ITP-UH-02/94

# ON THE BETHE ANSATZ SOLUBLE DEGENERATE HUBBARD MODEL

Holger Frahm[1] and Andreas Schadschneider[2]

[1]Institut für Theoretische Physik, Universität Hannover
D–30167 Hannover, Germany
[2]Institut für Theoretische Physik, Universität zu Köln
D–50937 Köln, Germany

## INTRODUCTION

Studies of exactly soluble models for correlated electrons in one dimension have attracted wide spread interest in recent years. The reason for this is simple: they provide rigourous results on the behaviour of these systems in the presence of strong quantum fluctuations and thus may give some guidance at how to interpret observations in the much less well understood models in higher dimensions.

The prototype of models in this field is of course the one-dimensional Hubbard model which is soluble by the Bethe Ansatz [1] as the $N = 2$ lattice version of Yang-Sutherland gas of fermions with a $\delta$-function interaction carrying SU(*N*) spin [2, 3]. An obvious question is whether there exist integrable lattice models for general $N$. Such a degenerate Hubbard model has first been proposed by Choy for $N = 4$ [4] and Haldane in the limit $N \to \infty$ [5] and many properties (such as excitation spectrum, existence of a Mott transition at density $n_c = 1$ and finite coupling strength, critical exponents) of the model are known from the investigation of the corresponding Bethe Ansatz equations.

There is, however, one unresolved problem with this generalization of the SU(2) Hubbard model: usually the Bethe Ansatz relies on the fact that there are not more than two particle interactions. In the SU(2) case this is guaranteed by the Pauli principle, and for the Yang-Sutherland model points where more than two particles meet are of measure zero in phase space. In the lattice model for $N > 2$ such configurations have to be considered.

Here we first present a review of the properties of the degenerate Hubbard model and the controversy arising from the problem of mutliply occupied sites. Then, from the *complete* solution of the Bethe Ansatz equations with only a few electrons present together with some assumptions on the symmetries of the model we construct a Hamiltonian operator that reproduces the Bethe Ansatz spectrum for the minimal chain of length $L = 2$. While this turns out not to be sufficient to identify the Hamiltonian for general $L$ it indicates what types of interactions have to be taken into account in this model.

Talk given at the NATO Advanced Research Workshop on "The Physics and Mathematical Physics of the Hubbard model", held in San Sebastian, Spain, October 1993

## BETHE ANSATZ AND BASIC PROPERTIES OF THE MODEL

The generalization of the Hubbard model to as lattice system of fermions carrying SU(*N*) spin on the level of the Bethe Ansatz equations is straightforward. The inhomogeneous SU(2) spin problem arising within the Bethe Ansatz is replaced by the corresponding one for the SU(*N*) Heisenberg spin chain leading to the following set of equations

$$
\begin{aligned}
\mathrm{e}^{ik_jL} &= \prod_{\alpha=1}^{M_1} \frac{4(\sin k_j - \lambda_\alpha^{(1)}) + iU}{4(\sin k_j - \lambda_\alpha^{(1)}) - iU}\,, \qquad j = 1,\ldots,N_c \\
\prod_{\beta=1}^{M_{r-1}} \frac{4(\lambda_\alpha^{(r)} - \lambda_\beta^{(r-1)}) + iU}{4(\lambda_\alpha^{(r)} - \lambda_\beta^{(r-1)}) - iU} \cdot \prod_{\beta=1}^{M_{r+1}} \frac{4(\lambda_\alpha^{(r)} - \lambda_\beta^{(r+1)}) + iU}{4(\lambda_\alpha^{(r)} - \lambda_\beta^{(r+1)}) - iU} & \\
&= \prod_{\beta\neq\alpha} \frac{2(\lambda_\alpha^{(r)} - \lambda_\alpha^{(r)}) + iU}{2(\lambda_\alpha^{(r)} - \lambda_\alpha^{(r)}) - iU}\,, \qquad \alpha = 1,\ldots,M_r
\end{aligned} \tag{1}
$$

for $r = 1,\ldots,N-1$ where we have put $M_0 = N_c$, $M_N = 0$ and $\lambda_\alpha^{(0)} = \sin k_\alpha$. To each solution of these equations there corresponds a state with energy $E = -2\sum_j \cos k_j$. As mentioned above the equations (1) have first been studied by Choy and Haldane for special choices of $N$. Later, the case of arbitrary $N$ has been independently studied by Lee and Schlottmann [6] and Schadschneider [7]. In the limit $N \to \infty$ one can consider states where all particles carry a different SU(*N*) colour. In this "bosonic" limit the $\lambda_\alpha^{(r)}$ for $r > 0$ can be eliminated from the Bethe Ansatz equations (1) resulting in

$$
\mathrm{e}^{ik_jL} = \prod_{\ell\neq j} \frac{2(\sin k_j - \sin k_\ell) + iU}{2(\sin k_j - \sin k_\ell) - iU}, \qquad j = 1,\ldots,N_c\,. \tag{2}
$$

