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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 superconducting 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

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

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 $\tilde{c}_{j\uparrow}^\dagger = e_j^\dagger(1 - a_j^\dagger a_j)$, $\tilde{c}_{j\downarrow}^\dagger = e_j^\dagger a_j^\dagger a_j$ 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 $\tilde{c}_{j\downarrow}^\dagger = h_j^\dagger(1 - a_j^\dagger a_j)$, $\tilde{c}_{j\uparrow}^\dagger = h_j^\dagger a_j^\dagger a_j$ and their adjoints.

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

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

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

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

The second term in H' is given by

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

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.

\mathcal{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^\dagger, 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^\dagger, e_i) respectively hole (h_i^\dagger, h_i) operators. Γ_{sc} governs the dynamics of the $SO(3)-\sigma$ 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 $O(3)-\sigma$ 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 $SO(3)-\sigma$ model in terms of $O(3)-\sigma$ models has been given in [3]. This suggest a simple explanation of the development of superconducting states in the $SO(3)-\sigma$ model along the lines given in [4] for the $O(3)-\sigma$ 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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