PHYSICAL REVIEW B VOLUME 38, NUMBER 1 1 JULY 1988

SU(2) gauge symmetry of the large-U limit of the Hubbard model

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(Received 28 December 1987; revised manuscript received 24 March 1988)

We demonstrate explicitly the SU(2) gauge invariance of the large-U limit of the Hubbard model, i.e., the Heisenberg model written in terms of electron operators with a constraint of one particle per site. We use this result to demonstrate the equivalence of two apparently very different mean-field theories.

The strong-coupling, near-half-filled Hubbard model has received considerable attention lately as a model for the high-T_c superconductors.[1] It has been pointed out that the large-U limit with half filling has a local SU(2) gauge invariance.[2] This may be important for understanding the proposed gapless spinon spectrum[3] and also the superconductivity-destroying phase coherence at exactly half filling. This gauge symmetry is also useful for analyzing various mean-field theories.[4,5] The physical reason that motivated us to study this SU(2) symmetry lies in the fact that the spinons in the resonating-valence-bond (RVB) state have to be created or destroyed in pairs. The physical effect of $c_{i\sigma}^\dagger$ is the same as that of $c_{i-\sigma}$.[6]

In this report, we give an explicit proof of invariance under *time-dependent* SU(2) gauge transformations. We then use the gauge invariance to show the equivalence, at half filling, of two apparently quite different mean-field solutions: d-wave superconductivity and the "flux phase" found in the large-n limit of the Heisenberg model.

The Mott limit of the half-filled Hubbard model (with $J=t^2/U$) is the Heisenberg model

$$H=(J/4)\sum_{\mathbf{x},\mathbf{y}}(c_{\mathbf{x}}^{\alpha\dagger}\sigma_\alpha^\beta c_{\mathbf{x}\beta})\cdot(c_{\mathbf{y}}^{\alpha\dagger}\sigma_\alpha^\beta c_{\mathbf{y}\beta})\,, \tag{1}$$

with the constraint $c_{\mathbf{x}}^{\alpha\dagger}c_{\mathbf{x}\alpha}=1$. H is, of course, invariant under the usual global rotational symmetry under which the electron operators (c_1,c_2) transform as an SU(2) doublet: $c_\alpha\rightarrow c_\beta g_\alpha^\beta$. Here g_α^β is an SU(2) matrix. We can form a second SU(2) doublet out of the creation operators $(c_2^\dagger,-c_1^\dagger)$. It is convenient to combine these two doublets into a 2×2 matrix:

$$\psi_{\alpha\beta}\equiv\begin{pmatrix}c_1 & c_2\\ c_2^\dagger & -c_1^\dagger\end{pmatrix}. \tag{2}$$

Under a global SU(2) transformation, $\psi_{\alpha\beta}$ transforms as

$$\psi_{\alpha\beta}\rightarrow\psi_{\alpha\gamma}g_\beta^\gamma\,.$$

We now define a second local SU(2) by left matrix multiplication of ψ

$$:\psi_{\alpha\beta}\rightarrow h_\alpha^\gamma\psi_{\gamma\beta}\,.$$

Clearly, these two SU(2)'s commute. The [global SU(2)] spin operators can be written $\mathbf{S}=\frac{1}{4}\,\mathrm{tr}\psi^\dagger\psi\boldsymbol{\sigma}^T$, where $\boldsymbol{\sigma}^T$ is the transpose of $\boldsymbol{\sigma}$. Since

$$\psi^\dagger\rightarrow g^\dagger\psi^\dagger h^\dagger\,,$$

it follows that $\mathbf{S}$ is invariant under the local SU(2). Thus, the Heisenberg interaction

$$(J/16)\sum_{\mathbf{x},\mathbf{y}}(\mathrm{tr}\psi_{\mathbf{x}}^\dagger\psi_{\mathbf{x}}\boldsymbol{\sigma}^T)\cdot(\mathrm{tr}\psi_{\mathbf{y}}^\dagger\psi_{\mathbf{y}}\boldsymbol{\sigma}^T)$$

is invariant under *local gauge* transformations: $\psi_{\mathbf{x}}\rightarrow h_{\mathbf{x}}\psi_{\mathbf{x}}$, where the transformation matrices $h_{\mathbf{x}}$ depend on the site $\mathbf{x}$.