### Ground state

In absence of any symmetry breaking fields the rapidities $\lambda_\alpha^{(r)}$ can be eliminated from the equations. In the thermodynamic limit $L \to \infty$ the ground state ist characterized by the density of the $k_j$ alone, which is given as the solution of the integral equation

$$
\begin{aligned}
\rho(k) &= \frac{1}{2\pi} + \frac{\cos k}{2\pi} \int_{-k_0}^{k_0} d\bar{k}\, h_N(\sin k - \sin \bar{k}) \rho(\bar{k}), \\
h_N(x) &= \frac{4}{NU}\, \mathrm{Re} \left\{ \psi\left(1 + \frac{2ix}{NU}\right) - \psi\left(\frac{1}{N} + \frac{2ix}{NU}\right) \right\}.
\end{aligned} \tag{3}
$$

The domain of integration is fixed by the relation $\int_{-k_0}^{k_0} dk \rho(k) = N_c/L = n_c$. From (3) it follows that this integral evaluates to 1 for $k_0 = \pi$. For this value a closed expression for the ground state energy can be given ($J_n$ are Bessel functions):

$$
\frac{E_0}{L} = -2 \int_{-k_0}^{k_0} dk \cos k \rho(k) = -2 \int_{-\infty}^{+\infty} \frac{d\omega}{\omega} e^{-U|\omega|/4} \frac{\sinh(N-1)U\omega/4}{\sinh NU\omega/4} J_0(\omega) J_1(\omega)\,.
$$

For $N = 2$, the choice $k_0 = \pi$ corresponds to $n_c = 1$ for arbitrary values of the Coulomb repulsion $U$. This is not true for $N > 2$: solving Eq. (3) for sufficiently small $U$ one finds that $\rho$ is not positive definite, hence representing an unphysical solution of the integral equation. The condition that min$\rho(k) \geq 0$ defines an $N$-dependent critical value $U_c$ of the coupling constant at which the system undergoes a first order Mott-transition from a metallic to an insulating ground state (see [5] and the discussion below).

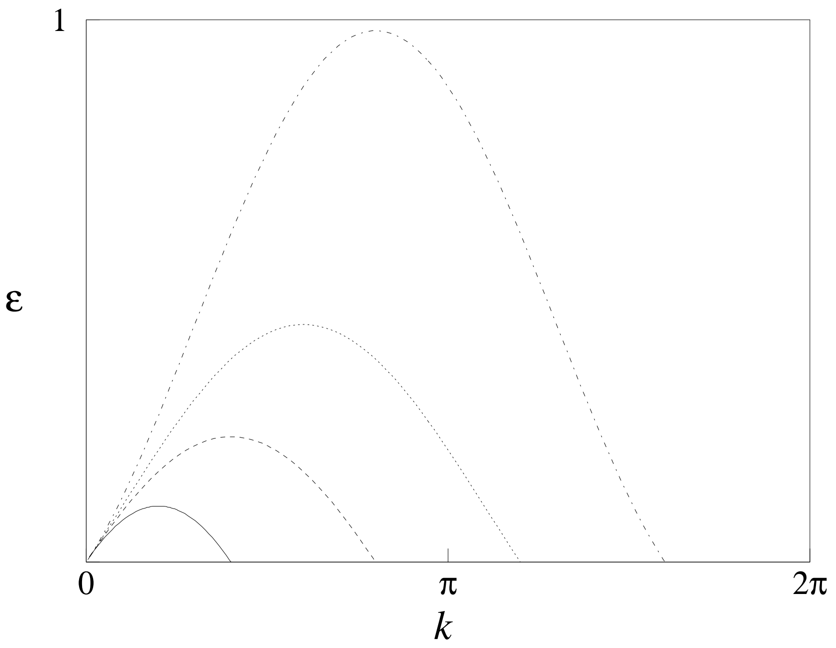


**Figure 1**: Dispersion of the elementary spinon excitations $\epsilon^{(r)}(k)$ for $N = 5$ at filling $n_c = 1$. The physical excitations are scattering states of spinons, hence the curves define lower bounds of various continua of spin waves.

