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MAGNETIC PROPERTIES OF THE HUBBARD MODEL WITH INFINITE INTERACTION

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Abstract. The problem of the ground state multiplicity of the Hubbard model with the infinite interaction is considered for the systems of segments of length n.

Introduction.

The simplest model of strong correlated systems is the Hubbard model with the infinite repulsion described by the Hamiltonian

$$H = \Sigma\, t_{ij}(c^{+}_{i\sigma}c_{j\sigma} + c^{+}_{j\sigma}c_{i\sigma})(1-c^{+}_{i,-\sigma}c_{i,-\sigma})(1-c^{+}_{j,-\sigma}c_{j,-\sigma}) \qquad (1)$$

One of the most important problems is to find the dependence of the ground state multiplicity on the electron density ρ.(Nagaoka problem [1]). We consider this problem for special kind of systems,consisting of ladders of n-sites segments with different intra- and intersegment hopping integrals, t and $t_{\perp}$.

Spin Hamiltonian (SH).

If $\alpha = t_{\perp}/t \ll 1$ one can make use of the perturbation theory in α. For $t_{\perp} = 0$ energetic levels are spin degenerated. The resolve of degeneracy (up to α^2) leads to Hamiltonian acting upon the spin variables of the neighbouring segments [2]. It turns out that the energy of two neighbouring segments with equal (inequal) non-zero numbers of electrons is minimal at total minimal (maximal) spin. Thus, SH describes the competing interactions of ferro (F)- and antiferromagnetic (AF) types. For $\rho<1/n$ there cannot be more than one electron at each segment and the ground state is singlet. For $\rho>1/n$ the competion interactions leads to a separation of phases with F and AF ordering. For example, for the system with n=2 (ladders of dimers) and for $\rho>1/2$ F-polaron is created. Its size is proportional to $\alpha^{-1/3}$,and at $\rho_c=(2\pi)^{-1}(3\pi\alpha\ln 2)^{1/3}$is equal to the ladder length. Thus, the system is saturated ferromagnet. For the case with n>2 polarons may be both F-and AF-type leading to the "cascade" of transitions with the alteration of total spin. Equally to the ladders a more complicated system may be considered. It consists of dimers packed up a 2d lattice. For $\rho\leq 1/2$ SH is equivalent to Hamiltonian of the 2d t-J model which magnetic properties have been discussed in [3]. As in the case of the ladder model for $\rho>1/2$ the F polaron appears as well as the critical density ρ_c above which the system becomes a saturated ferromagnet.

The variotional approach.

For ladders with arbitrary α we seek the wave function Ψ in the following form(for simplicity we consider the model with n=2):

$$\Psi = \prod_i N_{i\alpha} N_{i\beta} (x_i + y_{i\alpha} \psi_{\alpha\alpha}(i) + y_{i\beta} \psi_{\beta\beta}(i) + \psi_{\alpha\beta}(i) b^+_{i\alpha} b^+_{i\beta} + b^+_{i\alpha} \psi_\beta (i) + b^+_{i\beta} \psi_\alpha(i)),$$

where

$$\psi_{\sigma\sigma}(i) = c^+_{1\sigma} c^+_{2\sigma}; \quad \psi_{\alpha\beta}(i) = \lambda_s \varphi_s(i) + \lambda_t \varphi_t(i); \quad \varphi_{s,t} = (2)^{-1/2} (c^+_{1\alpha} c^+_{2\beta} \mp c^+_{1\beta} c^+_{2\alpha}); \quad \psi_\sigma(i) = (2)^{-1/2} (c^+_{1\sigma} + c^+_{2\sigma}).$$

1,2 are the numbers of sites of a i-th segment; λ_s,λ_t are the variational parameters at $\lambda_s^2 + \lambda_t^2 = 1$; $x_i^2 + y_{i\alpha}^2 + y_{i\beta}^2 = 1$ ($y_{i\sigma}$ = 0 or 1). $N_{i\sigma} = b^+_{i\sigma} b_{i\sigma}$; $b^+_{i\sigma}$ are the operators of pseudo-fermi-particles.

Effective Hamiltonian for pseudoparticles is $H_{eff} = \langle\Psi H \Psi\rangle$ where $\langle..\rangle$ means an average on c-operators. Analysing H_{eff} we have reproduced the results obtained by SH method for $\alpha<<1$. In isotropic case, $\alpha=1$, and for $\rho<1/2$ a ground state is singlet. At $\rho \rightarrow 1$ a ground state spin is maximal. At $\rho=0.67$ this state becomes unstable with respect to overturning single up-spin electron. However, it turns out that at $\rho=0.73$ F state is unstable against multimagnon excitations. Note that in Gutzwiller approximation F state in this model is stable at all values of ρ.

We also studied the dependence $S(\rho)$ using the exact diagonalization of small ladders of dimers (up to 16 sites). The agreement between analytical and numerical results is fairly good.

References.

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