

SU(2) gauge invariance and order parameters in strongly coupled electronic systems

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We show that the spin- $\frac{1}{2}$ Heisenberg model (the strong-coupling limit of the Hubbard model) is also the strong-coupling limit of an SU(2) lattice gauge theory with fermions. The local SU(2) gauge symmetry is manifest. The role of this gauge invariance is investigated in both the Hamiltonian and path-integral formulations. Off half-filling, our results reveal the existence of a lattice SU(2) bosonic matrix field which is a natural candidate for a condensate order parameter.

The recent discovery of high-temperature superconductors¹ have renewed the interest in the theoretical study of purely electronic models. Anderson and collaborators have developed the idea of the “resonating valence-bond” (RVB) states² in the framework of the Hubbard model at strong coupling and near half-filling.³ Magnetism probably plays an essential role in the new superconducting mechanism. In addition to that, it has been recently claimed that the Hubbard model in that limit (i.e., the Heisenberg model) has a local U(1) symmetry⁴ later enlarged to a local SU(2) symmetry⁵ after analyzing the “spinon” degrees of freedom.

Very little is known about the Hubbard and the spin= $\frac{1}{2}$ Heisenberg models in two and three dimensions. We believe that the analysis of this local symmetry is worthwhile since it may lead to the development of new techniques to study these models (probably borrowing some insight from the analysis of gauge theories in particle physics). In particular, there may be strong analogies between the process of pairing in the Hubbard model and confinement in lattice gauge theories. Also, the gauge symmetry may help in the construction of order parameters as shown below.

The purpose of this paper is to further discuss the SU(2) local symmetry pointed out in Refs. 2-5 making an analogy to lattice gauge theories in both the Hamiltonian and Lagrangian formulations. In particular, we present an exact expression for the partition function of the Heisenberg model as a path integral resembling a lattice gauge theory with SU(2) gauge variables and dynamical fermions. In a recent paper, Affleck, Zou, Hsu, and Anderson⁶ have independently given a discussion of this symmetry from a somewhat different point of view.

The Hubbard model in the strong-coupling limit ($U \gg t$) and at half-filling is equivalent to an antiferromagnetic Heisenberg model (spin $\frac{1}{2}$) with a Hamiltonian given by

$$H_{\text{Heisenberg}} = \frac{J}{2} \sum_{\mathbf{x}, \hat{\mathbf{i}}} \mathbf{S}_{\mathbf{x}} \cdot \mathbf{S}_{\mathbf{x}+\hat{\mathbf{i}}}, \tag{1}$$

where $J > 0$, \mathbf{x} labels sites of a d -dimensional cubic lattice, and $\hat{\mathbf{i}} = \hat{\mathbf{1}}, \hat{\mathbf{2}}, \dots, \hat{\mathbf{d}}$ are unit vectors in the different directions. This result can be easily deduced using degenerate perturbation theory. The spin variables at every site

are defined as

$$S_{\mathbf{x}}^{\alpha} = \frac{1}{2} c_{\mathbf{x},a}^{\dagger} \sigma_{ab}^{\alpha} c_{\mathbf{x},b}, \tag{2}$$

where $\sigma^{\alpha} (\alpha = 1, 2, 3)$ are Pauli matrices and $c_{\mathbf{x},a}^{\dagger}, c_{\mathbf{x},a}$ are fermionic operators. The index a represents spin ($a = \uparrow, \downarrow$). The coupling J is related with the standard parameters of the Hubbard model through $J = 2t^2/U$. In this strong-coupling limit, the fermionic variables satisfy the constraint $c_{\mathbf{x},\uparrow}^{\dagger} c_{\mathbf{x},\uparrow} + c_{\mathbf{x},\downarrow}^{\dagger} c_{\mathbf{x},\downarrow} = 1$ at every site. The model defined by Eq. (1) has a well-known SU(2) global symmetry that corresponds to simultaneous rotations of the spin degrees of freedom. This model is supposed to describe the CuO₂ planes⁷ of the undoped La₂CuO₄ as well as the insulating phase of Y₁Ba₂Cu₃O_{7- δ} . At low hole concentration these materials become superconductors so from the study of the undoped limit we may get some insight about the superconductivity mechanism.

