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Magnetic orderings and phase separations in a simple model of insulating systems

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HIGHLIGHTS

- A simple effective electronic model for (anti-)ferromagnetic insulators is studied.
- Methods of analyses: variational MFA, MC simulations, rigorous solutions and others.
- Phase diagrams for various lattice dimensions and electron densities are derived.
- The interplay of different energy scales generates interesting critical behaviour.
- This (magnetic) system exhibits phase separation phenomenon and tricritical points.

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ABSTRACT

A simple effective model for a description of magnetically ordered narrow-band insulators is studied. The Hamiltonian considered consists of the effective on-site interaction (U) and intersite magnetic exchange interactions (J^z, J^{xy}) between nearest-neighbours. The phase diagrams and properties of this model for arbitrary chemical potential μ and arbitrary electron density n have been determined within several approaches: (i) the variational method (which treats the on-site interaction term exactly and the intersite interactions within the mean-field approximation) for any $J^z, J^{xy} \neq 0$ (exact in the limit of infinite dimensions), (ii) the Monte Carlo simulations on a square lattice with periodic boundary conditions for $J^{xy} = 0$, and (iii) other approximate methods (inter alia: random phase approximation and spin-wave approximation) as well as (iv) rigorous treatment to obtain results concerning the ground state phase diagrams (the two last also for $J^z, J^{xy} \neq 0$). The investigations of the general case show that, depending on the values of interaction parameters and electron concentration n, the system can exhibit not only homogeneous phases: (anti-)ferromagnetic (F_α, $\alpha = z, xy$) and nonordered (NO), but also phase separated states (PS_α: F_α/NO). For a fixed n one finds the following phase transitions (both continuous and discontinuous ones) and their sequences, which can occur with increasing temperature: $F_\alpha \rightarrow$ NO, $PS_\alpha \rightarrow$ NO, $PS_\alpha \rightarrow F_\alpha \rightarrow$ NO, $PS_\alpha \rightarrow F_\alpha \rightarrow PS_\alpha \rightarrow$ NO. The system analysed exhibits also tricritical behaviour.

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1. Introduction

The extended Hubbard model with anisotropic direct magnetic exchange interactions (the t–U–J^{xy}–J^z model) is a conceptually simple phenomenological model for studying correlations and for description of magnetism and other types of electron orderings in narrow band systems with easy-axis or easy-plane magnetic anisotropy [1–18]. The special feature of this model is that the magnetic coupling J is not related to the Hubbard U ($J \approx t^2/U$ as in the Hubbard model [19,20]) allowing finite exchange interactions even for $U \to +\infty$ and an independent treatment of J does not need the $U \to +\infty$ limit (in contrast to the t–J model in which charge fluctuations are strongly suppressed [21–25]). Actually, the t–U–J model connects the two limiting cases smoothly. In large U limit this model is reduced to the t–J model while it recovers the t–U model in small J limit.

The model t–U–J^{xy}-J^zHamiltonian on the lattice is of the following form:

$$\hat{H} = \sum_{i,j,\sigma} t_{ij}\left(\hat{c}^{+}_{i\sigma}\hat{c}_{j\sigma} + \hat{c}^{+}_{j\sigma}\hat{c}_{i\sigma}\right) + U\sum_{i}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} - J^{xy}\sum_{\langle i,j\rangle}\left(\hat{s}^{+}_{i}\hat{s}^{-}_{j} + \hat{s}^{+}_{j}\hat{s}^{-}_{i}\right) - 2J^{z}\sum_{\langle i,j\rangle}\hat{s}^{z}_{i}\hat{s}^{z}_{j} - \mu\sum_{i}\hat{n}_{i}, \tag{1}$$

where t_{ij} is the single electron hopping integral, U is the on-site density–density interaction, J^{xy} and J^z are xy- and z-components of the intersite magnetic exchange interaction, respectively. $\sum_{\langle i,j\rangle}$ restricts the summation to the nearest neighbours independently. $\hat{c}^{+}_{i\sigma}$ ($\hat{c}_{i\sigma}$) denotes the creation (annihilation) operator of an electron with spin σ at the site i, $\hat{n}_i = \sum_\sigma \hat{n}_{i\sigma}$, and $\hat{n}_{i\sigma} = \hat{c}^{+}_{i\sigma}\hat{c}_{i\sigma}$ (is the number of electrons with spin σ at site i). Spin operators $\hat{\vec{s}}_i$ at site i are defined by $\hat{s}^{z}_{i} = \frac{1}{2}(\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})$, $\hat{s}^{+}_{i} = \hat{c}^{+}_{i\uparrow}\hat{c}_{i\downarrow} = (\hat{s}^{-}_{i})^{\dagger}$. μ is the chemical potential associated with concentration of electrons n by the following relation:

$$n = \frac{1}{N}\sum_{i}\langle\hat{n}_i\rangle, \tag{2}$$

with $0 \le n \le 2$ and N is the total number of lattice sites. $\langle\hat{n}_i\rangle$ denotes an average value of operator $\hat{n}_i$.