**Excitations**

The low-lying excitations have been studied by Schadschneider and by Schlottmann [7, 8]. Three types of excitations have to be taken into account: As in the $N = 2$ Hubbard model there are particle-hole excitations leading to a single branch of gapless charge density waves as long as $k_0 < \pi$ (note that unlike in the *N*=2 model this includes the case of density $n_c = 1$ for coupling $U < U_c$!).

Corresponding to the *N*–1 levels in the hierarchy of Bethe Ansätze for the SU(*N*) spin-problem there are *N*–1 types of elementary spin excitations corresponding to holes in the distribution of the $\lambda^{(r)}$. For large $U$ the dispersion relations of these quasiparticles are

$$\epsilon^{(r)}(k_r) = \frac{4\pi}{NU} n_c \left(1 - \frac{\sin 2\pi n_c}{2\pi n_c}\right) \frac{\cos\left(\pi r/N - k_r/n_c\right) - \cos \pi r/N}{\sin \pi r/N} \tag{4}$$

where $k_r \leq 2\pi n_c \frac{N-r}{N}$ (see Figure 1). For filling $n_c = 1$ these dispersion relations reduce to the results known for the SU(*N*) Heisenberg magnet (see e.g. [9]). As in the latter model the physical excitations are scattering states of the quasiparticles (4), e.g. pairs of quasiparticles carrying SU(*N*) color $r$ and $N - r$ respectively.

Finally there are bound states corresponding to configurations including multiple occupancies. These bound states correspond to solutions of the Bethe Ansatz equations (1) including complex values of $k_j$ or $\lambda_\alpha^{(r)}$. The simplest excitations of this type are pairs of complex conjugate pseudomomenta bound to a rapidity at level $r = 1$: $\sin k_\alpha^{\pm} = \lambda_\alpha^{(1)} \pm iU/4$. Studying their spectrum at $n_c = 1$ and $U > U_c$ one finds that these excitations have a gap $\Delta(U)$ which remains *finite* as $U$ approaches $U_c$ from above for any $N > 2$ [7]. This proves that the metal insulator transition at $U_c$ is of first order.

## Critical exponents

Using exact finite-size calculations within the framework of the Bethe Ansatz together with the predictions from conformal field theory the long distance asymptotics of correlation functions of the model can be studied [10]. Using these results one obtains for example the exponent of the momentum distribution function $\langle c_{k\sigma} c_{k\sigma}^\dagger \rangle = |k - k_F|^\alpha$ near the Fermi momentum $k_F = \pi / N n_c$. In absence of external fields $\alpha$ depends on the density of electrons $n_c$ and the coupling strength $U$ only in a combination related to the compressibility of the electron gas. It varies in the interval

$$0 = \alpha(U \to 0) \leq \alpha \leq \alpha(U \to \infty) = \frac{1}{2} - \frac{1}{N} + \frac{1}{2N^2}.$$

Near the Mott transition $n_c = 1$, $U \lesssim U_c$ the exponent $\alpha$ approaches its $U \to \infty$ value with a square-root dependence on the coupling constant. In the limit $N \to \infty$ one finds

$$\alpha = \frac{1}{2} - \frac{4\sqrt{14}}{7\pi} \sqrt{1 - \frac{U}{U_c}} + \ldots$$

Similarly, one can study different correlation functions. In particular one finds the exponents of the SU(*N*) Heisenberg model for spin spin correlation functions at $n_c = 1$ and $U > U_c$ and the behaviour of free $N$-component fermions as $U \to 0$.

## THE HAMILTONIAN OF THE DEGENERATE HUBBARD MODEL

Up to now we have not given an expression for the Hamiltonian of the model studied here—and this is for a good reason. The Bethe Ansatz for the model has been introduced in analogy to the generalization of the gas with repulsive $\delta$-function interaction and *not* as e.g. for the SU(2) Hubbard model by explicit construction of solutions of the Schrödinger equation for a given Hamiltonian making an explicit Ansatz for the eigenfunctions. There have been several attempts to write down a Hamiltonian for the degenerate ($N > 2$) model, however none of them is actually solved by the Bethe Ansatz (1). In this section we shortly review the proposed expressions for the Hamiltonian together with a discussion of why they fail, since this sheds some light on the question how the correct Hamiltonian may look like.