We will prove below that there is another hidden (local) SU(2) symmetry in the Heisenberg Hamiltonian. To prove this it is convenient to make a particle-hole transformation in, for example, the spin-down operators, i.e., we make the operatorial change of variables

$$c_{\mathbf{x},1}, c_{\mathbf{x},1}^{\dagger} \rightarrow \psi_{\mathbf{x},1}, \psi_{\mathbf{x},1}^{\dagger}; c_{\mathbf{x},2}, c_{\mathbf{x},2}^{\dagger} \rightarrow \psi_{\mathbf{x},2}^{\dagger}, \psi_{\mathbf{x},2}. \tag{3}$$

The notation 1,2 is introduced here replacing the up and down components because they will represent the “color” degrees of freedom in the resulting SU(2) gauge theory. Note that now the “vacuum” state (annihilated by $\psi_{1,2}$) has N particles in the original variables (N is the number of sites), i.e., the system is half-filled. This is like filling the negative energy sea of the Dirac equation. Using the transformation Eq. (3) the Heisenberg Hamiltonian can be exactly rewritten as

$$H = \frac{J}{8} \sum_{\mathbf{x}, \hat{\mathbf{i}}} [M_{\mathbf{x}} M_{\mathbf{x}+\hat{\mathbf{i}}} + 2(B_{\mathbf{x}}^{\dagger} B_{\mathbf{x}+\hat{\mathbf{i}}} + B_{\mathbf{x}+\hat{\mathbf{i}}}^{\dagger} B_{\mathbf{x}})] - \frac{Jd}{4} \sum_{\mathbf{x}} (M_{\mathbf{x}} - \frac{1}{2}), \tag{4}$$

where antiperiodic boundary conditions have been assumed for the fermionic operators and the “meson” and

“baryon” operators M and B are defined as

$$M_x = \sum_a \psi_{x,a}^\dagger \psi_{x,a},$$

$$B_x = \sum_{a,b} \frac{\epsilon_{ab}}{2} \psi_{x,a} \psi_{x,b} = \psi_{x,1} \psi_{x,2}. \quad (5)$$

$\sum_x M_x$ corresponds to the total protection of spin S^3 (plus a constant). Usually, we are interested in the $S^3=0$ case. Note that now the Heisenberg Hamiltonian is expressed only as a function of the SU(2) gauge-invariant operators at every site so the local symmetry is obvious.⁸ In other words, the theory is invariant under the change

$$\psi_{x,a} \rightarrow \sum_b V_x^{ab} \psi_{x,b}, \quad (6)$$

where the matrix V belongs to SU(2), i.e., it has the properties $V^\dagger = V^{-1}$ and $\det V = 1$ [note that the local U(1) symmetry found in Ref. 4 is, in fact, only the diagonal part of this larger SU(2) symmetry]. It is important to note that the local SU(2) symmetry appears through a transformation of the new vector $\psi = \text{col}(c_1, c_2)$ (rewriting it in the original variables) and not in terms of the vector $\text{col}(c_1, c_2)$. The constraint $c_x^\dagger c_x = 1$ is, in the new language, $n_{x,1} = n_{x,2}$ (where $n_{x,a}$ is the number operator corresponding to color a) or, in other words, $\psi_x^\dagger \sigma_3 \psi_x = 0$. [In fact, this is equivalent to imposing the constraints $\psi_x^\dagger \sigma_i \psi_x = 0$ ($i=1,2,3$) since the extra conditions are simply $c_1^\dagger c_1 = c_2^\dagger c_2 = 0$ which are automatically satisfied in the strong-coupling limit.] This constraint means that at every site we have the same number of particles with color 1 and 2. This is reasonable since at each site we should have singlets under the SU(2) local symmetry and $|0\rangle, B^\dagger|0\rangle$ are those singlets.⁹

Although the local symmetry is clearly present in the Heisenberg model when it is written as in Eq. (4), it is convenient to introduce a gauge field in this formulation to make the local symmetry even more apparent. For that purpose, we will first work with the Hamiltonian formulation of lattice gauge theories¹⁰ and later with the path-integral formulation.

