Local canonical transformations of fermions

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By permitting canonical transformations that are nonlinear in fermion creation and annihilation operators, we show that the space of canonical transformations of ordinary spin-$\frac{1}{2}$ operators local to a point in space is $SU(2)\otimes SU(2)\otimes U(1)\otimes Z_2$. We identify those subgroups that form local and global gauge symmetries of the Hubbard-Heisenberg model on and off half filling. Our systematic method of generating *all* local canonical transformations enables us to discover a "nonlinear" local U(1) gauge symmetry of the Heisenberg-Hubbard model that remains a local symmetry away from half filling. The paper presents this group together with all other known canonical transformations in a unified framework.

There has been considerable work done on spin-$\frac{1}{2}$ quantum models and several gauge symmetries have been observed.[1,2] This paper will show how to systematically enumerate *all* possible point-local gauge transformation acting on spin-$\frac{1}{2}$ operators. With this method we will show that there is an apparently previously unnoticed hidden local gauge symmetry of a variant of the t-J model. This U(1) transformation appears as a "nonlinear" transformation, i.e., a gauge transformation transforming a creation or annihilation operator into a sum of nonlinear polynomials of such operators.

To understand these ideas we begin by considering the multiparticle states available to spin-$\frac{1}{2}$ particles in a universe consisting of exactly one point. There are four possibilities: $\Psi_1 = |0>, \Psi_2 = |\uparrow\downarrow>, \Psi_3 = |\uparrow>, \Psi_4 = |\downarrow>$, corresponding to an empty site, a doubly occupied site, or a singly occupied site with spin up or down. Since an overall phase multiplying all the states cannot change any matrix elements, the most general nontrivial unitary transformation in this space is SU(4). We shall explore how the action of this unitary transformation can be described by an equivalent canonical transformation defined solely in terms of second quantized operators.

Let us define the matrix $m_{i,j}$ which obeys $m_{i,j}\Psi_k = \Psi_i\delta_{jk}$. After a bit of algebra[3] it can be shown that the action of the matrix m can be equivalently written using normal ordered Fermi operators as the matrix

$$m = \begin{pmatrix} 1-n_\uparrow-n_\downarrow+n_\uparrow n_\downarrow & c_\downarrow c_\uparrow & (1-n_\downarrow)c_\uparrow & (1-n_\uparrow)c_\downarrow \\ c_\uparrow^\dagger c_\downarrow^\dagger & n_\uparrow n_\downarrow & -c_\downarrow^\dagger n_\uparrow & c_\uparrow^\dagger n_\downarrow \\ c_\uparrow^\dagger(1-n_\downarrow) & -n_\uparrow c_\downarrow & n_\uparrow(1-n_\downarrow) & c_\uparrow^\dagger c_\downarrow \\ c_\downarrow^\dagger(1-n_\uparrow) & n_\downarrow c_\uparrow & c_\downarrow^\dagger c_\uparrow & n_\downarrow(1-n_\uparrow) \end{pmatrix}, \tag{1}$$

where $c_\sigma^\dagger$ and c_σ are the ordinary second quantized creation and destruction operators of a particle with spin σ. A general SU(4) matrix x acting on Ψ can then be represented as a polynomial X of Fermi operators by

$$X = \sum_{i,j} x_{i,j}m_{j,i} \equiv P(x) \equiv \mathrm{Tr}\,(xm)\ . \tag{2}$$

It then follows that $P(x)P(y) = P(xy)$ with matrix multiplication implied by xy. The matrix m also satisfies $(m_{i,j})^\dagger = m_{j,i}$ so that

$$[P(x)]^\dagger = P(x^\dagger)\ , \tag{3}$$

where $x^\dagger$ denotes Hermitian conjugate. We therefore see that there is a one-to-one relation between all local nonscalar unitary operators and elements of SU(4).