When the Bethe Ansatz was first introduced by Choy [4] and Haldane [5] they gave the following expression for the corresponding Hamiltonian

$$\mathcal{H} = -\sum_{j=1}^{L} \sum_{\sigma=1}^{N} \left( c_{j+1,\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{j+1,\sigma} \right) + U \sum_{j=1}^{L} f(\sum_{\sigma=1}^{N} n_{j\sigma}) \tag{5}$$

where $f$ is a function of the total number of electrons on a single site only ($f(0) = 0$, $f(n) = n - 1$ for $n \geq 1$). Later [11] they noticed, however, that their proposed Bethe Ansatz wavefunctions did not solve Schrödinger's equation at points in configuration space with more than double occupancies. They even proved that this problem can not be resolved if the Bethe Ansatz states are complete. By now, it is well understood that the Bethe Ansatz alone actually does *not* give the full spectrum in models with an internal symmetry. For the SU(2) model only the Bethe Ansatz extended using the full SO(4) symmetry of the model yields the complete spectrum [12].

Later Lee and Schlottmann [13] claimed that the problem of mutliple occupancies could be resolved by studying the model (5) in a Hilbert space with more than double occupancies forbidden. This amounts to changing the hopping term to

$$-\mathcal{P}_2 \sum_{j=1}^{L} \sum_{\sigma=1}^{N} \left( c_{j+1,\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{j+1,\sigma} \right) \mathcal{P}_2 \tag{6}$$

where $\mathcal{P}_2$ is the operator projection onto the restricted Hilbertspace. With this restriction the interaction then takes the Hubbard form $U \sum_j \sum_{\sigma<\sigma'} n_{j\sigma} n_{j\sigma'}$.

At this point a few remarks concerning this form of the Hamiltonian are at place. The basic properties as known from the investigation of the Bethe Ansatz equations (1) already allow a brief discussion of the expressions for $\mathcal{H}$ with (6):
(1) In the SU(2) Hubbard model for spin $\frac{1}{2}$ electrons more than double occupancies are forbidden by the Pauli exclusion principle, and the operator $\mathcal{P}_2$ drops from the expression (6).
(2) In a dilute limit the projection operator is irrelevant and the lattice model reduces to the Yang–Sutherland model for SU(*N*) fermion gas with $\delta$-interaction — as it should.
(3) In the limit $U \to \infty$ the finite energy sector of the model is that of free spinless fermions, the strong repulsion eliminates states with more than single occupancy.
(4) Finally, in the limit $U \to 0$, however, the Bethe Ansatz equations describe a system of *free* $N$-component fermions (this is also reflected in the critical exponents of the model in this limit). This is in obvious contradiction to the Hamiltonian (6) where the projection operator should introduce strong correlations.

On further step towards the identification of the correct Hamiltonian of the SU(*N*) system was taken by Schlottmann [14] who noticed that the two-particle phase-shift function in absence of symmetry breaking fields

$$\delta(k_1, k_2) = \int^{\sin k_1 - \sin k_2} dx\ h_N(x)$$

in the continuum limit ($k_i \ll 1$) is characteristic for a long-ranged two-body interaction

$$V(r) \propto \frac{1}{\sinh^2 ar}$$

which indicates a more complicated interaction term for the lattice than the purely local one given in the original expression (5).

In the remainder of this report we shall present some new results from studies aiming at the determination of the correct lattice Hamiltonian for the SU(*N*) Hubbard model. Our strategy is as follows:

We start by solving the Bethe Ansatz equations (1) *completely* for small chains. It is well known that the Bethe Ansatz gives the states of highest weight with respect to the global symmetries of the model. In the present case that means that the results from the analysis of the Bethe Ansatz equations have to be extended using the SU(*N*) symmetry of the system and a possible generalization of the $\eta$-pairing symmetry in the SU(2) model. Once we have generated the complete spectrum (together with the eigenstates) of the model within this approach it is possible to reconstruct the Hamiltonian from the spectral data.

