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Autor(en): **Holz, A.**

Objekttyp: **Article**

Zeitschrift: **Helvetica Physica Acta**

Band (Jahr): **65 (1992)**

Heft 2-3

PDF erstellt am: **24.05.2024**

Persistenter Link: https://doi.org/10.5169/seals-116467

SO(3)-σ MODEL OF DOPED TWO-DIMENSIONAL SPIN-1/2 HEISENBERG ANTIFERROMAGNET

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Abstract. A theory of the doped spin-1/2 Heisenberg antiferromagnet (HA) is developed within the concept of a SO(3)-σ model, recently studied [1] for the undoped system. Disordered states of the HA are discussed via topological defects of the SO(3)-σ model supplemented by line defects due to discrete nature of lattice structure.

Introduction. A semiclassical action Γ_{sc} of a doped spin-1/2 HA based on the gauge group $G_D = SO(3) \times SU(2)$ is derived according to a method suggested in ref. 1. Some qualitative features of the resulting SO(3)-σ model with respect to mobility and superconding properties of charge are discussed within the context of the defect structure of the model.

The Hamiltonian of the electron doped two-dimensional (2-D) spin-1/2 HA may be represented in the form

$$H = J\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j(1-e_i^{\dagger}e_i)(1-e_j^{\dagger}e_j)+\frac{t}{2}\sum_{\langle i,j\rangle}\tilde{c}^{\dagger}_{i,\sigma}\tilde{c}_{j\sigma}+\mu\sum_i e_i^{\dagger}e_i+s\sum_i e_i^{\dagger}e_i(a_i+a_i^{\dagger}). \tag{1}$$

The first term refers to the spin-1/2 HA ($J > 0$) and $e_i^{\dagger}e_i = 0,1$ measures occupancy of spin sites by extra electrons, where $\{e_i,e_j^{\dagger}\} = \delta_{ij}$. The spin operators are expressed in the form $\mathbf{S}_i = \hbar\left[\frac{1}{2}(a_i^{\dagger}+a_i)\mathbf{e}_x+\frac{1}{2}i(-a_i^{\dagger}+a_i)\mathbf{e}_y+(a_i^{\dagger}a_i-\frac{1}{2})\mathbf{e}_z\right]$. The operators $a_i^{\dagger}, a_i$ obey for $i \neq j$ and $i = j$ Bose and Fermi commutation relations, respectively. The second and third term in (1) refer to the hopping motion of extra electrons and their chemical potential, respectively. Referring $(a_i^{\dagger},a_i)$ to a state, where all spins point down, one may use the identities $\tilde{c}^{\dagger}_{j\uparrow} = e_j^{\dagger}(1-a_j^{\dagger}a_j)$, $\tilde{c}^{\dagger}_{j\downarrow} = e_j^{\dagger}a_j^{\dagger}a_j$ and their adjoints. The sets of operators $(a_i^{\dagger},a_i)$ and $(e_i^{\dagger},e_i)$ commute among each other. The last term in (1) allows for a stochastic change of $n_i = a_i^{\dagger}a_i$ during times when the site is in a singlet state ($e_i^{\dagger}e_i = 1$). For hole doping one replaces $(e_i^{\dagger},e_i)$ by hole operators $(h_i^{\dagger},h_i)$ and uses $\tilde{c}_{j\downarrow} = h_j^{\dagger}(1-a_j^{\dagger}a_j)$, $\tilde{c}_{j\uparrow} = h_j^{\dagger}a_j^{\dagger}a_j$ and their adjoints.

Gauge Transformation. Eq. (1) will be subject to an unitary transformation $H \to H' = U^{\dagger}HU - i\hbar U^{\dagger}\partial_t U$, of the type (applying to all electrons), $c_{j,\sigma} \to c'_{j,\sigma} = \mathcal{R}^{(1/2)}_{j,\sigma\sigma'}c_{j,\sigma'}$, where $\mathcal{R}^{(1/2)}_j \in SU(2)$. The first term of H' can be expressed in the form

$$H'^{(1)} = J\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{R}^{ji}\cdot\mathbf{S}_j(1-e_i^{\dagger}e_i)(1-e_j^{\dagger}e_j)+\frac{t}{2}\sum_{\langle i,j\rangle}\tilde{c}^{\dagger}_{i,\sigma}\mathcal{R}^{ji(1/2)}_{\sigma'\sigma}\tilde{c}_{j,\sigma'}+\dots, \tag{2}$$

where the third and fourth term in (1) remain invariant, and

$$\mathbf{R}^{ji} \equiv \mathbf{R}_j^{t}\cdot\mathbf{R}_i, \qquad \mathbf{R}_i \in SO(3), \qquad \mathcal{R}^{ji(1/2)} \equiv \mathcal{R}^{(1/2)}_j\cdot\mathcal{R}^{\dagger(1/2)}_i. \tag{3}$$

