Applications of gauge invariance to quantum disordered many-spin systems

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We show that in contrast to the classical case, there is no local Mattis transformation for many-spin quantum systems. However, it is possible to construct a class of local unitary transformations that provides an extension of the concept of gauge invariance to quantum disordered systems. Interesting differences are found between classical and quantum systems, even in the large-spin limit.

In the last few years, quantum spin systems have been extensively investigated. Interest for them, for instance, has been stimulated by the recent discovery of high-temperature superconductivity.[1] However, most of the work has been concentrated on uniform and isotropic interacting spin Hamiltonians. Very few exact analytical results have been obtained there,[2] so it seems to be very important to look for some simple and general methods that would be valid for a large class of spin Hamiltonians. In classical systems, the concept of gauge invariance has been found to be very powerful and useful. The concept of a Mattis transformation has been quite crucial in showing that many disordered classical systems can be mapped onto a simple ordered model, by contrast to frustrated systems.[3] In this framework, frustration is an intrinsic, gauge-invariant quantity which may dramatically change the behavior of the system, as, for example, in spin glasses.

In this paper, we investigate the possibility of generalizing such concepts to quantum spin systems. The question of the existence of a quantum Mattis transformation is discussed and then illustrated with some applications of gauge invariance to disordered quantum models.

Let us consider a system of N quantum spins, with the following Hamiltonian:

$$H=\sum_{i,j=1}^{N} J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j . \tag{1}$$

The quantized values of the operator $\mathbf{S}_i^2$ can be chosen arbitrarily for each site. Classically, the system is invariant under the Mattis transformation

$$\begin{aligned} &S_i\rightarrow \eta_i S_i , \\ &J_{ij}\rightarrow \eta_i\eta_j J_{ij} , \end{aligned} \tag{2}$$

where $\eta_i=\pm 1$.

Quantum random Mattis models have already been studied by Sherrington.[4] However, here we will focus on properties which do not depend on averaging over the disorder.

In the case of quantum system, one would like to find a set of unitary operators U_i such that

$$U_i S_i U_i^{-1}=\eta_i S_i . \tag{3}$$

However, when $\eta_i=-1$, there exists no such transformation, since if we assume that $USU^{-1}=-S$ for an arbitrary operator U, then

$$U[S^\alpha,S^\beta]U^{-1}=i\epsilon_{\alpha\beta\gamma}US^\gamma U^{-1}=-i\epsilon_{\alpha\beta\gamma}S^\gamma . \tag{4}$$

On the other hand,

$$\begin{aligned} U[S^\alpha,S^\beta]U^{-1}&=[US^\alpha U^{-1},US^\beta U^{-1}] \\ &=[S^\alpha,S^\beta]=i\epsilon_{\alpha\beta\gamma}S^\gamma , \end{aligned} \tag{5}$$

and this assumption is inconsistent.

In fact, the spin commutation rules constrain such a transformation (actually time reversal) to be represented by an *antilinear operator* T. More precisely, let $\mathcal{C}$ denote the complex conjugation in the standard representation for spin operators, where S^z, S^+, and S^- have simultaneously real matrix elements. Then we have[5]

$$T=\exp(-iS^y)\mathcal{C} . \tag{6}$$

A general Mattis transformation (η_i depending on i) would be represented by a time-reversal operation applied only to the spins for which $\eta_i=-1$. However, for many spin systems, time reversal has to be applied globally, since it is not possible to define an operator which is partially linear and antilinear. So, we conclude that for a quantum many-spin system, the energy spectrum is not invariant under the transformation $J_{ij}\rightarrow\eta_i\eta_j J_{ij}$. This is already seen, for example, in a system of two coupled spins $\frac{1}{2}$. If $H=J\mathbf{S}_1\cdot\mathbf{S}_2$ and $H'=-J\mathbf{S}_1\cdot\mathbf{S}_2$, their energy spectra are respectively $\{-\frac{3}{4}J;\frac{1}{4}J\}$ and $\{-\frac{1}{4}J;\frac{3}{4}J\}$ which are not identical. In this situation, the global change in the sign of the Hamiltonian cannot be compensated by a redefinition of, say, S_2, as would be the case for classical spins.

