

An Exact Mapping of the t - J Model to the Unrestricted Hilbert space

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We present an exact mapping of the thermodynamical properties of the t - J model to the unrestricted fermionic Hilbert space. At half filling this is accomplished by the introduction of a complex chemical potential. At finite hole concentration we generalize the t - J model to a particle-hole symmetric form. Identifying a symmetrized combination of a hole and a doubly-occupied site with the charge carrier, we prove that the thermodynamical properties of original and the generalized t - J model are identical.

1. Introduction

The t - J Hamiltonian has the form:

$$-t \sum_{\langle i,j \rangle, \sigma} (1 - c_{i,-\sigma}^+ c_{i,-\sigma}) c_{i,\sigma}^+ c_{j,\sigma} (1 - c_{j,-\sigma}^+ c_{j,-\sigma}) + J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j. \quad (1)$$

Here $c_{i,\sigma}^+$ is the creation operator for an electron with spin $\sigma = \uparrow, \downarrow$ on the lattice site i , and $\langle i, j \rangle$ denotes pairs of nearest neighbor (n.n.) sites. The \mathbf{S}_i are the spin operators for the antiferromagnetic ($J \geq 0$) nearest-neighbor interaction. The operators in parentheses in the first term in Eq.(1) (the kinetic energy, with $t > 0$) are the constraints that enforce single occupancy. Doubly occupied sites are assumed to be so high in energy, due to a strong on-site Coulomb repulsion, that they are out of the Hilbert space.

To compute the thermodynamics, we must compute the partition function as a trace of $e^{-\beta H}$ over the projected, or singly-occupied, Hilbert space. We will show that this is equivalent to the trace of a more complicated operator, with the trace extended over all fermionic states (including states with doubly-occupied sites). As we have shown in previous work¹, this allow for standard Green's function techniques, whereas the use of a restricted Hilbert space causes Wick's theorem to fail.

2. Particle-Hole Symmetrization

It is first necessary to make the dynamics completely particle-hole symmetric. Here a hole is an empty site and a particle is a doubly-occupied site, or doublon. The spin parts of Eq.(1) act symmetrically on holons and doublons, since both are singlets.

We can construct a particle-hole-symmetric extension of the kinetic energy by adding, for each $\langle ij \rangle$, an extra term in which the particle \leftrightarrow hole replacement is made simultaneously in both the i, j operators. This gives

$$T = -t \sum_{\langle i,j \rangle, \sigma} [(1 - n_{i,-\sigma}) c_{i,\sigma}^+ c_{j,\sigma} (1 - n_{j,-\sigma}) + n_{i,\sigma} c_{i,-\sigma} c_{j,-\sigma}^+ n_{j,\sigma}]. \quad (2)$$

In this extended model there are two types of charged objects, $|0\rangle$ and $|\uparrow\downarrow\rangle$, which are treated identically. Suppose we have N_h holes and N_d doublons. The dynamics of the extended Hamiltonian (including Eq.(2)) with a total number of charged objects $N_c = N_h + N_d$ is identical to the original t - J Hamiltonian (in the projected subspace) with N_c holes. The second piece in T hops a doublon exactly the way the first term moves a hole:

$$\bigcirc \uparrow \Rightarrow \uparrow \bigcirc \quad ; \quad \uparrow\downarrow \uparrow \Rightarrow \uparrow \uparrow\downarrow.$$

Note that T does not mix the two types of charges.

3. Partition Function

The partition function is a trace over the projected Hilbert space; i.e., on each site the allowed states are $|0\rangle$, $|\uparrow\rangle$, and $|\downarrow\rangle$. That is, the desired partition function is

$$Z_{proj} = \text{Tr} \left(e^{-\beta(H - \mu N_h)} \right)_{proj} \quad (3)$$

where we have included a chemical potential μ for holes. This Z_{proj} is exactly equivalent to the thermodynamics of holes plus doublons under the extended or symmetrized Hamiltonian, and with an unrestricted trace, as we will show.