We can now employ this representation of SU(4) to generate the canonical transformations preserving the anticommutator $\{c_\sigma^\dagger, c_{\sigma'}\}_+ = \delta_{\sigma,\sigma'}$. Let x be a unitary matrix, obeying $xx^\dagger = 1$, and $U = P(x)$. Then it is trivial to verify that the transformation

$$c_\sigma \to U^\dagger c_\sigma U\ ,\quad c_\sigma^\dagger \to U^\dagger c_\sigma^\dagger U\ , \tag{4}$$

is canonical. Since no subgroup of this SU(4) commutes with all of $\{c_\uparrow^\dagger, c_\downarrow^\dagger, c_\uparrow, c_\downarrow\}$ there is a one-to-one relation between elements of SU(4) and the point-localized canonical transformations.

Thus far we have only considered canonical transformations in a universe consisting of one point, say r. If we want to build up a many-particle wave function we have to preserve the more general anticommutation relation

$$\{c_\sigma^\dagger(r), c_{\sigma'}(r')\}_+ = \delta_{\sigma,\sigma'}\delta_{r,r'} \ . \tag{5}$$

This imposes additional constraints on x so that $U = P(x)$ preserves Eq. (5). To discover these constraints we write the transformation in Eq. (4) as

$$c_\uparrow^\dagger \rightarrow P_{\text{even}}(r) + P_{\text{odd}}(r) \ , \tag{6}$$

where $P_{\text{even}}(r)$ is a polynomial which has terms each of which is a product of an even number of creation and destruction operators at point r, and $P_{\text{odd}}(r)$ consists of terms with odd numbers of operators. Clearly, $P_{\text{even}}(r)$ commutes with *all* polynomial operators $P_{\text{even}}(r')$ and $P_{\text{odd}}(r')$ at site $r' \neq r$. Therefore, the only possibility of preserving anticommutators between particles at distinct points in space is that $P_{\text{even}}=0$.[4] It can be checked that the Lie algebra generated by this constraint corresponds to SU(2)⊗SU(2)⊗U(1). The resulting Lie group can be represented through Eq. (2) by the matrix

$$x = \begin{pmatrix} ue^{i\chi/2} & -v^* e^{i\chi/2} & 0 & 0 \\ ve^{-3i\chi/2} & u^* e^{-3i\chi/2} & 0 & 0 \\ 0 & 0 & ge^{i\chi/2} & -h^* e^{i\chi/2} \\ 0 & 0 & he^{i\chi/2} & g^* e^{i\chi/2} \end{pmatrix} , \tag{7}$$

where $|u|^2+|v|^2=1$ and $|g|^2+|h|^2=1$. The entire symmetry group also contains the discrete transformations generating particle-hole exchanges separately in each spin component. However, one of these suffices to represent the entire group, since a simultaneous particle-hole transformation in each spin is a special case of Eq. (7). The entire group is then generated by Eq. (7) together with the matrix performing particle-hole exchange in the down component of spin:

$$x_{\text{particle-hole},\downarrow} = \begin{pmatrix} 0&0&0&1 \\ 0&0&1&0 \\ 0&1&0&0 \\ 1&0&0&0 \end{pmatrix} \ . \tag{8}$$

(The spin up particle-hole transformation is obtained from the above by multiplying by the matrix with $u=0$, $v=1$, $g=0$, $h=1$, $\chi=0$, which is already in the Lie group.) Thus, the full group of permissible unitary transformations for spin-$\frac{1}{2}$ fermions is $G \equiv$SU(2)⊗SU(2)⊗U(1)⊗Z_2.

We now label and list the action through Eq. (4) of each of these natural subgroups of G. We use the obvious notation that $u=1$, $v=0$, $g=1$, $h=0$, and $\chi=0$ in Eq. (7) unless explicitly defined.

