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LETTER TO THE EDITOR

Superconductivity and topological terms arising from magnetic interactions

D Schmeltzer

Department of Physics, Bar-Ilan University, Ramat-Gan 52100, Israel

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Abstract. The Kondo lattice Hamiltonian used for the CuO_2 layers is investigated. A new derivation of the Wess–Zumino term in magnetic systems, and a new model for super-conductivity are presented. Holes belonging to the same copper site interact ferromagnetically, in contrast to holes belonging to different copper sites which interact anti-ferromagnetically. The presence of holes leads to a frustrated Heisenberg lattice. In a frustrated lattice, the individual Wess–Zumino terms of individual spins may combine to provide a non-trivial topological term for the 2D case.

We investigate the Kondo lattice Hamiltonian derived for the CuO_2 layers [1–9]. The path integral based on the coherent states is constructed [10]. The complex Grassman field [11] representation is used for the fermion oxygen holes and the bilinear real Grassman coherent representation [12] is used for the spin- $\frac{1}{2}$ copper (Cu) system. The latter representation is used in order to derive an alternative solution of the Wess–Zumino (wz) term [13, 14] in quantum magnetic systems.

The effective action obtained from the coherent path integral leads to the following new mean-field picture of pairing of oxygen holes. As a result of doping, a ferromagnetic (F) interaction is induced between the oxygen holes (O^{1-}) around Cu^{2+} and an antiferromagnetic (AF) interaction between O^{1-} holes belonging to different Cu^{2+} sites. This leads to a BCS potential for the holes.

When we go beyond the mean-field approximation (elimination of double occupancy induced by the ferromagnetic short-range interactions), we recover the solution obtained in the one-band Hubbard model—separation of charge and spin [13–16]. In the slave-boson picture, the kinetic energy is controlled by a hopping term proportional to the hole concentration (the holons), and in addition we have a frustrated Heisenberg lattice. Contrary to the case for the 2D Heisenberg square lattice [15], we find that individual wz terms of individual spins may combine to provide a non-trivial topological term.

The basic model assumes [4–9] that the Cu $3d_{x^2-y^2}$ bonding band remains half-filled in the presence of a dopant, while the additional holes go into the oxygen band O^{1-} of type p_{σ} or p_{π} . This leads to a square lattice of spins with spin- $\frac{1}{2}$ AF Heisenberg interaction with a coupling constant J between the spins S(n) ($n = (n_x, n_y)$) and to a Kondo coupling K (K > 0 for p_{σ} orbitals and K < 0 for p_{π}) between the Cu²⁺ and O¹⁻:

$$H = H_{\rm O} + H_{\rm M} \tag{1a}$$

$$H_{\rm O} = \sum_{\alpha = \uparrow, \downarrow} \sum_{k} (E_k - E_{\rm F}) P_{\alpha}^+(k) P_{\alpha}(k) \tag{1b}$$

$$H_{\rm M} = J \sum_{n,n'} S(n) \cdot S(n') + K \sum_{n} S(n) \cdot R(n).$$
(1c)

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 H_0 is the oxygen hole's kinetic energy and H_M is the magnetic part [4–9]. $\mathbf{R}(n)$ is the total O operator in the cell *n*. In each unit cell we have three atoms, one Cu and two O at positions $n + v_x$ and $n + v_y$. The microscopic [14] form of $\mathbf{R}(n)$ is

$$\mathbf{R}(n) = \sum_{n+v,n'+v'} (-1)^{\alpha(n+v,n'+v')} P^+(n+v) \boldsymbol{\sigma} P(n'+v')$$

(α is even or odd and is determined by the phases of the p and d orbitals [14, 17]). In the limit of a large band width $8t \ge K$, we make a long-wave approximation and make the replacements

$$\mathbf{R}(n) \simeq P^+(n)\boldsymbol{\sigma} P(n) \qquad E(k) \simeq tk^2$$

where

$$P(n) \simeq 4(P(n+v_x) + P(n-1_x+v_x) + P(n+v_y) + P(n-1_y+v_y))^{-1/2}.$$

(According to the microscopic derivation [4] based on the $d-p_{\sigma}$ hybridisation, $8t \approx 1.04 \text{ eV}$, K = 1.3 eV and $J = 0.1 - 0.44\delta$ where δ is the oxygen hole concentration.) These values of the parameters justify our using the long-wave approximation. When we consider p_{π} orbitals the $t \rightarrow 0$ limit is more reasonable. In this case we integrate out the oxygen fermion. We use the approximation

$$K\sum_{n} \mathbf{R}(n) \cdot \mathbf{S}(n) \approx K\sum_{n} P^{+}(n+v_{x})\boldsymbol{\sigma} P(n+v_{x}) \cdot (\mathbf{S}(n) + \mathbf{S}(n+1_{x}))$$
$$+ P^{+}(n+v_{y})\boldsymbol{\sigma} P(n+v_{y}) \cdot (\mathbf{S}(n) + \mathbf{S}(n+1_{y}))$$

(each hole couples to two copper ions).