Hamiltonian (1) with $t_{ij} = 0$ can be considered as a simplified model for the family of $A_{0.5}M_2X_4$ compounds (where A is Ga or Al, M is one of the transition metals V or Mo, and X is S, Se, or Te). These cluster compounds exhibit very interesting ferromagnetic behaviour [26–29]. Moreover, model (1) can be used to description of the proximity effects of magnetic and superconducting (triplet) orderings [1–7] in Sr_2RuO_4 [30], UGe_2 [31], $(TMTSF)_2X$ [32,33] and the exotic spin liquid states (RVB [34] or gossamer [9–11,23]). In addition, a large number of quasi-one dimensional insulating compounds, like Sr_3ZnIrO, $CsMnBr_3$, $CuGeO_3$, $Sr_3CuPt_xIr_{1-x}O_6$ and Ca_3CoRhO_6 show magnetic behaviour that can be described by the introduction of an intersite magnetic interactions [35–37].

For the strong on-site repulsion ($U \to +\infty$) and the isotropic antiferromagnetic exchange ($J^z = J^{xy} = J < 0$) model (1) was extensively studied in the context of high T_c superconductivity [23–25]. For finite values of U the t–U-J model has been also considered [9–18] as a model for gossamer superconductivity [9–11], iron-pnictides [15] and superconductivity on optical lattices [17,18]. The t–U-J model with ferromagnetic $J > 0$ has been also extensively used to describe ferromagnetism in metals, e.g. [38–43]. Model (1) with the transverse (XY-type) anisotropic exchange has been proposed in Ref. [1–3] as a suitable approach for description of narrow band systems with easy-plane magnetic anisotropy. In particular, the authors studied the weak-coupling ground state phase diagram of the one-dimensional t–U–J^{xy}–J^zmodel at $n = 1$ and $n \neq 1$ using the continuum-limit (infinite band) field theory approach [1,3] as well as (for $U > 0$ and $J^z = 0$) the density matrix renormalization group (DMRG) method [2]. Extensions of the studies of the half-filled t–U–J^{xy}-J^zmodels at $T = 0$ to the case of d-dimensional hypercubic lattices, including $d = 1$, 2 and $d = \infty$, by means of the (broken symmetry) Hartree–Fock approximation supplemented, for $d = \infty$, by the slave boson mean-field approach (SBMFA) and, for $d = 1$, by the level-crossing approach for finite-size clusters, have been also performed [4–6].

Because of the complexity of the model there are no exact solutions for the t–U–J^{xy}-J^z Hamiltonian and only few results are known beyond the weak coupling regime or away from half-filling ($n = 1$).

In this work we will focus on the zero-bandwidth limit of model (1): $t_{ij} = 0$, for the case of arbitrary electron density $0 < n < 2$. The (zero-bandwidth) U–J^{xy}–J^zHamiltonian considered in the following has the form

$$\hat{H} = U\sum_{i}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} - J^{xy}\sum_{\langle i,j\rangle}\left(\hat{s}^{+}_{i}\hat{s}^{-}_{j} + \hat{s}^{+}_{j}\hat{s}^{-}_{i}\right) - 2J^{z}\sum_{\langle i,j\rangle}\hat{s}^{z}_{i}\hat{s}^{z}_{j} - \mu\sum_{i}\hat{n}_{i}, \tag{3}$$

where concentration n can be calculated from (2). Notice that the model is different from the well-known $S = 1/2$ Heisenberg–Ising model of magnetism, because four different states are possible on every site (which are: $|0\rangle_i$ – no electrons (empty), $|\uparrow\rangle_i$, $|\downarrow\rangle_i$ – states with one electron with spin up or down, and $|\uparrow\downarrow\rangle_i$ – two electrons (full)) and the $\left\{\hat{\vec{s}}_i\right\}$ operators are the $S = 1$ spin operators with the 0-eigenvalue degenerated twice. In addition, in our analyses we involve the on-site U interaction. Notice that only for $U \to +\infty$ and $n = 1$ model (3) is equivalent with the anisotropic $S = 1/2$ Heisenberg model (for $J^{xy} = 0$ – with $S = 1/2$ Ising model). In such a limit only two states: $|\uparrow\rangle_i$ and $|\downarrow\rangle_i$ are possible at every site. Interesting equivalences of model (3) with several other pseudospin models in particular limits are pointed out in Appendix A.

In the analysis presented in Sections 2–4 we have used a variational approach (VA) which treats the on-site interaction U exactly and the intersite interactions (J^z,J^{xy}) within the mean-field approximation (MFA) for hypercubic lattices. In Section 5