This is an important *difference* between classical and quantum systems. A possible interpretation of this fact is the following. Classically, the partition function is calculated using the Hamiltonian H which does not provide any specific information about the dynamics. As a result, the partition function is unchanged after "local" time-reversal transformations (i.e., applied to a fraction of the spins only). However, this invariance is lost already at the classical level, when a realistic *dynamics* is investigated. For instance, the classical Bloch's equations of motion

$$\frac{d\mathbf{S}_i}{dt}=\sum_j J_{ij}\mathbf{S}_i\times\mathbf{S}_j \tag{7}$$

are not invariant under a local transformation $S_i \rightarrow \eta_i S_i$.

In quantum mechanics, dynamics is completely determined by the eigenstates and the eigenvalues. The invariance under a local gauge transformation is then no longer expected to hold for quantum spins.

In spite of this restriction on gauge invariance in quantum spin systems, we would like to stress the fact that usual continuous symmetries (rotations) are still available and may even be quite useful and powerful, especially in the investigation of the properties of disordered systems. The idea is that a rotation of π around the x axis, for instance, changes the spin operators according to

$$\begin{aligned} &S_x \rightarrow S_x , \\ &S_y \rightarrow -S_y , \\ &S_z \rightarrow -S_z . \end{aligned} \tag{8}$$

When different rotations operate on neighboring spins, a new Hamiltonian is generated, in which the spectrum is identical to the original one. Furthermore, the eigenstates of both Hamiltonians are related by a unitary transformation. The main purpose of this paper is to show that this class of local symmetry operations is large enough so that nontrivial information can be deduced from them.

Before discussing explicit applications of this special kind of gauge invariance, we shall first give a few notations and formulas that will be useful in the following. We will concentrate on local rotations with an angle of π along the x, y, and z axis. As will be discussed, such transformations do not mix the different spin components in the Hamiltonian, but generate random anisotropic couplings. This is not a fundamental restriction, but may simplify the presentation.

A rotation of π around the α ($\alpha=1$, 2, or 3) axis is described by the unitary operator $U(\alpha,\pi)=\exp(-i\pi S_\alpha)$, and therefore we have

$$U(\alpha,\pi)S^\beta U^{-1}(\alpha,\pi)=(2\delta_{\alpha\beta}-1)S^\beta \equiv \eta_\alpha(\beta)S^\beta . \tag{9a}$$

Starting from $H=\sum_{ij}\sum_{\beta=1}^{3} J_{ij}^{\beta} S_i^\beta S_j^\beta$, we can apply local rotations as defined above, and this transforms H into

$$H'=\sum_{i,j} J_{ij}'^{\beta} S_i^\beta S_j^\beta , \tag{9b}$$

where

$$J_{ij}'^{\beta}=J_{ij}^{\beta}\eta_{\alpha_i}(\beta)\eta_{\alpha_j}(\beta) \quad (\alpha_i=1,\ 2,\ \text{or}\ 3) . \tag{9c}$$

In the spin-$\frac{1}{2}$ case the $U(\alpha,\pi)$ take a very simple form

$$U(\alpha,\pi)=\exp[-i(\pi/2)\sigma_\alpha]=-i\sigma_\alpha , \tag{10}$$

where σ_α are the usual Pauli matrices. The connection between the eigenfunctions of H and H' is then quite simple in this case.

Let us now discuss the application of the gauge transformation [Eq. (9)] to one-dimensional spin systems.