In order to investigate the Hamiltonian given in (1) we construct the path integral using the coherent states

$$|\tau_{\rm p}\rangle = |Z(\tau_{\rm p})\rangle \otimes |S(\tau_{\rm p})\rangle$$
 $P = 1 - N$ $N\delta t = \beta = 1/T.$

 $|Z(\tau_p)\rangle$ is the coherent state for the fermion oxygen holes:

$$|Z(\tau_{\rm p})\rangle = \exp\left(\sum_{\alpha=\uparrow,\downarrow}\sum_{n+\nu}\psi_{\alpha}(n+\nu,\tau_{\rm p})P_{\alpha}^{+}(n+\nu,\tau_{\rm p})\right)|0).$$
(2a)

 ψ_{α} , ψ_{α}^{+} are complex Grassman fields, P_{α}^{+} is a hole creation operator, and $|0\rangle$ is the vacuum state for the double-occupied oxygen. The coherent state $|S(\tau_{p})\rangle$ for Cu²⁺ is

$$|S(\tau_{\rm p})\rangle \propto \exp\left(\sum_{n}\sum_{r=1}^{\infty} {\rm i}S_r(n,\tau_{\rm p})\sum_{\alpha,\beta=\uparrow,\downarrow} d^+_{\alpha}(n,\tau_{\rm p})\sigma^r_{\alpha,\beta}d_{\beta}(n,\tau_{\rm p})\right)|\Phi_0\rangle$$
(2b)

where d_{α} , d_{α}^{+} are the Cu fermion variables, S_r is the 3-component spin, $|\Phi_0\rangle$ is the vacuum state of Cu²⁺ (at each site we have one fermion). A useful representation for S_r is the 3-component real Grassman field [12]:

$$S_r = -\frac{1}{2}i\varepsilon_{rlm}\eta_l\eta_m \qquad r = 1, 2, 3$$

The partition function is computed with the aid of the Trotter formula [10] and the resolution operator, $\int d\mu(\tau_p) |\tau_p\rangle \langle \tau_p | = 1$, where $d\mu = d\psi^+ d\psi d\eta_1 d\eta_2 d\eta_3$. When we decouple the $S(n) \cdot S(n')$ interaction we use the Hubbard–Stratonovici transformation and introduce the collective field M. The partition function is

$$Z = \int \mathrm{d}\mu \, D^3 M \,\mathrm{e}^{-A} \tag{3a}$$

$$A = A_0 + A_{\rm M} \tag{3b}$$

$$A_{0} = \int_{0}^{\beta} \mathrm{d}\tau \left(\sum_{\alpha=\uparrow,\downarrow} \sum_{k} \psi_{\alpha}^{+}(k,\tau) (\partial_{\tau} - E(k) + E_{\mathrm{F}}) \psi_{\alpha}(k,\tau) \right)$$
(3c)

$$A_{\rm M} = \int_{0}^{\beta} \mathrm{d}\tau \left(\frac{1}{2} \sum_{n} \eta_{l}(n,\tau) (\partial_{\tau} - \mathrm{i}\phi_{r}(n,\tau)\varepsilon_{rlm}) \eta_{m}(n,\tau) + J \sum_{n,n'} M(n,\tau) \cdot M(n',\tau) \right)$$
(3d)

where $\phi(n, \tau) = KR(n, \tau) + 2iJ\Omega(n, \tau)$ and $\Omega(n, \tau) = \sum_n M(n', \tau)$, in which n' are nearest-neighbour sites to n. We will integrate the real Grassman fields (it is important to note that the use of the fields η_r avoids constraint fields required when we use normal fermions). This is useful for obtaining the O(3) non-linear σ -model for spin $\frac{1}{2}$ when K = 0 as well for the case when we integrate the Cu²⁺ variables and obtain an effective action in terms of the hole variables. We find

$$A_{\text{eff}} = A_0 + \int_0^\beta \mathrm{d}\tau \left(J \sum_{n,n'} M(n,\tau) \cdot M(n',\tau) \right) + \sum_n \Gamma[\phi(n,\tau)]$$
(3e)

where the last term in (3e) is the result of the real Grassman integration,

$$\Gamma[\boldsymbol{\phi}(n,\tau)] = -\frac{1}{2} \operatorname{Tr} \ln(\partial_{\tau} - \mathrm{i}\phi_{r}(n,\tau)\varepsilon_{rlm}).$$
(3f)