Pseudospin SU(2): ≡"SU(2)$_P$":

$$c_{r,\uparrow}^\dagger \rightarrow uc_{r,\uparrow}^\dagger - vc_{r,\downarrow} \ ,$$

$$c_{r,\downarrow}^\dagger \rightarrow uc_{r,\downarrow}^\dagger + vc_{r,\uparrow} \ .$$

Spin SU(2): ≡"SU(2)$_S$":

$$c_{r,\uparrow}^\dagger \rightarrow g^* c_{r,\uparrow}^\dagger + h^* c_{r,\downarrow}^\dagger \ ,$$

$$c_{r,\downarrow}^\dagger \rightarrow g c_{r,\downarrow}^\dagger - h c_{r,\uparrow}^\dagger \ .$$

Nonlinear U(1): "U(1)$_{NL}$":

$$c_{r,\uparrow}^\dagger \rightarrow c_{r,\uparrow}^\dagger(1-n_\downarrow) + e^{2i\chi}c_{r,\uparrow}^\dagger n_\downarrow \ ,$$

$$c_{r,\downarrow}^\dagger \rightarrow c_{r,\downarrow}^\dagger(1-n_\uparrow) + e^{2i\chi}c_{r,\downarrow}^\dagger n_\uparrow \ .$$

Z_2: "hole-particle up":

$$c_{r,\uparrow}^\dagger \rightarrow c_{r,\uparrow} \ ,$$

$$c_{r,\downarrow}^\dagger \rightarrow c_{r,\downarrow}^\dagger \ .$$

Each subgroup except possibly U(1)$_{NL}$ has previously been clearly identified in the literature. The group SU(2)$_S$ is of course the usual spin rotations. The group SU(2)$_P$ was noted by Affleck and Marston.[2] Conjugation by the group Z_2 exchanges spin and pseudospin. This group was noted by Shiba;[5] its generator is the *only* generator of G which does not preserve S^2, and in fact changes the sign of this operator. This fact has been used to convert the positive-U Hubbard model to negative-U Hubbard with a chemical potential dependent magnetic field which vanishes at half filling.

In order to discover which subgroups of G are symmetries of a given Hamiltonian, it is convenient to know which local operators remain invariant under which local subgroup. By representing each local operator $O(r)$ in the form $O(r) = \sum_{i,j} o_{i,j}(r)m_{i,j}(r)$ it is simple to check the commutativity of the matrix $o_{i,j}$ with the elements of the Lie algebra of G. Defining the ordinary U(1) gauge subgroup of electromagnetism as U(1)$_Q$, we see that it is a subgroup of SU(2)$_P$ with the transformation $c_\sigma^\dagger \rightarrow e^{i\phi}c_\sigma^\dagger$. We define the spin operators $\mathbf{S}$ in the usual way: $S_r = \sum_{\alpha,\beta} c_{r,\alpha}^\dagger \gamma_{\alpha,\beta} c_{r,\beta}$ and γ is the vector of Pauli matrices. With these definitions, it is not difficult to show the following.

$\mathbf{S}^2(x)$ is invariant under SU(2)$_P$⊗SU(2)$_S$⊗U(1)$_{NL}$, that is, under the entire group of transformations *except* the discrete Z_2 part.[5]

All components of $\mathbf{S}(x)$ are invariant under SU(2)$_P$⊗U(1)$_{NL}$.

The number operator n is invariant under

$SU(2)_S \otimes U(1)_{NL} \otimes U(1)_Q$.

$c^\dagger_\sigma(1-n_{-\sigma})$ is invariant under $U(1)_{NL}$.

Equipped with this information we investigate what gauge transformations are symmetries of the t-J-U-μ model defined by the Hamiltonian

$$H = -t \sum_{<r,r',\sigma>} c^\dagger_{r,\sigma} c_{r',\sigma} + J \sum_{<r,r'>} S_r \cdot S_{r'} - U \sum_r S_r^2 - \mu N . \quad (9)$$

The summation is over all grid points r and nearest neighbors r' of a lattice, and N is the total particle number.

