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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

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

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

Gauge Transformation. Eq. (1) will be subject to an unitary transformation $H \to H' = U^+ H U - i\hbar U^+ \partial_t U$, 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

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

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

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

The second term in H' is given by

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

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.

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