The computation of (3f) is a non-trivial calculation. We substitute $\phi(n, \tau) = \phi_0(n) + \delta \phi(n, \tau)$ and expand (3f) to second order in $\delta \phi$. Using methods similar to the one used in [18] for the ϕ^4 model we find

$$\Gamma[\boldsymbol{\phi}(n,\tau)] \simeq \int_0^\beta \mathrm{d}\tau \left[-\frac{1}{2} (\boldsymbol{\phi}^2(n,\tau))^{1/2}\right] + \frac{1}{2} \mathrm{i} S_{\mathrm{WZ}}[\boldsymbol{\phi}(n)] \tag{4a}$$

where the second term has the form of the wz or Berry phase [19]

$$S_{WZ}[\boldsymbol{\phi}(n)] = \int_{0}^{\beta} \mathrm{d}\tau \, \frac{1}{2} \varepsilon_{rlm} \, \frac{\boldsymbol{\phi}_{r}(n)}{|\boldsymbol{\phi}(n)|^{3}} \, \delta \boldsymbol{\phi}_{l}(n,\tau) \partial_{\tau} \boldsymbol{\phi}_{m}(n,\tau). \tag{4b}$$

The result given in (4) is obtained after some extended calculation. The justification of this result can be seen from the adiabatic theorem which allows us to compute (3f). The problem which we have to solve is described by a time-dependent Hamiltonian $h(\tau) = \frac{1}{2}\sigma \cdot \phi(\tau)$. But this is exactly the problem solved by Berry [17] with the first term in (4a) being the instantaneous eigenvalue and (4b) corresponding to the non-adiabatic corrections, called the Berry phase. In the absence of holes K = 0, we put $\phi(n) = \sum_{n'en} M(n') \simeq (-1) 4M(n)$. Expanding around the minimum |M| = 1 we obtain an alternative derivation to the topological term given in [15] for the Heisenberg spin- $\frac{1}{2}$ AF. In the presence of holes we investigate (3) and (4) in the limit $|K| \ge J$ (this limit is in agreement with the microscopic parameters [4]). To leading order J/|K| we replace the wz term $S_{WZ}[\phi] \simeq S_{WZ}[R]$ and expand $(\phi^2(n, \tau))^{1/2}$ to first order in J/|K|. We replace $R^2 = \langle R^2 \rangle + (R^2 - \langle R^2 \rangle)$ and obtain for $J/|K|\langle R^2 \rangle < 1$ the formula

$$A_{\text{eff}} \simeq A_0 + \int_0^\beta \mathrm{d}\tau \left(J \sum_{n,n'} M(n,\tau) \cdot M(n',\tau) - \frac{1}{4} |K| \sum_n \frac{R^2(n,\tau)}{\langle R^2(n) \rangle^{1/2}} + \mathrm{i}J \sum_n \frac{\mathrm{sgn}\,K}{\langle R^2(n) \rangle^{1/2}} R(n,\tau) \cdot \Omega(n,\tau) \right) + \frac{1}{2} \mathrm{i} \sum_n S_{\text{WZ}}[R(n)].$$
(5)

(Formally, we can replace $(\phi^2(n))^{1/2}$ by a Gaussian integration, $(\phi^2(n))^{1/2} \rightarrow \sigma^2(n) + \phi^2(n)/\sigma^2(n)$. The minimum of the Gaussian field occurs at $4\sigma^2 = \langle \phi^2 \rangle^{1/2} \simeq K \langle R^2 \rangle$ for K/J > 1). In the long-wavelength approximation

$$\mathbf{R}(n) \simeq \psi^+(n)\boldsymbol{\sigma}\psi(n)$$
$$\mathbf{R}^2(n) = \frac{3}{4} \sum_{\alpha=\uparrow,\downarrow} \left(\psi^+_\alpha(n)\psi_\alpha(n) - \psi^+_\alpha(n)\psi_\alpha(n)\psi^+_{-\alpha}(n)\psi_{-\alpha}(n) \right).$$