As the simplest example let us consider the degenerate Hubbard model with SU(3) electrons on a two-site lattice. As outlined above we require the system to have a global SU(3) symmetry, which determines the degeneracies in the spectrum at constant particle number. In addition, if only electrons with two different colours are present, we require the Hamiltonian to reduce to the usual Hubbard model with spin $\frac{1}{2}$ electrons. The spectrum of the latter model for the two-site lattice is sketched in Figure 2.

Note that only the states which are highest weight with respect to the global SO(4)= SU(2)$\otimes$SU(2)/$Z_2$-symmetry of the SU(2)-Hubbard model are obtained from the regular Bethe

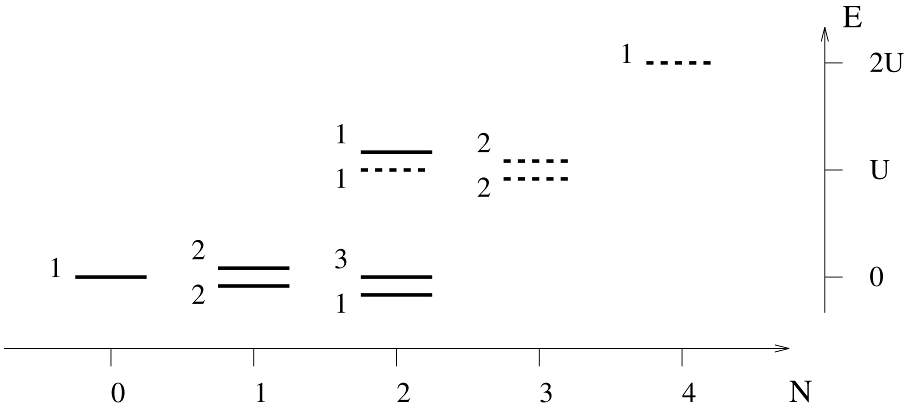


**Figure 2**: Spectrum of the SU(2) Hubbard model for large $U$ on a two-site lattice as a function of the particle number (schematic). The numbers indicate the degeneracy of the eigenvalues. Energy levels drawn as solid lines are obtained from the Bethe Ansatz directly, the dashed ones are not highest weight with respect to the $\eta$-pairing SU(2).

Ansatz [12]. In particular, the states with more than two electrons are accessible only after extending the Bethe Ansatz with the $\eta$-pairing SU(2)-symmetry.

As mentioned above we require these eigenenergies to be present in the spectrum of the SU(3) system as well, with the degeneracies replaced by those of the corresponding SU(3)-multiplets (see Figure 3). Clearly, this identification of eigenstates of the SU(2) model with the ones in the degenerate model gives only a small part of the spectrum. To obtain *all* eigenvalues additional assumptions on the symmetries of the system are necessary.

Since the Hamiltonian is unknown so far, we do not know the analog of the $\eta$-pairing algebra for the degenerate model. However, a reasonable assumption is that there should exist some generalized particle-hole symmetry in the model. As in the SU(2) model we require the spectrum to be invariant (up to a chemical potential term) under the transformation $c_j^\dagger = (-1)^j \tilde{c}_j$, $c_j = (-1)^j \tilde{c}_j^\dagger$. The known energies for the two SU(3) sextets fix the chemical potential term that is added to the Hamiltonian when performing this transformation.

Counting states we find that there are still four SU(3)-singlets in the three-particle sector missing. These SU(3)-singlets are obtained from the $L = 2$ Bethe Ansatz equations by choosing $N_c = 3$, $M_1 = 2$, and $M_2 = 1$. For this configuration they reduce to the "bosonic" equations (2) which can be written as polynomials in the unknowns $z_j = \exp ik_j$ and hence be solved completely. It turns out that there are, in fact, exactly four nondegenerate solutions of this type: two with momentum $K = 0$ and two with momentum $K = \pi$. The three Bethe Ansatz roots $k_j$ are all real for small $U$ while two of them form a pair of complex conjugate numbers for sufficiently strong interaction.[1] The corresponding energies are

$$\varepsilon_\pm(K) = -2\cos K + \frac{1}{2}\left(3U \pm \sqrt{U^2+64}\right) .$$

Requiring the corresponding states to be eigenvectors of an operator linear in the Coulomb repulsion $U$ (i.e. $\mathcal{H} = \mathcal{T} + U\mathcal{V}$) together with their known total momentum we can uniquely determine the corresponding wavefunctions.