Let us first remark that the Heisenberg Hamiltonian can be obtained as the strong coupling limit of the Kogut-Susskind (KS) Hamiltonian of a SU(2) lattice gauge theory which is defined as

$$H = \frac{8}{3J} \sum_{x,l,a} E_{x,l,a}^\dagger E_{x,l,a} + \frac{i}{2} \sum_{x,l,a,b} (\psi_{x,a}^\dagger \hat{U}_{x,l}^{ab} \psi_{x+l,b} - \text{H.c.}), \quad (7)$$

where x and \hat{l} denote sites and directions of the same d -dimensional lattice where the Heisenberg model is defined. The operators \hat{U} are gauge fields and E^a are momentumlike operators with the algebra

$$[E_{x,\hat{l}}^a, \hat{U}_{y,\hat{j}}^{ab}] = \frac{\delta_{xy} \delta_{\hat{l}\hat{j}}}{2} \sum_c \sigma_{ac}^a \hat{U}_{x,\hat{l}}^{cb}, \quad (8a)$$

$$[E_{x,\hat{l}}^a, E_{y,\hat{j}}^\beta] = i \delta_{xy} \delta_{\hat{l}\hat{j}} \sum_\gamma \epsilon^{a\beta\gamma} E_{x,\hat{l}}^\gamma. \quad (8b)$$

The relation between the Heisenberg coupling constant and the coupling constant g of the gauge theory is $J = 16/3g^2$. For more details, we refer the reader to the literature on lattice gauge theories.¹¹

To show the equivalence of this model with the Heisen-

berg Hamiltonian we use perturbation theory in J (“strong-coupling” limit). We consider as zero-order Hamiltonian the electric term. Since the fermions do not appear in it, then the ground state is highly degenerate since (as mentioned before) at every site there are two possible singlets (no fermions and a “baryon”). Then the degeneracy is 2^N . The electric term is minimized by having no flux of electric field at any link. Using degenerate perturbation theory up to second order we can remove the degeneracy. The intermediate states have a link with one unit of flux. The corresponding intermediate energy can be obtained using the result $E^a E^a \hat{U}|0\rangle = \frac{3}{4} \hat{U}|0\rangle$. Following this method, it is easy to show that beginning with the KS Hamiltonian and using perturbation theory in J we recover the Heisenberg Hamiltonian Eq. (4) (up to a constant).¹² Of course, the relation between these two models exists only in the small J limit. The Hamiltonian Eq. (7) has a local SU(2) symmetry if we define that the link operator transforms as $\hat{U}_{x+\hat{l}} \rightarrow V_x \hat{U}_{x,\hat{l}} V_{x+\hat{l}}^\dagger$ and the matter fields as in Eq. (6).

Anderson and collaborators²⁻⁵ have argued that operators such as $\Delta_+(\mathbf{x}, \mathbf{x}+\hat{l}) = c_l^\dagger(\mathbf{x}) c_l(\mathbf{x}+\hat{l})$ may play the role of order parameters in these systems (specially off half-filling). In our notation Δ_+ takes the form $\Delta_+(\mathbf{x}, \mathbf{x}+\hat{l}) = \psi_l^\dagger(\mathbf{x}) \psi_l(\mathbf{x}+\hat{l})$. This operator is invariant under the global SU(2) symmetry of the Heisenberg model. Under the local SU(2) symmetry discussed above Δ_+ transforms nontrivially. Elitzur’s theorem, which states that only locally gauge-invariant operators can acquire an expectation value, rules out any possibility of a Δ_+ condensate at half-filling.