Therefore the third term in (5) (the F term) produces an on-site repulsion of strength $\frac{3}{8}|K|\langle R^2\rangle^{-1/2}$. Having no wz term for the *M* variables allows us to perform a Gaussian integration and to obtain an effective action in terms of hole variables,

$$A_{\text{eff}} \approx A_0 + \int_0^\beta \mathrm{d}\tau \left(J \sum_{n,n'} \frac{4}{(\langle R^2(n) \rangle \langle R^2(n') \rangle)^{1/2}} \mathbf{R}(n,\tau) \cdot \mathbf{R}(n',\tau) - \frac{1}{4} |K| \sum_n \frac{R^2(n,\tau)}{\langle R^2(n) \rangle^{1/2}} + \frac{1}{2} \mathrm{i} \sum_n S_{\text{WZ}}[\mathbf{R}(n)].$$

$$(6)$$

Equation (6) represents our new effective interaction for the oxygen holes. We have an AF term for next-nearest-neighbour holes and an F interaction for nearest-neighbour holes. In addition we have a wz term which may lead to a non-trivial Hopf term [19–21]. As I have suggested [20], doping may lead to statistical transmutation and non-conventional superconductivity (sc) may occur. In the long-wave approximation we replace $\mathbf{R}(n) = \psi^+(n)\boldsymbol{\sigma}\psi(n)$. Using the Grassman fields ψ^+_{α} , ψ_{α} the wz term restores the time derivative term in (3c)

$$\left(\frac{1}{2} \mathbf{i} \, S_{\mathrm{WZ}}[\mathbf{R}] = \sum_{\alpha = \uparrow, \downarrow} \int_{0}^{\beta} \mathrm{d} \, \tau \, \psi_{\alpha}^{+} \partial_{\tau} \psi_{\alpha}\right)$$

and the magnetic interaction is represented as a BSC potential

$$V(K-K' = q) = \frac{3}{8} |K| / \langle R^2 \rangle^{1/2} - (4J/\langle R^2 \rangle) (\cos q_x + \cos q_y).$$
(7)

Such a potential gives rise to anisotropic pairing [1, 22]. (For small hole concentrations the repulsion part of R^2 is negligible leading to anisotropic S waves.) The potential given in (7) is identical to the one considered in [22] (see equation (7.46) therein). The d-wave critical temperature (for large hole concentrations) BCS is given by $T_c \simeq 4T_F e^{-1/\lambda}$ (where $T_F \simeq tk_F^2$, $\lambda \simeq \frac{8}{7}J/\pi t \langle R^2 \rangle$ and $\delta = k_F^2/2\pi$ is the oxygen hole concentration). The presence of the repulsive term of strength $3|K|/8\langle R^2\rangle^{1/2}$ suggests that in a non-mean-field approximation we have to integrate out the double occupancy [11-15] or to work in the limit $|K| \rightarrow \infty$. This will lead to a charge and spin separation introduced with the aid of the slave bosons [11–15] and the term $\langle R^2 \rangle = \frac{3}{4}\delta$ is the oxygen hole concentration (note that equations (5)–(7) are valid for $\delta > \delta_{\min} = J/|K|$). We find a result in agreement with the one-band model [23], a Heisenberg AF interaction and a kinetic term which contains holons and spinons [16, 20, 24]. The difference consists in the fact that R(n) is defined with respect to the oxygen variables and not Cu. Considering the short-wavelength behaviour, we substitute for R(n) the microscopic representation which is a function of the oxygen sites. The result of this is that the term $R(n) \cdot R(n')$ leads to frustration! Therefore, in contrast to the 2D AF, where the total wz vanishes [15], we have $\sum_{n} S_{WZ}[\mathbf{R}(n)] \neq 0$. In order to consider in detail the short-wave behaviour, we consider the limit $t \rightarrow 0$ and integrate out the oxygen variable in (1). The effective action in terms of the S(n) variables which are mapped into the O(3) non-linear σ -model with a wz term $S_{WZ}[M(n)]$ and $M^2 = 1$ is

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$$\tilde{A}_{\text{eff}} = \int_{0}^{\beta} \mathrm{d}\tau J \sum_{n,n'} M(n,\tau) \cdot M(n',\tau) + \frac{1}{2} \mathrm{i} \sum_{n} S_{\text{WZ}}[M(n)] - \operatorname{Tr} \ln[\partial_{\tau} + E_{\text{F}} + K\sigma(n+v) \cdot (M(n,\tau) + M(n+1,\tau)) - t(n+v,n+v')].$$
(8a)