Note that this gauge symmetry is *not* a symmetry of the Heisenberg model per se, since it acts trivially on the spin operators. Rather, it is a symmetry of the large-U limit of the Hubbard model. It is a consequence of the redundancy of parametrizing spin operators in terms of electron operators. As discussed below, projecting out gauge-invariant states corresponds to the Gutzwiller projection on the states with singly occupied sites. For large but finite U, there is an approximate gauge symmetry, in the sense that the symmetry is only broken in the sector of the Hilbert space containing high-energy states [energies of $O(U)$].

The Langrangian, $L=[\sum_{\mathbf{x}}c_{\mathbf{x}}^{\dagger\alpha}(id/dt)c_{\mathbf{x}\alpha}-H]$, can also be written in a gauge-invariant way:

$$L=\tfrac{1}{2}\sum_{\mathbf{x}}\mathrm{tr}\psi_{\mathbf{x}}^\dagger(id/dt)\psi_{\mathbf{x}}-H\,, \tag{3}$$

upon integrating by parts with respect to time and throwing away a constant anticommutator term. However, there seem to be two problems with this gauge invariance. First of all, to complete our specification of the Heisenberg model we want to impose the constraint to one particle per site: $c^{\dagger\alpha}c_\alpha-1=\frac{1}{2}\,\mathrm{tr}\psi^\dagger\sigma^z\psi=0$. This constraint is not gauge invariant. Furthermore, L is not invariant under time-dependent gauge transformations: $\psi_{\mathbf{x}}(t)\rightarrow h_{\mathbf{x}}(t)\psi_{\mathbf{x}}(t)$. Miraculously, these two difficulties cancel each other. We make L invariant under time-dependent gauge transformations by adding the temporal component of a gauge field:

$$L\rightarrow\tfrac{1}{2}\sum_{\mathbf{x}}\mathrm{tr}\psi_{\mathbf{x}}^\dagger(id/dt+A_{0\mathbf{x}})\psi_{\mathbf{x}}-H\,. \tag{4}$$

Here, A_0 is an SU(2) gauge field, i.e., a traceless, Hermitian matrix which can be written $A_0 = \frac{1}{2}\sigma\cdot\mathbf{A}_0$. Under gauge transformations, A_0 transforms as $A_0 \rightarrow h[A_0 + i(d/dt)]h^\dagger$. L is now manifestly gauge invariant. However, we seem to have changed the Lagrangian in an unjustified way by adding the gauge field. Fortunately, we have simply introduced Langrange multipliers which enforce the constraint of one particle per site. The three components $\mathbf{A}_0$ of the matrix A_0 are Lagrange multipliers, since they appear only linearly in L. They constrain to 0 the three quantities, $\mathrm{tr}\psi^\dagger\sigma\psi$. Observing that $\mathrm{tr}\psi^\dagger\sigma^+\psi = 2c^{1\dagger}c^{2\dagger}$, we see that the three constraints are $c^{\dagger 1}c^{\dagger 2}=0$, $c_1c_2=0$, $c^{\dagger\alpha}c_\alpha=1$. These constraints mean, respectively, that there are no vacant sites, no doubly occupied sites, and one particle per site. The first two are, of course, implied by the third, so this is simply a redundant way of imposing the third constraint. This completes our proof of the SU(2) gauge invariance of the Heisenberg model, when written in terms of electron operators.

Next, we consider the nature of the gauge symmetry breaking that occurs for finite U/t and other than half filling. For finite U/t we promote $\mathbf{A}_0$ from Lagrange multipliers to Hubbard-Stratonovich fields by adding an extra term to L: $L \rightarrow +(3/8U)\sum_{\mathbf{x}}\mathrm{tr}A_0^2$. Integrating out A_0 shifts H by the Hubbard interaction

$$H \rightarrow H + (U/2)\sum_{\mathbf{x}}(c_{\mathbf{x}}^{\dagger\alpha}c_{\mathbf{x}\alpha}-1)^2 . \qquad (5)$$

This corresponds to a mass term for the gauge field, A_0, which breaks the gauge invariance. Invariance under time-independent gauge transformations is, in fact, preserved by this mass term. The addition of a chemical potential to move away from half filling corresponds to adding a term to L: $L \rightarrow L + (3U\mu/8)\sum_{\mathbf{x}}\mathrm{tr}A_0\sigma^z$. This term breaks the invariance under time-independent gauge transformations down to the U(1) subgroup: $\psi \rightarrow \exp(i\theta\sigma^z)\psi$, or equivalently, $c_\alpha \rightarrow e^{i\theta}c_\alpha$. Naively adding a hopping term completely destroys all remnants of the gauge symmetry. However, when U/t is large, and the doping is small, the hopping term has a small effect and the gauge invariance is only broken by a small amount. This approximate gauge invariance may still be useful for describing the effective low-energy theory of spin excitations. Furthermore, by introducing separate spinon and holon operators, a related U(1) gauge invariance can be defined in the theory with finite U/t and the non-doubly-occupied sector projected out.[6]