Having studied the Hamiltonian formulation now we show the existence of the SU(2) local symmetry in the path-integral formulation. We begin again with the Heisenberg Hamiltonian written in terms of the new field ψ [Eq. (4)]. Following very well-known standard rules of quantum field theory we can write the partition function of the model as a functional integral over Grassmann variables:¹³

$$Z_{\text{Heisenberg}} = \text{tr}(e^{-\beta H}) = \left(\prod_x \int d\bar{\psi}_x d\psi_x dU_{\hat{0}} \right) \times \exp[-S(\bar{\psi}, \psi, U_{\hat{0}})], \quad (9a)$$

where the action is

$$-S(\bar{\psi}, \psi, U_{\hat{0}}) = \sum_x \bar{\psi}_x (\psi_x - U_{x,\hat{0}} \psi_{x+\hat{0}}) - \epsilon \sum_{x,\hat{l}} \mathcal{H}_{x,x+\hat{l}} + \frac{J\epsilon d}{4} \sum_x (M_x - \frac{1}{2}), \quad (9b)$$

$x = (\mathbf{x}, t)$ is now a space-time index, t is the new “time” direction introduced in the partition function using the Trotter formula: $\beta = \epsilon N_t$ and ϵ and N_t are the lattice spacing and the number of layers in the time direction. $\hat{0}$ is the unit vector in that direction. Equation (9) is an identity if we work in the limit $\epsilon \rightarrow 0$ and $N_t \rightarrow \infty$. The Grassmann fields have antiperiodic boundary conditions in the time direction. The matrix $U_{x,\hat{0}}$ is a SU(2) matrix that has been introduced to enforce the constraint that the number of particles of each color at every site is the same.¹⁴

The operator \mathcal{H} contains the spatial interactions and it

is defined as

$$\mathcal{H}_{x,x+\hat{i}} = \frac{J}{8} [M_x M_{x+\hat{i}} + 2(\bar{B}_x B_{x+\hat{i}} + \bar{B}_{x+\hat{i}} B_x)], \quad (10)$$

i.e., we have simply formally replaced the fermionic operators ψ^\dagger of Eq. (4) by the Grassmann fields $\bar{\psi}$. This term is diagonal in time.¹⁵

The quartic interaction is usually decoupled using a real variable by means of the Hubbard-Stratonovich identity. However, in our case, it is more useful to make the decoupling by means of an SU(2) matrix at every link. The approximate identity that we used is

$$\begin{aligned} \exp(-\epsilon \mathcal{H}_{x,x+\hat{i}}) \\ \approx \int_{\text{SU}(2)} dU_{x,\hat{i}} \exp \left[\frac{i\sqrt{J}\epsilon}{2} (\bar{\psi}_x U_{x,\hat{i}} \psi_{x+\hat{i}} - \text{H.c.}) \right]. \end{aligned} \quad (11)$$

$$\exp(-\epsilon \mathcal{H}_{x,x+\hat{i}}) = \int dW_{x,\hat{i}} \exp \left[-\text{tr}(W_{x,\hat{i}}^\dagger W_{x,\hat{i}}) + \frac{i\sqrt{J}\epsilon}{2} (\bar{\psi}_x W_{x,\hat{i}} \psi_{x+\hat{i}} - \text{H.c.}) \right]. \quad (13)$$

This formulation is equivalent to Eq. (11) at low temperatures. To understand this point, note that the matrix W can be written as $W = \sqrt{\alpha\alpha + \beta\beta} U$, where U is a SU(2) matrix. At low temperatures, the “radial” degree of freedom will be frozen to a mean value given by the saddle-point approximation. The fluctuations will survive in the unbroken SU(2) sector. In this way, we recover Eq. (11) (up to a constant). The local symmetries are present also in this formulation (they simply do not affect the radial component).

$$-S = \sum_x \bar{\psi}_x (\psi_x - U_{x,0} \psi_{x+0}) + \sum_{x,\hat{i}} \left[-\text{tr}(W_{x,\hat{i}}^\dagger W_{x,\hat{i}}) + \frac{i\sqrt{J}\epsilon}{2} (\bar{\psi}_x W_{x,\hat{i}} \psi_{x+\hat{i}} - \text{H.c.}) \right] + \frac{J\epsilon d}{4} \sum_x (\bar{\psi}_x \psi_x - \frac{1}{2}). \quad (14b)$$

This result is valid not only for a square lattice but also for a triangular lattice. Equation (14) can be the starting point of a numerical simulation of the Heisenberg model (it is also useful for the Hubbard model at half-filling if J is small). In fact, Eq. (14) resembles a lattice quantum field theory with dynamical fermions¹⁷ (the main differences are that here the W fields have a “radial” component and the hopping in the time direction is asymmetric). We can integrate the fermions exactly. If the determinant coming from the Grassmann integration is positive then we can apply stochastic differential equations methods to attack the problem.¹⁸

