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SO(3)-6 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)-6 model, recently studied [1] for the undoped system. Disordered states of the HA are discussed via topological defects of the SO(3)-6 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

$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_{i} \cdot \mathbf{S}_{j} (1 - e_{i}^{\dagger} e_{i}) (1 - e_{j}^{\dagger} e_{j}) + \frac{\mathbf{t}}{2} \sum_{\langle i,j \rangle} \widetilde{c}_{i,\sigma}^{\dagger} \widetilde{c}_{j\sigma}^{\dagger} + \mu \sum_{i} e_{i}^{\dagger} e_{i} + s \sum_{i} e_{i}^{\dagger} e_{i} (a_{i} + a_{i}^{\dagger}). \tag{1}$$

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 $\mathbf{S}_i=\hbar\left[\frac{1}{2}(a_i^{\dagger}+a_i)\mathbf{e}_{\chi}+\frac{1}{2}i(-a_i^{\dagger}+a_i)\mathbf{e}_{\chi}+(a_i^{\dagger}a_i^{}-\frac{1}{2})\mathbf{e}_{z}^{}\right]$. 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 $\widetilde{C}_{j\uparrow}^{}=e_j^{\dagger}(1-a_j^{\dagger}a_j)$, $\widetilde{C}_{j\downarrow}^{}=e_j^{\dagger}a_j^{\dagger}a_j^{}$ 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 $(e_i^{}e_i^{}=1)$. For hole doping one replaces (e_i^{\dagger},e_i) by hole operators (h_i^{\dagger},h_i) and uses $\widetilde{C}_{j\downarrow}=h_j^{\dagger}(1-a_j^{\dagger}a_j)$, $\widetilde{C}_{j\uparrow}=h_j^{\dagger}a_j^{\dagger}a_j^{}$ and their adjoints.

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

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

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

$$\mathbf{R}^{ji} = \mathbf{R}_{i}^{t} \cdot \mathbf{R}_{i}, \qquad \mathbf{R}_{i} \in SO(3), \quad \mathbf{R}^{ji(1/2)} = \mathbf{R}_{i}^{(1/2)} \cdot \mathbf{R}_{i}^{+(1/2)}. \tag{3}$$

The second term in H' is given by

$$H^{'(2)} = H^{'}_{(1/2)} - i\hbar \sum_{j} \{ \mathcal{R}^{\dagger (1/2)}_{j,\sigma\sigma'} \partial_{t} \mathcal{R}^{(1/2)}_{j,\sigma'\sigma''} \, \widetilde{c}^{\dagger}_{j,\sigma''} \, \widetilde{c}^{\dagger}_{j,\sigma''} + \mathcal{R}^{(1/2)}_{j,\sigma'\sigma} \partial_{t} \mathcal{R}^{\dagger (1/2)}_{j,\sigma''\sigma'} \, \widetilde{c}^{\dagger}_{j,\sigma''\sigma'} \}. \eqno(4)$$

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

$$H'_{(1/2)} = -i\hbar \sum_{i} |m_{i}\rangle (\Re_{i}^{\dagger (1/2)} \partial_{t} \Re_{i}^{(1/2)})_{m_{i}n_{i}} \langle n_{i} | (1 - e_{i}^{\dagger} e_{i}), \{ |n_{i}\rangle \langle m_{i}| \} \equiv \begin{bmatrix} a_{i}^{\dagger} a_{i} & a_{i}^{\dagger} \\ a_{i} & a_{i}a_{i}^{\dagger} \end{bmatrix}, (5)$$

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 $\mathbf{R}_i^{(1/2)}$ 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

$$R_{i}^{(1/2)} = R^{(1/2)}(\alpha_{i}, \beta_{i}, \gamma_{i}) \cdot \begin{cases} R^{(1/2)}(\pi, \pi, 0), & i \in L_{\mathbf{A}} \\ I^{(1/2)}, & i \notin L_{\mathbf{A}} \end{cases}$$
(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)-6 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)-6 model in terms of O(3)-6 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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