In order to enlarge the trace to the complete fermionic space, i.e. including states such as $|\downarrow\uparrow\rangle$, we must first construct a particle-hole symmetrization operator:

$$P_{p-h} = \prod_i (1 + c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger + c_{i\downarrow} c_{i\uparrow}) \quad (4)$$

This operator will allow us to identify the symmetric superposition of $|0\rangle$ and $|\downarrow\uparrow\rangle$ with the holes, thus reducing the unwanted degree of freedom. This is simply because both $P_{p-h}|0\rangle$ and $P_{p-h}|\downarrow\uparrow\rangle$ yield $|0\rangle + |\downarrow\uparrow\rangle$. Since we want to use it in connection with a partition function, it might be desirable to write P_{p-h} in an exponential form:

$$P_{p-h} = \lim_{\epsilon \rightarrow 0} e^{\left(\frac{1}{2} \sum_i \ln((2-\epsilon)/2) (c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger + c_{i\downarrow} c_{i\uparrow})\right)} \times e^{\left(\frac{1}{2} \sum_i \ln((2-\epsilon)\epsilon) [n_{i\downarrow} n_{i\uparrow} + (1-n_{i\downarrow})(1-n_{i\uparrow})]\right)}, \quad (5)$$

where $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$. Define

$$Z = \text{Tr} \left(P_{p-h} e^{-\beta H} e^{i(\pi/2 - \alpha\beta) \sum_i (n_{i\uparrow} + n_{i\downarrow} - 1)} \right). \quad (6)$$

Here the trace is over the unrestricted Hilbert space (including $|\downarrow\uparrow\rangle$ on each site). We will show that $Z = Z_{proj}$ whenever a given Hamiltonian has identical dynamics for holes and doubly occupied sites. The system can be pushed to half-filling by setting $\alpha = 0$ in Eq.(6). Hence α plays the role of a chemical potential, as we will see more clearly below.

The extra exponential in Eq.(6) is quite unlike approaches in which a constraint such as $n_{i\uparrow} + n_{i\downarrow} = 1$ is enforced by an expression like $\int_0^{2\pi} d\lambda (e^{-\beta H} e^{i\lambda(n_{i\uparrow} + n_{i\downarrow} - 1)})$. In our approach, a particular state ($|\downarrow\uparrow\rangle$ here) is unwanted. Because of the Hamiltonian's particle-hole symmetry, the contribution of the unwanted state combines with the contribution from $|0\rangle$ so as to give Z_{proj} .

Now we will show that $Z = Z_{proj}$. Let $|n\rangle$ be a state which is in the projected Hilbert space. In general $|n\rangle$ has some singly-occupied sites and some vacant sites. In the unrestricted Hilbert space there exists another state in which one of these sites is doubly occupied instead of being vacant. These two states have the same matrix element $\langle n | P_{p-h} e^{-\beta H} | n \rangle$, by virtue of the particle-hole symmetry of H . This is most easily seen in a path integral expansion. By construction, the propagation, i.e. the dynamics, of the empty and the doubly occupied site are identical. At the end of the path, all holes and the doublon return to their original sites. The amplitude for this process is the same as for the holes-only case. For all charges to be indistinguishable, we must also let the doublon exchange places with a hole during

propagation. Due to the particle-hole symmetrization operator P_{p-h} , this process too contributes with the same amplitude as the others.

Including the extra exponential in Eq.(6), the contribution of these two related states to Z is

$$2 \sin \alpha \beta \langle n | e^{-\beta H} | n \rangle.$$

In particular, when $\alpha \rightarrow 0$, the contribution of these two states cancels, and only states in which all sites are singly occupied contribute. That is, $\alpha = 0$ gives half filling.

Generalizing the above, consider the set of 2^{N_c} states with a given configuration of singly-occupied sites. These are the states which arise by letting each of the N_c charges be either a hole or a doublon. These states contribute $(2 \sin \alpha \beta)^{N_h} \langle n | e^{-\beta H} | n \rangle$ to Z . In the restricted trace, Eq.(3), the contribution of $|n\rangle$ to Z_{proj} is $e^{\beta \mu N_h} \langle n | e^{-\beta H} | n \rangle$. Hence we can ensure that $Z = Z_{proj}$ if we choose

$$2 \sin \alpha \beta = e^{\beta \mu}. \quad (7)$$

Thus as claimed α plays the role of a chemical potential.

3. Comments and Conclusions

Some comments: First, for the special case of half-filling, when one can do without the generalized kinetic energy, some of the above formulae have already appeared in literature². Second, the expectation value of any operator defined in the projected Hilbert space can be computed using the unrestricted trace, if the operator is first particle-hole symmetrized. Third, one can show that at half filling the above formulation leads to half-statistics Matsubara frequencies for holes and doublons in our Greens-function approach¹.

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References

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