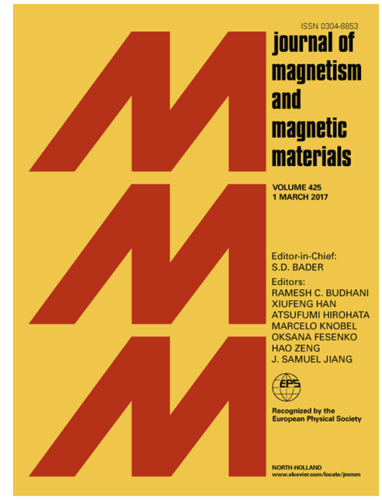
Accepted Manuscript



Research articles

Magnetic phase transitions and unusual antiferromagnetic states in the Hubbard model

P.A. Igoshev, M.A. Timirgazin, A.K. Arzhnikov, V.Yu. Irkhin

PII: S0304-8853(17)31984-4
DOI: https://doi.org/10.1016/j.jmmm.2017.10.007
Reference: MAGMA 63221

To appear in: *Journal of Magnetism and Magnetic Materials*

Please cite this article as: P.A. Igoshev, M.A. Timirgazin, A.K. Arzhnikov, V.Yu. Irkhin, Magnetic phase transitions and unusual antiferromagnetic states in the Hubbard model, *Journal of Magnetism and Magnetic Materials* (2017), doi: https://doi.org/10.1016/j.jmmm.2017.10.007

Magnetic phase transitions and unusual antiferromagnetic states in the Hubbard model

P.A. Igoshev[a,c], M.A. Timirgazin[b], A. K. Arzhnikov[b], V. Yu. Irkhin[a]

[a] *Institute of Metal Physics, Russian Academy of Sciences, 620108 Ekaterinburg, Russia*
[b] *Physical-Technical Institute, 426000, Kirov str. 132, Izhevsk, Russia*
[c] *Ural Federal University, 620002 Ekaterinburg, Russia*

Abstract

Ground state magnetic phase diagrams of the square and simple cubic lattices are investigated for the narrow band Hubbard model within the slave-boson approach by Kotliar and Ruckenstein. The transitions between saturated (half-metallic) and non-saturated ferromagnetic phases as well as similar transition in antiferromagnetic (AFM) state are considered in the three-dimensional case. Two types of saturated antiferromagnetic state with different concentration dependences of sublattice magnetization are found in the two-dimensional case in the vicinity of half-filling: the state with a gap between AFM subbands and AFM state with large electron mass. The latter state is hidden by the phase separation in the finite-U case.

Keywords: Hubbard model, slave bosons, non-collinear magnetism, antiferromagnetism, frustration
PACS: 71.27.+a, 75.10.Lp, 71.30.+h, 75.50.Ee

1. Introduction

As first demonstrated by Nagaoka, in the limit of infinite Hubbard's repulsion U the ground state for simple bipartite lattices in the nearest-neighbour approximation is a saturated ferromagnetic state for a low density δ of current carriers (doubly occupied states ("doubles") or empty states ("holes") in an almost half-filled band) [1]. Nagaoka considered the stability of saturated ferromagnetic state (sFM) and found its spin-wave instability with increasing δ and decreasing U. Roth applied a variational principle to this problem and obtained two critical concentrations [2]. The first one, δ_c, corresponds to instability of saturated ferromagnetic state, and the second one, δ_c', to the second-order transition from non-saturated ferromagnetism into paramagnetic state.

Zarubin and Irkhin [3, 4] have applied the $1/z$-expansion of the Green's functions in the many-electron representation [5, 6] for the Hubbard model and obtained an interpolation description of saturated and non-saturated ferromagnetism.

When introducing the Heisenberg exchange J ($t-J$ model) a tendency to antiferromagnetism occurs since the ground state at $n = 1$ is AFM insulator. The hole states in AFM matrix (for empty conduction band) in the nearest-neighbor hopping approximation at $J = 0$ were found to be incoherent [7, 8, 9]. For finite J the states near the band bottom form a narrow coherent band with small residue of order $|J/t| \ll 1$ and heavy mass $\sim |t/J|$ [9]. However, this picture is broken by different ways: (i) in the presence of next-nearest neighbor hopping which strongly affects the form of magnetic order; (ii) for finite density of carriers which makes Neel AFM order to be unfavorable; (iii) for finite Hubbard U when a large number of spin excitation can be involved.

Email address: valentin.irkhin@imp.uran.ru (V. Yu. Irkhin)

The competition of FM and AFM ordering results in occurrence of spiral magnetic ordering [10] or the magnetic phase separation [11, 10, 12]. These results were obtained under the assumption that saturated ferromagnetism is the ground state at finite doping and sufficiently large U. Here we present a more general physical picture taking into account finite next-nearest electron hopping which results, in particular, in occurrence of an unusual correlated antiferromagnetic state even at infinite U.

2. Formalism

We consider the Hubbard model [13]

$$H = \sum_{ij\sigma\sigma'} t_{ij}\delta_{\sigma\sigma'} c^\dagger_{i\sigma} c_{j\sigma'} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \qquad (1)$$

with the electron hopping $t_{ij} = -t$ for the nearest neighbors and t' for the next-nearest neighbors (we assume $t > 0$), $c^\dagger_{i\sigma}, c_{i\sigma}$ are the electron creation and annihilation operators, respectively, $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$, i is the site number, σ is the spin projection.

The local spin space rotation around x axis, matching different site magnetization vectors along, say, z axis, by the angle $\mathbf{QR}_i$ (where $\mathbf{Q}$ is a spiral wave vector, $\mathbf{R}_i$ is the site position) is applied for the consideration of plane magnetic spirals. This maps the spiral magnetic state into an effective ferromagnetic one, but the hopping term in the Hamiltonian becomes non-diagonal with respect to index σ: $t_{ij}\delta_{\sigma\sigma'} \to t^{\sigma\sigma'}_{ij} = \exp[i\mathbf{Q}(\mathbf{R}_i - \mathbf{R}_j)\sigma^x]_{\sigma\sigma'} t_{ij}$ in Eq. (1). The Hartree–Fock treatment of the many–particle Coulomb interaction term replaces it to some effective field $U\langle n_{i\bar{\sigma}}\rangle$ which mixes the averaged contributions from singly and doubly occupied states. However, this is not satisfactory even qualitatively, especially at large U.

A simple way of taking into account the correlation effects is an extension of the configuration space to a bosonic sector