The first case is an anisotropic nearest-neighbor linear chain of N spins, described by the Hamiltonian

$$\begin{aligned} H=\sum_{i=1}^{N} &(-1)^{l_i} J_{ix} S_i^x S_{i+1}^x \\ &+(-1)^{m_i} J_{iy} S_i^y S_{i+1}^y + (-1)^{n_i} J_{iz} S_i^z S_{i+1}^z , \end{aligned} \tag{11}$$

where $J_{ix}=J_{iy}=J_{iz}>0$ and where periodic boundary conditions are imposed, so $S_{N+1}=S_1$. The sign of the interactions are fixed by the *random* numbers $\{l_i,m_i,n_i\}_{i=1}^{N}$, which could be **0** or 1 under the following constraints:

$$l_i+m_i+n_i=0 \text{ or } 2 \quad \text{for } i=1,2,\ldots,N , \tag{12}$$

$$\sum_{i=1}^{N} l_i=\sum_{i=1}^{N} m_i=\sum_{i=1}^{N} n_i=k , \quad 0\le k\le \lfloor 2N/3 \rfloor . \tag{13}$$

After the action of the gauge transformation [Eq. (9)] not more than N times on the system, one can verify that the system is identical to a uniform one dimensional antiferromagnetic chain. Therefore, the energy spectrum of the system (11)–(13) is identical to the energy spectrum of a uniform antiferromagnetic chain. The eigenstates of the system can be easily found from the eigenstates of the uniform chain according to the transformations (9a).

One can generalize this picture to the case where $|J_{ix}|=|J_{iy}|=|J_{iz}|$ and $|J_{ix}|\neq|J_{jx}|$ for $i\neq j$. Using the transformation (9), one can verify that the system is mapped onto an isotropic random antiferromagnetic quantum spin chain. Such systems were solved approximately for several different distribution of bonds. For general class of distribution of bonds there are qualitatively universality properties.[6] The critical exponents γ and α depend on the distribution of bonds but not strongly.

It is worthwhile to stress that these rotations can be used to map a model with a nonuniform magnetic field onto a simpler one with a homogeneous field. For instance, rotation of π around the z direction changes h_x into $-h_x$, h_y into h_y, and h_z into h_z. Starting from the exactly solved case of the antiferromagnetic spin-$\frac{1}{2}$ Heisenberg chain in the presence of a uniform field,[7] one can generate then a class of solvable Hamiltonians with nonuniform interactions and magnetic field by application of local rotations.

Generalization of (9) to systems in higher dimensions is straightforward. However, one must remember that the disorder in the system is now limited by the appearance of *loops* in the system. In two dimensions, for example, one can choose a random system where $J_{i,j;i+1,j}^{l}=J_{i,j;i,j+1}^{l}=J_{i,j;i-1,j}^{l}=J_{i,j;i,j-1}^{l}\equiv J_{i,j}^{l}$, where i,j are odd numbers, $l=x,y,z$, and one or three components of each J_{ij} are positive.

The above mentioned results indicate that the energy spectrum of an antiferromagnetic system does not change in many cases under the presence of strong ferromagnetic interactions and anisotropy.

The local rotation symmetry is also relevant to frustrated quantum systems. The sources of a frustration in quantum system could be either frustrated J_x, J_y, or J_z plaquets. One can verify that the frustration in these three different plaquets is a quantity which is *invariant* under the gauge transformation (9). For example, if in the system there are only J_x frustrated plaquets, than after any number of transformations of the form (9), *only the same* J_x plaquets are frustrated.

In an Ising system that consists of one frustrated loop, the energy of the system is a summation of all the bonds, minus twice the weakest bond (in the absolute value) in the loop. The energy of the loop is independent of the *sign* of the weakest bond and on the *location* of this bond among the other. One may ask similar questions about

the behavior of a quantum frustrated loop. By using the gauge transformation (9), we can partially answer these questions.

Assume a frustrated loop where all the bonds $J^{\alpha}_{i,i+1}$ ($\alpha=x,y,z$), except J^{x}_{12} and J^{y}_{12}, are weak ferromagnetic bonds. J^{x}_{12} and J^{y}_{12} are the strongest antiferromagnetic bonds, which are responsible to the frustration in the system. As a result of the action of π rotation along the z axis on the spin S_2, the signs of the bonds J^{x}_{12}, J^{y}_{12}, J^{x}_{23}, and J^{y}_{23} are changed. Therefore, after this transformation the bonds which are responsible to the frustration are *weak* antiferromagnetic bonds (J^{x}_{23},J^{y}_{23}). One can apply the transformation many times in order to fix the weak antiferromagnetic bonds among weak ferromagnetic bonds, and far away from the strong ferromagnetic bonds (J^{x}_{12},J^{y}_{12}). It is important to note again that the energy spectrum of the system is invariant under the transformation (9). Therefore, this example indicates that in many frustrated loops the energy spectrum and the dynamics of the system is independent of the sign of the weakest bond and on the location of the bond which is responsible for the frustration. This behavior is similar to the behavior of the classical Ising system.