It is simple to show $\frac{4}{3}S^2 = n_\uparrow + n_\downarrow - 2n_\uparrow n_\downarrow$ so that indeed by suitably redefining the chemical potential μ we can recover the more conventional Hubbard term $Un_\uparrow n_\downarrow$. When $\mu = 0$ and $U \to \infty$, Eq. (9) corresponds to Heisenberg model at half filling, but for finite U allows charge fluctuations. Using the list above, it is now trivial to read off the local gauge symmetries: $SU(2)_P$ is local gauge symmetry for μ=0 and t=0; $U(1)_{NL}$ is local gauge symmetry for H when $t = 0$ *and* for the t-J model projected to singly occupied sites where $c^\dagger_{\sigma,x}$ is replaced by $c^\dagger_{\sigma,x}(1-n_{-\sigma})$; and $SU(2)_S$ is a local gauge symmetry for H when t=0 and J=0.

We now ask what local gauge symmetries can be coupled together to generate a global symmetry. The term that most thoroughly destroys all local gauge symmetries is of course the kinetic energy term, since all other terms depend on the local operators $\mathbf{S}_r$.

Under local pseudospin SU(2), the hopping term becomes

$$\sum_\sigma c^\dagger_{\sigma,r} c_{\sigma,r'} \to (u_r v_{r'} + v_r u_{r'})(c_{\downarrow,r} c_{\uparrow,r'} - c_{\uparrow,r} c_{\downarrow,r'}) + \text{ c.c.}$$
$$+(u_r u^*_{r'} - v_r v^*_{r'})(c^\dagger_{\uparrow,r} c_{\uparrow,r'} + c^\dagger_{\downarrow,r} c_{\downarrow,r'}) + \text{ c.c.} \quad (10)$$

Hence, the hopping term is preserved if

$$u_r v_{r'} + v_r u_{r'} = 0 \ , \quad u_r u^*_{r'} - v_r v^*_{r'} = 1 \ . \quad (11)$$

In order to solve these equations for u and v together with the normalization condition on u and v, we must have that $u_r = u_{r'}$ and $v_r = -v_{r'}$. Therefore, given an arbitrary SU(2) transformation parametrized by u and v, we see that for a global SU(2) pseudospin symmetry $v_r = (-1)^r v_0$, and $u_r = u_0$, where -1^r is even or odd for each of the two sublattices of a bipartite lattice.

By noting the connection between the the local pseudospin transformation and the operator description via Eq. (2), it can be seen this global gauge symmetry is exactly generated by the sum of local operators identified by Zhang.[6] The SU(2) algebra he identified lifts the local SU(2) pseudospin gauge symmetry of the Heisenberg-Hubbard model pointed out by Affleck and Marston to a global gauge symmetry in the presence of a hopping term. As was also noted by Zhang, we see here also that second nearest-neighbor hopping destroys the global symmetry.

One can ask whether or not there is some clever way to tie together local spin and pseudospin transformations to generate another global symmetry. It is a straightforward exercise to check that this does not work and that this global $SU(2)_P$ symmetry together with the ordinary global $SU(2)_S$ exhausts the global symmetries built up from point-localized gauge transformations continuously connected to the identity transformation.

There is a second global symmetry that is discretely generated. It is given by the product of the local generator of Z_2 multiplied by the transformation $c^\dagger_{r,\downarrow} \to -1^r c^\dagger_{r,\downarrow}$. The entire global symmetry of the hopping is then $SU(2)_P \otimes SU(2)_S \otimes Z_2$.

The replacement of $c^\dagger_\sigma$ by the "projected operators"[1] $c^\dagger_\sigma(1-n_{-\sigma})$ yields a theory with local $U(1)_{NL}$ gauge symmetry, as well as Zhang's global SU(2). In a converse argument, if one begins with the ordinary the t-J-U model, applies a local element of $U(1)_{NL}$, and then integrates over the local gauge fields, the surviving gauge invariant terms then coincides exactly with the projected Hamiltonian.