There are results in the literature of lattice gauge theories that can be analyzed from the point of view of the Heisenberg model. These are numerical and mean-field studies for the SU(2) gauge theory with a chemical potential and a fermionic mass¹⁹ in the strong-coupling sector⁸ all in 3+1 dimensions. They were obtained in the Lagrangian formulation of lattice gauge theories (recently, they were also obtained in the Hamiltonian formulation²⁰). The numerical results showed clearly that the ground state of this SU(2) model (at zero temperature

To derive Eq. (11) it is necessary to expand both terms and perform the integration over the SU(2) Haar measure.¹⁶ We have neglected terms of order J^2 that correspond to density-density interactions.⁸ The model rewritten as in Eq. (11) has the same local symmetries discussed for the Hamiltonian version but now including the time direction (i.e., using matrices V that are also time dependent).

Another possibility is to make the decoupling using a more general matrix of the form

$$W = \begin{pmatrix} \alpha & \beta \\ -\beta & \bar{\alpha} \end{pmatrix} \quad (12)$$

(where α and β are complex numbers) by means of the exact identity

Combining Eq. (9) and (13), we arrive to an exact expression for the partition function of the Heisenberg model as a function of variables usually used in lattice gauge theories. There are no assumptions on the value of J . The final result is

$$Z_{\text{Heisenberg}} = \int \mathcal{D}\bar{\psi} \mathcal{D}\psi \int \mathcal{D}W \int_{\text{SU}(2)} \mathcal{D}U_0 \exp(-S), \quad (14a)$$

where

and external field) in 3+1 dimensions has antiferromagnetic properties (Néel state) since the “chiral” order parameter was nonzero ($\langle \bar{\psi}\psi \rangle \neq 0$) in the massless limit. This order parameter of the staggered fermions corresponds to a staggered magnetization $\langle (-1)^{(x+y+z)} S_x^3 \rangle$ for the Heisenberg model (see, for example, Ref. 21). Increasing the temperature and/or the external fields it was found numerically and analytically in the SU(2) gauge theory that the symmetry is restored. For more results see Ref. 8.

Away from half-filling a hole kinetic-energy (KE) term should be added to the Hamiltonian. In the presence of an electromagnetic field, this term acquires a phase factor at each link. After the particle-hole transformation [Eq. (3)], it has the form

$$H_{\text{KE}} = t \sum_{x,\hat{i}} \psi_x^\dagger \sigma_3 e^{i\sigma_3 A_{x,\hat{i}}} \psi_{x+\hat{i}} + \text{H.c.}, \quad (15)$$

where $A_{x,\hat{i}}$ is the gauge field at every link. The constraint is now $Q = \sum_x \psi_x^\dagger \sigma_3 \psi_x = -N\delta$ ($\delta \ll 1$) and the charge at every site can take the values 0 or -1 (for a hole). Note that in the new formulation the charge operator involves a

σ_3 matrix and it is not simply given by $\psi^\dagger\psi$ (in other words, the two components of ψ have opposite charges).

Now the Hamiltonian $H = H_{\text{Heisenberg}} + H_{\text{KE}}$ is gauge invariant under electromagnetic gauge transformations. However, it is not invariant under the local SU(2) symmetry previously discussed. This invariance can be recovered by noting that any noninvariance can be regarded as the result of an implicit gauge fixing. Take, for example, the case of the Bardeen-Cooper-Schrieffer (BCS) theory. Studying the Landau free energy in the London gauge, where the order parameter is real, it is immediate to see the generation of a mass term for the gauge field, but this is not a good starting point for the analysis of order parameters. To do that it is necessary to keep the gauge symmetry intact.