The last term represents the effect of the integration of the oxygen holes (each oxygen hole couples to two nearest neighbours Cu^{2+} by the coupling K). t(n + v, n + v') is the oxygen hole hopping integral. We compute the Tr ln[] to order t^2/K . For $|E_F| < |K|$ we obtain

$$\int_{0}^{\beta} \mathrm{d}\tau \left(\sum_{n} \sum_{1 = \pm 1_{x}, \pm 1_{y}} -\frac{1}{2} |K| [(M(n, \tau) + M(n + 1, \tau))^{2}]^{1/2} + \frac{t^{2}}{|K|} \sum_{n, n''} M(n, \tau) \cdot M(n'', \tau) \right) + \frac{1}{2} \mathrm{i} \sum_{n} S_{\mathrm{WZ}}[F(M)].$$
(8b)

The first term represents the t = 0 approximation which gives rise to an F interaction and the second one $t^2/|K|$ represents the AF next-nearest-neighbour interaction. The last term is the wz term which is a function of the effective field which acts on the oxygen spin. Using the adiabatic theorem [17] we have an effective time-dependent Hamiltonian $h(\tau) = \frac{1}{2}\sigma F[M(\tau)]$. In the limit t = 0 we have F(M) = M(n) + M(n + 1) which leads to the wz term $S_{WZ}[M(n) + M(n \pm 1_x)] + S_{WZ}[M(n) + M(n \pm 1_y)]$. Combining the results of (8a) and (8b) we find a frustrated lattice, a nearest-neighbour interaction of strength $J_1 = J - \frac{1}{2}|K|$ and a next-nearest-neighbour AF interaction $J_2 = t_2/|K|$. In addition we have two wz terms $S_{WZ}[M]$ and $S_{WZ}[F(M)]$. The first one arises from the mapping of the spin- $\frac{1}{2}$ to the O(3) non-linear σ -model, the second one is an induced wz term. The evaluation of the wz term $S_{WZ}[M]$ is possible with the aid of the polar representation of the vector M ($0 \le \varphi < 2\pi, 0 \le \Theta < \pi$) from which we find

$$\frac{1}{2}\mathrm{i} S_{\mathrm{WZ}}[M] = \frac{1}{2}\mathrm{i} \sum_{n} \int \mathrm{d} \tau \, \dot{\varphi}(n) \{1 - \cos[\Theta(n)]\}.$$

For $J_2 \ge |J_1|$, the classical minimum is obtained for AF order in the x direction and a modulated F order in the y direction. For this case we choose

$$\cos[\Theta(n_x, n_y)] \simeq (-1)^{n_x} \cos[\Theta(n_x, n_y)] \simeq (-1)^{n_x} f(n_y)$$

and find

$$\frac{1}{2}$$
i $\sum_{n} S_{WZ}[M] \simeq -i\pi \sum_{n_y} f(n_y)$

where $f(n_y)$ is a slowly varying function of the co-latitude Θ in the y direction. As a result the modulo 2π of the sum is finite, giving rise to a non-trivial topological term. The presence of the non-trivial topological term (see the 1D AF) suppresses the long-range Néel order in 2D and stabilises the RVB state proposed by Anderson.

Using the mapping O(3) to CP^1

$$M(n) = Z^+(n)\boldsymbol{\sigma} Z(n)$$

where $Z = (Z_1, Z_2), |Z_1|^2 + |Z_2|^2 = 1, Z_1 = e^{i\varphi} \sin(\frac{1}{2}\Theta)$ and $Z_2 = e^{i\varphi} \cos(\frac{1}{2}\Theta)$ we replace the wz term by

$$\frac{1}{2}i\sum_{n} S_{WZ}[M] = \int_{0} \mathrm{d}\tau \sum_{n} Z^{+}(n) \,\partial_{\tau} Z(n)$$

and obtain a Bose action. We have a 2D quantum frustrated system for which the Néel state is destabilised in favour of the RVB for $J_2/|J_1| > (J_2/|J_1|)_c$ and which may lead to superconductivity. It is important to note that this result is in agreement with general concepts in quantum mechanics. The wZ term is equivalent to the canonical phase of the action in a coherent state representation $|\tau\rangle = |M\rangle \otimes |F(M)\rangle$ where $|F(M)\rangle$ is an adiabatic eigenstate of the oxygen hole Hamiltonian as a function of M. Constructing the path integral with the aid of the coherent state $|\tau\rangle$, we find that the action is composed of two parts: (i) the copper magnetic energy plus the oxygen hole eigenvalues which depend on the instantaneous configuration of the copper variables, and (ii) the canonical phase

$$A_{c} = \int_{0}^{\beta} \mathrm{d}\tau \left(\langle M | \partial_{\tau} | M \rangle + \langle F(M) | \partial_{\tau} | F(M) \rangle \right)$$

which is equal to the sum of the two wz terms.

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