A consequence of this global symmetry for the Hubbard model at half filling is that any observed broken global $U(1)_Q$ gauge symmetry is in fact a signature of broken $SU(2)_P$ symmetry, since the choice of axis that is singled out can point arbitrarily in SU(2) space. In a familiar analogue, if an isotropic magnetic system is observed with spontaneous magnetization along the z axis, we know that a state with equivalent energy is obtained by an arbitrary orientation of this vector. The global $SU(2)_P$ symmetry vanishes off half filling and/or with second neighbor hopping, all of which either promote or suppress the expectation value of the charge density wave expectation value.

Under $SU(2)_P$ it can be checked that the triad of operators

$$(\Delta^*_{k+Q} - \Delta_k, i(\Delta^*_{k+Q} + \Delta_k), \rho_{k,k-Q}) \ , \quad (12)$$

where $Q = (\pi,\pi)$ and $\Delta_k = < c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow} - c^\dagger_{k,\downarrow} c^\dagger_{-k,\uparrow} >$ and $\rho_{k,k-Q} = < c^\dagger_{-k,\downarrow} c_{Q-k,\downarrow} > + < c^\dagger_{-k,\uparrow}, c_{Q-k,\uparrow} > + < c^\dagger_{k,\downarrow} c_{Q+k,\downarrow} > + < c^\dagger_{k,\uparrow} c_{Q+k,\uparrow} >$, transforms like a vector under global $SU(2)_P$. With the special choice of $k = (\pi, 0)$ this triad corresponds to $< d, is, \rho_{\pi,\pi} >$, the triplet consisting of the d-wave order parameter, i times the s-wave order parameter, and a charge density wave populating preferentially one sublattice. The direction of the spontaneously broken symmetry selects a direction $SU(2)_P$ space that can be measured by this triplet. This triplet can therefore be identified as the "order parameter" for broken SU(2) pseudospin symmetry, and all other expectation values of operators that are not invariant with $SU(2)_P$ are tied to the direction singled out by the vector $(d, is, \rho_{k,Q})$. By writing Eq. (12) we have implicitly imposed a coordinate system on SU_P where $U(1)_Q$ represents a rotation around the pseudospin z axis.

The motivation for this work was the desire to systematically enumerate all gauge symmetries of the t-J

model to see if any had been missed in previous unsystematic studies. We have shown that at least in the space of symmetries generated by direct products of point-local gauge transformations, the entire global symmetry group of the Heisenberg-Hubbard model with a kinetic energy term has been previously identified, and we have nothing to add to the arguments. However, it is certainly possible to build up local gauge transformations that mix Fermi operators on say, a pair of nearest-neighbor sites. The ordinary Bogoliubov transformation in BCS theory is an example of such a canonical transformation, although in that case operators are mixed in momentum space rather than in real space. We have in no way addressed the wider freedom this gives in constructing well-localized symmetries for these spin models. This problem can, however, be systematically attacked in the manner described here; one enumerates all states accessible to a pair of lattice sites, and constructs the operator which effects unitary operations in this space. This problem rapidly grows in complexity as more sites are used to build a transformation. In fact, including only a pair of sites in the construction of canonical transformations already results in searching for subgroups of SU(16) instead of SU(4).

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[3] Fabian Wenger (unpublished) has noticed that this matrix can be systematically generated. The top row $m_{1,k}$ maps each state k precisely to the vacuum. The element $m_{1,k}$ is therefore a product of creation operators, which raises the state k to the fully occupied state followed by the operator, which lowers the fully occupied state to the vacuum. The first column is then obtained using $m_{k,1} = m^\dagger_{1,k}$. The interior of the matrix from the relation $m_{i,j} = m_{i,1}m_{1,j}$.

[4] It is easy to check this statement in the case of spinless fermions. In that case, the simplistic argument results in the SU(2) transformation $c^\dagger \rightarrow uv(2n-1) + u^2c^\dagger - v^2c$ which rotates empty and a singly occupied state into each other. The constraint of $P_{\text{even}}=0$, implies either $u=0$ or $v=0$, giving the ordinary U(1) electromagnetic gauge transformation together with the discrete Z_2 particle-hole interchange.

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