At this point we have collected all the information necessary to reconstruct the Hamiltonian for the SU(3) degenerate Hubbard model on the two-site lattice from $\mathcal{H} = \sum |n\rangle E_n \langle n|$

[1]This appears to be closely related to the observed Mott-transition at $n_c = 1$ and finite $U$: For small values of $U$ the Bethe Ansatz $k_j$ are all real, while beyond $U = 6$ two of them form a complex conjugate pair.

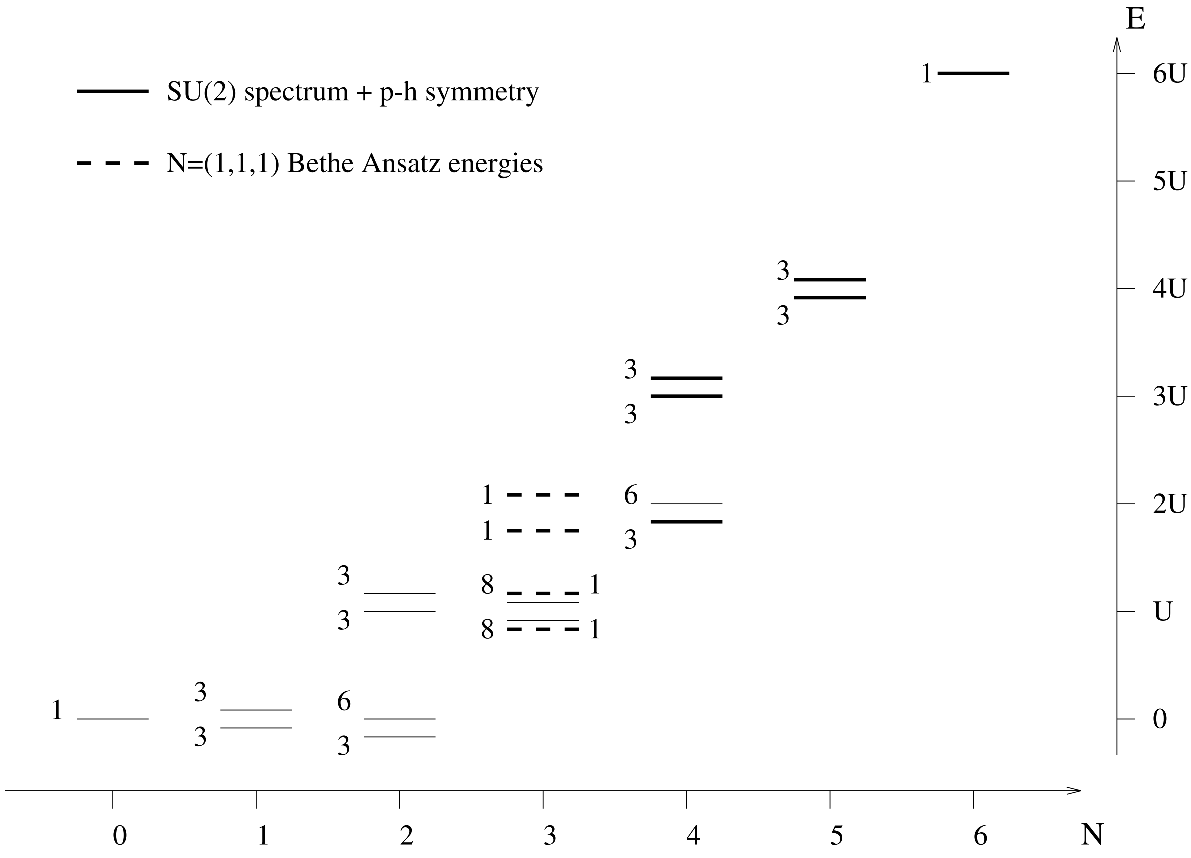


**Figure 3**: Spectrum of the SU(3) degenerate Hubbard model for large $U$ on a two-site lattice as a function of the particle number (schematic). The SU(2) spectrum has been completed using the proposed particle-hole symmetry and the four 3-particle solutions of the Bethe Ansatz equations as discussed in the main text. Again, the numbers indicate the (SU(3)-) degeneracy of the eigenvalues.

where the sum runs over all the eigenstates of the model (known from the SU(2) case, particle-hole symmetry and requiring the Hamiltonian to be linear in $U$). The resulting Hamiltonian reduces to the free hopping term in (5) as $U \to 0$. In addition to on site and nearest neighbour interaction terms that depend only on the occupation numbers one finds bond-charge interaction

$$\propto \prod_{\sigma' \neq \sigma} (n_{1\sigma'} - n_{2\sigma'}) \left( c_{1\sigma}^\dagger c_{2\sigma} + h.c. \right),$$

nearest neighbour spin exchange terms

$$\propto (n_{1\sigma} - n_{2\sigma})^2 \left( c_{1\sigma'}^\dagger c_{2\sigma''}^\dagger c_{1\sigma''} c_{2\sigma'} + h.c \right),$$

and three particle hopping amplitudes.