As an application of this gauge invariance we will now show the equivalence of two apparently very different mean-field theories of the half-filled Hubbard model. Baskaran, Zou, and Anderson[4] (BZA), and also Ruckenstein, Hirschfeld, and Appel,[4] applied a Bardeen-Cooper-Schrieffer-type factorization to the Heisenberg interaction, assuming that

$$\langle (c_{\uparrow\mathbf{x}}c_{\downarrow\mathbf{y}} - c_{\downarrow\mathbf{x}}c_{\uparrow\mathbf{y}})\rangle \equiv \Delta_{\mathbf{xy}} \qquad (6)$$

was nonzero for nearest-neighbor points $\mathbf{x}$ and $\mathbf{y}$. Although BZA assumed that $\Delta_{\mathbf{xy}}$ was the same for all nearest-neighbor pairs, Kotliar[4] later considered the possibility that $\Delta_{\mathbf{xy}}$ might have a different phase for links running in the x or y directions. Defining Δ_x and Δ_y to be the value of $\Delta_{\mathbf{xy}}$ for these two cases, Kotliar then discussed the s wave, $\Delta_x = \Delta_y$; the d wave, $\Delta_x = -\Delta_y$; and mixed, $\Delta_x = i\Delta_y$. At half filling, he found that the s-wave and d-wave cases were equivalent. This equivalence follows from making a U(1) gauge transformation on every second row: $c_{\mathbf{x}} \rightarrow i^y c_{\mathbf{x}}$. This changes the sign of Δ_x but not Δ_y. However, we cannot map the mixed state into the s-wave state by a gauge transformation.

Affleck and Marston[5] considered a different mean-field theory based on the large-n limit. They considered a nonzero expectation value for

$$\langle c_{\mathbf{x}}^{\dagger\alpha}c_{\mathbf{y}\alpha}\rangle \equiv \chi_{\mathbf{xy}} . \qquad (7)$$

They considered general configurations invariant under translations across diagonals of the square lattice. This permits four different χ's since there are two inequivalent points as well as two inequivalent directions. Labeling the four points around a plaquette 1, 2, 3, and 4, they discussed two relevant phases:

$$\text{uniform: } \chi_{12} = \chi_{23} = \chi_{43} = \chi_{14} ,$$

and

$$\text{flux: } \chi_{12} = \chi_{23} = \chi_{43}^* = \chi_{14}^* = e^{i\pi/4}|\chi| .$$

Using the U(1) gauge invariance they observed that only the phase of $\chi_{12}\chi_{23}\chi_{43}^*\chi_{14}^*$, the flux, is observable.[7] [For the SU(n) models with $n > 2$ there is only a U(1) gauge invariance.]

BZA and Kotliar found a gapless Fermi surface in the s-wave or d-wave phase, but a gap vanishing only at $(\pm\pi/2, \pm\pi/2)$ in the mixed phase. Affleck and Marston found a gapless Fermi surface in the uniform phase and a gap vanishing only at $(\pm\pi/2, \pm\pi/2)$ in the flux phase. They also found that the four points where the gap vanishes can be shifted in wave-vector space by a gauge transformation. Only the dispersion relation for particle-hole excitations is meaningful. In fact, using an SU(2) gauge transformation, we can show that BZA's or Kotliar's s-wave or d-wave state is equivalent to Affleck and Marston's uniform phase and Kotliar's mixed phase is equivalent to Affleck and Marston's flux phase. To show this, we make a gauge transformation on the even sublattice, points 2 and 4: $c_\uparrow \rightarrow c_\downarrow^\dagger$, $c_\downarrow \rightarrow -c_\uparrow^\dagger$. This has the following effect on the order parameters:

$$\Delta_{12} \rightarrow \chi_{12}^*,\ \Delta_{23} \rightarrow \chi_{23},\ \Delta_{43} \rightarrow \chi_{43},\ \Delta_{14} \rightarrow \chi_{14}^* . \qquad (8)$$

Thus, we see that the s-wave state (all Δ real) maps into the uniform phase. The mixed state maps into $\chi_{12} = \chi_{43} = 1$, $\chi_{23} = -\chi_{14} = i$. This has flux π, and can be mapped into the form given above by a further U(1) gauge transformation.