We have previously stressed what appears to be an important difference between quantum mechanics and classical statistical mechanics. In the former case, time-reversal transformations can only be applied globally whereas in the latter, local-spin inversions lead to the full group of Mattis transformation. However, when the spin S become large, we may expect some kind of correspondence principle between the quantum system and its classical version. We would like to address this question briefly here. For instance, let us consider a system of two coupled spins S with $H=J\mathbf{S}_1\cdot\mathbf{S}_2$. The eigenvalues of H are $E(\sigma)=(J/2)[\sigma(\sigma+1)-2S(S+1)]$ with degeneracies $g(\sigma)=2\sigma+1$, σ taking all the values between 0 and $2S$. The partition function is

$$Z(\beta)=\exp[\beta JS(S+1)] \times\sum_{\sigma=0}^{2S}(2\sigma+1)\exp\left[-\frac{\beta J}{2}\sigma(\sigma+1)\right]. \quad (14)$$

In the high-temperature limit ($\beta\rightarrow 0$), we get

$$[Z(\beta,J)]_{\beta\rightarrow 0}=\frac{4}{\beta J}\sinh\{\beta J[S(S+1)+\tfrac{1}{4}]\}. \quad (15)$$

In this limit, $Z(\beta,J)=Z(\beta,-J)$ as is the case when S_1 and S_2 are classical, from the Mattis transformation $S_1\rightarrow S_1$ and $S_2\rightarrow -S_2$.

This simple example actually shows that the invariance of the partition function under a local Mattis transformation is recovered only at large temperature [$T\sim O(JS^2)$], rather than at large S. Another example is provided by the crucial difference between the low-lying excitation spectra of quantum ferromagnets and antiferromagnets. For ferromagnets, spin-wave theory gives $\varepsilon(k)\sim k^2$ at small k, but for antiferromagnets[8] we have $\varepsilon(k)\sim k$. These different dispersion relations are reflected in the thermodynamics. For instance, the low-temperature magnetization curves behave differently, where the $T^{3/2}$ behavior in ferromagnets is to be compared to the T^2 law in antiferromagnets.[8] It is important to note that these features are already valid for large values of S. As a result, the low-temperature partition functions for both systems will be different, even at large S. This behavior is in contrast to the case of classical spins where the partition functions for a ferromagnetic and an antiferromagnetic Hamiltonian on an unfrustrated lattice are identical (since one can flip the spins on a given sublattice and change the sign of J). The fact that a many-spin quantum system recovers the invariance of $Z(\beta)$ under a local Mattis transformation only at large temperature is related to the fact that eigenstates in quantum mechanics contain the full information about the dynamics of the system as previously discussed. Low-energy excitations reflect the low-temperature dynamics that is invariant only under a global time-reversal symmetry in general. So, the full Mattis invariance does not appear in the low-temperature partition function.

In conclusion, we have shown some applications of gauge invariance to quantum disordered spin systems and stressed some important differences between quantum and classical statistical mechanics. Directions for future work involve many open questions. Is there some similarity between quantum systems which corresponding classical Hamiltonians are related by Mattis transformation? How does this similarity emerge as a function of increasing temperature? Do phase transitions occur in both systems? Also, in the XY limit, Mattis transformations can be exactly implemented in quantum systems, by rotations around the z axis. It is interesting then to investigate whether such invariance can be extended beyond the strict XY limit, to the case of a weak coupling in the z direction. These considerations do not hold for the general Heisenberg symmetry, which deserves a special treatment. In that case, the difference between classical and quantum behavior under a Mattis transformation is expected to be the most dramatic.

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