In the next step we have studied the SU(3) model on a chain of length $L = 4$. We have solved the Bethe Ansatz equations for the singlets in the 3-particle sector completely. Among the 20 possible SU(3) singlets there should be four states each with single and triple occupancies on a single site and twelve with double occupancies. This counting should translate to the degeneracies present in the spectrum at large $U$. We find that the Bethe Ansatz equations have 14 solutions in this sector with energies and degeneracies $[0]^4$, $[U]^6$ and $[2U]^4$ as $U \to \infty$.

Assuming that the Hamiltonian for the degenerate Hubbard model contains terms involving operators on neighbouring sites only we write the $L = 2$ Hamiltonian as $\mathcal{H}_{L=2} = H_{12} + H_{21}$

from which we obtain the $L = 4$ Hamiltonian as $\mathcal{H}_{L=4} = \sum_j H_{j,j+1}$. Unfortunately, it is easily seen that this Hamiltonian does *not* reproduce the spectrum obtained from the Bethe Ansatz: diagonalizing $\mathcal{H}_{L=4}$ in the three particle SU(3) singlet subspace with momentum $K = 0$ we do not find a state with energy $\propto 2U$ asymptotically.

## SUMMARY

We have studied the Bethe Ansatz equations that arise from the substitution of the spin-problem of the SU(2) Hubbard model by an SU(*N*) spin problem. The solution of these equations shows that this system has one branch of gapless charge excitations and *N*–1 branches of gapless spinon excitations for filling $n_c < 1$ *and* for $n_c = 1$ and Coulomb interaction $U < U_c$. At the critical coupling $U_c$ a first order Mott transition takes place, beyond which the charge excitations are massive.

The lattice Hamiltonian that is solved by these equations is still unknown. In principle it should be possible to reconstruct the Hamiltonian from the Bethe Ansatz solution, however a number of questions arise in this program:
(1) How should the Bethe Ansatz spectrum (which contains only states of highest weight with respect to the global symmetry of the system) be completed?
(2) If the interaction is "long-ranged" the problem of rebuilding these terms from the results for small lattices is not unique.

Nevertheless, this problem is certainly worth the efforts as the model allows to study phenomena such as a Mott transition at finite coupling which is not present in the N=2 case and provides exact results that are useful in estimating the quality of asymptotic 1/*N* expansions.

## REFERENCES


1. E. H. Lieb and F. Y. Wu, *Phys. Rev. Lett.* **20**, 1445 (1968).
2. C. N. Yang, *Phys. Rev. Lett.* **19**, 1312 (1967).
3. B. Sutherland, *Phys. Rev. Lett.* **20**, 98 (1968).
4. T. C. Choy, *Phys. Lett.* **80A**, 49 (1980).
5. F. D. M. Haldane, *Phys. Lett.* **80A**, 281 (1980), *ibid.* **81A**, 545 (1981) (erratum).
6. K. Lee and P. Schlottmann, *Physica B* **163**, 398 (1990).
7. A. Schadschneider, Dissertation, Universität zu Köln, 1991.
8. P. Schlottmann, *Phys. Rev. B* **43**, 3101 (1991).
9. H. Johannesson, *Nucl. Phys. B* **270**, 235 (1986).
10. H. Frahm and A. Schadschneider, *J. Phys. A* **26**, 1463 (1993).
11. T. C. Choy and F. D. M. Haldane, *Phys. Lett.* **90A**, 83 (1982).
12. F. H. L. Eßler, V. E. Korepin, and K. Schoutens, *Nucl. Phys. B* **384**, 431 (1992).
13. K. Lee and P. Schlottmann, *Phys. Rev. Lett.* **63**, 2299 (1989).
14. P. Schlottmann, *Phys. Rev. B* **45**, 5784 (1992).