Since we have introduced the temporal component of a gauge field, it is natural to ask if we can also find the spatial components. These can be introduced by rewriting the Heisenberg interaction using a second Hubbard-Stratonovich transformation. First, it is convenient to rewrite the Heisenberg interaction as

$$H = (-J/8)\sum_{\mathbf{x},\mathbf{y}}\mathrm{tr}\psi_{\mathbf{x}}\psi_{\mathbf{y}}^\dagger\psi_{\mathbf{y}}\psi_{\mathbf{x}}^\dagger .$$

We now introduce a Hubbard-Stratonovich matrix field U_α^β (not to be confused with the Hubbard coupling constant), $U_{\mathbf{xy}}=(J/8)\psi_{\mathbf{x}}\psi_{\mathbf{y}}^\dagger$, by rewriting the Hamiltonian

$$H=\sum_{\mathbf{x},\mathbf{y}}\mathrm{tr}[(8/J)U_{\mathbf{xy}}^\dagger U_{\mathbf{xy}}+(\psi_{\mathbf{x}}^\dagger U_{\mathbf{xy}}\psi_{\mathbf{y}}+\mathrm{H.c.})]\,. \tag{9}$$

U transforms under gauge transformations as $U_{\mathbf{xy}}\to h_{\mathbf{x}}U_{\mathbf{xy}}h_{\mathbf{y}}^\dagger$. This is the same transformation as that of the lattice variables in a lattice gauge theory. In that case, the matrix U is restricted to be an SU(2) matrix and thus can be written $U_{\mathbf{xy}}=\exp(i\theta_{\mathbf{xy}})$, where the matrix θ is traceless and Hermitian. In the continuum limit, $\theta_{\mathbf{xy}}$ becomes the component of the gauge field corresponding to the direction of the link **xy**. The components of the matrix U are

$$(8/J)U_{\mathbf{xy}}=\begin{pmatrix}-\chi_{\mathbf{xy}}^\dagger & \Delta_{\mathbf{xy}}\\ \Delta_{\mathbf{xy}}^\dagger & \chi_{\mathbf{xy}}\end{pmatrix}=i(|\chi|^2+|\Delta|^2)^{1/2}\hat{U}\,, \tag{10}$$

where $\hat{U}$ is an SU(2) matrix. (Here, we are referring to the ordinary bosonic elements of the Hubbard-Stratonovich matrix.) The integral over χ, Δ can be written as the integral over $(|\chi|^2+|\Delta|^2)^{1/2}$ times the (normal Haar measure) integral over the SU(2) matrix $\hat{U}$. We expect that the integral over $(|\chi|^2+|\Delta|^2)^{1/2}$ will be dominated by a nonzero saddle point with fluctuations being unimportant at low energies. Thus the low-energy sector will be described entirely by normal lattice gauge theory variables.[8]

The phases of χ and Δ were interpreted as U(1) gauge fields previously.[3,5,8] We now see that χ and Δ together form an SU(2) gauge field. The essence of what we have done here is similar to field-theoretic descriptions of other problems in which the constraints on the physical variables are difficult to handle. The fermions can now be integrated out in principle since it is only a linear problem and the SU(2) gauge symmetry average takes care of the Gutzwiller projection. We may characterize the difference between the uniform and the flux phase (or s-wave state versus mixed state) in an SU(2) invariant way, by the sign of the SU(2) plaquette variable: $\mathrm{tr}U_{\mathbf{xy}}U_{\mathbf{yz}}U_{\mathbf{zw}}U_{\mathbf{wx}}$. This quantity is positive in the uniform phase and negative in the flux phase. The correlations among the gauge fields may, as suggested in Refs. 3 and 5, affect various lattice modes of the oxygens through the overlap charges on the links, leading to the orthorhombic-tetragonal transition in the high-T_c oxides.

In conclusion, we have explicitly demonstrated the local SU(2) gauge invariance of the Heisenberg model. With the help of this symmetry we have showed the equivalence of two apparently different mean-field theories. Further work on this non-Abelian gauge theory may be the best way to understand the mysteries of the RVB state.

We wish to thank D. Gross, J. B. Marston, G. Semenoff, W. Unruh, J. Wheatley, and L. Yaffe for useful discussions. One of us (I.A.) acknowledges financial support from the Canadian Institute for Advanced Research. Others of us (Z.Z., T.H., and P.W.A.) were supported in part by the National Science Foundation Grant No. DMR-8518163.

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