Similarly, in our case we must introduce a set of degrees of freedom on sites such that, upon fixing the gauge, it yields Eq. (15). This is very naturally achieved by the introduction of an SU(2) matrix at every site and redefining the kinetic-energy term as

$$H_{\text{KE}} = t \sum_{\mathbf{x}, \mathbf{l}} \psi_{\mathbf{x}}^\dagger g_{\mathbf{x}} \sigma_3 e^{i\sigma_3 A_{\mathbf{x}, \mathbf{l}}} g_{\mathbf{x}+\mathbf{l}}^\dagger \psi_{\mathbf{x}+\mathbf{l}} + \text{H.c.} \quad (16)$$

If the new field $g_{\mathbf{x}}$ transforms as $g_{\mathbf{x}} \rightarrow g_{\mathbf{x}} V_{\mathbf{x}}^\dagger$ and the fermionic field as in Eq. (6), then H_{KE} is SU(2) gauge in-

variant. [If we fix the gauge where $g_{\mathbf{x}}$ is equal to the identity, then we recover Eq. (15).] However, the field $g_{\mathbf{x}}$ does not commute with the electromagnetic link operator $e^{i\sigma_3 A_{\mathbf{x}, \mathbf{l}}}$. Hence, it transforms nontrivially under electromagnetic (em) gauge transformations, i.e., it is charged. It can easily be proved that in order to preserve both the SU(2) and U(1)_{em} symmetries in the KE term, the field g should, in fact, transform like $g \rightarrow V g e^{i\sigma_3 \phi}$ if $A_{\mathbf{x}, \mathbf{l}} \rightarrow A_{\mathbf{x}, \mathbf{l}} + \phi_{\mathbf{x}} - \phi_{\mathbf{x}+\mathbf{l}}$. Then the local symmetry group is finally SU(2) \times U(1)_{em}. The field ψ only transforms under SU(2) and it is neutral with respect to electromagnetism.²²

The field g may be a good candidate for a superconductivity order parameter since it is a charged site field noninvariant under SU(2). It also transforms nontrivially with respect to the standard SU(2) global rotations of the Heisenberg model so it can also describe antiferromagnetism.

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⁹The "asymmetric" way in which the transformation Eq. (3) treats the up and down components of the spin is just a special case of a more general transformation. In fact, applying a SU(2) matrix to the vector ψ we obtain another redefinition of variables that keeps invariant the Hamiltonian Eq. (4). So instead of Eq. (3), we can define the new fields in a more symmetric way like, for example, $\psi_1 = (1/\sqrt{2})(c_1 + c_1^\dagger)$ and $\psi_2 = (1/\sqrt{2})(-c_1 + c_1^\dagger)$ without changing our conclusions below.

¹⁰J. Kogut and L. Susskind, *Phys. Rev. D* **11**, 395 (1975).

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¹⁴Note that in the original variables to enforce the constraint at every site we would have needed to use currents in the time direction (Wilson lines in the language of lattice gauge theories). After the particle-hole transformation, Eq. (3a), the system is already half-filled and we do not need those Wilson lines. Away from half-filling, constraints will have to be imposed to fix particle number.

¹⁵Note that in Eq. (9b) we wrote the discrete version of the temporal derivative in such a way that there is no additional doubling of fermions in the continuum limit and also such that for a "constant" spatial interaction we obtain the correct results [for comments on these points see R. Blankenbecler, D. Scalapino, and R. Sugar, *Phys. Rev. D* **24**, 2278 (1981); U. Wolff, *Nucl. Phys. B* **225**, 391 (1983)].

¹⁶Remember that

$$\int_{\text{SU}(2)} dUU_i^\dagger U_{kl} = \frac{1}{2} \delta_{il} \delta_{jk}; \quad \int_{\text{SU}(2)} dUU_{ij} U_{kl} = \frac{1}{2} \epsilon_{ik} \epsilon_{jl}.$$

¹⁷Note that, in general, the Wilson loop is not a good order parameter for a gauge theory with light matter fields contrary to what is claimed in Ref. 4.

¹⁸R. Scalettar, D. Scalapino, R. Sugar, and D. Toussaint (unpublished).

¹⁹It can be shown that the mass term corresponds in the language of the Heisenberg model to a staggered external magnetic field while the chemical potential represents a uniform external magnetic field.

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²²Note that the introduction of the field g forces a new form for the constraint $\sum \psi^\dagger g \sigma_3 g^\dagger \psi = -N\delta$. Compare this with the definition given above.