The second term in H' is given by

$$H'^{(2)} = H'_{(1/2)} - i\hbar\sum_j\{\mathcal{R}^{\dagger(1/2)}_{j,\sigma\sigma'}\partial_t\mathcal{R}^{(1/2)}_{j,\sigma'\sigma''}\tilde{c}^{\dagger}_{j,\sigma}\tilde{c}_{j,\sigma''}+\mathcal{R}^{(1/2)}_{j,\sigma'\sigma}\partial_t\mathcal{R}^{\dagger(1/2)}_{j,\sigma''\sigma'}\tilde{c}_{j,\sigma}\tilde{c}^{\dagger}_{j,\sigma''}\}. \tag{4}$$

Here the first term refers to the doped spin-1/2 HA and can be expressed in the form [1]

$$H'_{(1/2)} = -i\hbar\sum_i |m_i\rangle(\mathcal{R}_i^{\dagger(1/2}\partial_t\mathcal{R}_i^{(1/2)})_{m_i n_i}\langle n_i|(1-e_i^\dagger e_i),\ \{|n_i\rangle\langle m_i|\} \equiv \begin{bmatrix} a_i^\dagger a_i & a_i^\dagger \\ a_i & a_i a_i^\dagger \end{bmatrix}, \quad (5)$$

and the second term of (5) refers to extra electrons. $H'^{(1)}$ and $H'^{(2)}$ will produce potential and kinetic as well as topological phase terms in Γ_{sc}, respectively.

$\mathbf{R}_i$ and $\mathcal{R}_i^{(1/2)}$ may be parametrized by Euler angles $(\alpha_i,\beta_i,\gamma_i)$. Due to the antiferromagnetic (AF) coupling of spins it is more convenient to use locally a staggered arrangement of spins. This suggests the use of

$$\mathcal{R}_i^{(1/2)} = R^{(1/2)}(\alpha_i,\beta_i,\gamma_i)\cdot\begin{cases} R^{(1/2)}(\pi,\pi,0), & i \in L_A \\ I^{(1/2)}, & i \notin L_A \end{cases} \quad (6)$$

where $I^{(1/2)}$ is a unit matrix in SU(2), and an analogous relation in SO(3). L_A represents the set of lattice points, where the spin has been rotated by 180° around the $\hat{x}$-axis. L_A may represent a Néel sublattice containing defects in the form of domain boundaries.

Integrating out the operators (a_i^+,a_i), will result [1] in an action Γ_{sc} depending on the set $\{\alpha_i,\beta_i,\gamma_i\}$ and its time derivative, on the defect structure of L_A and on the particle (e_i^+,e_i) respectively hole (h_i^+,h_i) operators. Γ_{sc} governs the dynamics of the SO(3)-σ model corresponding to the doped spin-1/2 HA.

Defect States and Mobility of Charge. The motion of charge in the doped spin-1/2 HA preferentially takes place along domain boundaries, which become displaced perpendicularly to their original orientation. In case of dilute doping ($c_d \cong 0$) domains may be small and disconnected, leading to hole localization (insulating states). For $c_d \cong O(1)$ the AF order may be destroyed leading to an interconnected system of domain boundaries and to extended charge orbits (metallic state). In addition the SO(3)-model features defects which may be classified by $\pi_1(SO(3)) = \mathbb{Z}_2$ and $\pi_3(SO(3)) = \mathbb{Z}$. The fundamental group refers to disclination like defects in 2+1-D space time, whereas $\pi_3(SO(3))$ measures the entanglement of "disclinations" of strengths $s \in \mathbb{Z}$ and $s \in \mathbb{Z}+1/2$, and allows a connection with the approach in ref. 2. A measure of $\pi_3(SO(3))$ is the Wess-Zumino term which replaces the Hopf term in a O(3)-σ model, and supposedly governs the statistics of the model. In Γ_{sc} for $c_d = 0$, only a phase term of Berry's type was found [1]. A discussion of the topological properties of the SO(3)-σ model in terms of O(3)-σ models has been given in [3]. This suggest a simple explanation of the development of superconducting states in the SO(3)-σ model along the lines given in [4] for the O(3)-σ model. In particular charge may form composite objects with disclination cores (encircling these objects along domain boundaries) leading to peculiar normal and superconducting properties.

The author acknowledges discussions with J. Madore and financial support by DFG.

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